



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:53 AM UTC

PDB ID : 2RG0 / pdb_00002rg0
Title : Crystal structure of cellobiohydrolase from *Melanocarpus albomyces* complexed with cellotetraose
Authors : Parkkinen, T.; Koivula, A.; Vehmaanper, J.; Rouvinen, J.
Deposited on : 2007-10-02
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

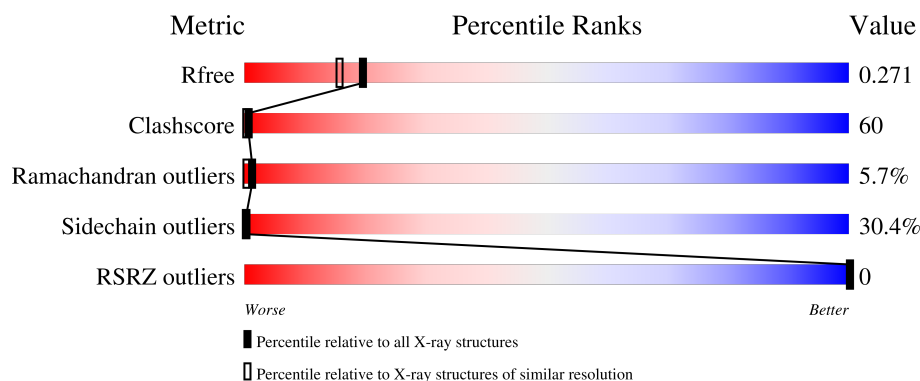
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	430	21% 53% 23% .
1	B	430	19% 51% 26% .
1	C	430	19% 56% 22% .
1	D	430	23% 51% 23% .
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	H	2	 50% 50%
2	I	2	 100%
2	J	2	 50% 50%
3	G	4	 25% 75%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PCA	A	1	-	-	X	-
1	PCA	B	1	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13956 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 Cellulose 1,4-beta-cellobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	B	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	C	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	D	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	0	0	0
			23	12	11			
2	F	2	Total	C	O	0	0	0
			23	12	11			
2	H	2	Total	C	O	0	0	0
			23	12	11			
2	I	2	Total	C	O	0	0	0
			23	12	11			
2	J	2	Total	C	O	0	0	0
			23	12	11			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	G	4	Total	C	O	0	0	0
			45	24	21			

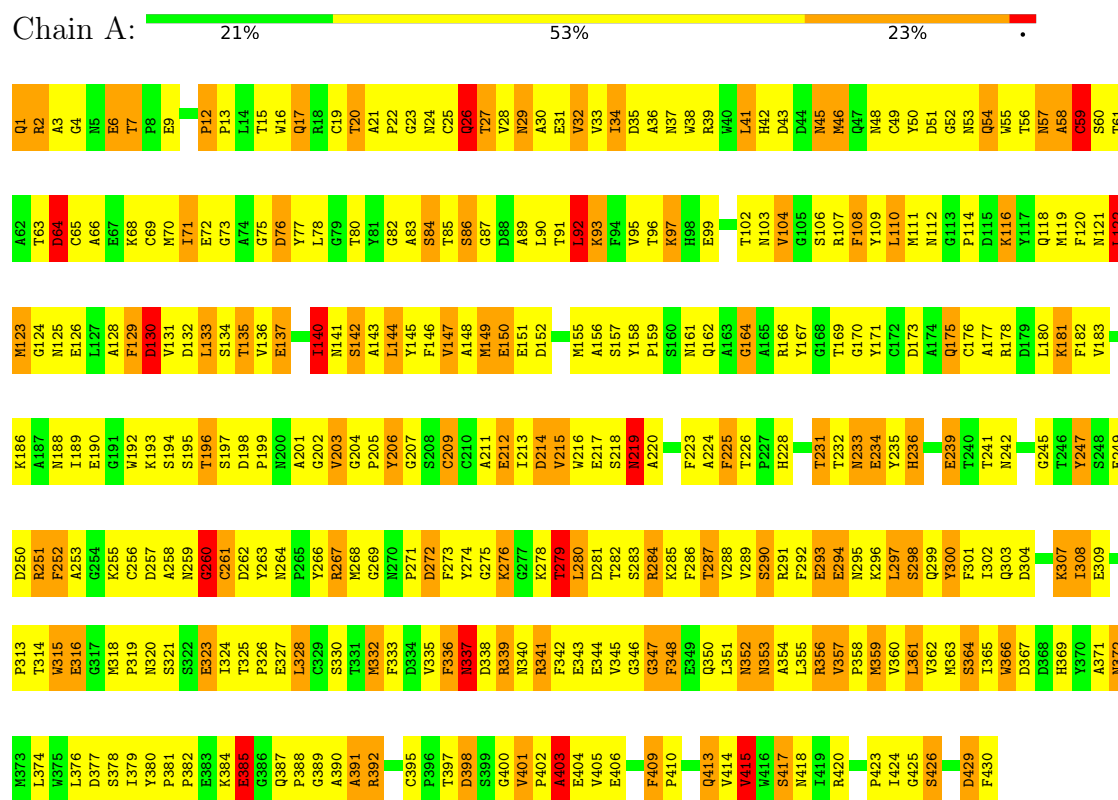
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total	O	0	0
			101	101		
4	B	109	Total	O	0	0
			109	109		
4	C	122	Total	O	0	0
			122	122		
4	D	132	Total	O	0	0
			132	132		

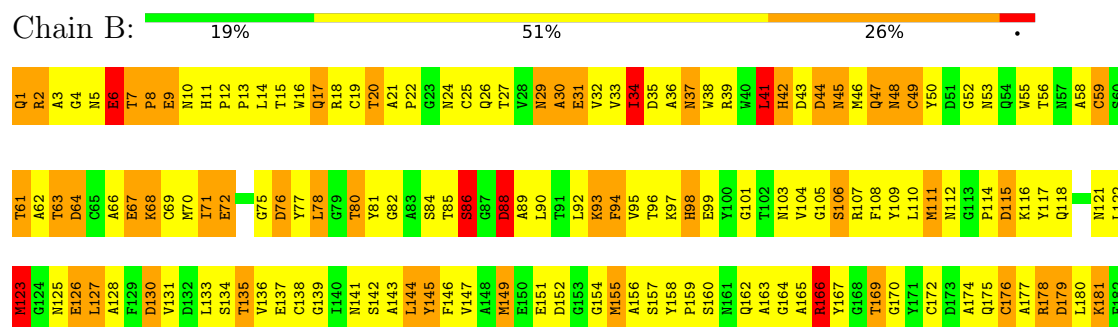
3 Residue-property plots

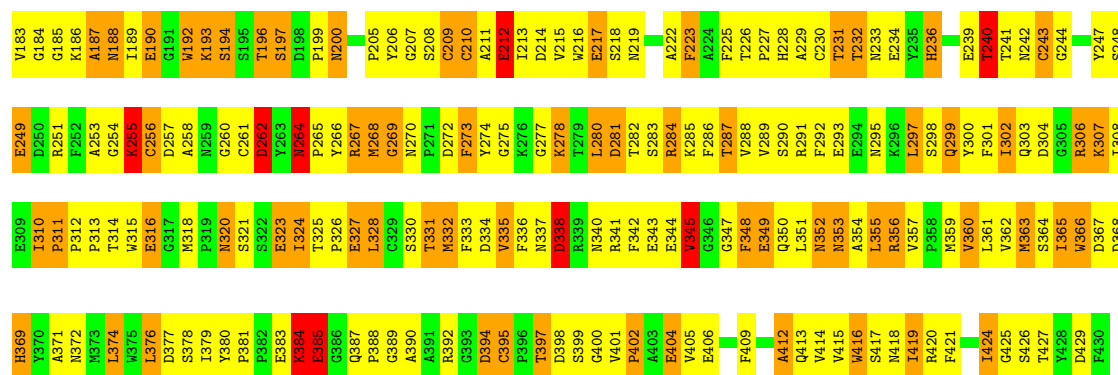
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Cellulose 1,4-beta-cellobiosidase



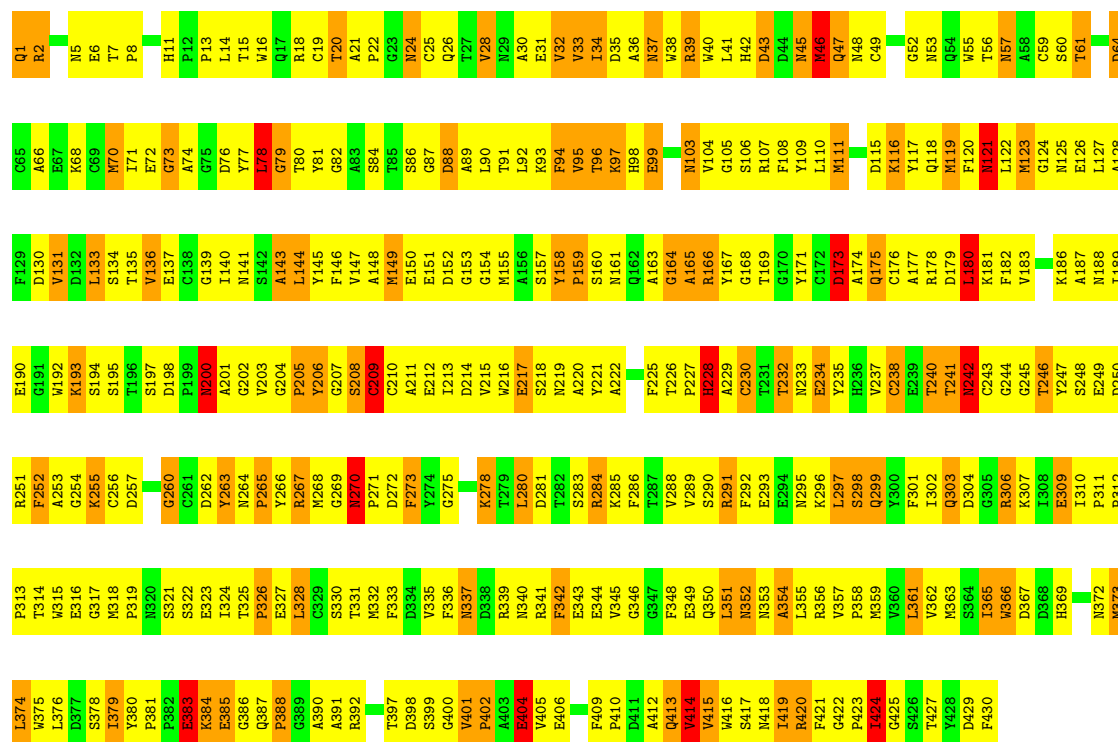
- Molecule 1: Cellulose 1,4-beta-cellobiosidase





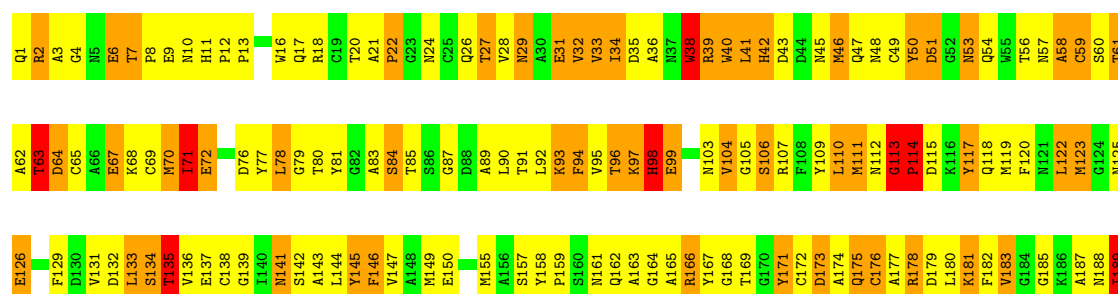
• Molecule 1: Cellulose 1,4-beta-cellobiosidase

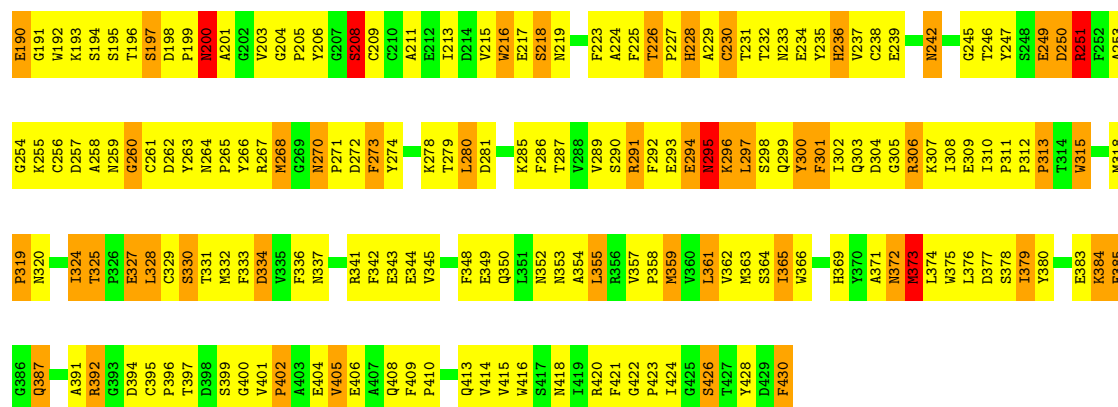
Chain C: 19% 56% 22%



• Molecule 1: Cellulose 1,4-beta-cellobiosidase

Chain D: 23% 51% 23%





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

Chain E:  100%

BGC1
BGC2

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

Chain F:  100%

BGC1
BGC2

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

Chain H:  50%

BGC1
BGC2

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

Chain I:  100%

BGC1
BGC2

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

Chain J:  50%

BGC1
BGC2

- Molecule 3: beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose-(1-4)-beta-D-glucopyranose

Chain G:  25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.98Å 94.81Å 190.43Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.6 (20.00-2.10) 98.1 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.10Å)	Xtriage
Refinement program	SHELX, SHELXL-97	Depositor
R, R_{free}	0.211 , 0.282 0.210 , 0.271	Depositor DCC
R_{free} test set	5265 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	10.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.428 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13956	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.53% 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: PCA, BGC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/3416	1.47	33/4648 (0.7%)
1	B	0.41	0/3416	1.56	57/4648 (1.2%)
1	C	0.40	0/3416	1.46	43/4648 (0.9%)
1	D	0.40	0/3416	1.49	53/4648 (1.1%)
All	All	0.40	0/13664	1.49	186/18592 (1.0%)

There are no bond length outliers.

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	ALA	CA-C-N	13.34	132.72	119.92
1	B	3	ALA	C-N-CA	13.34	132.72	119.92
1	B	366	TRP	CA-C-N	11.91	142.81	122.81
1	B	366	TRP	C-N-CA	11.91	142.81	122.81
1	C	228	HIS	CA-CB-CG	10.51	124.31	113.80
1	B	34	ILE	CA-C-N	10.32	135.37	120.82
1	B	34	ILE	C-N-CA	10.32	135.37	120.82
1	A	64	ASP	CA-CB-CG	10.11	122.70	112.60
1	B	264	ASN	CA-CB-CG	9.80	122.41	112.60
1	D	301	PHE	CA-CB-CG	9.60	123.40	113.80
1	A	216	TRP	CA-C-N	9.52	136.38	121.72
1	A	216	TRP	C-N-CA	9.52	136.38	121.72
1	A	219	ASN	CA-CB-CG	8.65	121.25	112.60
1	A	225	PHE	CA-CB-CG	8.46	122.26	113.80
1	D	251	ARG	CD-NE-CZ	8.31	136.04	124.40
1	B	98	HIS	CA-C-N	8.14	133.73	120.63
1	B	98	HIS	C-N-CA	8.14	133.73	120.63
1	D	113	GLY	CA-C-N	8.04	129.89	119.84
1	D	113	GLY	C-N-CA	8.04	129.89	119.84
1	A	409	PHE	CA-CB-CG	8.01	121.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	374	LEU	CA-C-N	7.98	131.77	120.28
1	C	374	LEU	C-N-CA	7.98	131.77	120.28
1	B	42	HIS	CA-C-N	7.92	136.98	122.02
1	B	42	HIS	C-N-CA	7.92	136.98	122.02
1	C	143	ALA	CA-C-N	7.62	134.86	122.29
1	C	143	ALA	C-N-CA	7.62	134.86	122.29
1	D	26	GLN	CA-C-N	7.53	135.92	121.54
1	D	26	GLN	C-N-CA	7.53	135.92	121.54
1	D	173	ASP	CA-CB-CG	7.52	120.12	112.60
1	D	268	MET	CA-C-N	7.24	131.54	121.26
1	D	268	MET	C-N-CA	7.24	131.54	121.26
1	A	26	GLN	CA-C-N	7.09	131.56	121.42
1	A	26	GLN	C-N-CA	7.09	131.56	121.42
1	C	34	ILE	CA-C-N	6.97	130.72	120.95
1	C	34	ILE	C-N-CA	6.97	130.72	120.95
1	D	189	ILE	CA-C-N	6.85	134.62	121.54
1	D	189	ILE	C-N-CA	6.85	134.62	121.54
1	A	12	PRO	O-C-N	6.83	124.45	121.31
1	A	260	GLY	CA-C-N	6.80	132.36	122.16
1	A	260	GLY	C-N-CA	6.80	132.36	122.16
1	A	236	HIS	CA-CB-CG	6.78	120.58	113.80
1	D	273	PHE	CA-C-N	6.71	132.23	122.77
1	D	273	PHE	C-N-CA	6.71	132.23	122.77
1	B	384	LYS	CA-C-N	6.66	134.26	121.54
1	B	384	LYS	C-N-CA	6.66	134.26	121.54
1	B	8	PRO	CA-C-N	6.61	132.88	122.17
1	B	8	PRO	C-N-CA	6.61	132.88	122.17
1	D	40	TRP	CA-C-N	6.52	130.12	120.87
1	D	40	TRP	C-N-CA	6.52	130.12	120.87
1	D	58	ALA	CA-C-N	6.50	132.77	122.36
1	D	58	ALA	C-N-CA	6.50	132.77	122.36
1	B	29	ASN	CA-C-N	6.48	133.92	121.54
1	B	29	ASN	C-N-CA	6.48	133.92	121.54
1	A	415	VAL	CA-C-N	6.47	130.67	121.42
1	A	415	VAL	C-N-CA	6.47	130.67	121.42
1	D	236	HIS	CA-CB-CG	6.41	120.21	113.80
1	B	331	THR	CA-C-N	6.37	129.10	120.44
1	B	331	THR	C-N-CA	6.37	129.10	120.44
1	B	231	THR	CA-C-N	6.31	130.66	121.26
1	B	231	THR	C-N-CA	6.31	130.66	121.26
1	B	338	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	16	TRP	CA-C-N	-6.30	110.93	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	TRP	C-N-CA	-6.30	110.93	121.64
1	B	218	SER	CA-C-N	6.23	134.16	121.95
1	B	218	SER	C-N-CA	6.23	134.16	121.95
1	A	58	ALA	CA-C-N	6.20	133.38	121.54
1	A	58	ALA	C-N-CA	6.20	133.38	121.54
1	D	333	PHE	CA-CB-CG	-6.12	107.69	113.80
1	B	262	ASP	CA-CB-CG	6.06	118.66	112.60
1	D	250	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	164	GLY	CA-C-N	6.00	128.33	120.28
1	A	164	GLY	C-N-CA	6.00	128.33	120.28
1	B	236	HIS	CA-CB-CG	5.97	119.77	113.80
1	C	401	VAL	O-C-N	5.95	127.88	121.10
1	B	242	ASN	CA-C-N	5.90	131.60	121.86
1	B	242	ASN	C-N-CA	5.90	131.60	121.86
1	D	58	ALA	O-C-N	5.87	129.34	122.24
1	C	242	ASN	CA-CB-CG	5.87	118.47	112.60
1	D	384	LYS	CA-C-N	5.84	132.70	121.54
1	D	384	LYS	C-N-CA	5.84	132.70	121.54
1	C	270	ASN	CA-C-N	5.81	125.50	119.05
1	C	270	ASN	C-N-CA	5.81	125.50	119.05
1	B	42	HIS	N-CA-C	5.79	115.89	108.24
1	A	108	PHE	CA-C-N	5.75	131.59	122.62
1	A	108	PHE	C-N-CA	5.75	131.59	122.62
1	D	373	MET	CA-C-N	5.69	128.69	120.38
1	D	373	MET	C-N-CA	5.69	128.69	120.38
1	A	279	THR	O-C-N	5.68	128.16	122.08
1	C	366	TRP	O-C-N	5.67	128.94	123.04
1	C	24	ASN	CA-CB-CG	5.67	118.27	112.60
1	A	372	ASN	CA-C-N	5.67	131.95	123.05
1	A	372	ASN	C-N-CA	5.67	131.95	123.05
1	D	200	ASN	CA-CB-CG	5.66	118.26	112.60
1	B	41	LEU	CA-C-N	-5.63	112.42	122.32
1	B	41	LEU	C-N-CA	-5.63	112.42	122.32
1	B	61	THR	CA-C-N	5.60	129.64	120.63
1	B	61	THR	C-N-CA	5.60	129.64	120.63
1	D	218	SER	CA-C-N	5.59	132.97	123.01
1	D	218	SER	C-N-CA	5.59	132.97	123.01
1	B	429	ASP	CA-C-N	5.58	131.75	121.70
1	B	429	ASP	C-N-CA	5.58	131.75	121.70
1	B	255	LYS	CA-C-N	5.58	132.33	121.63
1	B	255	LYS	C-N-CA	5.58	132.33	121.63
1	D	7	THR	CA-C-N	5.57	126.00	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7	THR	C-N-CA	5.57	126.00	119.99
1	B	223	PHE	CA-CB-CG	5.56	119.36	113.80
1	C	273	PHE	CA-C-N	5.56	131.57	122.07
1	C	273	PHE	C-N-CA	5.56	131.57	122.07
1	A	403	ALA	CA-C-N	5.55	127.99	120.38
1	A	403	ALA	C-N-CA	5.55	127.99	120.38
1	D	113	GLY	O-C-N	5.55	127.32	121.77
1	C	401	VAL	CA-C-N	5.53	126.75	119.84
1	C	401	VAL	C-N-CA	5.53	126.75	119.84
1	C	260	GLY	CA-C-N	5.52	131.11	122.17
1	C	260	GLY	C-N-CA	5.52	131.11	122.17
1	A	130	ASP	CA-CB-CG	5.52	118.12	112.60
1	D	135	THR	CA-C-N	5.51	128.56	122.22
1	D	135	THR	C-N-CA	5.51	128.56	122.22
1	D	50	TYR	CA-C-N	5.49	132.03	121.54
1	D	50	TYR	C-N-CA	5.49	132.03	121.54
1	D	141	ASN	N-CA-C	5.48	117.67	108.73
1	D	295	ASN	CA-CB-CG	5.48	118.08	112.60
1	B	88	ASP	CA-C-N	5.44	130.23	122.72
1	B	88	ASP	C-N-CA	5.44	130.23	122.72
1	C	366	TRP	CA-C-N	5.43	130.80	122.93
1	C	366	TRP	C-N-CA	5.43	130.80	122.93
1	B	323	GLU	CA-C-O	-5.42	115.80	121.55
1	C	57	ASN	CA-CB-CG	5.42	118.02	112.60
1	D	217	GLU	CA-C-N	-5.35	112.15	122.09
1	D	217	GLU	C-N-CA	-5.35	112.15	122.09
1	C	354	ALA	CA-C-N	5.34	127.97	120.28
1	C	354	ALA	C-N-CA	5.34	127.97	120.28
1	C	37	ASN	CA-C-N	5.34	131.64	122.09
1	C	37	ASN	C-N-CA	5.34	131.64	122.09
1	C	326	PRO	CA-C-N	5.33	127.69	120.44
1	C	326	PRO	C-N-CA	5.33	127.69	120.44
1	B	316	GLU	CB-CG-CD	5.31	121.63	112.60
1	A	92	LEU	CA-C-N	5.30	128.37	120.95
1	A	92	LEU	C-N-CA	5.30	128.37	120.95
1	B	269	GLY	CA-C-N	-5.29	116.31	123.46
1	B	269	GLY	C-N-CA	-5.29	116.31	123.46
1	D	38	TRP	CA-CB-CG	5.29	123.64	113.60
1	C	45	ASN	CA-C-N	5.26	131.58	121.54
1	C	45	ASN	C-N-CA	5.26	131.58	121.54
1	D	300	TYR	CA-C-O	-5.25	115.06	121.78
1	B	17	GLN	CA-C-N	5.23	130.12	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	17	GLN	C-N-CA	5.23	130.12	122.85
1	C	252	PHE	CA-CB-CG	-5.20	108.60	113.80
1	D	216	TRP	CA-C-N	5.20	129.90	122.72
1	D	216	TRP	C-N-CA	5.20	129.90	122.72
1	B	256	CYS	CA-C-O	-5.20	115.17	120.89
1	D	53	ASN	CA-CB-CG	5.20	117.80	112.60
1	C	414	VAL	CA-C-N	-5.18	116.38	123.12
1	C	414	VAL	C-N-CA	-5.18	116.38	123.12
1	B	311	PRO	CA-C-N	5.18	125.72	120.38
1	B	311	PRO	C-N-CA	5.18	125.72	120.38
1	D	208	SER	CA-C-N	-5.17	114.35	122.73
1	D	208	SER	C-N-CA	-5.17	114.35	122.73
1	D	218	SER	O-C-N	5.13	128.42	123.29
1	D	46	MET	CA-C-N	-5.13	113.65	121.66
1	D	46	MET	C-N-CA	-5.13	113.65	121.66
1	C	121	ASN	CA-C-N	5.13	129.28	120.71
1	C	121	ASN	C-N-CA	5.13	129.28	120.71
1	B	166	ARG	CA-C-N	5.12	128.78	120.23
1	B	166	ARG	C-N-CA	5.12	128.78	120.23
1	D	42	HIS	CA-C-N	5.11	131.30	121.54
1	D	42	HIS	C-N-CA	5.11	131.30	121.54
1	B	363	MET	CA-C-N	-5.07	114.07	122.39
1	B	363	MET	C-N-CA	-5.07	114.07	122.39
1	D	67	GLU	CA-C-N	5.07	131.22	121.54
1	D	67	GLU	C-N-CA	5.07	131.22	121.54
1	A	272	ASP	CA-CB-CG	5.07	117.67	112.60
1	B	192	TRP	CA-C-N	-5.07	115.67	122.86
1	B	192	TRP	C-N-CA	-5.07	115.67	122.86
1	C	194	SER	CA-C-N	-5.05	116.27	122.84
1	C	194	SER	C-N-CA	-5.05	116.27	122.84
1	C	209	CYS	CA-C-N	5.05	131.21	122.32
1	C	209	CYS	C-N-CA	5.05	131.21	122.32
1	B	262	ASP	CA-C-O	5.03	125.77	120.54
1	C	103	ASN	CA-C-N	5.03	129.95	123.11
1	C	103	ASN	C-N-CA	5.03	129.95	123.11
1	C	158	TYR	CA-C-N	5.01	126.10	119.84
1	C	158	TYR	C-N-CA	5.01	126.10	119.84
1	B	366	TRP	O-C-N	5.00	128.29	123.29
1	A	140	ILE	CA-C-N	-5.00	114.99	122.39
1	A	140	ILE	C-N-CA	-5.00	114.99	122.39

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3333	0	3028	381	0
1	B	3333	0	3028	417	0
1	C	3333	0	3028	404	0
1	D	3333	0	3028	372	0
2	E	23	0	21	3	0
2	F	23	0	21	7	0
2	H	23	0	21	2	0
2	I	23	0	21	5	0
2	J	23	0	21	5	0
3	G	45	0	39	8	0
4	A	101	0	0	12	0
4	B	109	0	0	11	0
4	C	122	0	0	12	0
4	D	132	0	0	12	0
All	All	13956	0	12256	1552	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 60.

All (1552) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:HE3	1:D:6:GLU:HB3	1.39	1.04
1:B:37:ASN:HA	1:B:181:LYS:HE2	1.38	1.02
1:D:21:ALA:HB3	1:D:24:ASN:HD22	1.18	1.01
1:C:250:ASP:HB3	1:C:253:ALA:HB2	1.42	1.01
1:B:2:ARG:HA	1:B:162:GLN:HB2	1.40	0.99
1:A:296:LYS:HE3	1:A:323:GLU:HB3	1.44	0.98
1:B:32:VAL:HG11	1:B:90:LEU:HD22	1.46	0.97
1:A:297:LEU:HB2	1:A:324:ILE:HB	1.47	0.94
1:C:155:MET:HA	1:C:161:ASN:HB3	1.49	0.94
1:D:77:TYR:HB3	1:D:83:ALA:HB3	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:MET:HG3	1:D:376:LEU:HB3	1.49	0.94
1:C:39:ARG:HH22	1:C:74:ALA:HB2	1.31	0.93
1:C:318:MET:HE2	1:C:332:MET:HA	1.49	0.92
1:B:111:MET:HA	1:B:118:GLN:H	1.36	0.91
1:C:267:ARG:HG3	1:C:392:ARG:HG3	1.51	0.88
1:B:230:CYS:HA	1:B:256:CYS:HA	1.56	0.87
1:C:372:ASN:HB3	1:C:400:GLY:HA3	1.55	0.87
1:A:146:PHE:HB3	1:A:359:MET:HB3	1.55	0.86
1:D:361:LEU:HD23	1:D:363:MET:HE2	1.59	0.85
1:D:291:ARG:HG3	1:D:298:SER:HB3	1.58	0.84
1:B:105:GLY:HA2	1:B:365:ILE:HG22	1.60	0.82
1:D:250:ASP:HB3	1:D:253:ALA:HB2	1.62	0.82
1:C:32:VAL:HG13	1:C:110:LEU:HD13	1.61	0.82
1:C:139:GLY:HA3	1:C:400:GLY:HA2	1.58	0.81
1:D:226:THR:HG23	1:D:262:ASP:HB3	1.61	0.81
1:D:297:LEU:HD11	1:D:355:LEU:HD11	1.62	0.81
1:D:408:GLN:HG3	1:D:409:PHE:HD1	1.46	0.81
1:D:135:THR:HB	1:D:413:GLN:H	1.45	0.81
1:D:110:LEU:HD12	1:D:111:MET:H	1.46	0.80
1:A:128:ALA:HB3	1:A:420:ARG:HB2	1.64	0.80
1:D:228:HIS:HB3	1:D:257:ASP:HB3	1.61	0.80
1:B:147:VAL:HG12	1:B:212:GLU:HB2	1.64	0.80
1:B:227:PRO:HG3	1:B:324:ILE:HG21	1.64	0.80
1:B:42:HIS:HA	1:B:49:CYS:HB2	1.65	0.79
1:B:146:PHE:HB3	1:B:359:MET:HB3	1.62	0.79
1:D:36:ALA:HA	1:D:39:ARG:HD2	1.64	0.78
1:D:129:PHE:HA	1:D:418:ASN:O	1.83	0.78
1:D:16:TRP:O	1:D:28:VAL:HB	1.83	0.78
1:A:342:PHE:HD2	1:A:343:GLU:HG3	1.48	0.78
1:D:396:PRO:O	1:D:399:SER:HB3	1.84	0.78
1:C:254:GLY:HA3	4:C:500:HOH:O	1.83	0.78
1:C:306:ARG:HH21	1:D:305:GLY:H	1.28	0.78
1:D:91:THR:O	1:D:92:LEU:HD23	1.84	0.77
1:A:2:ARG:HG3	1:A:69:CYS:O	1.84	0.77
1:A:137:GLU:O	1:A:140:ILE:HG13	1.84	0.77
1:D:227:PRO:HD2	1:D:261:CYS:O	1.83	0.77
1:B:177:ALA:HB3	1:B:208:SER:OG	1.85	0.77
1:B:178:ARG:HA	1:B:206:TYR:O	1.84	0.77
1:C:175:GLN:OE1	1:C:246:THR:HB	1.84	0.77
1:C:176:CYS:O	1:C:178:ARG:HG2	1.85	0.77
1:C:265:PRO:HA	1:C:270:ASN:HD22	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:PHE:HA	1:B:360:VAL:O	1.83	0.77
1:A:17:GLN:HB2	1:A:27:THR:HA	1.65	0.77
1:A:175:GLN:OE1	1:A:258:ALA:HB1	1.85	0.77
1:A:257:ASP:HA	1:A:341:ARG:HD3	1.66	0.76
1:A:293:GLU:HG2	1:A:296:LYS:O	1.84	0.76
1:B:97:LYS:HD2	1:C:6:GLU:OE2	1.85	0.76
1:A:341:ARG:O	1:A:345:VAL:HG22	1.86	0.76
1:B:420:ARG:HB2	1:B:427:THR:HG22	1.68	0.76
1:B:269:GLY:HA3	1:B:314:THR:OG1	1.84	0.76
1:C:36:ALA:HA	1:C:39:ARG:HG3	1.65	0.76
1:B:318:MET:HE2	1:B:332:MET:HA	1.67	0.76
1:A:104:VAL:HG23	2:F:2:BGC:O6	1.86	0.76
1:B:379:ILE:HA	1:B:390:ALA:O	1.85	0.76
1:C:263:TYR:HA	1:C:268:MET:HE3	1.67	0.76
1:D:95:VAL:HG22	1:D:104:VAL:HG13	1.68	0.76
1:B:126:GLU:HB2	1:B:290:SER:O	1.86	0.76
1:C:41:LEU:HA	1:C:70:MET:O	1.86	0.76
1:D:295:ASN:H	1:D:352:ASN:ND2	1.84	0.76
1:B:274:TYR:HA	1:B:280:LEU:HB3	1.67	0.76
1:C:127:LEU:HD12	1:C:420:ARG:O	1.86	0.76
1:D:96:THR:OG1	1:D:103:ASN:HB3	1.85	0.76
1:D:104:VAL:HG21	1:D:406:GLU:OE1	1.86	0.76
1:A:34:ILE:HB	1:A:77:TYR:OH	1.86	0.75
1:A:343:GLU:HA	1:A:347:GLY:H	1.50	0.75
1:A:267:ARG:HG3	1:A:392:ARG:HG3	1.67	0.75
1:B:147:VAL:O	1:B:360:VAL:HG23	1.86	0.75
1:D:125:ASN:HD22	1:D:423:PRO:HA	1.51	0.75
1:D:175:GLN:O	1:D:245:GLY:HA3	1.85	0.75
1:C:111:MET:HA	1:C:117:TYR:HA	1.69	0.75
1:C:41:LEU:HD23	1:C:70:MET:O	1.86	0.75
1:D:158:TYR:HB3	1:D:185:GLY:HA3	1.68	0.75
1:B:88:ASP:O	1:B:417:SER:HA	1.87	0.75
1:B:134:SER:HB3	4:B:510:HOH:O	1.86	0.75
1:C:188:ASN:HB3	1:C:204:GLY:HA3	1.67	0.75
1:B:292:PHE:HB3	1:B:355:LEU:HD11	1.68	0.74
1:C:226:THR:HG23	1:C:262:ASP:HB3	1.68	0.74
1:A:251:ARG:HH22	2:E:2:BGC:H2	1.52	0.74
1:A:276:LYS:HG3	1:A:283:SER:HB3	1.69	0.74
1:B:325:THR:OG1	1:B:328:LEU:HB2	1.88	0.74
1:B:41:LEU:HD23	1:B:71:ILE:HG23	1.69	0.74
1:C:379:ILE:HA	1:C:390:ALA:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:VAL:HA	1:B:109:TYR:O	1.88	0.74
1:B:123:MET:HE1	1:B:356:ARG:HE	1.51	0.74
1:B:268:MET:HA	1:B:315:TRP:NE1	2.03	0.74
1:C:206:TYR:HA	1:C:238:CYS:O	1.88	0.74
1:A:89:ALA:HA	1:A:417:SER:HB3	1.70	0.73
1:D:349:GLU:HA	1:D:352:ASN:OD1	1.88	0.73
1:A:356:ARG:HH11	1:A:356:ARG:HB2	1.53	0.73
1:A:107:ARG:HG3	1:A:364:SER:HB2	1.70	0.73
1:B:229:ALA:O	1:B:345:VAL:HG21	1.88	0.73
1:D:27:THR:HG23	1:D:29:ASN:HD21	1.53	0.73
1:B:277:GLY:HA2	1:B:281:ASP:OD1	1.88	0.73
1:D:120:PHE:O	1:D:358:PRO:HA	1.88	0.73
1:D:231:THR:OG1	1:D:255:LYS:HB3	1.88	0.73
1:D:264:ASN:HD21	1:D:266:TYR:HB3	1.52	0.73
1:D:354:ALA:O	1:D:357:VAL:HG23	1.88	0.73
1:A:17:GLN:OE1	1:A:420:ARG:HD3	1.89	0.73
1:D:92:LEU:HB2	1:D:414:VAL:HG12	1.71	0.73
1:D:111:MET:HE1	1:D:114:PRO:HA	1.71	0.73
1:D:211:ALA:HB2	1:D:233:ASN:HB3	1.69	0.73
1:A:2:ARG:HH22	1:A:70:MET:HE2	1.51	0.73
1:D:122:LEU:O	1:D:292:PHE:HB2	1.89	0.73
1:A:110:LEU:HB3	1:A:118:GLN:HB3	1.71	0.73
1:B:267:ARG:HB3	1:B:268:MET:HE2	1.69	0.72
1:A:296:LYS:HA	1:A:324:ILE:O	1.88	0.72
1:A:296:LYS:HG3	1:A:325:THR:HG22	1.72	0.72
1:B:240:THR:O	1:B:243:CYS:HB2	1.89	0.72
1:A:266:TYR:HB3	1:A:392:ARG:O	1.89	0.72
1:B:59:CYS:HB3	1:B:189:ILE:HD13	1.70	0.72
1:B:127:LEU:HD11	1:B:419:ILE:HG23	1.70	0.72
1:A:335:VAL:HG23	4:A:467:HOH:O	1.88	0.72
1:D:254:GLY:HA3	4:D:491:HOH:O	1.89	0.72
1:A:19:CYS:HB3	1:A:426:SER:O	1.89	0.72
1:A:354:ALA:O	1:A:357:VAL:HG23	1.90	0.72
1:B:117:TYR:O	1:B:151:GLU:HG3	1.90	0.72
1:B:175:GLN:NE2	3:G:2:BGC:H4	2.05	0.72
1:D:105:GLY:HA2	1:D:365:ILE:HG23	1.71	0.72
1:A:38:TRP:HD1	1:A:103:ASN:HD21	1.38	0.72
1:B:53:ASN:O	1:B:194:SER:HB3	1.89	0.72
1:B:222:ALA:HB3	1:B:376:LEU:O	1.89	0.72
1:D:53:ASN:HA	1:D:200:ASN:O	1.89	0.72
1:C:84:SER:O	1:C:90:LEU:HD12	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ILE:HG22	1:D:39:ARG:NH2	2.05	0.72
1:B:374:LEU:HD23	1:B:378:SER:HB3	1.70	0.71
1:D:39:ARG:HB3	1:D:71:ILE:HG22	1.71	0.71
1:D:41:LEU:HD13	1:D:49:CYS:HB2	1.71	0.71
1:A:32:VAL:HG12	1:A:109:TYR:O	1.90	0.71
1:C:293:GLU:OE1	1:C:296:LYS:HE3	1.89	0.71
1:A:356:ARG:HD3	1:B:20:THR:HB	1.71	0.71
1:B:212:GLU:O	1:B:228:HIS:HB2	1.90	0.71
1:C:19:CYS:HA	1:C:25:CYS:HA	1.72	0.71
1:B:111:MET:HB2	1:B:116:LYS:O	1.89	0.71
1:A:292:PHE:HA	1:A:297:LEU:HD12	1.73	0.71
1:B:101:GLY:HA3	4:B:513:HOH:O	1.90	0.71
1:A:379:ILE:HG21	1:A:385:GLU:HB2	1.72	0.71
1:D:319:PRO:HD3	1:D:331:THR:OG1	1.91	0.71
1:D:401:VAL:HB	1:D:404:GLU:HB2	1.71	0.71
1:B:75:GLY:HA2	1:C:78:LEU:HD12	1.73	0.70
1:D:350:GLN:O	1:D:353:ASN:HB2	1.91	0.70
1:A:275:GLY:O	1:A:281:ASP:HA	1.90	0.70
1:C:1:PCA:HA	1:C:66:ALA:O	1.91	0.70
1:D:39:ARG:HA	4:D:583:HOH:O	1.91	0.70
1:D:189:ILE:HG23	1:D:190:GLU:H	1.56	0.70
1:A:295:ASN:H	1:A:352:ASN:HD21	1.37	0.70
1:D:177:ALA:O	1:D:180:LEU:HG	1.90	0.70
1:B:22:PRO:HD3	1:B:426:SER:HA	1.73	0.70
1:A:59:CYS:HA	1:A:68:LYS:HD3	1.74	0.70
1:B:144:LEU:HD21	1:B:361:LEU:HG	1.74	0.70
1:B:281:ASP:HB3	1:B:284:ARG:HG3	1.73	0.70
1:B:384:LYS:HD2	1:B:387:GLN:HB2	1.74	0.70
1:C:149:MET:SD	1:C:171:TYR:HA	2.32	0.70
1:D:192:TRP:HA	1:D:203:VAL:O	1.91	0.70
1:D:79:GLY:O	1:D:98:HIS:HB3	1.92	0.70
1:D:249:GLU:HG2	4:D:490:HOH:O	1.90	0.70
1:B:6:GLU:OE1	1:C:97:LYS:HG3	1.92	0.69
1:A:173:ASP:HB2	1:A:212:GLU:OE1	1.92	0.69
1:D:361:LEU:CD2	1:D:363:MET:HE2	2.21	0.69
1:A:49:CYS:HA	1:A:58:ALA:O	1.92	0.69
1:D:96:THR:HG23	1:D:103:ASN:O	1.91	0.69
1:A:295:ASN:OD1	1:A:348:PHE:HB3	1.92	0.69
1:C:39:ARG:NH2	1:C:74:ALA:HB2	2.06	0.69
1:C:292:PHE:HB3	1:C:355:LEU:HD22	1.74	0.69
1:C:49:CYS:HA	1:C:56:THR:OG1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:GLU:H	1:C:140:ILE:HD12	1.57	0.69
1:D:62:ALA:HA	1:D:187:ALA:HB3	1.74	0.69
1:D:239:GLU:H	1:D:242:ASN:ND2	1.91	0.69
1:D:372:ASN:HB3	1:D:400:GLY:HA3	1.74	0.69
1:B:156:ALA:O	1:B:159:PRO:HD3	1.93	0.69
1:B:372:ASN:HB2	1:B:374:LEU:HD12	1.75	0.69
1:C:141:ASN:O	1:C:365:ILE:HA	1.93	0.69
1:A:37:ASN:HD22	2:F:1:BGC:H6C2	1.56	0.68
1:A:295:ASN:H	1:A:352:ASN:ND2	1.91	0.68
1:A:269:GLY:O	1:A:271:PRO:HD3	1.92	0.68
1:B:4:GLY:HA2	1:B:70:MET:HE3	1.75	0.68
1:D:251:ARG:NH1	1:D:258:ALA:HB1	2.08	0.68
1:A:84:SER:O	1:A:90:LEU:HD12	1.93	0.68
1:A:319:PRO:HG3	1:A:327:GLU:HG3	1.75	0.68
1:B:34:ILE:HD13	1:B:35:ASP:H	1.59	0.68
1:C:32:VAL:HG12	1:C:109:TYR:O	1.93	0.68
1:C:345:VAL:O	1:C:350:GLN:HG2	1.94	0.68
1:D:163:ALA:HB1	1:D:167:TYR:HB2	1.75	0.68
1:B:110:LEU:O	1:B:118:GLN:HB3	1.94	0.68
1:B:111:MET:HA	1:B:118:GLN:N	2.09	0.68
1:A:149:MET:HE2	1:A:360:VAL:HG21	1.75	0.68
1:C:61:THR:OG1	1:C:64:ASP:HB3	1.92	0.68
1:C:150:GLU:OE2	1:C:157:SER:HB3	1.93	0.68
1:B:12:PRO:HB3	1:B:85:THR:HG21	1.76	0.68
1:C:143:ALA:HB2	1:C:217:GLU:HA	1.76	0.68
1:D:273:PHE:O	1:D:279:THR:HB	1.94	0.68
1:A:177:ALA:O	1:A:207:GLY:HA2	1.93	0.68
1:D:280:LEU:HD22	1:D:303:GLN:OE1	1.94	0.68
1:A:289:VAL:O	1:A:299:GLN:HA	1.94	0.68
1:A:7:THR:HG21	1:A:73:GLY:O	1.95	0.67
1:C:31:GLU:O	1:C:111:MET:HB2	1.93	0.67
1:C:148:ALA:HB2	1:C:359:MET:HG2	1.76	0.67
1:C:183:VAL:HG13	1:C:235:TYR:OH	1.95	0.67
1:C:373:MET:HA	1:C:375:TRP:NE1	2.08	0.67
1:A:132:ASP:HB3	1:A:415:VAL:HG22	1.76	0.67
1:D:176:CYS:HA	1:D:208:SER:O	1.94	0.67
1:D:267:ARG:HA	1:D:391:ALA:O	1.94	0.67
1:B:372:ASN:O	1:B:400:GLY:HA3	1.93	0.67
1:C:302:ILE:HA	1:C:306:ARG:O	1.95	0.67
1:A:224:ALA:HA	1:A:263:TYR:O	1.94	0.67
1:A:340:ASN:HD21	1:A:342:PHE:HB3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASP:OD2	1:B:371:ALA:HB3	1.95	0.67
1:C:37:ASN:HD21	1:C:180:LEU:HA	1.60	0.67
1:C:131:VAL:O	1:C:285:LYS:HA	1.94	0.67
1:A:68:LYS:HG3	1:A:69:CYS:SG	2.35	0.67
1:B:155:MET:HG3	1:B:164:GLY:HA3	1.77	0.67
1:B:374:LEU:O	1:B:380:TYR:HB2	1.94	0.67
1:B:36:ALA:HA	1:B:39:ARG:HG3	1.74	0.66
1:D:35:ASP:HB2	1:D:109:TYR:OH	1.96	0.66
1:A:122:LEU:HG	1:A:359:MET:HG3	1.76	0.66
1:A:325:THR:OG1	1:A:327:GLU:HG2	1.95	0.66
1:C:207:GLY:O	1:C:237:VAL:HG13	1.95	0.66
1:D:71:ILE:HD12	1:D:167:TYR:HB3	1.76	0.66
1:D:251:ARG:HG3	1:D:251:ARG:HH11	1.60	0.66
1:B:36:ALA:HB2	1:B:169:THR:HG22	1.77	0.66
1:A:83:ALA:HA	1:A:91:THR:O	1.96	0.66
1:A:196:THR:HG23	4:A:511:HOH:O	1.94	0.66
1:D:401:VAL:O	1:D:405:VAL:HG22	1.95	0.66
1:A:64:ASP:O	1:A:68:LYS:HG2	1.96	0.66
1:B:154:GLY:HA2	1:B:157:SER:OG	1.96	0.66
1:C:384:LYS:HE3	1:C:387:GLN:HE22	1.60	0.66
1:D:264:ASN:ND2	1:D:267:ARG:H	1.94	0.66
1:B:94:PHE:HA	1:B:365:ILE:HG21	1.77	0.66
1:D:149:MET:HG2	1:D:171:TYR:HA	1.77	0.66
1:D:268:MET:O	1:D:313:PRO:HA	1.96	0.66
1:B:401:VAL:HG12	1:B:404:GLU:HB2	1.78	0.66
1:C:173:ASP:HB2	1:C:212:GLU:OE1	1.96	0.66
1:B:350:GLN:HA	1:B:353:ASN:OD1	1.95	0.65
1:B:376:LEU:O	1:B:376:LEU:HG	1.95	0.65
1:D:166:ARG:HD2	1:D:167:TYR:HE2	1.61	0.65
1:B:401:VAL:HG11	1:B:404:GLU:OE2	1.96	0.65
1:C:349:GLU:O	1:C:352:ASN:HB2	1.95	0.65
1:D:155:MET:SD	1:D:164:GLY:HA2	2.36	0.65
1:D:230:CYS:HB2	1:D:232:THR:O	1.96	0.65
1:A:57:ASN:HB2	4:A:457:HOH:O	1.97	0.65
1:D:110:LEU:HD12	1:D:111:MET:N	2.12	0.65
1:A:2:ARG:HA	1:A:162:GLN:OE1	1.96	0.65
1:B:134:SER:OG	1:B:283:SER:HA	1.96	0.65
1:D:64:ASP:OD1	1:D:68:LYS:HD2	1.97	0.65
1:C:39:ARG:HA	1:C:39:ARG:HH11	1.62	0.64
1:A:257:ASP:OD2	1:A:260:GLY:HA2	1.96	0.64
1:B:111:MET:HE2	1:B:116:LYS:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:SER:O	1:A:392:ARG:HB2	1.97	0.64
1:C:307:LYS:HD3	1:D:304:ASP:HB3	1.79	0.64
1:D:134:SER:O	1:D:135:THR:HG23	1.98	0.64
1:B:141:ASN:HB3	1:B:366:TRP:NE1	2.12	0.64
1:C:306:ARG:HH21	1:D:305:GLY:N	1.94	0.64
1:A:146:PHE:HA	1:A:360:VAL:O	1.98	0.64
1:B:76:ASP:OD1	1:C:76:ASP:HA	1.97	0.64
1:C:91:THR:OG1	1:C:415:VAL:HB	1.97	0.64
1:C:182:PHE:HA	1:C:186:LYS:O	1.97	0.64
1:A:2:ARG:NH2	1:A:70:MET:HE2	2.13	0.64
1:B:81:TYR:HA	1:B:103:ASN:ND2	2.12	0.64
1:B:275:GLY:HA3	1:B:278:LYS:HD2	1.80	0.64
1:D:263:TYR:OH	1:D:313:PRO:HD3	1.97	0.64
1:A:133:LEU:HD11	1:A:286:PHE:HZ	1.63	0.64
1:A:257:ASP:OD1	1:A:341:ARG:HB3	1.98	0.64
1:A:340:ASN:O	1:A:344:GLU:HB2	1.97	0.64
1:C:40:TRP:O	1:C:71:ILE:HA	1.98	0.64
1:D:13:PRO:O	1:D:85:THR:HG21	1.98	0.64
1:D:49:CYS:HA	1:D:58:ALA:HB3	1.79	0.64
1:B:230:CYS:HB3	1:B:255:LYS:O	1.97	0.64
1:D:147:VAL:O	1:D:359:MET:HB3	1.98	0.64
1:D:264:ASN:HB3	1:D:267:ARG:HB3	1.80	0.64
1:A:61:THR:HB	1:A:190:GLU:OE1	1.98	0.63
1:B:205:PRO:HA	1:B:240:THR:HG23	1.80	0.63
1:B:227:PRO:HB2	1:B:351:LEU:HD11	1.80	0.63
1:C:39:ARG:HD2	1:C:167:TYR:HB3	1.80	0.63
1:B:48:ASN:OD1	1:C:99:GLU:HG3	1.98	0.63
1:B:183:VAL:HG21	1:B:206:TYR:O	1.98	0.63
1:B:21:ALA:HA	1:B:426:SER:HB3	1.81	0.63
1:B:117:TYR:HB2	1:B:151:GLU:HA	1.79	0.63
1:C:130:ASP:HA	1:C:286:PHE:O	1.98	0.63
1:A:146:PHE:O	1:A:147:VAL:HG13	1.98	0.63
1:C:95:VAL:HG22	1:C:104:VAL:HG22	1.79	0.63
1:C:353:ASN:O	1:C:357:VAL:HG23	1.98	0.63
1:D:295:ASN:H	1:D:352:ASN:HD21	1.46	0.63
1:B:31:GLU:O	1:B:31:GLU:HG2	1.99	0.63
1:A:38:TRP:CD1	1:A:103:ASN:HD21	2.16	0.63
1:D:329:CYS:O	1:D:332:MET:HB3	1.98	0.63
1:C:153:GLY:HA3	1:C:165:ALA:N	2.14	0.63
1:A:215:VAL:HA	1:A:225:PHE:CD2	2.33	0.62
1:B:64:ASP:O	1:B:68:LYS:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:ASN:HA	1:A:348:PHE:CD2	2.34	0.62
1:B:88:ASP:HB2	1:B:418:ASN:H	1.63	0.62
1:C:288:VAL:HG13	1:C:299:GLN:NE2	2.14	0.62
1:C:35:ASP:OD2	1:C:37:ASN:HB2	1.99	0.62
1:A:164:GLY:O	1:A:169:THR:HG23	1.99	0.62
1:B:109:TYR:CE1	1:B:149:MET:HE1	2.35	0.62
1:D:149:MET:SD	1:D:171:TYR:HA	2.39	0.62
1:A:151:GLU:HB2	4:A:439:HOH:O	1.98	0.62
1:C:198:ASP:HB2	1:C:369:HIS:CD2	2.34	0.62
1:C:317:GLY:O	1:C:331:THR:HB	2.00	0.62
1:B:6:GLU:HA	4:B:507:HOH:O	1.98	0.62
1:B:384:LYS:HD3	1:B:385:GLU:N	2.14	0.62
1:C:195:SER:HB3	1:C:201:ALA:O	2.00	0.62
1:C:366:TRP:HB3	4:C:493:HOH:O	1.98	0.62
1:D:31:GLU:HG3	1:D:111:MET:HB2	1.81	0.62
1:A:37:ASN:OD1	1:A:181:LYS:HD3	1.99	0.62
1:B:286:PHE:HB3	1:B:303:GLN:NE2	2.14	0.62
1:C:115:ASP:HA	1:C:166:ARG:HG2	1.82	0.62
1:B:123:MET:HE1	1:B:356:ARG:HH21	1.64	0.61
1:C:141:ASN:HB2	1:C:373:MET:SD	2.40	0.61
1:A:144:LEU:HD21	1:A:361:LEU:HD11	1.80	0.61
1:A:343:GLU:HG2	1:A:347:GLY:HA2	1.81	0.61
1:C:95:VAL:HA	1:C:103:ASN:O	2.00	0.61
1:C:136:VAL:HG22	1:C:413:GLN:O	2.00	0.61
1:C:265:PRO:HG3	1:C:310:ILE:HG23	1.80	0.61
1:D:203:VAL:HG12	1:D:204:GLY:O	2.00	0.61
1:A:141:ASN:O	1:A:365:ILE:HA	1.99	0.61
1:A:286:PHE:HB3	1:A:303:GLN:NE2	2.15	0.61
1:C:264:ASN:H	1:C:268:MET:HE3	1.66	0.61
1:C:420:ARG:HD2	1:C:427:THR:HB	1.82	0.61
1:A:4:GLY:HA2	1:A:70:MET:SD	2.40	0.61
1:C:18:ARG:HB3	1:C:26:GLN:HG2	1.82	0.61
1:C:232:THR:HG22	1:C:234:GLU:HG2	1.83	0.61
1:A:84:SER:O	1:A:90:LEU:HA	2.01	0.61
1:D:34:ILE:HG23	1:D:35:ASP:O	2.00	0.61
1:D:179:ASP:HB3	1:D:247:TYR:CE1	2.36	0.61
1:A:141:ASN:HB3	1:A:366:TRP:NE1	2.15	0.61
1:A:264:ASN:HB3	1:A:267:ARG:HB2	1.83	0.61
1:C:92:LEU:O	1:C:413:GLN:HA	2.00	0.61
1:D:163:ALA:HB3	1:D:169:THR:HG21	1.82	0.61
1:D:50:TYR:O	1:D:51:ASP:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:PRO:HD2	1:D:399:SER:HB2	1.82	0.61
1:A:42:HIS:HA	1:A:48:ASN:HA	1.83	0.61
1:C:89:ALA:HB2	1:C:417:SER:HB3	1.81	0.61
1:A:114:PRO:O	1:A:166:ARG:HB2	2.00	0.60
1:A:377:ASP:HB2	1:A:395:CYS:SG	2.41	0.60
1:B:315:TRP:CH2	1:B:388:PRO:HB3	2.37	0.60
1:C:22:PRO:HG3	1:C:425:GLY:O	2.00	0.60
1:C:346:GLY:HA3	1:C:350:GLN:HB2	1.83	0.60
1:B:126:GLU:OE1	1:B:291:ARG:HG2	2.01	0.60
1:D:239:GLU:H	1:D:242:ASN:HD22	1.46	0.60
1:A:50:TYR:HA	1:A:55:TRP:HA	1.82	0.60
1:A:73:GLY:O	1:D:99:GLU:HG3	2.01	0.60
1:A:336:PHE:CD1	1:A:388:PRO:HB2	2.37	0.60
1:A:380:TYR:CD1	1:A:382:PRO:HD3	2.36	0.60
1:B:267:ARG:HG2	1:B:389:GLY:HA2	1.83	0.60
1:C:34:ILE:HG22	1:C:77:TYR:OH	2.02	0.60
1:D:206:TYR:CD2	1:D:239:GLU:HG3	2.36	0.60
1:A:188:ASN:OD1	1:A:206:TYR:HB2	2.01	0.60
1:C:41:LEU:HG	1:C:71:ILE:HG22	1.84	0.60
1:A:55:TRP:HB3	1:A:189:ILE:HD12	1.84	0.60
1:C:155:MET:HG3	1:C:161:ASN:O	2.02	0.60
1:C:264:ASN:O	1:C:268:MET:HG2	2.02	0.60
1:A:1:PCA:HG2	1:A:71:ILE:HD11	1.84	0.60
1:A:110:LEU:HD12	1:A:111:MET:H	1.67	0.60
1:A:268:MET:HE2	1:A:332:MET:HE3	1.83	0.60
1:A:262:ASP:O	1:A:332:MET:HE1	2.01	0.59
1:A:357:VAL:HG12	1:A:358:PRO:HD2	1.83	0.59
1:B:255:LYS:HG2	4:B:578:HOH:O	2.01	0.59
1:C:133:LEU:HD11	1:C:286:PHE:CZ	2.37	0.59
1:B:301:PHE:O	1:B:307:LYS:HG2	2.02	0.59
1:D:125:ASN:HB3	1:D:422:GLY:O	2.02	0.59
1:D:182:PHE:O	1:D:183:VAL:HG23	2.01	0.59
1:A:377:ASP:O	1:A:395:CYS:HB2	2.02	0.59
1:B:42:HIS:ND1	1:B:46:MET:HA	2.17	0.59
1:B:144:LEU:HD23	1:B:362:VAL:O	2.02	0.59
1:D:375:TRP:CH2	2:I:2:BGC:H5	2.37	0.59
1:D:385:GLU:O	1:D:387:GLN:HG3	2.02	0.59
1:A:119:MET:HA	1:A:359:MET:O	2.02	0.59
1:D:107:ARG:HH11	2:J:1:BGC:H2	1.67	0.59
1:B:35:ASP:O	1:B:38:TRP:HB2	2.02	0.59
1:C:183:VAL:HG13	1:C:208:SER:OG	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HG23	1:A:35:ASP:O	2.02	0.59
1:B:179:ASP:HB3	1:B:247:TYR:CE2	2.38	0.59
1:C:122:LEU:HD23	1:C:292:PHE:CD2	2.38	0.59
1:C:183:VAL:O	1:C:186:LYS:HG2	2.03	0.59
1:C:225:PHE:O	1:C:262:ASP:HA	2.03	0.59
1:C:307:LYS:HB2	1:C:430:PHE:CE2	2.38	0.59
1:D:17:GLN:O	1:D:420:ARG:HA	2.03	0.59
1:A:1:PCA:HA	1:A:66:ALA:O	2.02	0.58
1:A:231:THR:HG21	4:A:480:HOH:O	2.02	0.58
1:B:11:HIS:HB3	1:B:31:GLU:HG3	1.83	0.58
1:A:288:VAL:HG22	1:A:301:PHE:HE2	1.67	0.58
1:B:122:LEU:HD11	1:B:146:PHE:CE1	2.37	0.58
1:A:147:VAL:HG12	1:A:212:GLU:HA	1.83	0.58
1:B:213:ILE:HG21	1:B:292:PHE:HE2	1.68	0.58
1:C:126:GLU:OE1	1:C:424:ILE:HA	2.04	0.58
1:B:111:MET:HE1	1:B:165:ALA:HB1	1.85	0.58
1:B:265:PRO:O	1:B:270:ASN:HB2	2.02	0.58
1:B:353:ASN:HA	1:B:356:ARG:HG3	1.85	0.58
1:D:47:GLN:HG2	1:D:58:ALA:HB2	1.86	0.58
1:B:30:ALA:HB1	1:B:111:MET:O	2.03	0.58
1:B:291:ARG:HD3	1:B:424:ILE:HG23	1.86	0.58
1:C:209:CYS:O	1:C:235:TYR:HA	2.04	0.58
1:C:381:PRO:HD3	4:C:433:HOH:O	2.02	0.58
1:D:366:TRP:CD1	2:J:1:BGC:H3	2.39	0.58
1:B:374:LEU:HD23	1:B:378:SER:CB	2.34	0.58
1:C:402:PRO:O	1:C:406:GLU:HG3	2.04	0.58
1:A:142:SER:HA	1:A:364:SER:O	2.03	0.58
1:A:296:LYS:O	1:A:297:LEU:HD13	2.03	0.58
1:D:111:MET:HA	1:D:117:TYR:HA	1.86	0.58
1:C:33:VAL:O	1:C:108:PHE:HA	2.03	0.58
1:D:132:ASP:OD1	1:D:134:SER:HB3	2.03	0.58
1:D:155:MET:CE	1:D:164:GLY:HA2	2.34	0.58
1:B:209:CYS:HB2	1:B:236:HIS:NE2	2.18	0.58
1:A:148:ALA:HB2	1:A:359:MET:HE2	1.85	0.58
1:A:251:ARG:NH2	2:E:2:BGC:H2	2.17	0.58
1:B:231:THR:HG23	1:B:345:VAL:HB	1.85	0.58
1:C:306:ARG:NH2	1:D:305:GLY:H	2.00	0.58
1:C:341:ARG:O	1:C:341:ARG:HG3	2.04	0.58
1:D:144:LEU:HD23	1:D:144:LEU:O	2.04	0.58
1:D:155:MET:HG3	1:D:161:ASN:O	2.03	0.58
1:A:250:ASP:HB3	1:A:253:ALA:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:PHE:CZ	1:B:297:LEU:HD23	2.39	0.57
1:C:211:ALA:HB2	1:C:233:ASN:OD1	2.04	0.57
1:D:31:GLU:OE2	1:D:114:PRO:HD3	2.04	0.57
1:A:183:VAL:HG21	1:A:206:TYR:O	2.04	0.57
1:C:143:ALA:CB	1:C:217:GLU:HA	2.33	0.57
1:A:29:ASN:N	1:A:29:ASN:HD22	2.01	0.57
1:A:90:LEU:HD12	1:A:91:THR:H	1.69	0.57
1:A:111:MET:HE1	1:A:166:ARG:HA	1.86	0.57
1:A:295:ASN:N	1:A:352:ASN:HD21	2.02	0.57
1:A:307:LYS:HD3	1:A:430:PHE:HB3	1.86	0.57
1:B:122:LEU:HD21	1:B:146:PHE:CD1	2.39	0.57
1:B:128:ALA:CB	1:B:289:VAL:HG22	2.35	0.57
1:B:149:MET:HB2	1:B:360:VAL:HG21	1.85	0.57
1:B:327:GLU:O	1:B:331:THR:HG23	2.04	0.57
1:D:163:ALA:HB1	1:D:167:TYR:CB	2.34	0.57
1:B:151:GLU:HG2	1:B:151:GLU:O	2.04	0.57
1:B:105:GLY:HA2	1:B:365:ILE:CG2	2.34	0.57
1:C:325:THR:HG21	4:C:453:HOH:O	2.04	0.57
1:B:335:VAL:HG12	1:B:336:PHE:HD1	1.70	0.57
1:C:127:LEU:HG	1:C:128:ALA:H	1.69	0.57
1:D:35:ASP:HB2	1:D:109:TYR:CZ	2.39	0.57
1:A:351:LEU:O	1:A:355:LEU:HG	2.05	0.57
1:C:381:PRO:HB2	1:C:383:GLU:OE2	2.05	0.57
1:C:106:SER:HG	1:C:108:PHE:HE1	1.53	0.57
1:A:177:ALA:HB1	1:A:180:LEU:HG	1.85	0.57
1:C:121:ASN:O	1:C:421:PHE:HZ	1.88	0.57
1:B:335:VAL:HG12	1:B:336:PHE:CD1	2.39	0.57
1:C:296:LYS:HD2	1:C:323:GLU:OE2	2.05	0.57
1:C:401:VAL:CG1	1:C:404:GLU:HB2	2.35	0.57
1:D:264:ASN:ND2	1:D:266:TYR:HB3	2.18	0.57
1:A:77:TYR:HB3	1:A:83:ALA:HB3	1.86	0.56
1:A:202:GLY:O	1:A:203:VAL:HG23	2.04	0.56
1:C:295:ASN:H	1:C:352:ASN:HD21	1.52	0.56
1:A:280:LEU:HD22	1:A:308:ILE:HG21	1.87	0.56
1:B:295:ASN:HA	1:B:348:PHE:CE2	2.40	0.56
1:A:39:ARG:HA	1:D:99:GLU:OE2	2.05	0.56
1:A:112:ASN:O	1:A:116:LYS:HD2	2.05	0.56
1:A:257:ASP:CB	1:A:341:ARG:HG2	2.35	0.56
1:B:144:LEU:HA	1:B:362:VAL:O	2.04	0.56
1:B:213:ILE:HG21	1:B:292:PHE:CE2	2.41	0.56
1:B:217:GLU:O	1:B:376:LEU:HD11	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:PHE:CB	1:B:355:LEU:HD11	2.35	0.56
1:B:301:PHE:HB2	1:B:308:ILE:HB	1.87	0.56
1:D:3:ALA:HB1	1:D:167:TYR:OH	2.04	0.56
1:A:155:MET:HG3	1:A:161:ASN:O	2.06	0.56
1:B:42:HIS:HB2	1:B:47:GLN:O	2.04	0.56
1:B:71:ILE:HD11	1:B:163:ALA:CB	2.35	0.56
1:D:111:MET:CE	1:D:114:PRO:HA	2.35	0.56
1:D:423:PRO:HD2	1:D:426:SER:OG	2.04	0.56
1:D:18:ARG:HA	1:D:421:PHE:O	2.05	0.56
1:D:81:TYR:O	1:D:96:THR:HG21	2.06	0.56
1:D:265:PRO:HA	1:D:268:MET:HB2	1.87	0.56
1:D:195:SER:HB3	1:D:198:ASP:HB3	1.87	0.56
1:A:178:ARG:HB2	1:A:247:TYR:HB2	1.87	0.56
1:B:350:GLN:O	1:B:350:GLN:HG3	2.05	0.56
1:D:125:ASN:HD22	1:D:423:PRO:CA	2.19	0.56
1:D:372:ASN:HD22	1:D:402:PRO:HD3	1.71	0.56
1:A:233:ASN:N	1:A:233:ASN:HD22	2.04	0.56
1:D:61:THR:HG22	1:D:190:GLU:OE1	2.06	0.56
1:D:215:VAL:HG22	1:D:225:PHE:CE2	2.40	0.56
1:A:133:LEU:HD11	1:A:286:PHE:CZ	2.40	0.56
1:A:288:VAL:HG22	1:A:301:PHE:CE2	2.40	0.56
1:B:42:HIS:CE1	1:B:46:MET:HA	2.41	0.56
1:B:368:ASP:O	1:B:372:ASN:HA	2.06	0.56
1:D:2:ARG:HE	1:D:67:GLU:HA	1.71	0.56
1:C:122:LEU:HB3	1:C:292:PHE:CG	2.41	0.55
1:A:170:GLY:O	1:A:235:TYR:HE1	1.88	0.55
1:A:281:ASP:OD2	1:A:284:ARG:HD2	2.06	0.55
1:A:353:ASN:N	1:A:353:ASN:HD22	2.03	0.55
1:B:135:THR:O	1:B:412:ALA:HB1	2.05	0.55
1:B:301:PHE:O	1:B:307:LYS:HA	2.06	0.55
1:C:125:ASN:HB3	1:C:422:GLY:O	2.06	0.55
1:D:132:ASP:HB3	1:D:415:VAL:CG1	2.37	0.55
1:B:318:MET:HE3	1:B:335:VAL:HG11	1.89	0.55
1:D:141:ASN:O	1:D:365:ILE:HA	2.06	0.55
1:A:1:PCA:HG3	1:A:182:PHE:CE1	2.42	0.55
1:C:125:ASN:HD22	1:C:422:GLY:C	2.15	0.55
1:C:182:PHE:CE1	1:C:187:ALA:HB2	2.42	0.55
1:D:391:ALA:HB3	4:D:549:HOH:O	2.06	0.55
1:B:130:ASP:HA	1:B:286:PHE:O	2.06	0.55
1:A:252:PHE:HB3	1:A:341:ARG:HH11	1.72	0.55
1:A:289:VAL:HG21	1:A:300:TYR:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ALA:HB1	1:C:160:SER:OG	2.07	0.55
1:C:110:LEU:HD23	1:C:361:LEU:O	2.06	0.55
1:C:233:ASN:OD1	1:C:354:ALA:HB2	2.06	0.55
1:C:265:PRO:CA	1:C:270:ASN:HD22	2.17	0.55
1:C:95:VAL:CG2	1:C:104:VAL:HG22	2.36	0.55
1:B:163:ALA:O	1:B:166:ARG:HD2	2.07	0.55
1:C:340:ASN:OD1	1:C:343:GLU:HB2	2.07	0.55
1:A:367:ASP:OD2	1:A:402:PRO:HB3	2.07	0.55
1:B:379:ILE:HB	1:B:397:THR:CG2	2.37	0.55
1:B:401:VAL:CG1	1:B:404:GLU:HB2	2.35	0.55
1:D:21:ALA:HB3	1:D:24:ASN:ND2	2.04	0.55
1:D:342:PHE:CZ	1:D:348:PHE:HA	2.41	0.55
1:A:37:ASN:ND2	2:F:1:BGC:H6C2	2.22	0.55
1:A:324:ILE:HG22	1:A:348:PHE:CZ	2.42	0.55
1:B:175:GLN:HE22	3:G:2:BGC:H4	1.72	0.55
1:B:233:ASN:HB2	1:B:357:VAL:HG21	1.88	0.55
1:B:297:LEU:HB2	1:B:324:ILE:HB	1.88	0.55
1:D:95:VAL:CG1	1:D:97:LYS:HE2	2.37	0.55
1:D:109:TYR:CD1	1:D:362:VAL:HG22	2.42	0.55
1:D:377:ASP:HB2	1:D:395:CYS:SG	2.47	0.55
1:C:263:TYR:CZ	1:C:322:SER:HA	2.41	0.54
1:C:292:PHE:HB3	1:C:355:LEU:CD2	2.37	0.54
1:D:267:ARG:HG2	1:D:267:ARG:O	2.06	0.54
1:A:350:GLN:O	1:A:353:ASN:HB2	2.07	0.54
1:B:13:PRO:HA	1:B:31:GLU:CB	2.37	0.54
1:B:175:GLN:OE1	1:B:258:ALA:HB1	2.07	0.54
1:B:223:PHE:O	1:B:264:ASN:HB2	2.07	0.54
1:B:374:LEU:HD21	1:B:397:THR:HA	1.88	0.54
1:D:206:TYR:CE2	1:D:239:GLU:HG3	2.42	0.54
1:A:55:TRP:CE3	1:A:189:ILE:HD12	2.43	0.54
1:B:50:TYR:HD1	1:B:55:TRP:HA	1.72	0.54
1:B:122:LEU:CD2	1:B:213:ILE:HD13	2.38	0.54
1:C:94:PHE:CE2	1:C:95:VAL:HG23	2.42	0.54
1:C:128:ALA:HA	1:C:288:VAL:O	2.07	0.54
1:C:306:ARG:HE	1:D:305:GLY:N	2.05	0.54
1:C:369:HIS:HA	1:C:402:PRO:HG3	1.90	0.54
1:D:96:THR:HG1	1:D:103:ASN:HB3	1.72	0.54
1:B:42:HIS:HE1	1:B:46:MET:HE3	1.73	0.54
1:C:109:TYR:CD1	1:C:362:VAL:HG13	2.42	0.54
1:C:229:ALA:HB1	1:C:233:ASN:OD1	2.08	0.54
1:A:141:ASN:OD1	1:A:143:ALA:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:PHE:CE2	1:A:340:ASN:HA	2.43	0.54
1:B:59:CYS:HB3	1:B:189:ILE:CD1	2.36	0.54
1:C:375:TRP:H	1:C:375:TRP:CD1	2.25	0.54
1:D:198:ASP:OD1	1:D:201:ALA:HB3	2.08	0.54
1:D:289:VAL:HB	1:D:300:TYR:CE2	2.43	0.54
1:D:291:ARG:CG	1:D:298:SER:HB3	2.34	0.54
1:A:41:LEU:HD12	1:A:49:CYS:HB2	1.89	0.54
1:A:295:ASN:H	1:A:352:ASN:CG	2.15	0.54
1:C:14:LEU:HD12	1:C:15:THR:H	1.73	0.54
1:C:230:CYS:HB3	1:C:256:CYS:HA	1.90	0.54
1:C:6:GLU:HB3	1:C:72:GLU:OE2	2.08	0.54
1:B:82:GLY:HA3	1:B:93:LYS:HB3	1.88	0.54
1:C:198:ASP:HB2	1:C:369:HIS:NE2	2.23	0.54
1:A:65:CYS:HA	1:A:68:LYS:HG2	1.90	0.54
1:A:197:SER:O	1:A:199:PRO:HD3	2.08	0.54
1:B:95:VAL:HG22	1:B:104:VAL:HG22	1.89	0.54
1:B:112:ASN:HB2	1:B:118:GLN:OE1	2.07	0.54
1:A:36:ALA:HA	1:A:39:ARG:HD2	1.88	0.53
1:A:82:GLY:O	1:A:93:LYS:HG3	2.08	0.53
1:A:217:GLU:O	1:A:223:PHE:HB2	2.09	0.53
1:B:92:LEU:HD22	1:B:106:SER:HB3	1.90	0.53
1:B:287:THR:HB	1:B:302:ILE:HB	1.90	0.53
1:B:333:PHE:CD2	1:B:340:ASN:HA	2.43	0.53
1:D:27:THR:HG23	1:D:29:ASN:ND2	2.21	0.53
1:D:107:ARG:HA	1:D:364:SER:HB3	1.90	0.53
1:D:272:ASP:HA	1:D:278:LYS:HD3	1.88	0.53
1:A:319:PRO:CG	1:A:327:GLU:HG3	2.38	0.53
1:B:19:CYS:HA	1:B:25:CYS:HA	1.88	0.53
1:B:117:TYR:CE2	1:B:149:MET:HE2	2.42	0.53
1:C:31:GLU:HG3	1:C:111:MET:CE	2.38	0.53
1:D:11:HIS:CD2	1:D:33:VAL:HB	2.44	0.53
1:A:372:ASN:HB3	1:A:400:GLY:HA3	1.91	0.53
1:B:127:LEU:HD12	1:B:420:ARG:O	2.08	0.53
1:B:384:LYS:HE2	1:B:384:LYS:HA	1.90	0.53
1:A:92:LEU:HD22	1:A:108:PHE:CE1	2.44	0.53
1:B:34:ILE:HG12	1:B:108:PHE:CE1	2.43	0.53
1:C:126:GLU:CD	1:C:425:GLY:H	2.16	0.53
1:C:135:THR:HG22	1:C:412:ALA:HA	1.90	0.53
1:D:58:ALA:O	1:D:68:LYS:HD3	2.08	0.53
1:D:149:MET:CG	1:D:171:TYR:HA	2.39	0.53
1:A:82:GLY:O	1:A:93:LYS:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASN:O	1:A:400:GLY:HA3	2.08	0.53
1:A:46:MET:HB3	4:A:526:HOH:O	2.08	0.53
1:B:142:SER:HB2	1:B:414:VAL:HG11	1.90	0.53
1:B:178:ARG:HH11	1:B:178:ARG:HB3	1.73	0.53
1:B:340:ASN:CG	1:B:343:GLU:HB2	2.34	0.53
1:D:77:TYR:O	1:D:81:TYR:HB2	2.08	0.53
1:D:377:ASP:O	1:D:395:CYS:HB2	2.07	0.53
1:A:37:ASN:O	2:F:2:BGC:H3	2.09	0.53
1:A:99:GLU:HG3	1:D:40:TRP:CD1	2.42	0.53
1:B:22:PRO:CD	1:B:426:SER:HA	2.38	0.53
1:B:55:TRP:HE1	1:B:192:TRP:CG	2.27	0.53
1:B:68:LYS:HG3	1:B:68:LYS:O	2.09	0.53
1:D:65:CYS:HB3	1:D:182:PHE:CZ	2.44	0.53
1:D:297:LEU:HB2	1:D:324:ILE:HB	1.89	0.53
1:B:123:MET:HE1	1:B:356:ARG:NE	2.21	0.53
1:C:286:PHE:HB3	1:C:303:GLN:HG3	1.90	0.53
1:C:319:PRO:CG	1:C:328:LEU:HD23	2.39	0.53
1:D:40:TRP:O	1:D:72:GLU:HG2	2.09	0.53
1:A:38:TRP:CE2	2:F:2:BGC:H5	2.44	0.53
1:A:233:ASN:HD22	1:A:233:ASN:H	1.56	0.53
1:B:193:LYS:HA	4:B:501:HOH:O	2.09	0.53
1:B:226:THR:OG1	1:B:262:ASP:HB2	2.09	0.53
1:C:130:ASP:OD2	1:C:418:ASN:HB3	2.09	0.53
1:C:188:ASN:O	1:C:192:TRP:HE3	1.92	0.53
1:C:193:LYS:HB2	1:C:203:VAL:HB	1.90	0.53
1:C:198:ASP:HB3	1:C:201:ALA:HB3	1.90	0.53
1:C:384:LYS:CE	1:C:387:GLN:HE22	2.21	0.53
1:D:20:THR:OG1	1:D:24:ASN:HB3	2.09	0.53
1:D:92:LEU:HB2	1:D:414:VAL:CG1	2.38	0.53
1:A:132:ASP:HB3	1:A:415:VAL:HG13	1.90	0.53
1:C:13:PRO:HA	1:C:31:GLU:HB3	1.90	0.53
1:C:384:LYS:CD	1:C:387:GLN:HE22	2.22	0.53
1:D:92:LEU:O	1:D:413:GLN:HB2	2.08	0.53
1:D:122:LEU:HD11	1:D:146:PHE:CD1	2.44	0.53
1:B:229:ALA:HB3	4:B:557:HOH:O	2.07	0.52
1:C:133:LEU:O	1:C:220:ALA:HB2	2.09	0.52
1:B:146:PHE:HE2	1:B:361:LEU:HB2	1.73	0.52
1:D:266:TYR:HB2	4:D:512:HOH:O	2.08	0.52
1:A:195:SER:HB3	4:A:518:HOH:O	2.09	0.52
1:A:336:PHE:HD1	1:A:388:PRO:HB2	1.75	0.52
1:C:143:ALA:HA	1:C:216:TRP:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:ARG:O	1:C:344:GLU:HB3	2.09	0.52
1:C:369:HIS:CE1	1:C:402:PRO:HB3	2.43	0.52
1:B:92:LEU:HD22	1:B:106:SER:CB	2.39	0.52
1:B:141:ASN:HD21	1:B:217:GLU:HB3	1.75	0.52
1:C:288:VAL:HG22	1:C:301:PHE:CE2	2.45	0.52
1:A:50:TYR:CA	1:A:56:THR:HG23	2.40	0.52
1:B:274:TYR:CD1	1:B:280:LEU:HD12	2.45	0.52
1:C:120:PHE:HB2	1:C:146:PHE:CE2	2.44	0.52
1:D:213:ILE:HG22	1:D:213:ILE:O	2.09	0.52
1:A:86:SER:HB3	1:A:89:ALA:HB3	1.92	0.52
1:D:2:ARG:HB2	1:D:70:MET:HB3	1.90	0.52
1:B:1:PCA:O	1:B:162:GLN:HG3	2.10	0.52
1:B:267:ARG:HB3	1:B:268:MET:CE	2.37	0.52
1:C:147:VAL:HG12	1:C:212:GLU:CB	2.40	0.52
1:A:356:ARG:HH11	1:A:356:ARG:CB	2.23	0.52
1:B:379:ILE:HB	1:B:397:THR:HG21	1.91	0.52
1:C:144:LEU:HD11	1:C:361:LEU:HD21	1.90	0.52
1:A:17:GLN:O	1:A:17:GLN:HG2	2.07	0.52
1:A:226:THR:HG22	1:A:228:HIS:CD2	2.45	0.52
1:A:292:PHE:HA	1:A:297:LEU:CD1	2.39	0.52
1:B:130:ASP:CG	1:B:418:ASN:HD22	2.17	0.52
1:B:176:CYS:O	1:B:178:ARG:HG2	2.10	0.52
1:B:420:ARG:HB2	1:B:427:THR:CG2	2.38	0.52
1:D:95:VAL:HG11	1:D:97:LYS:HE2	1.90	0.52
1:A:173:ASP:HB2	1:A:212:GLU:CD	2.35	0.52
1:D:12:PRO:HD2	1:D:32:VAL:O	2.10	0.52
1:A:41:LEU:O	1:A:48:ASN:HA	2.10	0.51
1:C:19:CYS:HB3	1:C:24:ASN:O	2.11	0.51
1:C:32:VAL:HG12	1:C:109:TYR:C	2.35	0.51
1:C:257:ASP:CG	1:C:260:GLY:H	2.18	0.51
1:A:20:THR:HG23	1:A:24:ASN:O	2.10	0.51
1:A:132:ASP:HB3	1:A:415:VAL:CG2	2.40	0.51
1:A:287:THR:O	1:A:301:PHE:HA	2.09	0.51
1:A:324:ILE:HG22	1:A:348:PHE:CE1	2.45	0.51
1:B:10:ASN:O	1:B:77:TYR:HE1	1.93	0.51
1:B:172:CYS:HB2	1:B:209:CYS:O	2.10	0.51
1:B:345:VAL:HG23	1:B:345:VAL:O	2.10	0.51
1:C:34:ILE:HD12	1:C:108:PHE:CZ	2.46	0.51
1:C:110:LEU:HD21	1:C:363:MET:HE2	1.92	0.51
1:D:41:LEU:O	1:D:42:HIS:HB3	2.10	0.51
1:D:139:GLY:HA2	1:D:373:MET:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:ALA:HA	1:D:216:TRP:O	2.09	0.51
1:D:299:GLN:O	1:D:299:GLN:HG2	2.09	0.51
1:A:198:ASP:HB3	1:A:201:ALA:HB3	1.91	0.51
1:C:131:VAL:HG22	1:C:133:LEU:HG	1.92	0.51
1:C:193:LYS:HD2	1:C:203:VAL:CG1	2.40	0.51
1:D:211:ALA:CB	1:D:233:ASN:HB3	2.39	0.51
1:D:4:GLY:HA3	1:D:72:GLU:OE2	2.10	0.51
1:D:80:THR:HG23	1:D:98:HIS:CD2	2.45	0.51
1:A:268:MET:CE	1:A:332:MET:HE3	2.40	0.51
1:B:325:THR:HB	1:B:326:PRO:HD2	1.92	0.51
1:C:147:VAL:HG23	1:C:149:MET:CG	2.40	0.51
1:D:47:GLN:CG	1:D:58:ALA:HB2	2.40	0.51
1:D:166:ARG:HD2	1:D:167:TYR:CE2	2.45	0.51
1:A:256:CYS:O	1:A:341:ARG:HD3	2.10	0.51
1:C:92:LEU:HD22	4:C:490:HOH:O	2.09	0.51
1:C:163:ALA:HB1	1:C:167:TYR:CD2	2.45	0.51
1:C:319:PRO:HG3	1:C:328:LEU:HA	1.92	0.51
1:D:310:ILE:HG23	1:D:311:PRO:HD2	1.93	0.51
1:B:39:ARG:HH21	1:B:167:TYR:C	2.18	0.51
1:B:232:THR:HG22	1:B:232:THR:O	2.11	0.51
1:B:377:ASP:HB2	1:B:395:CYS:SG	2.50	0.51
1:C:80:THR:HB	1:C:81:TYR:CD2	2.46	0.51
1:C:373:MET:HG2	1:C:376:LEU:HD22	1.93	0.51
1:D:396:PRO:HD2	1:D:399:SER:CB	2.41	0.51
1:B:122:LEU:HD21	1:B:146:PHE:HD1	1.76	0.51
1:B:136:VAL:HG23	1:B:413:GLN:O	2.11	0.51
1:C:153:GLY:HA3	1:C:165:ALA:H	1.76	0.51
1:B:366:TRP:CG	3:G:4:BGC:H3	2.46	0.51
1:C:37:ASN:ND2	1:C:180:LEU:HA	2.25	0.51
1:C:178:ARG:HD3	1:C:248:SER:OG	2.11	0.51
1:C:385:GLU:HG3	1:C:386:GLY:N	2.26	0.51
1:D:107:ARG:HD3	2:J:1:BGC:H2	1.93	0.51
1:D:379:ILE:O	1:D:379:ILE:HG22	2.10	0.51
1:A:144:LEU:HD21	1:A:361:LEU:CD1	2.40	0.50
1:A:225:PHE:CE1	1:A:297:LEU:HB3	2.46	0.50
1:A:319:PRO:CB	1:A:327:GLU:HG3	2.41	0.50
1:B:16:TRP:CD1	1:B:30:ALA:HB3	2.46	0.50
1:B:21:ALA:HB1	1:B:22:PRO:HD2	1.92	0.50
1:B:107:ARG:HA	1:B:363:MET:O	2.10	0.50
1:B:226:THR:HG23	1:B:261:CYS:C	2.36	0.50
1:B:315:TRP:CZ2	1:B:388:PRO:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ARG:HB3	4:B:498:HOH:O	2.10	0.50
1:B:379:ILE:HG22	1:B:379:ILE:O	2.10	0.50
1:C:14:LEU:HB3	1:C:32:VAL:HG22	1.93	0.50
1:C:295:ASN:HA	1:C:348:PHE:CE2	2.46	0.50
1:D:17:GLN:CG	1:D:420:ARG:HG2	2.40	0.50
1:A:122:LEU:O	1:A:125:ASN:HB2	2.11	0.50
1:B:7:THR:O	1:B:72:GLU:OE1	2.30	0.50
1:B:94:PHE:CD2	1:B:95:VAL:HG23	2.46	0.50
1:C:232:THR:HG22	1:C:234:GLU:CG	2.41	0.50
1:D:209:CYS:SG	1:D:238:CYS:HB3	2.52	0.50
1:A:173:ASP:HB2	1:A:212:GLU:HG3	1.93	0.50
1:B:233:ASN:O	1:B:357:VAL:HG11	2.11	0.50
1:B:268:MET:HA	1:B:315:TRP:CD1	2.47	0.50
1:A:23:GLY:HA2	4:A:487:HOH:O	2.11	0.50
1:A:129:PHE:O	1:A:130:ASP:OD1	2.30	0.50
1:B:318:MET:HE3	1:B:335:VAL:CB	2.41	0.50
1:C:34:ILE:HA	1:C:107:ARG:O	2.10	0.50
1:C:133:LEU:HD11	1:C:286:PHE:HZ	1.76	0.50
1:A:209:CYS:HB2	1:A:236:HIS:CE1	2.47	0.50
1:A:220:ALA:HB1	1:A:276:LYS:CE	2.41	0.50
1:B:123:MET:CE	1:B:356:ARG:HE	2.24	0.50
1:B:186:LYS:O	1:B:187:ALA:O	2.30	0.50
1:B:262:ASP:OD1	1:B:262:ASP:O	2.30	0.50
1:B:287:THR:O	1:B:287:THR:HG22	2.10	0.50
1:B:289:VAL:O	1:B:299:GLN:HB2	2.12	0.50
1:C:242:ASN:O	1:C:254:GLY:HA2	2.12	0.50
1:D:401:VAL:HB	1:D:404:GLU:CB	2.40	0.50
1:A:294:GLU:OE1	1:A:352:ASN:OD1	2.30	0.50
1:A:346:GLY:O	1:A:347:GLY:O	2.30	0.50
1:A:401:VAL:O	1:A:405:VAL:HG22	2.11	0.50
1:B:43:ASP:HB2	1:B:47:GLN:O	2.11	0.50
1:B:143:ALA:HB1	1:B:216:TRP:O	2.11	0.50
1:B:197:SER:HB3	1:B:369:HIS:HB2	1.93	0.50
1:C:35:ASP:OD1	1:C:109:TYR:OH	2.30	0.50
1:C:96:THR:HG23	4:C:529:HOH:O	2.11	0.50
1:D:59:CYS:HA	1:D:68:LYS:HD3	1.93	0.50
1:D:112:ASN:O	1:D:113:GLY:O	2.30	0.50
1:D:133:LEU:HD21	1:D:216:TRP:HZ2	1.77	0.50
1:A:261:CYS:HB2	1:A:342:PHE:CD1	2.47	0.50
1:B:13:PRO:HA	1:B:31:GLU:HB2	1.93	0.50
1:B:121:ASN:O	1:B:125:ASN:OD1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:CYS:O	1:B:253:ALA:HB3	2.12	0.50
1:B:315:TRP:HB2	1:B:318:MET:SD	2.52	0.50
1:C:31:GLU:HG3	1:C:111:MET:HE3	1.92	0.50
1:C:110:LEU:HD23	1:C:361:LEU:HB3	1.94	0.50
1:C:188:ASN:HB2	1:C:192:TRP:HZ3	1.76	0.50
1:C:265:PRO:HA	1:C:270:ASN:ND2	2.21	0.50
1:C:289:VAL:O	1:C:289:VAL:HG12	2.11	0.50
1:C:349:GLU:OE2	1:C:352:ASN:OD1	2.30	0.50
1:A:155:MET:O	1:A:158:TYR:O	2.30	0.50
1:A:182:PHE:HB3	1:A:186:LYS:O	2.12	0.50
1:A:218:SER:O	1:A:219:ASN:HB3	2.12	0.50
1:B:20:THR:OG1	1:B:24:ASN:O	2.30	0.50
1:B:379:ILE:HD12	1:B:397:THR:HG23	1.94	0.50
1:C:157:SER:HG	1:C:158:TYR:HD2	1.60	0.50
1:C:264:ASN:HB3	1:C:267:ARG:HB2	1.94	0.50
1:C:295:ASN:OD1	1:C:352:ASN:OD1	2.30	0.50
1:A:228:HIS:HB3	1:A:257:ASP:O	2.12	0.50
1:B:178:ARG:HB3	1:B:178:ARG:NH1	2.27	0.50
1:B:354:ALA:HA	1:B:357:VAL:CG2	2.42	0.50
1:C:38:TRP:CZ2	1:C:106:SER:HA	2.47	0.50
1:C:206:TYR:HB3	1:C:237:VAL:CG1	2.42	0.50
1:C:379:ILE:HD11	4:C:533:HOH:O	2.11	0.50
1:D:237:VAL:HG12	1:D:237:VAL:O	2.11	0.50
1:D:380:TYR:HE2	2:I:1:BGC:HB	1.56	0.50
1:A:65:CYS:HA	1:A:68:LYS:CG	2.42	0.49
1:A:268:MET:SD	1:A:313:PRO:HB3	2.52	0.49
1:A:380:TYR:CD1	1:A:381:PRO:HA	2.46	0.49
1:B:29:ASN:O	1:B:30:ALA:O	2.30	0.49
1:B:41:LEU:HD23	1:B:71:ILE:CG2	2.41	0.49
1:B:123:MET:CE	1:B:356:ARG:HH21	2.25	0.49
1:B:179:ASP:HB3	1:B:247:TYR:CZ	2.47	0.49
1:C:193:LYS:CB	1:C:203:VAL:HB	2.42	0.49
1:D:17:GLN:HG3	1:D:420:ARG:HG2	1.94	0.49
1:D:245:GLY:O	1:D:251:ARG:HG3	2.12	0.49
1:D:251:ARG:O	1:D:251:ARG:HG2	2.12	0.49
1:A:59:CYS:HB3	1:A:189:ILE:CD1	2.42	0.49
1:A:135:THR:O	1:A:135:THR:OG1	2.30	0.49
1:A:276:LYS:HD3	1:A:276:LYS:N	2.27	0.49
1:B:380:TYR:HB3	1:B:392:ARG:CZ	2.41	0.49
1:C:264:ASN:C	1:C:268:MET:HG2	2.37	0.49
1:D:259:ASN:O	1:D:260:GLY:O	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:OD1	1:A:354:ALA:HB2	2.12	0.49
1:A:267:ARG:HE	1:A:389:GLY:HA2	1.78	0.49
1:A:273:PHE:HA	1:A:279:THR:HB	1.95	0.49
1:B:215:VAL:HA	1:B:225:PHE:CE2	2.47	0.49
1:B:378:SER:O	1:B:392:ARG:HD2	2.12	0.49
1:C:390:ALA:O	1:C:392:ARG:HD2	2.11	0.49
1:D:35:ASP:HB3	1:D:38:TRP:CZ3	2.47	0.49
1:A:86:SER:CB	1:A:89:ALA:HB3	2.42	0.49
1:A:263:TYR:OH	1:A:313:PRO:HD3	2.12	0.49
1:A:357:VAL:O	1:A:359:MET:HG2	2.12	0.49
1:B:126:GLU:O	1:B:421:PHE:HA	2.12	0.49
1:C:204:GLY:O	1:C:205:PRO:O	2.30	0.49
1:D:51:ASP:O	1:D:54:GLN:O	2.30	0.49
1:D:215:VAL:HG21	1:D:292:PHE:CZ	2.47	0.49
1:D:302:ILE:HG23	1:D:306:ARG:O	2.11	0.49
1:A:188:ASN:O	1:A:192:TRP:HE3	1.96	0.49
1:C:173:ASP:O	1:C:210:CYS:O	2.29	0.49
1:A:64:ASP:OD2	1:A:68:LYS:HD2	2.11	0.49
1:A:400:GLY:O	1:A:402:PRO:HD3	2.12	0.49
1:B:90:LEU:O	1:B:416:TRP:HD1	1.95	0.49
1:B:127:LEU:HG	1:B:128:ALA:N	2.26	0.49
1:B:135:THR:OG1	1:B:412:ALA:HA	2.13	0.49
1:B:189:ILE:O	1:B:192:TRP:HB2	2.12	0.49
1:B:199:PRO:HG2	1:B:200:ASN:OD1	2.12	0.49
1:B:424:ILE:O	1:B:424:ILE:HG22	2.11	0.49
1:C:152:ASP:O	1:C:164:GLY:HA3	2.12	0.49
1:C:214:ASP:OD1	1:C:217:GLU:OE1	2.30	0.49
1:D:159:PRO:O	1:D:162:GLN:OE1	2.30	0.49
1:D:372:ASN:ND2	1:D:402:PRO:HD3	2.26	0.49
1:C:18:ARG:HB2	1:C:28:VAL:HG21	1.93	0.49
1:C:226:THR:HG21	2:H:2:BGC:O2	2.12	0.49
1:C:293:GLU:HG3	1:C:296:LYS:HB3	1.95	0.49
1:C:325:THR:HB	1:C:326:PRO:HD2	1.95	0.49
1:C:373:MET:HG3	1:C:375:TRP:CZ2	2.48	0.49
1:D:64:ASP:O	1:D:68:LYS:HB2	2.12	0.49
1:D:315:TRP:HD1	1:D:318:MET:HE3	1.77	0.49
1:A:145:TYR:HB2	1:A:213:ILE:O	2.12	0.49
1:A:290:SER:HB3	1:A:299:GLN:HG3	1.95	0.49
1:B:155:MET:O	1:B:158:TYR:O	2.30	0.49
1:D:366:TRP:HB3	4:D:599:HOH:O	2.11	0.49
1:A:48:ASN:O	1:A:58:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:TYR:CE1	1:A:362:VAL:HG13	2.48	0.49
1:B:187:ALA:O	1:B:188:ASN:HB2	2.13	0.49
1:C:55:TRP:CG	1:C:189:ILE:HG13	2.47	0.49
1:C:122:LEU:O	1:C:292:PHE:HB2	2.13	0.49
1:C:206:TYR:HB3	1:C:237:VAL:HG11	1.94	0.49
1:D:34:ILE:HG22	1:D:39:ARG:HH21	1.76	0.49
1:A:378:SER:OG	1:A:395:CYS:O	2.30	0.49
1:A:418:ASN:O	1:A:420:ARG:HG2	2.13	0.49
1:B:99:GLU:OE1	1:C:81:TYR:OH	2.30	0.49
1:B:172:CYS:HB2	1:B:209:CYS:C	2.38	0.49
1:C:1:PCA:HG3	1:C:182:PHE:CD2	2.47	0.49
1:C:148:ALA:HA	1:C:359:MET:HA	1.94	0.49
1:C:384:LYS:O	1:C:385:GLU:O	2.31	0.49
1:A:215:VAL:HA	1:A:225:PHE:HD2	1.78	0.48
1:A:340:ASN:HD21	1:A:342:PHE:CB	2.24	0.48
1:B:128:ALA:HA	1:B:288:VAL:O	2.12	0.48
1:B:142:SER:O	1:B:142:SER:OG	2.30	0.48
1:D:49:CYS:O	1:D:56:THR:HG23	2.13	0.48
1:D:373:MET:SD	1:D:376:LEU:HD23	2.52	0.48
1:A:15:THR:HA	1:A:28:VAL:O	2.12	0.48
1:B:145:TYR:CD1	1:B:362:VAL:HB	2.49	0.48
1:B:180:LEU:HB2	1:B:183:VAL:HG23	1.96	0.48
1:B:188:ASN:HB3	1:B:192:TRP:CZ3	2.47	0.48
1:B:353:ASN:O	1:B:357:VAL:HG23	2.12	0.48
1:C:40:TRP:HB3	1:C:72:GLU:HB2	1.94	0.48
1:A:257:ASP:HB2	1:A:341:ARG:HG2	1.95	0.48
1:B:209:CYS:HB2	1:B:236:HIS:CD2	2.48	0.48
1:B:264:ASN:OD1	1:B:266:TYR:HB3	2.13	0.48
1:D:27:THR:HG22	1:D:27:THR:O	2.12	0.48
1:D:36:ALA:O	1:D:39:ARG:HB2	2.13	0.48
1:A:177:ALA:CB	1:A:180:LEU:HG	2.43	0.48
1:A:178:ARG:HE	1:A:205:PRO:HA	1.79	0.48
1:B:80:THR:HG22	1:B:81:TYR:CG	2.48	0.48
1:B:152:ASP:CG	1:B:155:MET:H	2.22	0.48
1:C:18:ARG:CB	1:C:26:GLN:HG2	2.43	0.48
1:C:39:ARG:HA	1:C:39:ARG:NH1	2.25	0.48
1:C:41:LEU:HD23	1:C:70:MET:C	2.38	0.48
1:C:384:LYS:HD2	1:C:384:LYS:HA	1.52	0.48
1:D:327:GLU:O	1:D:331:THR:HG23	2.13	0.48
1:B:14:LEU:HD23	1:B:110:LEU:HD11	1.95	0.48
1:C:139:GLY:CA	1:C:400:GLY:HA2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:GLU:O	1:C:330:SER:OG	2.30	0.48
1:D:2:ARG:HH21	1:D:68:LYS:N	2.11	0.48
1:D:4:GLY:HA3	1:D:72:GLU:CD	2.38	0.48
1:D:80:THR:O	1:D:80:THR:HG22	2.13	0.48
1:D:182:PHE:CD1	1:D:187:ALA:HA	2.49	0.48
1:A:3:ALA:C	1:A:70:MET:HB2	2.38	0.48
1:A:316:GLU:OE2	1:A:316:GLU:HA	2.14	0.48
1:B:4:GLY:HA2	1:B:70:MET:CE	2.42	0.48
1:B:114:PRO:HG2	1:B:115:ASP:OD2	2.13	0.48
1:B:244:GLY:HA3	1:B:254:GLY:H	1.78	0.48
1:C:264:ASN:H	1:C:268:MET:CE	2.26	0.48
1:D:93:LYS:HE3	1:D:413:GLN:OE1	2.12	0.48
1:D:129:PHE:HE2	1:D:131:VAL:HB	1.78	0.48
1:A:391:ALA:O	1:A:392:ARG:HG3	2.13	0.48
1:B:48:ASN:O	1:B:56:THR:HG21	2.14	0.48
1:C:35:ASP:HB3	1:C:38:TRP:CZ3	2.48	0.48
1:C:119:MET:HE2	1:C:119:MET:HB3	1.70	0.48
1:D:414:VAL:HG21	1:D:416:TRP:CZ2	2.48	0.48
1:D:423:PRO:O	1:D:426:SER:HB3	2.13	0.48
1:A:6:GLU:OE1	1:A:46:MET:HE1	2.13	0.48
1:A:50:TYR:N	1:A:56:THR:HG23	2.29	0.48
1:A:55:TRP:HB3	1:A:189:ILE:CD1	2.44	0.48
1:A:131:VAL:HA	1:A:415:VAL:O	2.14	0.48
1:A:280:LEU:HD21	1:A:301:PHE:CG	2.48	0.48
1:A:326:PRO:O	1:A:330:SER:OG	2.30	0.48
1:B:115:ASP:OD2	1:B:115:ASP:N	2.47	0.48
1:B:136:VAL:HG21	1:B:414:VAL:HB	1.95	0.48
1:B:249:GLU:H	1:B:249:GLU:HG2	1.51	0.48
1:C:14:LEU:H	1:C:31:GLU:HA	1.78	0.48
1:C:18:ARG:HD2	1:C:26:GLN:OE1	2.14	0.48
1:D:93:LYS:HE2	4:D:530:HOH:O	2.13	0.48
1:D:330:SER:O	1:D:334:ASP:OD2	2.31	0.48
1:D:352:ASN:HA	1:D:355:LEU:HB2	1.95	0.48
1:D:401:VAL:C	1:D:405:VAL:HG22	2.38	0.48
1:B:80:THR:OG1	1:C:76:ASP:HB2	2.13	0.48
1:B:92:LEU:HD21	1:B:108:PHE:CD1	2.49	0.48
1:C:94:PHE:CD2	1:C:95:VAL:HG23	2.49	0.48
1:B:10:ASN:O	1:B:12:PRO:HD3	2.14	0.47
1:B:41:LEU:HD13	1:B:69:CYS:HB3	1.96	0.47
1:C:119:MET:SD	1:C:151:GLU:HG3	2.54	0.47
1:C:275:GLY:C	1:C:278:LYS:HG3	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:VAL:HG22	1:D:225:PHE:HE2	1.78	0.47
1:D:272:ASP:C	1:D:278:LYS:HD3	2.38	0.47
1:A:164:GLY:HA2	1:A:169:THR:OG1	2.15	0.47
1:B:183:VAL:HG11	1:B:206:TYR:HB3	1.95	0.47
1:C:134:SER:HB2	1:C:283:SER:HA	1.95	0.47
1:A:320:ASN:O	1:A:321:SER:HB3	2.14	0.47
1:B:135:THR:O	1:B:137:GLU:HG2	2.14	0.47
1:C:106:SER:OG	1:C:108:PHE:HE1	1.96	0.47
1:C:387:GLN:O	1:C:390:ALA:HB3	2.13	0.47
1:A:96:THR:OG1	1:A:103:ASN:O	2.30	0.47
1:A:308:ILE:O	1:A:308:ILE:HG22	2.15	0.47
1:B:126:GLU:OE1	1:B:424:ILE:HA	2.14	0.47
1:C:309:GLU:HG2	4:C:525:HOH:O	2.15	0.47
1:A:389:GLY:HA3	4:A:495:HOH:O	2.15	0.47
1:B:1:PCA:HA	1:B:66:ALA:O	2.15	0.47
1:B:117:TYR:H	1:B:151:GLU:HG2	1.78	0.47
1:B:128:ALA:HB1	1:B:289:VAL:HG22	1.95	0.47
1:B:318:MET:HE3	1:B:335:VAL:CG1	2.45	0.47
1:C:7:THR:O	1:C:73:GLY:HA3	2.15	0.47
1:C:275:GLY:CA	1:C:278:LYS:HG3	2.45	0.47
1:D:2:ARG:H	1:D:2:ARG:HG2	1.34	0.47
1:D:115:ASP:O	1:D:165:ALA:HB3	2.15	0.47
1:D:374:LEU:HD21	1:D:399:SER:O	2.13	0.47
1:A:22:PRO:O	1:A:429:ASP:OD2	2.32	0.47
1:A:95:VAL:HG23	1:A:410:PRO:HA	1.97	0.47
1:A:178:ARG:HG2	1:A:204:GLY:O	2.15	0.47
1:A:379:ILE:CG2	1:A:385:GLU:HB2	2.43	0.47
1:B:181:LYS:HE3	1:B:181:LYS:HB2	1.29	0.47
1:C:82:GLY:O	1:C:93:LYS:HB2	2.15	0.47
1:C:230:CYS:HB3	1:C:255:LYS:O	2.14	0.47
1:C:241:THR:O	1:C:253:ALA:HB1	2.15	0.47
1:C:363:MET:HE3	1:C:363:MET:HB2	1.79	0.47
1:C:375:TRP:O	1:C:392:ARG:HG2	2.14	0.47
1:D:107:ARG:HG2	1:D:109:TYR:CE1	2.50	0.47
1:D:189:ILE:HG23	1:D:190:GLU:HG3	1.95	0.47
1:D:315:TRP:CD1	1:D:318:MET:HE3	2.49	0.47
1:D:336:PHE:O	1:D:337:ASN:HB2	2.14	0.47
1:C:245:GLY:H	1:C:251:ARG:HA	1.79	0.47
1:D:27:THR:CG2	1:D:29:ASN:HD21	2.23	0.47
1:A:149:MET:HE2	1:A:360:VAL:CG2	2.44	0.47
1:A:252:PHE:HE2	1:A:259:ASN:ND2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:PRO:HG2	1:A:328:LEU:HD23	1.97	0.47
1:C:117:TYR:OH	1:C:168:GLY:HA2	2.15	0.47
1:D:341:ARG:HD2	1:D:345:VAL:HG13	1.97	0.47
1:D:415:VAL:HG13	1:D:415:VAL:O	2.14	0.47
1:B:133:LEU:HD13	1:B:219:ASN:C	2.40	0.47
1:B:231:THR:CG2	1:B:345:VAL:HB	2.44	0.47
1:B:244:GLY:O	1:B:248:SER:OG	2.30	0.47
1:B:306:ARG:HE	1:B:306:ARG:HB3	1.56	0.47
1:C:147:VAL:HG23	1:C:149:MET:HG2	1.97	0.47
1:C:263:TYR:OH	1:C:321:SER:O	2.33	0.47
1:D:31:GLU:HG3	1:D:111:MET:CB	2.43	0.47
1:D:94:PHE:CD1	1:D:104:VAL:HG12	2.50	0.47
1:D:145:TYR:OH	1:D:171:TYR:OH	2.30	0.47
1:D:266:TYR:CZ	1:D:271:PRO:HB3	2.50	0.47
1:A:343:GLU:HA	1:A:347:GLY:N	2.26	0.46
1:B:15:THR:HB	1:B:27:THR:CG2	2.45	0.46
1:B:175:GLN:O	1:B:176:CYS:HB2	2.15	0.46
1:C:155:MET:HA	1:C:161:ASN:CB	2.33	0.46
1:D:105:GLY:CA	1:D:365:ILE:HG23	2.42	0.46
1:B:196:THR:O	1:B:196:THR:OG1	2.30	0.46
1:C:230:CYS:HB3	1:C:255:LYS:C	2.40	0.46
1:D:136:VAL:HG11	1:D:142:SER:OG	2.15	0.46
1:A:379:ILE:HA	1:A:391:ALA:HA	1.96	0.46
1:B:82:GLY:O	1:B:93:LYS:HB2	2.14	0.46
1:B:97:LYS:HD2	1:C:6:GLU:CD	2.40	0.46
1:B:126:GLU:HB3	1:B:291:ARG:HG2	1.95	0.46
1:C:26:GLN:HG3	1:C:28:VAL:HG22	1.98	0.46
1:C:122:LEU:HB3	1:C:292:PHE:CB	2.45	0.46
1:C:147:VAL:HG12	1:C:212:GLU:HB3	1.97	0.46
1:C:193:LYS:HB2	1:C:203:VAL:O	2.16	0.46
1:C:312:PRO:HB3	1:C:321:SER:HA	1.97	0.46
1:D:35:ASP:HB2	1:D:109:TYR:CE2	2.51	0.46
1:D:45:ASN:O	1:D:46:MET:HB2	2.16	0.46
1:D:280:LEU:HA	1:D:303:GLN:OE1	2.16	0.46
1:D:134:SER:O	1:D:134:SER:OG	2.29	0.46
1:D:223:PHE:O	1:D:224:ALA:HB2	2.15	0.46
1:D:229:ALA:O	1:D:257:ASP:HB2	2.15	0.46
1:D:307:LYS:HD2	1:D:430:PHE:CD2	2.51	0.46
1:A:22:PRO:HB2	1:A:429:ASP:CG	2.41	0.46
1:A:293:GLU:OE1	1:A:298:SER:OG	2.33	0.46
1:B:89:ALA:HA	1:B:416:TRP:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LEU:O	1:B:145:TYR:HB3	2.15	0.46
1:B:213:ILE:O	1:B:213:ILE:HG22	2.15	0.46
1:C:14:LEU:HD12	1:C:15:THR:N	2.31	0.46
1:C:48:ASN:O	1:C:56:THR:OG1	2.30	0.46
1:C:166:ARG:HB2	1:C:167:TYR:CD2	2.50	0.46
1:D:174:ALA:HB1	1:D:257:ASP:O	2.16	0.46
1:D:400:GLY:O	1:D:402:PRO:HD3	2.14	0.46
1:A:297:LEU:O	1:A:323:GLU:HA	2.16	0.46
1:A:380:TYR:HB3	1:A:392:ARG:CZ	2.46	0.46
1:B:9:GLU:OE2	1:B:9:GLU:HA	2.05	0.46
1:B:50:TYR:CD1	1:B:55:TRP:HA	2.51	0.46
1:B:257:ASP:CG	1:B:260:GLY:H	2.23	0.46
1:B:377:ASP:O	1:B:378:SER:HB2	2.16	0.46
1:C:146:PHE:O	1:C:212:GLU:HA	2.16	0.46
1:C:221:TYR:O	1:C:222:ALA:HB2	2.16	0.46
1:C:227:PRO:HG3	1:C:297:LEU:CD2	2.45	0.46
1:C:288:VAL:HG13	1:C:299:GLN:HE21	1.80	0.46
1:C:392:ARG:HD2	1:C:392:ARG:N	2.31	0.46
1:C:392:ARG:HG2	1:C:392:ARG:HH11	1.79	0.46
1:D:2:ARG:HA	1:D:162:GLN:HB2	1.98	0.46
1:D:7:THR:HA	1:D:8:PRO:HD3	1.67	0.46
1:D:96:THR:OG1	1:D:96:THR:O	2.33	0.46
1:D:126:GLU:HB2	1:D:291:ARG:HA	1.96	0.46
1:A:114:PRO:HB2	1:A:166:ARG:CZ	2.45	0.46
1:C:105:GLY:HA3	1:C:365:ILE:O	2.16	0.46
1:C:263:TYR:OH	1:C:322:SER:HA	2.16	0.46
1:D:113:GLY:O	1:D:115:ASP:N	2.49	0.46
1:A:149:MET:CE	1:A:360:VAL:HG21	2.45	0.46
1:B:400:GLY:O	1:B:402:PRO:HD3	2.16	0.46
1:C:164:GLY:HA2	1:C:169:THR:OG1	2.15	0.46
1:C:208:SER:OG	1:C:235:TYR:OH	2.30	0.46
1:C:269:GLY:O	1:C:314:THR:HG21	2.16	0.46
1:C:319:PRO:HD3	1:C:331:THR:OG1	2.15	0.46
1:D:293:GLU:HB2	1:D:296:LYS:O	2.16	0.46
1:A:9:GLU:OE1	1:A:33:VAL:HG23	2.16	0.46
1:A:195:SER:N	4:A:518:HOH:O	2.48	0.46
1:D:105:GLY:O	1:D:106:SER:HB3	2.16	0.46
1:D:141:ASN:HB2	1:D:373:MET:SD	2.56	0.46
1:D:157:SER:O	1:D:159:PRO:HD3	2.15	0.46
1:D:172:CYS:O	1:D:173:ASP:HB3	2.16	0.46
1:A:39:ARG:NH1	1:A:73:GLY:HA2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:HB3	1:A:415:VAL:CG1	2.46	0.46
1:A:267:ARG:HE	1:A:389:GLY:CA	2.28	0.46
1:B:15:THR:O	1:B:15:THR:OG1	2.30	0.46
1:B:147:VAL:CG1	1:B:212:GLU:HB2	2.39	0.46
1:B:341:ARG:NH1	1:B:344:GLU:OE1	2.49	0.46
1:C:257:ASP:HA	1:C:341:ARG:HG2	1.98	0.46
1:A:211:ALA:HB2	1:A:233:ASN:HB3	1.99	0.45
1:B:227:PRO:CG	1:B:324:ILE:HG21	2.41	0.45
1:B:354:ALA:HA	1:B:357:VAL:HG23	1.98	0.45
1:C:94:PHE:CZ	1:C:104:VAL:HG13	2.52	0.45
1:C:121:ASN:ND2	1:C:121:ASN:H	2.14	0.45
1:C:266:TYR:CD2	1:C:271:PRO:HA	2.51	0.45
1:D:408:GLN:HG3	1:D:409:PHE:CD1	2.38	0.45
1:B:76:ASP:OD1	1:B:76:ASP:O	2.34	0.45
1:B:327:GLU:N	1:B:327:GLU:OE2	2.50	0.45
1:B:366:TRP:HE3	1:B:367:ASP:O	1.99	0.45
1:C:154:GLY:C	1:C:161:ASN:HD22	2.23	0.45
1:C:324:ILE:O	1:C:324:ILE:HG22	2.16	0.45
1:C:336:PHE:HA	1:C:388:PRO:HB2	1.98	0.45
1:A:225:PHE:CZ	1:A:297:LEU:HB3	2.50	0.45
1:B:126:GLU:OE2	1:B:427:THR:OG1	2.30	0.45
1:B:152:ASP:OD2	1:B:155:MET:HB2	2.16	0.45
1:B:291:ARG:HB3	1:B:424:ILE:HG12	1.98	0.45
1:C:78:LEU:O	1:C:80:THR:N	2.50	0.45
1:C:275:GLY:HA3	1:C:278:LYS:HG3	1.98	0.45
1:D:2:ARG:O	1:D:71:ILE:N	2.50	0.45
1:A:133:LEU:H	1:A:133:LEU:HD12	1.80	0.45
1:A:318:MET:HE3	1:A:335:VAL:HG11	1.98	0.45
1:B:1:PCA:O	1:B:162:GLN:N	2.50	0.45
1:B:175:GLN:NE2	3:G:3:BGC:O2	2.49	0.45
1:B:178:ARG:NE	1:B:248:SER:OG	2.49	0.45
1:B:200:ASN:ND2	4:B:504:HOH:O	2.50	0.45
1:B:227:PRO:HB2	1:B:351:LEU:CD1	2.46	0.45
1:B:299:GLN:HG3	1:B:300:TYR:N	2.31	0.45
1:B:384:LYS:HG3	1:B:387:GLN:HB2	1.98	0.45
1:C:160:SER:OG	1:C:160:SER:O	2.30	0.45
1:C:264:ASN:O	1:C:267:ARG:N	2.50	0.45
1:D:50:TYR:OH	1:D:192:TRP:NE1	2.50	0.45
1:D:264:ASN:O	1:D:268:MET:N	2.50	0.45
1:A:39:ARG:NE	1:A:167:TYR:O	2.50	0.45
1:B:39:ARG:NH2	1:B:167:TYR:HA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ARG:O	1:C:26:GLN:N	2.50	0.45
1:C:32:VAL:CG1	1:C:110:LEU:HA	2.45	0.45
1:C:135:THR:HG22	1:C:135:THR:O	2.17	0.45
1:D:38:TRP:HE3	1:D:38:TRP:H	1.64	0.45
1:D:181:LYS:HB2	1:D:181:LYS:HE2	1.66	0.45
1:D:371:ALA:O	1:D:373:MET:N	2.50	0.45
1:A:17:GLN:HE21	1:A:25:CYS:HB2	1.81	0.45
1:A:51:ASP:O	1:A:53:ASN:N	2.50	0.45
1:B:9:GLU:OE2	1:B:39:ARG:NH1	2.50	0.45
1:B:115:ASP:OD1	1:B:166:ARG:NH1	2.50	0.45
1:B:267:ARG:NH1	3:G:1:BGC:H6C1	2.32	0.45
1:B:380:TYR:CG	1:B:381:PRO:HA	2.51	0.45
1:C:212:GLU:O	1:C:212:GLU:HG3	2.16	0.45
1:C:265:PRO:O	1:C:270:ASN:ND2	2.50	0.45
1:D:270:ASN:OD1	1:D:311:PRO:HB2	2.16	0.45
1:A:19:CYS:O	1:A:426:SER:OG	2.30	0.45
1:A:252:PHE:O	1:A:341:ARG:NH1	2.50	0.45
1:A:348:PHE:HD2	1:A:352:ASN:ND2	2.15	0.45
1:B:112:ASN:ND2	1:B:118:GLN:OE1	2.50	0.45
1:B:251:ARG:NH2	3:G:2:BGC:O6	2.49	0.45
1:C:39:ARG:HH11	1:C:39:ARG:CA	2.29	0.45
1:C:42:HIS:HB2	1:C:47:GLN:O	2.17	0.45
1:C:188:ASN:HB2	1:C:192:TRP:CZ3	2.52	0.45
1:C:401:VAL:HG11	1:C:404:GLU:OE2	2.16	0.45
1:D:107:ARG:HD3	2:J:1:BGC:C2	2.46	0.45
1:D:178:ARG:HB2	1:D:203:VAL:HG13	1.99	0.45
1:D:215:VAL:HG21	1:D:292:PHE:HZ	1.81	0.45
1:D:239:GLU:O	1:D:242:ASN:ND2	2.50	0.45
1:D:274:TYR:C	1:D:278:LYS:HD2	2.42	0.45
1:D:401:VAL:O	1:D:404:GLU:N	2.50	0.45
1:B:77:TYR:HD2	1:B:81:TYR:HD2	1.65	0.45
1:B:402:PRO:O	1:B:405:VAL:HG22	2.17	0.45
1:C:124:GLY:N	1:C:292:PHE:O	2.49	0.45
1:D:296:LYS:HE3	4:D:545:HOH:O	2.16	0.45
1:D:409:PHE:N	1:D:410:PRO:HD3	2.32	0.45
1:A:123:MET:HE2	1:A:123:MET:HB2	1.85	0.45
1:A:158:TYR:HA	1:A:159:PRO:HD3	1.58	0.45
1:B:152:ASP:OD2	1:B:155:MET:N	2.50	0.45
1:B:180:LEU:HB2	1:B:183:VAL:CG2	2.47	0.45
1:B:228:HIS:ND1	1:B:257:ASP:O	2.50	0.45
1:C:32:VAL:CG1	1:C:110:LEU:HD22	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:LYS:HE3	1:C:96:THR:HG22	1.99	0.45
1:C:118:GLN:NE2	4:C:540:HOH:O	2.50	0.45
1:C:123:MET:HE3	1:C:123:MET:HB2	1.67	0.45
1:D:9:GLU:OE1	1:D:77:TYR:OH	2.30	0.45
1:D:35:ASP:OD2	1:D:38:TRP:HZ3	1.99	0.45
1:D:387:GLN:NE2	4:D:595:HOH:O	2.50	0.45
1:A:413:GLN:O	1:A:413:GLN:NE2	2.50	0.45
1:B:22:PRO:HD3	1:B:425:GLY:O	2.16	0.45
1:B:61:THR:N	1:B:64:ASP:OD2	2.50	0.45
1:B:123:MET:HE1	1:B:356:ARG:NH2	2.29	0.45
1:C:91:THR:HA	1:C:415:VAL:HA	1.98	0.45
1:C:401:VAL:HB	1:C:404:GLU:HB2	1.98	0.45
1:D:110:LEU:O	1:D:117:TYR:HB3	2.16	0.45
1:D:380:TYR:O	1:D:392:ARG:NH2	2.50	0.45
1:A:274:TYR:HA	1:A:280:LEU:O	2.17	0.44
1:A:280:LEU:CD2	1:A:308:ILE:HG21	2.47	0.44
1:A:300:TYR:CD1	1:A:307:LYS:HD2	2.52	0.44
1:B:349:GLU:HA	1:B:352:ASN:OD1	2.17	0.44
1:C:32:VAL:HG12	1:C:110:LEU:HA	2.00	0.44
1:C:116:LYS:H	1:C:116:LYS:HG2	1.38	0.44
1:C:198:ASP:OD1	1:C:201:ALA:N	2.50	0.44
1:C:267:ARG:HA	1:C:391:ALA:O	2.18	0.44
1:D:71:ILE:HD11	1:D:163:ALA:CB	2.47	0.44
1:D:163:ALA:HB1	1:D:167:TYR:CG	2.52	0.44
1:D:218:SER:OG	1:D:219:ASN:N	2.49	0.44
1:D:251:ARG:NH2	2:I:2:BGC:O6	2.50	0.44
1:A:1:PCA:HG3	1:A:182:PHE:CD1	2.52	0.44
1:A:12:PRO:O	1:A:32:VAL:N	2.50	0.44
1:A:55:TRP:HE3	1:A:189:ILE:HD12	1.81	0.44
1:A:133:LEU:HA	1:A:136:VAL:HG23	1.99	0.44
1:A:197:SER:OG	1:A:198:ASP:N	2.50	0.44
1:A:381:PRO:HA	1:A:382:PRO:HD3	1.83	0.44
1:B:26:GLN:NE2	1:B:27:THR:O	2.50	0.44
1:B:67:GLU:OE2	1:B:162:GLN:NE2	2.50	0.44
1:B:82:GLY:O	1:B:93:LYS:N	2.50	0.44
1:B:110:LEU:HA	1:B:110:LEU:HD12	1.79	0.44
1:B:175:GLN:NE2	3:G:2:BGC:O6	2.50	0.44
1:B:354:ALA:O	1:B:357:VAL:N	2.50	0.44
1:C:212:GLU:O	1:C:228:HIS:HD2	2.00	0.44
1:C:291:ARG:HE	1:C:424:ILE:CG2	2.30	0.44
1:D:16:TRP:HZ3	1:D:421:PHE:HB3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:TRP:CZ2	1:D:106:SER:HA	2.52	0.44
1:D:65:CYS:HB3	1:D:182:PHE:HZ	1.82	0.44
1:A:42:HIS:NE2	1:A:72:GLU:OE2	2.50	0.44
1:A:239:GLU:O	1:A:242:ASN:ND2	2.50	0.44
1:B:44:ASP:OD1	1:B:45:ASN:N	2.50	0.44
1:B:84:SER:O	1:B:90:LEU:HD12	2.18	0.44
1:B:94:PHE:CE2	1:B:95:VAL:HG23	2.52	0.44
1:B:178:ARG:HD2	1:B:207:GLY:HA3	2.00	0.44
1:B:243:CYS:O	1:B:254:GLY:N	2.50	0.44
1:C:34:ILE:HB	1:C:77:TYR:HE2	1.82	0.44
1:C:176:CYS:O	1:C:178:ARG:N	2.50	0.44
1:C:213:ILE:HD12	1:C:213:ILE:N	2.33	0.44
1:C:262:ASP:OD1	1:C:267:ARG:NH1	2.50	0.44
1:C:333:PHE:O	1:C:337:ASN:N	2.50	0.44
1:D:98:HIS:H	1:D:98:HIS:HD1	1.63	0.44
1:D:303:GLN:O	1:D:306:ARG:N	2.50	0.44
1:A:337:ASN:ND2	4:A:461:HOH:O	2.50	0.44
1:C:60:SER:HB3	1:C:64:ASP:CG	2.43	0.44
1:C:92:LEU:HB2	1:C:414:VAL:CG1	2.46	0.44
1:D:76:ASP:OD2	1:D:79:GLY:N	2.50	0.44
1:D:200:ASN:OD1	1:D:200:ASN:N	2.49	0.44
1:D:219:ASN:ND2	1:D:377:ASP:OD2	2.50	0.44
1:A:45:ASN:O	1:A:46:MET:HB2	2.17	0.44
1:A:376:LEU:O	1:A:392:ARG:HB3	2.18	0.44
1:B:48:ASN:ND2	1:B:50:TYR:O	2.50	0.44
1:B:174:ALA:O	1:B:258:ALA:HA	2.17	0.44
1:B:183:VAL:N	1:B:186:LYS:O	2.50	0.44
1:B:209:CYS:O	1:B:210:CYS:HB3	2.17	0.44
1:B:229:ALA:N	4:B:557:HOH:O	2.49	0.44
1:B:342:PHE:O	1:B:347:GLY:HA2	2.16	0.44
1:C:18:ARG:NH2	4:C:540:HOH:O	2.50	0.44
1:C:339:ARG:NH2	4:C:498:HOH:O	2.50	0.44
1:D:96:THR:N	1:D:103:ASN:O	2.50	0.44
1:D:342:PHE:HZ	1:D:348:PHE:HA	1.83	0.44
1:A:21:ALA:O	1:A:23:GLY:N	2.49	0.44
1:A:126:GLU:CD	1:A:425:GLY:H	2.25	0.44
1:C:18:ARG:O	1:C:25:CYS:HA	2.17	0.44
1:C:88:ASP:OD1	1:C:88:ASP:N	2.50	0.44
1:C:216:TRP:NE1	1:C:218:SER:OG	2.50	0.44
1:C:326:PRO:HG2	1:C:327:GLU:OE2	2.18	0.44
1:C:369:HIS:ND1	1:C:402:PRO:HG3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ARG:CB	1:D:70:MET:HB3	2.48	0.44
1:D:246:THR:OG1	1:D:251:ARG:NH1	2.50	0.44
1:D:280:LEU:HD23	1:D:308:ILE:HG21	1.99	0.44
1:D:334:ASP:OD2	1:D:334:ASP:N	2.50	0.44
1:A:50:TYR:O	1:A:51:ASP:HB2	2.18	0.44
1:A:380:TYR:HA	1:A:381:PRO:HA	1.61	0.44
4:A:463:HOH:O	1:B:116:LYS:HE2	2.17	0.44
1:B:17:GLN:O	1:B:420:ARG:HA	2.17	0.44
1:B:80:THR:HG22	1:B:81:TYR:CD1	2.52	0.44
1:B:197:SER:CB	1:B:369:HIS:HB2	2.47	0.44
1:C:126:GLU:OE2	1:C:427:THR:OG1	2.30	0.44
1:C:319:PRO:HG2	1:C:328:LEU:HD23	1.99	0.44
1:C:357:VAL:HA	1:C:358:PRO:HD2	1.78	0.44
1:D:129:PHE:CE2	1:D:131:VAL:HB	2.52	0.44
1:D:295:ASN:OD1	1:D:295:ASN:N	2.50	0.44
1:A:90:LEU:HD12	1:A:91:THR:N	2.31	0.44
1:A:262:ASP:OD1	1:A:262:ASP:N	2.50	0.44
1:A:267:ARG:NE	1:A:389:GLY:O	2.50	0.44
1:A:302:ILE:O	1:A:302:ILE:HG22	2.17	0.44
1:A:315:TRP:CH2	1:A:388:PRO:HB3	2.53	0.44
1:B:160:SER:OG	1:B:185:GLY:HA3	2.18	0.44
1:C:128:ALA:HB2	1:C:289:VAL:HG22	2.00	0.44
1:C:152:ASP:C	1:C:165:ALA:H	2.23	0.44
1:C:226:THR:CG2	1:C:262:ASP:HB3	2.42	0.44
1:C:244:GLY:HA2	1:C:253:ALA:HB3	2.00	0.44
1:C:268:MET:O	1:C:313:PRO:HB3	2.18	0.44
1:A:152:ASP:OD2	1:A:156:ALA:HB2	2.18	0.44
1:A:380:TYR:O	1:A:392:ARG:NH2	2.50	0.44
1:B:274:TYR:O	1:B:278:LYS:HD2	2.17	0.44
1:B:290:SER:OG	1:B:299:GLN:NE2	2.50	0.44
1:D:2:ARG:HG2	1:D:69:CYS:O	2.18	0.44
1:D:247:TYR:HB2	4:D:608:HOH:O	2.18	0.44
1:A:51:ASP:N	1:A:54:GLN:O	2.50	0.43
1:A:120:PHE:N	1:A:359:MET:O	2.50	0.43
1:A:146:PHE:HB3	1:A:359:MET:CB	2.38	0.43
1:B:130:ASP:OD1	1:B:130:ASP:N	2.50	0.43
1:C:89:ALA:HA	1:C:416:TRP:O	2.18	0.43
1:C:133:LEU:HD11	1:C:286:PHE:CE2	2.52	0.43
1:C:208:SER:HG	1:C:235:TYR:HH	1.61	0.43
1:D:375:TRP:CZ2	2:I:2:BGC:H5	2.53	0.43
1:D:428:TYR:O	1:D:430:PHE:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:CYS:HB3	1:A:189:ILE:HD13	1.99	0.43
1:A:150:GLU:H	1:A:150:GLU:HG3	1.29	0.43
1:B:63:THR:HG23	1:B:186:LYS:HE3	2.00	0.43
1:B:178:ARG:HH21	1:B:248:SER:HA	1.83	0.43
1:B:257:ASP:OD2	1:B:260:GLY:N	2.50	0.43
1:C:14:LEU:O	1:C:30:ALA:O	2.36	0.43
1:C:125:ASN:HD22	1:C:423:PRO:N	2.17	0.43
1:C:380:TYR:HE2	2:H:1:BGC:O2	2.01	0.43
1:D:133:LEU:H	1:D:133:LEU:HG	1.62	0.43
1:D:262:ASP:OD1	1:D:262:ASP:N	2.50	0.43
1:D:280:LEU:HD11	1:D:286:PHE:CD1	2.52	0.43
1:A:43:ASP:OD1	1:A:68:LYS:NZ	2.50	0.43
1:A:142:SER:HB3	1:A:414:VAL:HB	2.00	0.43
1:B:145:TYR:O	1:B:362:VAL:HG23	2.18	0.43
1:B:318:MET:HE3	1:B:335:VAL:HB	1.99	0.43
1:B:324:ILE:HG22	1:B:324:ILE:O	2.17	0.43
1:C:52:GLY:O	1:C:200:ASN:HA	2.17	0.43
1:D:77:TYR:HB3	1:D:83:ALA:CB	2.33	0.43
1:A:148:ALA:HB2	1:A:359:MET:CE	2.49	0.43
1:A:171:TYR:O	1:A:180:LEU:HD11	2.18	0.43
1:A:182:PHE:O	1:A:183:VAL:HG23	2.18	0.43
1:A:342:PHE:CD2	1:A:343:GLU:HG3	2.39	0.43
1:A:357:VAL:CG1	1:A:358:PRO:HD2	2.46	0.43
1:B:72:GLU:OE1	1:B:72:GLU:HA	2.17	0.43
1:B:133:LEU:HD13	1:B:219:ASN:O	2.19	0.43
1:B:144:LEU:HD23	1:B:145:TYR:H	1.83	0.43
1:C:43:ASP:OD2	1:C:47:GLN:N	2.49	0.43
1:C:192:TRP:HE1	1:C:202:GLY:HA3	1.84	0.43
1:C:228:HIS:ND1	1:C:257:ASP:O	2.50	0.43
1:C:409:PHE:N	1:C:410:PRO:HD3	2.33	0.43
1:D:181:LYS:O	1:D:188:ASN:HB2	2.18	0.43
1:A:60:SER:HB3	1:A:64:ASP:OD1	2.19	0.43
1:D:266:TYR:CD2	1:D:271:PRO:HA	2.54	0.43
1:A:46:MET:HA	1:A:46:MET:HE3	2.01	0.43
1:A:369:HIS:CG	1:A:402:PRO:HG2	2.54	0.43
1:B:384:LYS:O	1:B:385:GLU:HB3	2.18	0.43
1:C:82:GLY:CA	1:C:96:THR:HG21	2.49	0.43
1:C:144:LEU:HD23	1:C:215:VAL:HB	1.99	0.43
1:D:48:ASN:O	1:D:56:THR:OG1	2.29	0.43
1:D:63:THR:HB	1:D:64:ASP:H	1.69	0.43
1:D:137:GLU:O	1:D:219:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LEU:N	1:D:180:LEU:HD23	2.33	0.43
1:D:245:GLY:HA2	1:D:258:ALA:HB2	2.00	0.43
1:A:2:ARG:O	1:A:70:MET:HA	2.18	0.43
1:A:259:ASN:OD1	1:A:259:ASN:N	2.51	0.43
1:A:362:VAL:HG12	1:A:363:MET:N	2.34	0.43
1:B:312:PRO:HB3	1:B:320:ASN:C	2.44	0.43
1:B:354:ALA:O	1:B:357:VAL:HB	2.19	0.43
1:C:64:ASP:OD1	1:C:68:LYS:HD2	2.19	0.43
1:C:312:PRO:HB3	1:C:321:SER:CA	2.48	0.43
1:D:123:MET:HE1	1:D:352:ASN:HB3	2.01	0.43
1:D:263:TYR:OH	1:D:312:PRO:HA	2.19	0.43
1:A:17:GLN:HE21	1:A:25:CYS:CB	2.32	0.43
1:A:134:SER:HB2	1:A:283:SER:O	2.19	0.43
1:B:39:ARG:HH11	1:B:39:ARG:HD3	1.68	0.43
1:C:136:VAL:HG12	1:C:140:ILE:HB	2.00	0.43
1:D:61:THR:O	1:D:64:ASP:OD2	2.37	0.43
1:D:182:PHE:CZ	1:D:187:ALA:HB2	2.53	0.43
1:A:13:PRO:HA	1:A:31:GLU:HA	2.00	0.43
1:A:17:GLN:HB2	1:A:26:GLN:O	2.18	0.43
1:A:63:THR:HG22	1:A:63:THR:O	2.18	0.43
1:A:302:ILE:HG12	1:A:430:PHE:CE1	2.52	0.43
1:A:333:PHE:O	1:A:337:ASN:N	2.50	0.43
1:A:378:SER:O	1:A:392:ARG:HD2	2.18	0.43
1:B:17:GLN:HG3	4:B:520:HOH:O	2.19	0.43
1:D:135:THR:OG1	1:D:413:GLN:O	2.30	0.43
1:D:146:PHE:CE2	1:D:361:LEU:HB2	2.54	0.43
1:D:318:MET:HG2	1:D:331:THR:O	2.19	0.43
1:D:374:LEU:O	1:D:378:SER:HB3	2.19	0.43
1:A:83:ALA:HB2	1:A:108:PHE:HZ	1.83	0.43
1:A:318:MET:HE2	1:A:332:MET:HA	2.01	0.43
1:B:1:PCA:HB2	1:B:2:ARG:H	1.61	0.43
1:B:9:GLU:HB2	1:B:167:TYR:CZ	2.54	0.43
1:B:110:LEU:HB2	1:B:361:LEU:HD23	2.01	0.43
1:C:55:TRP:CZ2	1:C:181:LYS:HG2	2.54	0.43
1:C:315:TRP:O	1:C:318:MET:HB2	2.19	0.43
1:D:18:ARG:NH1	1:D:118:GLN:HE22	2.16	0.43
1:D:123:MET:SD	1:D:294:GLU:HG3	2.58	0.43
1:D:373:MET:HE3	1:D:373:MET:HB2	1.91	0.43
1:A:31:GLU:HG2	1:A:111:MET:HB2	2.01	0.42
1:A:114:PRO:HB2	1:A:166:ARG:NH2	2.34	0.42
1:A:300:TYR:CG	1:A:307:LYS:HE3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ILE:HG12	1:A:430:PHE:HE1	1.83	0.42
1:A:398:ASP:OD1	1:A:398:ASP:N	2.50	0.42
1:B:139:GLY:HA2	1:B:377:ASP:OD2	2.19	0.42
1:C:173:ASP:HB2	1:C:174:ALA:H	1.68	0.42
1:C:198:ASP:HB2	1:C:369:HIS:HE2	1.84	0.42
1:D:40:TRP:HB3	1:D:72:GLU:HB2	2.01	0.42
1:D:149:MET:SD	1:D:171:TYR:HD1	2.42	0.42
1:A:323:GLU:H	1:A:323:GLU:HG2	1.32	0.42
1:C:34:ILE:HD12	1:C:108:PHE:CE1	2.54	0.42
1:C:82:GLY:HA3	1:C:96:THR:HG21	2.01	0.42
1:C:176:CYS:HB3	1:C:207:GLY:HA3	2.01	0.42
1:C:197:SER:OG	1:C:198:ASP:N	2.50	0.42
1:C:263:TYR:HE1	1:C:328:LEU:HG	1.84	0.42
1:D:21:ALA:HB1	1:D:22:PRO:HD2	2.00	0.42
1:D:35:ASP:HB3	1:D:38:TRP:HZ3	1.84	0.42
1:D:91:THR:C	1:D:92:LEU:HD23	2.43	0.42
1:A:35:ASP:OD2	1:A:107:ARG:NH2	2.49	0.42
1:B:122:LEU:HB3	1:B:355:LEU:HD13	2.02	0.42
1:B:131:VAL:HG13	1:B:286:PHE:CE2	2.54	0.42
1:B:188:ASN:O	1:B:192:TRP:HE3	2.01	0.42
1:C:20:THR:OG1	1:C:21:ALA:N	2.51	0.42
1:C:133:LEU:HD21	1:C:216:TRP:CZ2	2.54	0.42
1:C:299:GLN:O	1:C:310:ILE:HD12	2.19	0.42
1:C:381:PRO:HB3	4:C:491:HOH:O	2.19	0.42
1:D:372:ASN:HB2	1:D:374:LEU:HG	2.01	0.42
1:D:379:ILE:HG12	1:D:391:ALA:HA	2.02	0.42
1:A:21:ALA:HB1	1:A:22:PRO:HD2	2.00	0.42
1:A:336:PHE:HD1	1:A:336:PHE:HA	1.70	0.42
1:B:99:GLU:HA	1:C:40:TRP:CE3	2.54	0.42
1:B:177:ALA:HB1	1:B:180:LEU:HG	1.99	0.42
1:B:254:GLY:O	1:B:256:CYS:N	2.50	0.42
1:C:145:TYR:CE2	1:C:362:VAL:HB	2.55	0.42
1:C:178:ARG:HB3	1:C:207:GLY:HA2	2.00	0.42
1:C:193:LYS:HD2	1:C:203:VAL:HG12	2.02	0.42
1:C:284:ARG:NH1	1:C:304:ASP:OD2	2.50	0.42
1:C:306:ARG:NH2	1:D:302:ILE:HG22	2.34	0.42
1:D:180:LEU:HB2	1:D:183:VAL:HG23	2.01	0.42
1:D:295:ASN:HA	1:D:348:PHE:CE2	2.54	0.42
1:B:155:MET:HG3	1:B:164:GLY:CA	2.47	0.42
1:C:38:TRP:CH2	1:C:107:ARG:HB2	2.54	0.42
1:C:155:MET:HB2	1:C:164:GLY:HA3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:LYS:HE3	1:C:387:GLN:NE2	2.31	0.42
1:D:40:TRP:CE3	1:D:72:GLU:HG3	2.54	0.42
1:D:109:TYR:CE1	1:D:362:VAL:HG13	2.54	0.42
1:A:339:ARG:HH11	1:A:339:ARG:HD2	1.61	0.42
1:B:58:ALA:HB1	1:B:68:LYS:CE	2.50	0.42
1:C:147:VAL:HG12	1:C:212:GLU:HB2	2.01	0.42
1:C:213:ILE:HA	1:C:227:PRO:HA	2.01	0.42
1:D:84:SER:O	1:D:90:LEU:HD12	2.20	0.42
1:D:133:LEU:HA	1:D:136:VAL:HG23	2.02	0.42
1:D:423:PRO:C	1:D:426:SER:HB3	2.44	0.42
1:A:77:TYR:O	1:A:82:GLY:N	2.52	0.42
1:A:106:SER:OG	1:A:108:PHE:HE1	2.02	0.42
1:A:149:MET:HE3	1:A:149:MET:HB2	1.93	0.42
1:B:58:ALA:HB1	1:B:68:LYS:HE2	2.02	0.42
1:B:134:SER:HA	1:B:282:THR:O	2.19	0.42
1:B:152:ASP:OD1	1:B:154:GLY:N	2.50	0.42
1:B:378:SER:O	1:B:392:ARG:HB2	2.19	0.42
1:C:430:PHE:HD2	1:D:304:ASP:OD1	2.02	0.42
1:D:12:PRO:HD3	1:D:77:TYR:CE1	2.54	0.42
1:D:39:ARG:HB3	1:D:71:ILE:CG2	2.47	0.42
1:D:93:LYS:HD2	1:D:413:GLN:OE1	2.19	0.42
1:D:117:TYR:OH	1:D:169:THR:O	2.30	0.42
1:D:232:THR:OG1	1:D:255:LYS:NZ	2.49	0.42
1:D:319:PRO:HG3	1:D:327:GLU:HB2	2.00	0.42
1:D:375:TRP:H	1:D:375:TRP:CD1	2.37	0.42
1:A:380:TYR:CG	1:A:381:PRO:HA	2.55	0.42
1:B:272:ASP:O	1:B:278:LYS:HB2	2.19	0.42
1:A:76:ASP:O	1:A:80:THR:N	2.50	0.42
1:B:18:ARG:O	1:B:26:GLN:N	2.50	0.42
1:B:183:VAL:CG1	1:B:206:TYR:HB3	2.50	0.42
1:B:302:ILE:O	1:B:302:ILE:HG22	2.20	0.42
1:C:60:SER:HB3	1:C:64:ASP:OD2	2.19	0.42
1:C:104:VAL:HG21	1:C:406:GLU:OE1	2.20	0.42
1:C:123:MET:HA	1:C:292:PHE:O	2.20	0.42
1:C:226:THR:O	1:C:226:THR:HG22	2.20	0.42
1:C:234:GLU:HG2	1:C:234:GLU:H	1.53	0.42
1:D:157:SER:C	1:D:159:PRO:HD3	2.45	0.42
1:A:77:TYR:O	1:A:83:ALA:N	2.50	0.42
1:A:206:TYR:HD2	1:A:206:TYR:HA	1.71	0.42
1:A:426:SER:O	1:A:426:SER:OG	2.37	0.42
1:B:149:MET:HE3	1:B:170:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:VAL:HG12	1:C:238:CYS:N	2.35	0.42
1:C:273:PHE:CE1	1:C:311:PRO:HD3	2.55	0.42
1:D:181:LYS:C	1:D:188:ASN:HB2	2.45	0.42
1:D:226:THR:HG23	1:D:262:ASP:CB	2.40	0.42
1:D:287:THR:O	1:D:301:PHE:HA	2.20	0.42
1:D:401:VAL:O	1:D:405:VAL:N	2.49	0.42
1:A:17:GLN:HB2	1:A:27:THR:CA	2.43	0.41
1:A:55:TRP:HH2	1:A:182:PHE:CE1	2.38	0.41
1:A:307:LYS:HD3	1:A:430:PHE:CG	2.54	0.41
1:B:39:ARG:HD2	1:B:72:GLU:O	2.20	0.41
1:B:117:TYR:N	1:B:151:GLU:O	2.50	0.41
1:B:122:LEU:HD23	1:B:213:ILE:HD13	2.02	0.41
1:B:205:PRO:O	1:B:239:GLU:HA	2.20	0.41
1:B:348:PHE:O	1:B:352:ASN:OD1	2.38	0.41
1:C:16:TRP:HB2	1:C:419:ILE:HB	2.02	0.41
1:C:148:ALA:HB2	1:C:359:MET:CG	2.48	0.41
1:C:179:ASP:HB3	1:C:247:TYR:CZ	2.55	0.41
1:C:293:GLU:O	1:C:296:LYS:N	2.50	0.41
1:C:353:ASN:HA	1:C:356:ARG:HD2	2.02	0.41
1:D:91:THR:HG23	1:D:415:VAL:HB	2.02	0.41
1:D:230:CYS:CB	1:D:256:CYS:HA	2.50	0.41
1:D:286:PHE:CB	1:D:303:GLN:HG2	2.50	0.41
1:A:41:LEU:HD11	1:A:182:PHE:HZ	1.84	0.41
1:A:83:ALA:HB2	1:A:108:PHE:CZ	2.55	0.41
1:A:274:TYR:CZ	1:A:282:THR:HG21	2.55	0.41
1:B:117:TYR:CZ	1:B:149:MET:HE2	2.55	0.41
1:B:384:LYS:HD2	1:B:387:GLN:CB	2.47	0.41
1:C:178:ARG:HB3	1:C:207:GLY:CA	2.51	0.41
1:D:197:SER:HB2	1:D:369:HIS:HD2	1.83	0.41
1:D:414:VAL:O	1:D:414:VAL:HG13	2.19	0.41
1:A:104:VAL:O	2:F:2:BGC:H6C2	2.20	0.41
1:A:295:ASN:N	1:A:352:ASN:OD1	2.51	0.41
1:A:340:ASN:ND2	1:A:342:PHE:H	2.17	0.41
1:B:82:GLY:HA3	1:B:93:LYS:CB	2.50	0.41
1:B:313:PRO:HD3	1:B:321:SER:O	2.21	0.41
1:B:374:LEU:CD2	1:B:397:THR:HA	2.51	0.41
1:C:7:THR:HA	1:C:8:PRO:HD2	1.94	0.41
1:C:275:GLY:O	1:C:281:ASP:HA	2.20	0.41
1:C:341:ARG:NH1	1:C:344:GLU:OE1	2.50	0.41
1:D:85:THR:HA	1:D:89:ALA:O	2.20	0.41
1:D:107:ARG:NH2	2:J:2:BGC:O6	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:HG23	1:A:190:GLU:N	2.35	0.41
1:B:181:LYS:O	1:B:187:ALA:HA	2.21	0.41
1:C:45:ASN:O	1:C:46:MET:HB2	2.19	0.41
1:C:78:LEU:HB3	1:C:79:GLY:H	1.58	0.41
1:C:80:THR:HB	1:C:81:TYR:CE2	2.56	0.41
1:C:127:LEU:HG	1:C:128:ALA:N	2.32	0.41
1:C:205:PRO:HB2	1:C:206:TYR:H	1.47	0.41
1:D:11:HIS:HD2	1:D:33:VAL:HB	1.84	0.41
1:D:115:ASP:C	1:D:165:ALA:HB3	2.44	0.41
1:D:408:GLN:C	1:D:410:PRO:HD3	2.45	0.41
1:A:33:VAL:HG22	1:A:34:ILE:N	2.35	0.41
1:A:196:THR:OG1	1:A:197:SER:N	2.53	0.41
1:A:343:GLU:CG	1:A:347:GLY:HA2	2.47	0.41
1:A:362:VAL:HG12	1:A:363:MET:H	1.85	0.41
1:B:189:ILE:HG23	1:B:190:GLU:N	2.36	0.41
1:B:219:ASN:O	1:B:274:TYR:OH	2.34	0.41
1:B:267:ARG:HH12	3:G:1:BGC:H6C1	1.85	0.41
1:B:325:THR:H	1:B:328:LEU:HB2	1.85	0.41
1:B:327:GLU:CD	1:B:327:GLU:H	2.28	0.41
1:C:6:GLU:H	1:C:72:GLU:CD	2.28	0.41
1:C:122:LEU:HD23	1:C:292:PHE:CE2	2.56	0.41
1:A:17:GLN:HB2	1:A:26:GLN:C	2.46	0.41
1:A:93:LYS:HG3	1:A:93:LYS:H	1.52	0.41
1:A:130:ASP:N	1:A:417:SER:O	2.50	0.41
1:A:143:ALA:N	1:A:364:SER:O	2.49	0.41
1:A:144:LEU:O	1:A:145:TYR:HB3	2.21	0.41
1:C:2:ARG:C	1:C:70:MET:HB3	2.46	0.41
1:C:158:TYR:HA	1:C:159:PRO:HD2	1.70	0.41
1:D:280:LEU:HD11	1:D:286:PHE:CG	2.56	0.41
1:A:41:LEU:CD1	1:A:49:CYS:HB2	2.51	0.41
1:A:403:ALA:O	1:A:406:GLU:N	2.53	0.41
1:B:95:VAL:CG2	1:B:104:VAL:HG13	2.51	0.41
1:B:137:GLU:HG3	1:B:409:PHE:CG	2.56	0.41
1:B:310:ILE:HA	1:B:311:PRO:HD2	1.85	0.41
1:B:325:THR:H	1:B:328:LEU:CB	2.34	0.41
1:B:387:GLN:HA	1:B:388:PRO:HD3	1.91	0.41
1:C:144:LEU:HG	1:C:145:TYR:N	2.36	0.41
1:C:383:GLU:H	1:C:383:GLU:HG2	1.51	0.41
1:D:36:ALA:HA	1:D:39:ARG:CD	2.43	0.41
1:D:230:CYS:HB3	1:D:256:CYS:HA	2.03	0.41
1:D:242:ASN:HA	4:D:524:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:LYS:O	1:D:308:ILE:HG13	2.21	0.41
1:B:394:ASP:OD2	1:B:394:ASP:N	2.53	0.41
1:C:230:CYS:HB3	1:C:256:CYS:CA	2.51	0.41
1:C:297:LEU:HD12	1:C:297:LEU:HA	1.79	0.41
1:D:2:ARG:HH21	1:D:68:LYS:CA	2.34	0.41
1:A:125:ASN:HD22	1:A:423:PRO:HA	1.85	0.41
1:A:145:TYR:CB	1:A:214:ASP:HA	2.51	0.41
1:A:145:TYR:O	1:A:362:VAL:N	2.50	0.41
1:A:250:ASP:OD2	1:A:253:ALA:HB2	2.20	0.41
1:B:86:SER:O	1:B:89:ALA:HB3	2.20	0.41
1:B:99:GLU:HG3	1:C:40:TRP:HB2	2.02	0.41
1:B:145:TYR:HE2	1:B:212:GLU:OE1	2.04	0.41
1:B:163:ALA:O	1:B:166:ARG:HG3	2.20	0.41
1:B:178:ARG:HD2	1:B:243:CYS:SG	2.60	0.41
1:B:255:LYS:HD2	4:B:499:HOH:O	2.20	0.41
1:B:328:LEU:HD13	1:B:328:LEU:HA	1.79	0.41
1:B:372:ASN:HB3	1:B:400:GLY:C	2.46	0.41
1:C:145:TYR:HB3	1:C:214:ASP:HA	2.02	0.41
1:C:174:ALA:HB2	1:C:212:GLU:HG2	2.02	0.41
1:C:351:LEU:O	1:C:354:ALA:N	2.52	0.41
1:D:325:THR:HB	1:D:327:GLU:OE1	2.20	0.41
1:D:350:GLN:OE1	1:D:353:ASN:OD1	2.38	0.41
1:A:85:THR:HG22	1:A:87:GLY:H	1.86	0.41
1:A:225:PHE:CZ	1:A:297:LEU:HG	2.56	0.41
1:A:371:ALA:O	1:A:374:LEU:HG	2.21	0.41
1:B:11:HIS:CD2	1:B:33:VAL:HG23	2.56	0.41
1:B:109:TYR:CZ	1:B:149:MET:HE1	2.55	0.41
1:B:141:ASN:HB3	1:B:366:TRP:CE2	2.56	0.41
1:B:273:PHE:HE2	1:B:301:PHE:HE1	1.69	0.41
1:C:144:LEU:HB3	1:C:216:TRP:HB3	2.03	0.41
1:C:280:LEU:HD22	1:C:280:LEU:HA	1.88	0.41
1:C:374:LEU:O	1:C:378:SER:N	2.50	0.41
1:D:45:ASN:ND2	4:D:488:HOH:O	2.50	0.41
1:A:38:TRP:NE1	2:F:2:BGC:H6C2	2.35	0.40
1:B:6:GLU:HB3	1:B:7:THR:H	1.57	0.40
1:B:42:HIS:CE1	1:B:46:MET:HE3	2.53	0.40
1:B:232:THR:HG22	1:B:234:GLU:HG2	2.03	0.40
1:C:2:ARG:O	1:C:70:MET:HB3	2.20	0.40
1:C:228:HIS:HA	1:C:342:PHE:HE1	1.85	0.40
1:C:346:GLY:CA	1:C:350:GLN:HB2	2.50	0.40
1:D:78:LEU:HD22	1:D:78:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:PHE:O	1:D:105:GLY:N	2.50	0.40
1:D:195:SER:CB	1:D:198:ASP:HB3	2.51	0.40
1:C:108:PHE:O	1:C:362:VAL:HG13	2.21	0.40
1:C:115:ASP:O	1:C:165:ALA:HB3	2.21	0.40
1:C:225:PHE:HE1	1:C:298:SER:O	2.03	0.40
1:A:97:LYS:HA	1:A:102:THR:HA	2.03	0.40
1:A:251:ARG:NH2	2:E:1:BGC:O3	2.55	0.40
1:A:336:PHE:CE1	1:A:388:PRO:HB2	2.56	0.40
1:D:35:ASP:HA	1:D:168:GLY:O	2.22	0.40
1:A:7:THR:HG21	1:A:73:GLY:C	2.45	0.40
1:A:75:GLY:O	1:A:77:TYR:N	2.55	0.40
1:A:212:GLU:OE2	1:A:214:ASP:OD1	2.40	0.40
1:A:228:HIS:ND1	1:A:257:ASP:O	2.54	0.40
1:A:232:THR:HG22	1:A:234:GLU:HG2	2.03	0.40
1:A:245:GLY:O	1:A:251:ARG:HG3	2.22	0.40
1:A:315:TRP:CZ3	1:A:388:PRO:HB3	2.57	0.40
1:B:143:ALA:O	1:B:364:SER:OG	2.36	0.40
1:B:325:THR:HB	1:B:327:GLU:OE2	2.22	0.40
1:C:307:LYS:HD2	1:C:430:PHE:HB3	2.04	0.40
1:D:198:ASP:OD1	1:D:201:ALA:N	2.50	0.40
1:D:380:TYR:HE2	2:I:1:BGC:O2	2.04	0.40
1:A:41:LEU:HD22	1:A:41:LEU:HA	1.88	0.40
1:A:124:GLY:O	1:A:125:ASN:ND2	2.54	0.40
1:B:55:TRP:H	1:B:55:TRP:CD1	2.40	0.40
1:C:193:LYS:N	1:C:193:LYS:NZ	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	428/430 (100%)	354 (83%)	57 (13%)	17 (4%)	2 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	428/430 (100%)	336 (78%)	64 (15%)	28 (6%)	1	0
1	C	428/430 (100%)	332 (78%)	69 (16%)	27 (6%)	1	0
1	D	428/430 (100%)	331 (77%)	71 (17%)	26 (6%)	1	0
All	All	1712/1720 (100%)	1353 (79%)	261 (15%)	98 (6%)	1	0

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	CYS
1	A	122	LEU
1	A	278	LYS
1	A	347	GLY
1	B	6	GLU
1	B	30	ALA
1	B	78	LEU
1	B	86	SER
1	B	187	ALA
1	B	188	ASN
1	B	240	THR
1	B	273	PHE
1	B	304	ASP
1	B	385	GLU
1	B	399	SER
1	C	46	MET
1	C	94	PHE
1	C	205	PRO
1	C	385	GLU
1	C	399	SER
1	C	402	PRO
1	D	43	ASP
1	D	51	ASP
1	D	94	PHE
1	D	114	PRO
1	D	135	THR
1	D	190	GLU
1	D	199	PRO
1	D	235	TYR
1	D	260	GLY
1	D	372	ASN
1	A	30	ALA
1	A	129	PHE

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Mol	Chain	Res	Type
1	A	176	CYS
1	B	210	CYS
1	B	335	VAL
1	C	43	ASP
1	C	73	GLY
1	C	79	GLY
1	C	87	GLY
1	C	165	ALA
1	C	180	LEU
1	C	200	ASN
1	C	240	THR
1	C	429	ASP
1	D	87	GLY
1	D	98	HIS
1	D	113	GLY
1	D	385	GLU
1	A	52	GLY
1	A	315	TRP
1	A	337	ASN
1	A	384	LYS
1	A	403	ALA
1	B	94	PHE
1	B	123	MET
1	B	184	GLY
1	B	212	GLU
1	B	338	ASP
1	C	78	LEU
1	C	173	ASP
1	C	206	TYR
1	C	383	GLU
1	C	388	PRO
1	C	404	GLU
1	D	63	THR
1	D	106	SER
1	D	191	GLY
1	D	205	PRO
1	D	319	PRO
1	A	385	GLU
1	B	62	ALA
1	B	211	ALA
1	B	412	ALA
1	B	424	ILE

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Mol	Chain	Res	Type
1	C	177	ALA
1	C	219	ASN
1	C	414	VAL
1	D	22	PRO
1	D	71	ILE
1	D	176	CYS
1	D	285	LYS
1	D	328	LEU
1	A	76	ASP
1	A	390	ALA
1	B	176	CYS
1	A	260	GLY
1	A	391	ALA
1	B	8	PRO
1	B	138	CYS
1	C	159	PRO
1	B	402	PRO
1	C	164	GLY
1	B	345	VAL
1	B	52	GLY
1	D	313	PRO
1	D	402	PRO
1	C	424	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/354 (100%)	238 (67%)	116 (33%)	0	0
1	B	354/354 (100%)	238 (67%)	116 (33%)	0	0
1	C	354/354 (100%)	258 (73%)	96 (27%)	0	0
1	D	354/354 (100%)	252 (71%)	102 (29%)	0	0
All	All	1416/1416 (100%)	986 (70%)	430 (30%)	0	0

All (430) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	GLU
1	A	7	THR
1	A	17	GLN
1	A	20	THR
1	A	26	GLN
1	A	27	THR
1	A	29	ASN
1	A	32	VAL
1	A	34	ILE
1	A	41	LEU
1	A	45	ASN
1	A	46	MET
1	A	54	GLN
1	A	57	ASN
1	A	59	CYS
1	A	64	ASP
1	A	71	ILE
1	A	78	LEU
1	A	84	SER
1	A	86	SER
1	A	92	LEU
1	A	93	LYS
1	A	97	LYS
1	A	104	VAL
1	A	110	LEU
1	A	116	LYS
1	A	121	ASN
1	A	122	LEU
1	A	123	MET
1	A	130	ASP
1	A	133	LEU
1	A	135	THR
1	A	137	GLU
1	A	140	ILE
1	A	142	SER
1	A	144	LEU
1	A	147	VAL
1	A	149	MET
1	A	150	GLU
1	A	157	SER
1	A	175	GLN
1	A	181	LYS

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Mol	Chain	Res	Type
1	A	193	LYS
1	A	194	SER
1	A	196	THR
1	A	203	VAL
1	A	206	TYR
1	A	209	CYS
1	A	212	GLU
1	A	214	ASP
1	A	215	VAL
1	A	219	ASN
1	A	231	THR
1	A	233	ASN
1	A	234	GLU
1	A	239	GLU
1	A	241	THR
1	A	247	TYR
1	A	249	GLU
1	A	251	ARG
1	A	252	PHE
1	A	255	LYS
1	A	261	CYS
1	A	267	ARG
1	A	272	ASP
1	A	276	LYS
1	A	279	THR
1	A	280	LEU
1	A	284	ARG
1	A	285	LYS
1	A	287	THR
1	A	290	SER
1	A	291	ARG
1	A	293	GLU
1	A	294	GLU
1	A	297	LEU
1	A	298	SER
1	A	300	TYR
1	A	304	ASP
1	A	307	LYS
1	A	308	ILE
1	A	309	GLU
1	A	314	THR
1	A	316	GLU

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Mol	Chain	Res	Type
1	A	323	GLU
1	A	328	LEU
1	A	332	MET
1	A	336	PHE
1	A	337	ASN
1	A	338	ASP
1	A	339	ARG
1	A	341	ARG
1	A	348	PHE
1	A	352	ASN
1	A	353	ASN
1	A	356	ARG
1	A	357	VAL
1	A	359	MET
1	A	361	LEU
1	A	364	SER
1	A	366	TRP
1	A	385	GLU
1	A	387	GLN
1	A	392	ARG
1	A	397	THR
1	A	398	ASP
1	A	401	VAL
1	A	404	GLU
1	A	409	PHE
1	A	413	GLN
1	A	415	VAL
1	A	417	SER
1	A	424	ILE
1	A	426	SER
1	A	429	ASP
1	B	2	ARG
1	B	5	ASN
1	B	6	GLU
1	B	7	THR
1	B	9	GLU
1	B	20	THR
1	B	31	GLU
1	B	34	ILE
1	B	37	ASN
1	B	41	LEU
1	B	44	ASP

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Mol	Chain	Res	Type
1	B	45	ASN
1	B	47	GLN
1	B	48	ASN
1	B	49	CYS
1	B	59	CYS
1	B	63	THR
1	B	64	ASP
1	B	67	GLU
1	B	68	LYS
1	B	71	ILE
1	B	72	GLU
1	B	76	ASP
1	B	78	LEU
1	B	80	THR
1	B	86	SER
1	B	88	ASP
1	B	93	LYS
1	B	96	THR
1	B	98	HIS
1	B	106	SER
1	B	111	MET
1	B	115	ASP
1	B	123	MET
1	B	126	GLU
1	B	127	LEU
1	B	130	ASP
1	B	135	THR
1	B	144	LEU
1	B	145	TYR
1	B	149	MET
1	B	155	MET
1	B	166	ARG
1	B	169	THR
1	B	178	ARG
1	B	179	ASP
1	B	181	LYS
1	B	190	GLU
1	B	193	LYS
1	B	194	SER
1	B	196	THR
1	B	197	SER
1	B	200	ASN

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Mol	Chain	Res	Type
1	B	209	CYS
1	B	212	GLU
1	B	214	ASP
1	B	217	GLU
1	B	232	THR
1	B	240	THR
1	B	241	THR
1	B	243	CYS
1	B	249	GLU
1	B	255	LYS
1	B	262	ASP
1	B	264	ASN
1	B	267	ARG
1	B	268	MET
1	B	278	LYS
1	B	280	LEU
1	B	281	ASP
1	B	284	ARG
1	B	285	LYS
1	B	287	THR
1	B	293	GLU
1	B	297	LEU
1	B	298	SER
1	B	299	GLN
1	B	302	ILE
1	B	306	ARG
1	B	307	LYS
1	B	310	ILE
1	B	316	GLU
1	B	320	ASN
1	B	323	GLU
1	B	324	ILE
1	B	327	GLU
1	B	328	LEU
1	B	330	SER
1	B	332	MET
1	B	334	ASP
1	B	337	ASN
1	B	338	ASP
1	B	345	VAL
1	B	348	PHE
1	B	349	GLU

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Mol	Chain	Res	Type
1	B	352	ASN
1	B	353	ASN
1	B	355	LEU
1	B	356	ARG
1	B	360	VAL
1	B	365	ILE
1	B	369	HIS
1	B	374	LEU
1	B	376	LEU
1	B	383	GLU
1	B	384	LYS
1	B	385	GLU
1	B	394	ASP
1	B	395	CYS
1	B	397	THR
1	B	398	ASP
1	B	404	GLU
1	B	406	GLU
1	B	415	VAL
1	B	416	TRP
1	B	419	ILE
1	C	2	ARG
1	C	5	ASN
1	C	11	HIS
1	C	20	THR
1	C	28	VAL
1	C	32	VAL
1	C	33	VAL
1	C	39	ARG
1	C	46	MET
1	C	47	GLN
1	C	53	ASN
1	C	57	ASN
1	C	59	CYS
1	C	61	THR
1	C	64	ASP
1	C	70	MET
1	C	78	LEU
1	C	86	SER
1	C	88	ASP
1	C	95	VAL
1	C	96	THR

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Mol	Chain	Res	Type
1	C	97	LYS
1	C	98	HIS
1	C	99	GLU
1	C	111	MET
1	C	116	LYS
1	C	119	MET
1	C	121	ASN
1	C	123	MET
1	C	131	VAL
1	C	133	LEU
1	C	136	VAL
1	C	144	LEU
1	C	149	MET
1	C	166	ARG
1	C	173	ASP
1	C	175	GLN
1	C	180	LEU
1	C	190	GLU
1	C	193	LYS
1	C	200	ASN
1	C	208	SER
1	C	209	CYS
1	C	217	GLU
1	C	228	HIS
1	C	230	CYS
1	C	232	THR
1	C	234	GLU
1	C	238	CYS
1	C	240	THR
1	C	241	THR
1	C	242	ASN
1	C	243	CYS
1	C	246	THR
1	C	249	GLU
1	C	252	PHE
1	C	255	LYS
1	C	263	TYR
1	C	265	PRO
1	C	267	ARG
1	C	270	ASN
1	C	272	ASP
1	C	278	LYS

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Mol	Chain	Res	Type
1	C	280	LEU
1	C	284	ARG
1	C	290	SER
1	C	291	ARG
1	C	297	LEU
1	C	298	SER
1	C	299	GLN
1	C	303	GLN
1	C	306	ARG
1	C	309	GLU
1	C	316	GLU
1	C	328	LEU
1	C	335	VAL
1	C	337	ASN
1	C	342	PHE
1	C	351	LEU
1	C	352	ASN
1	C	361	LEU
1	C	365	ILE
1	C	367	ASP
1	C	373	MET
1	C	379	ILE
1	C	383	GLU
1	C	384	LYS
1	C	397	THR
1	C	398	ASP
1	C	404	GLU
1	C	405	VAL
1	C	413	GLN
1	C	415	VAL
1	C	419	ILE
1	C	420	ARG
1	C	424	ILE
1	D	2	ARG
1	D	6	GLU
1	D	10	ASN
1	D	27	THR
1	D	29	ASN
1	D	31	GLU
1	D	32	VAL
1	D	33	VAL
1	D	34	ILE

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Mol	Chain	Res	Type
1	D	38	TRP
1	D	39	ARG
1	D	41	LEU
1	D	57	ASN
1	D	59	CYS
1	D	60	SER
1	D	61	THR
1	D	63	THR
1	D	64	ASP
1	D	70	MET
1	D	71	ILE
1	D	72	GLU
1	D	78	LEU
1	D	84	SER
1	D	93	LYS
1	D	96	THR
1	D	97	LYS
1	D	98	HIS
1	D	99	GLU
1	D	104	VAL
1	D	110	LEU
1	D	111	MET
1	D	114	PRO
1	D	117	TYR
1	D	119	MET
1	D	122	LEU
1	D	123	MET
1	D	126	GLU
1	D	133	LEU
1	D	134	SER
1	D	135	THR
1	D	138	CYS
1	D	145	TYR
1	D	146	PHE
1	D	150	GLU
1	D	166	ARG
1	D	171	TYR
1	D	175	GLN
1	D	178	ARG
1	D	181	LYS
1	D	183	VAL
1	D	189	ILE

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Mol	Chain	Res	Type
1	D	193	LYS
1	D	194	SER
1	D	196	THR
1	D	197	SER
1	D	200	ASN
1	D	208	SER
1	D	226	THR
1	D	228	HIS
1	D	230	CYS
1	D	234	GLU
1	D	236	HIS
1	D	242	ASN
1	D	249	GLU
1	D	251	ARG
1	D	270	ASN
1	D	280	LEU
1	D	281	ASP
1	D	290	SER
1	D	291	ARG
1	D	294	GLU
1	D	295	ASN
1	D	296	LYS
1	D	297	LEU
1	D	306	ARG
1	D	309	GLU
1	D	315	TRP
1	D	320	ASN
1	D	324	ILE
1	D	325	THR
1	D	327	GLU
1	D	328	LEU
1	D	330	SER
1	D	334	ASP
1	D	343	GLU
1	D	344	GLU
1	D	355	LEU
1	D	359	MET
1	D	361	LEU
1	D	365	ILE
1	D	373	MET
1	D	379	ILE
1	D	383	GLU

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Mol	Chain	Res	Type
1	D	384	LYS
1	D	387	GLN
1	D	392	ARG
1	D	394	ASP
1	D	397	THR
1	D	405	VAL
1	D	424	ILE
1	D	426	SER
1	D	430	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	24	ASN
1	A	26	GLN
1	A	29	ASN
1	A	48	ASN
1	A	103	ASN
1	A	121	ASN
1	A	125	ASN
1	A	236	HIS
1	A	270	ASN
1	A	303	GLN
1	A	320	ASN
1	A	337	ASN
1	A	340	ASN
1	A	353	ASN
1	A	372	ASN
1	A	408	GLN
1	A	413	GLN
1	B	5	ASN
1	B	26	GLN
1	B	45	ASN
1	B	125	ASN
1	B	141	ASN
1	B	175	GLN
1	B	270	ASN
1	B	299	GLN
1	B	320	ASN
1	B	340	ASN
1	B	372	ASN

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Mol	Chain	Res	Type
1	B	387	GLN
1	B	418	ASN
1	C	5	ASN
1	C	17	GLN
1	C	37	ASN
1	C	45	ASN
1	C	118	GLN
1	C	121	ASN
1	C	125	ASN
1	C	161	ASN
1	C	270	ASN
1	C	320	ASN
1	C	337	ASN
1	C	352	ASN
1	C	353	ASN
1	C	387	GLN
1	D	11	HIS
1	D	24	ASN
1	D	29	ASN
1	D	98	HIS
1	D	121	ASN
1	D	125	ASN
1	D	242	ASN
1	D	264	ASN
1	D	337	ASN
1	D	340	ASN
1	D	352	ASN
1	D	353	ASN
1	D	369	HIS
1	D	372	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	PCA	C	1	1	7,8,9	2.19	1 (14%)	9,10,12	1.50	2 (22%)
1	PCA	D	1	1	7,8,9	2.24	1 (14%)	9,10,12	1.52	2 (22%)
1	PCA	A	1	1	7,8,9	2.31	1 (14%)	9,10,12	1.84	3 (33%)
1	PCA	B	1	1	7,8,9	2.16	1 (14%)	9,10,12	1.56	2 (22%)

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
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CD-N	5.62	1.48	1.34
1	D	1	PCA	CD-N	5.48	1.48	1.34
1	B	1	PCA	CD-N	5.43	1.48	1.34
1	C	1	PCA	CD-N	5.39	1.47	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	OE-CD-CG	-3.28	120.87	126.72
1	A	1	PCA	CG-CD-N	-2.91	101.26	108.39
1	C	1	PCA	CB-CG-CD	2.61	108.44	104.41
1	D	1	PCA	CG-CD-N	-2.60	102.02	108.39
1	B	1	PCA	OE-CD-CG	-2.49	122.28	126.72
1	B	1	PCA	CB-CA-C	-2.40	109.37	112.66
1	D	1	PCA	CB-CG-CD	2.09	107.64	104.41
1	C	1	PCA	CB-CA-C	-2.08	109.81	112.66
1	A	1	PCA	CB-CA-C	-2.00	109.91	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	1	PCA	2	0
1	A	1	PCA	4	0
1	B	1	PCA	4	0

5.5 Carbohydrates [i](#)

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BGC	E	1	2	12,12,12	0.50	0	17,17,17	1.13	2 (11%)
2	BGC	E	2	2	11,11,12	0.39	0	15,15,17	0.80	1 (6%)
2	BGC	F	1	2	12,12,12	0.52	0	17,17,17	0.97	1 (5%)
2	BGC	F	2	2	11,11,12	0.33	0	15,15,17	1.31	2 (13%)
3	BGC	G	1	3	12,12,12	0.57	0	17,17,17	1.08	1 (5%)
3	BGC	G	2	3	11,11,12	0.46	0	15,15,17	1.10	1 (6%)
3	BGC	G	3	3	11,11,12	0.39	0	15,15,17	1.49	3 (20%)
3	BGC	G	4	3	11,11,12	0.43	0	15,15,17	0.90	0
2	BGC	H	1	2	12,12,12	0.56	0	17,17,17	1.03	0
2	BGC	H	2	2	11,11,12	0.45	0	15,15,17	1.03	1 (6%)
2	BGC	I	1	2	12,12,12	0.55	0	17,17,17	0.90	1 (5%)
2	BGC	I	2	2	11,11,12	0.40	0	15,15,17	1.15	1 (6%)
2	BGC	J	1	2	12,12,12	0.48	0	17,17,17	0.99	1 (5%)
2	BGC	J	2	2	11,11,12	0.41	0	15,15,17	0.99	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	E	1	2	-	2/2/22/22	0/1/1/1
2	BGC	E	2	2	-	0/2/19/22	0/1/1/1
2	BGC	F	1	2	-	2/2/22/22	0/1/1/1
2	BGC	F	2	2	-	2/2/19/22	0/1/1/1
3	BGC	G	1	3	-	2/2/22/22	0/1/1/1
3	BGC	G	2	3	-	0/2/19/22	0/1/1/1
3	BGC	G	3	3	-	0/2/19/22	0/1/1/1
3	BGC	G	4	3	-	2/2/19/22	0/1/1/1
2	BGC	H	1	2	-	1/2/22/22	0/1/1/1
2	BGC	H	2	2	-	2/2/19/22	0/1/1/1
2	BGC	I	1	2	-	0/2/22/22	0/1/1/1
2	BGC	I	2	2	-	2/2/19/22	0/1/1/1
2	BGC	J	1	2	-	0/2/22/22	0/1/1/1
2	BGC	J	2	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	BGC	O4-C4-C5	3.42	117.75	109.32
2	F	2	BGC	C1-O5-C5	-3.40	107.63	112.19
2	E	1	BGC	C4-C3-C2	-2.60	106.27	110.83
3	G	3	BGC	O5-C5-C6	2.57	112.67	107.66
2	H	2	BGC	C6-C5-C4	-2.50	106.88	113.02
3	G	1	BGC	O5-C5-C4	2.43	114.07	109.70
2	J	1	BGC	C1-O5-C5	-2.41	108.99	113.65
2	F	1	BGC	C3-C4-C5	-2.22	106.20	110.23
3	G	3	BGC	C3-C4-C5	-2.21	106.22	110.23
2	I	2	BGC	C2-C3-C4	-2.12	107.13	110.86
3	G	2	BGC	C1-O5-C5	-2.12	109.34	112.19
2	I	1	BGC	C1-O5-C5	-2.12	109.55	113.65
2	E	2	BGC	O5-C5-C6	2.09	111.72	107.66
2	E	1	BGC	C6-C5-C4	-2.03	108.03	113.02
2	F	2	BGC	O5-C5-C6	2.02	111.59	107.66

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	BGC	C4-C5-C6-O6
2	F	1	BGC	O5-C5-C6-O6
2	E	1	BGC	O5-C5-C6-O6
3	G	1	BGC	O5-C5-C6-O6
2	F	2	BGC	O5-C5-C6-O6
3	G	4	BGC	O5-C5-C6-O6
2	E	1	BGC	C4-C5-C6-O6
2	F	1	BGC	C4-C5-C6-O6
2	F	2	BGC	C4-C5-C6-O6
3	G	4	BGC	C4-C5-C6-O6
2	I	2	BGC	C4-C5-C6-O6
2	I	2	BGC	O5-C5-C6-O6
2	H	2	BGC	O5-C5-C6-O6
2	H	2	BGC	C4-C5-C6-O6
2	H	1	BGC	C4-C5-C6-O6

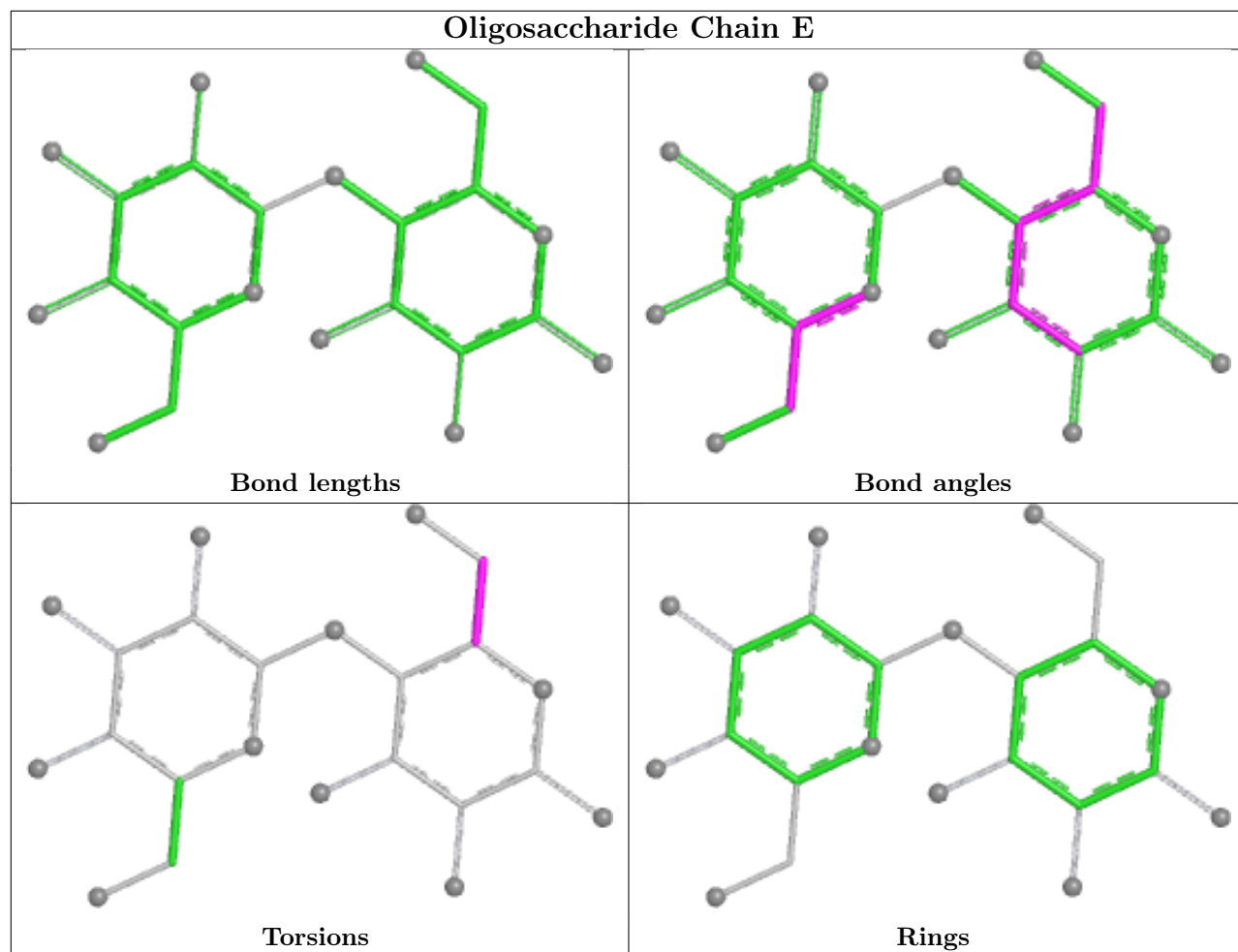
There are no ring outliers.

14 monomers are involved in 30 short contacts:

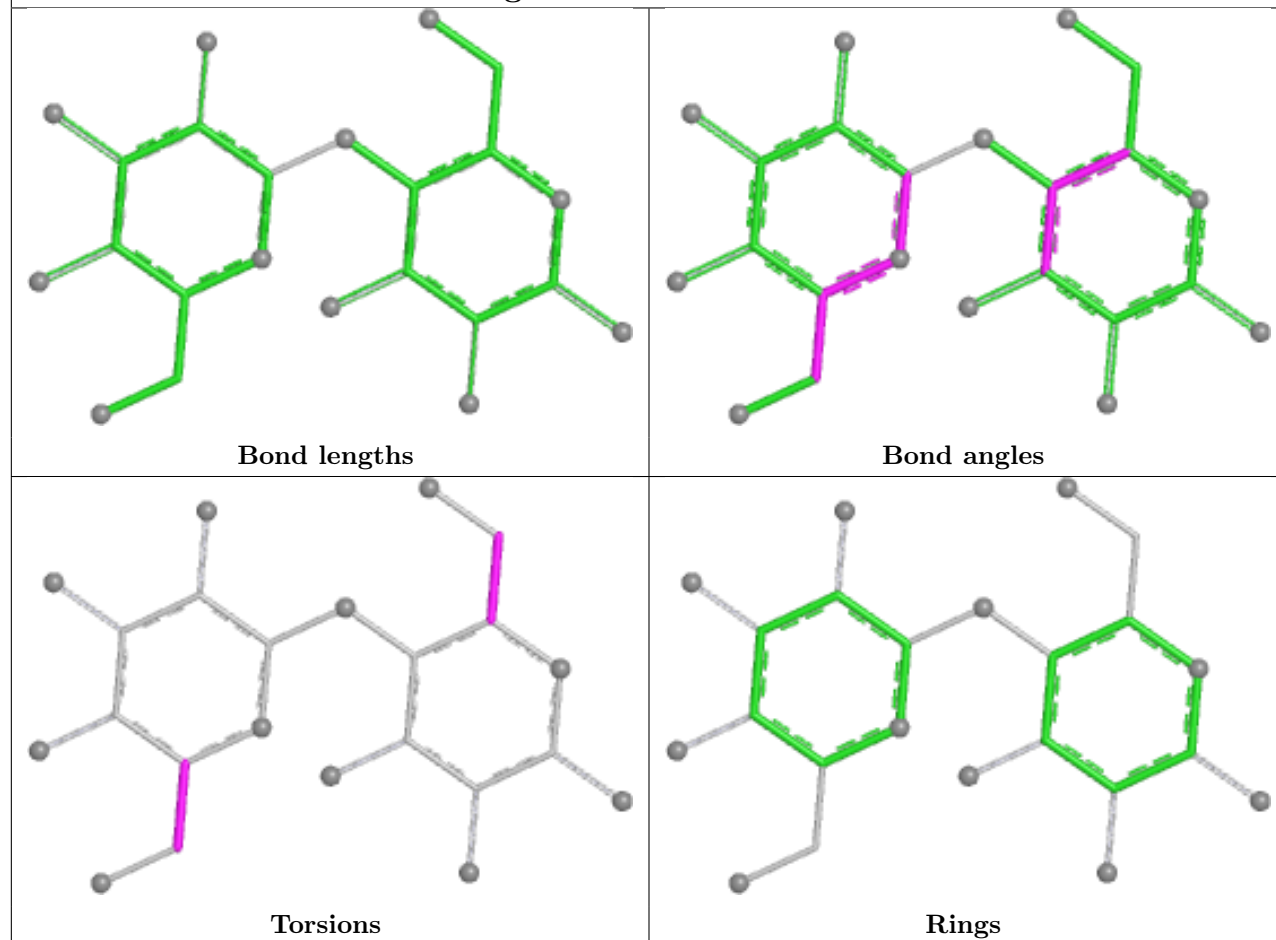
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	4	BGC	1	0
2	E	2	BGC	2	0
2	E	1	BGC	1	0
2	I	1	BGC	2	0
3	G	2	BGC	4	0
3	G	3	BGC	1	0
2	J	2	BGC	1	0
3	G	1	BGC	2	0
2	H	1	BGC	1	0
2	F	1	BGC	2	0
2	I	2	BGC	3	0
2	F	2	BGC	5	0
2	H	2	BGC	1	0
2	J	1	BGC	4	0

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

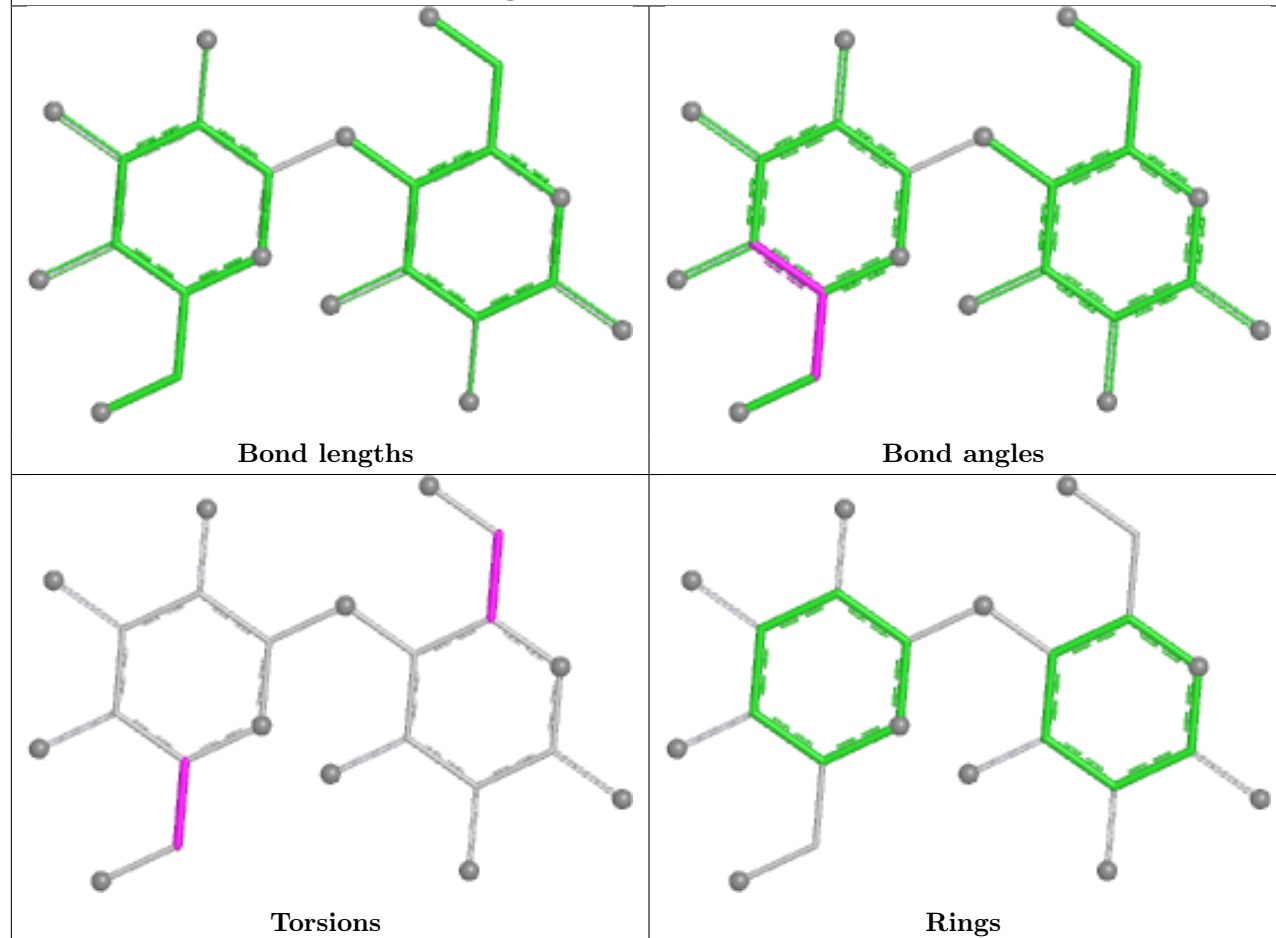
Oligosaccharide Chain E

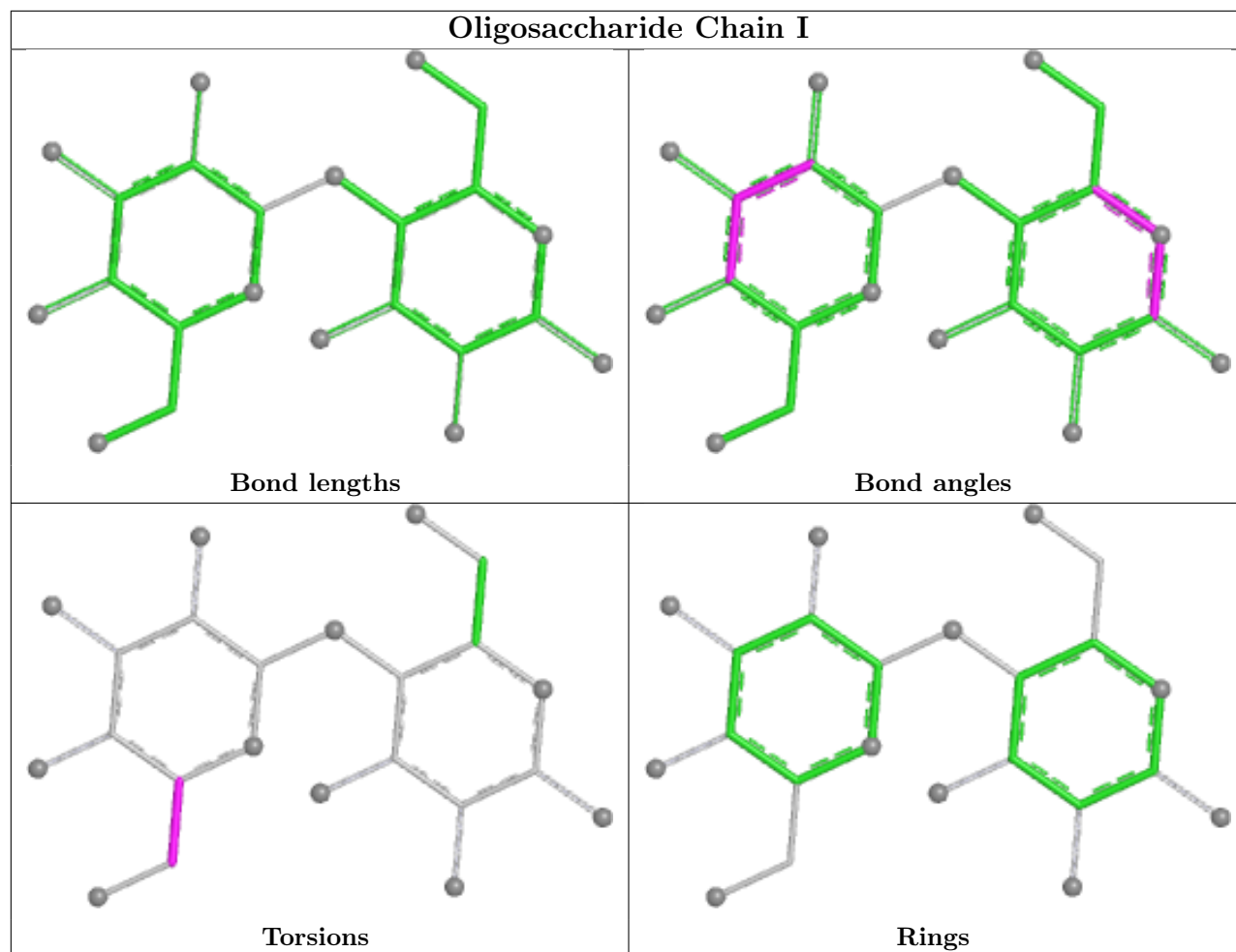


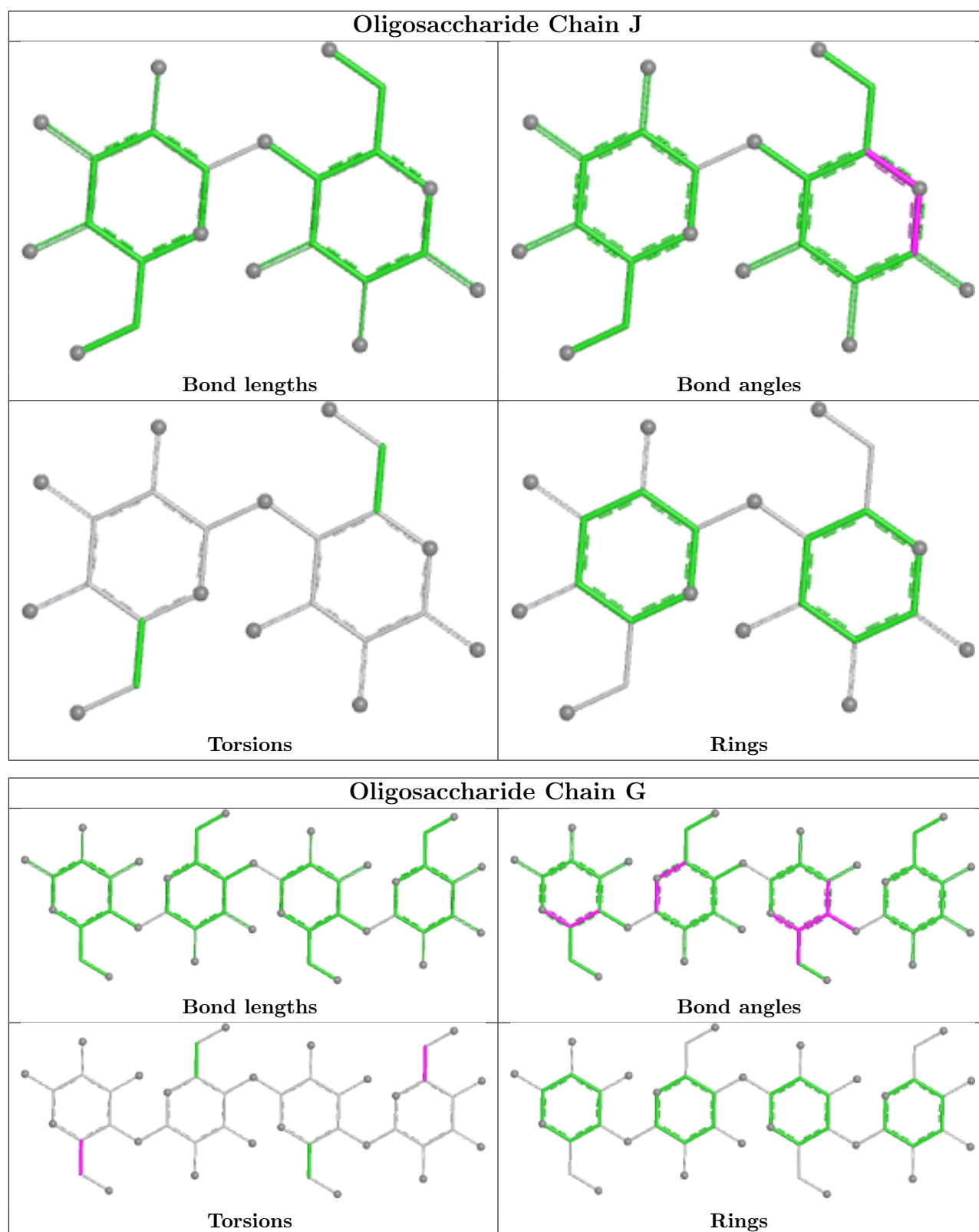
Oligosaccharide Chain F



Oligosaccharide Chain H







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	A	429/430 (99%)	-0.98	0 100 100	12, 32, 53, 70	0
1	B	429/430 (99%)	-0.95	0 100 100	11, 33, 55, 80	0
1	C	429/430 (99%)	-1.00	0 100 100	10, 31, 53, 83	0
1	D	429/430 (99%)	-1.01	0 100 100	10, 31, 49, 68	0
All	All	1716/1720 (99%)	-0.99	0 100 100	10, 32, 53, 83	0

There are no RSRZ outliers to report.

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

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

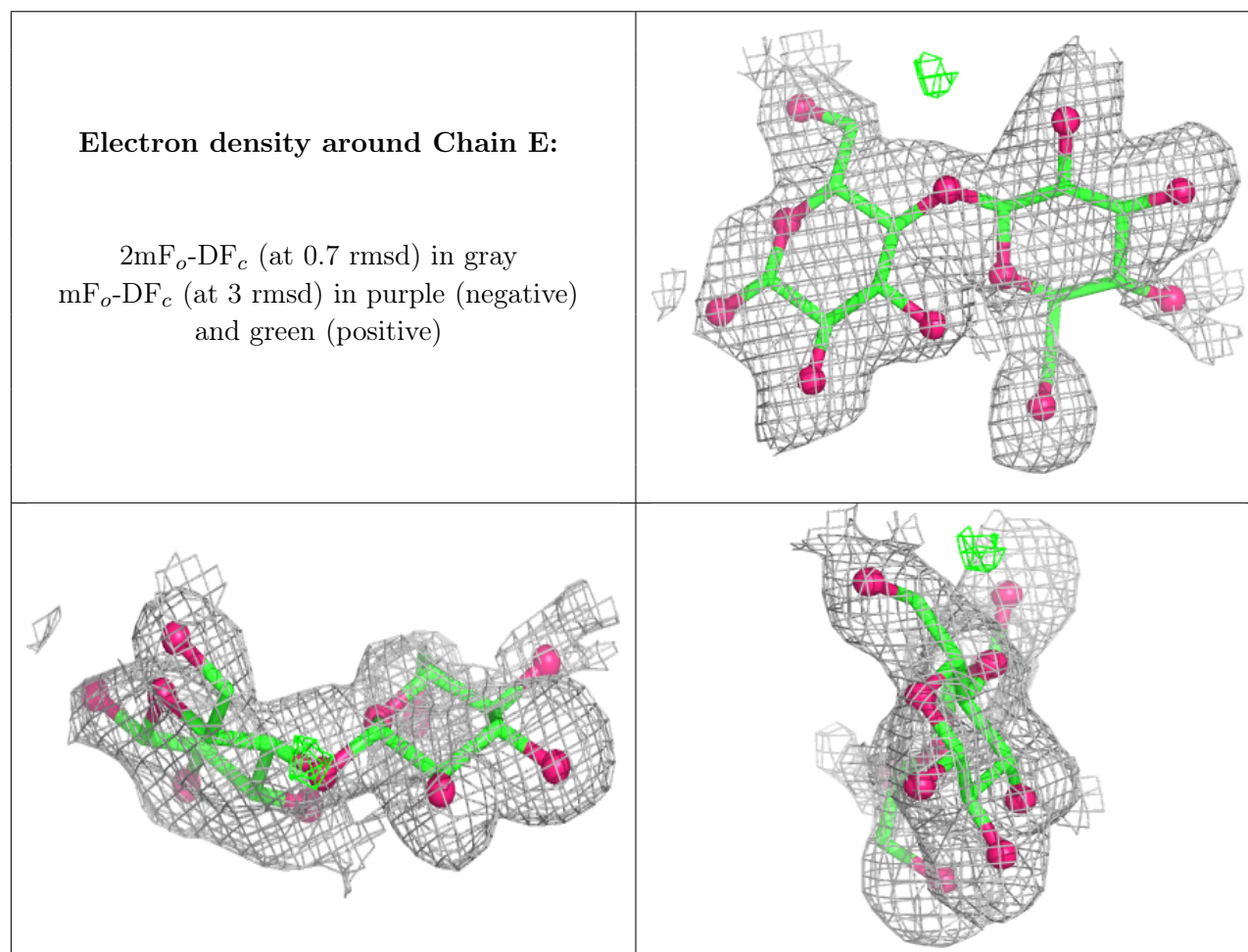
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PCA	B	1	8/9	0.98	0.05	28,41,48,52	0
1	PCA	C	1	8/9	0.98	0.05	21,32,43,57	0
1	PCA	A	1	8/9	0.99	0.04	15,28,31,49	0
1	PCA	D	1	8/9	0.99	0.04	19,25,30,40	0

6.3 Carbohydrates [i](#)

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

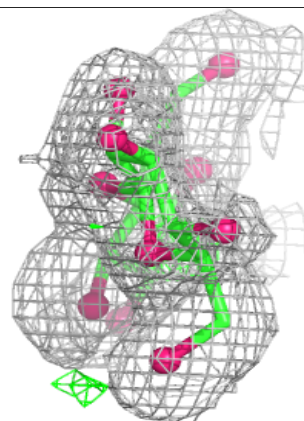
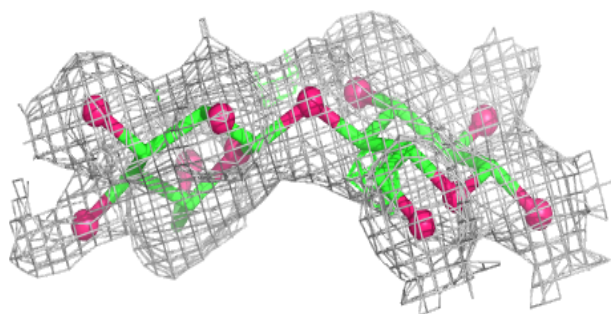
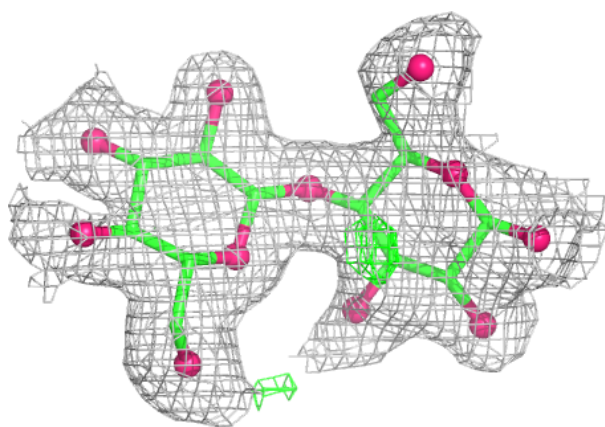
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BGC	E	1	12/12	0.98	0.06	28,41,49,49	0
2	BGC	F	1	12/12	0.98	0.06	21,26,44,50	0
3	BGC	G	2	11/12	0.98	0.05	22,35,44,60	0
2	BGC	F	2	11/12	0.99	0.04	12,20,31,48	0
2	BGC	H	1	12/12	0.99	0.04	19,22,37,50	0
2	BGC	H	2	11/12	0.99	0.04	17,23,30,45	0
2	BGC	I	2	11/12	0.99	0.04	22,25,33,43	0
2	BGC	J	1	12/12	0.99	0.04	21,27,42,51	0
2	BGC	J	2	11/12	0.99	0.05	7,31,39,42	0
3	BGC	G	1	12/12	0.99	0.04	15,24,29,31	0
2	BGC	E	2	11/12	0.99	0.05	18,30,40,57	0
3	BGC	G	3	11/12	0.99	0.05	17,41,48,49	0
3	BGC	G	4	11/12	0.99	0.05	16,33,45,53	0
2	BGC	I	1	12/12	1.00	0.03	6,19,36,59	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.

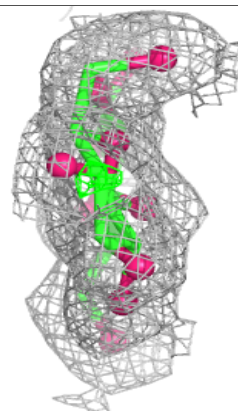
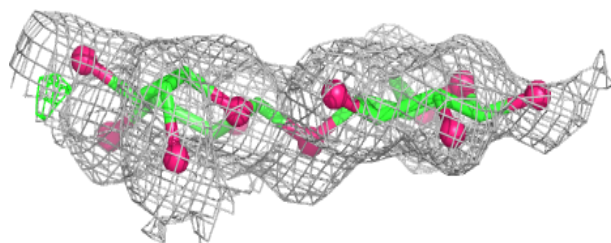
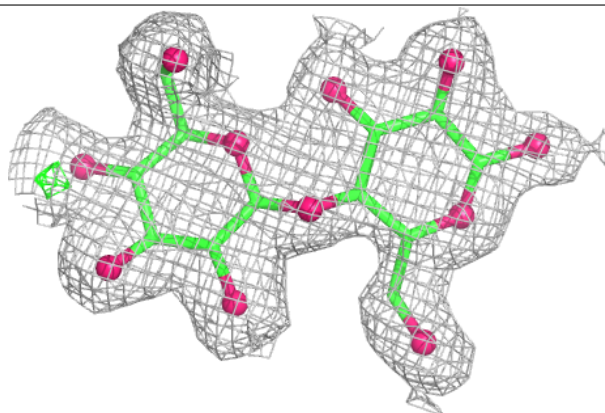


Electron density around Chain F:

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

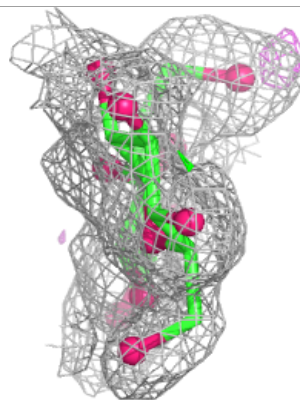
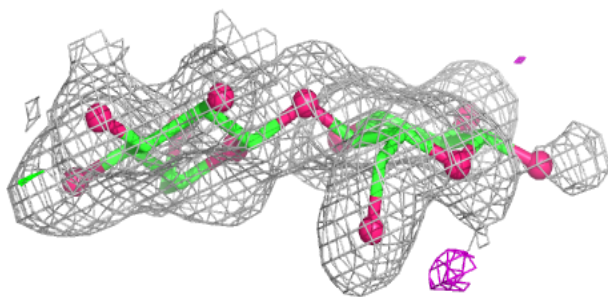
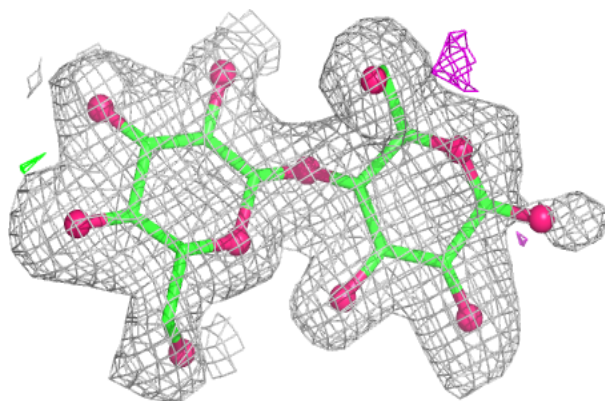
**Electron density around Chain H:**

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



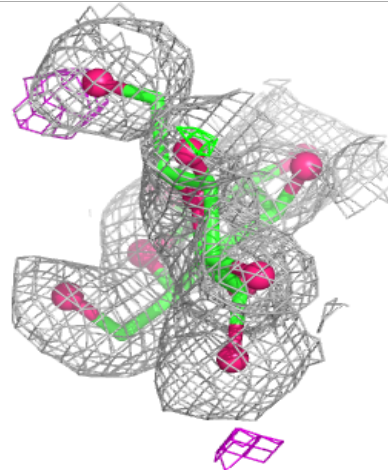
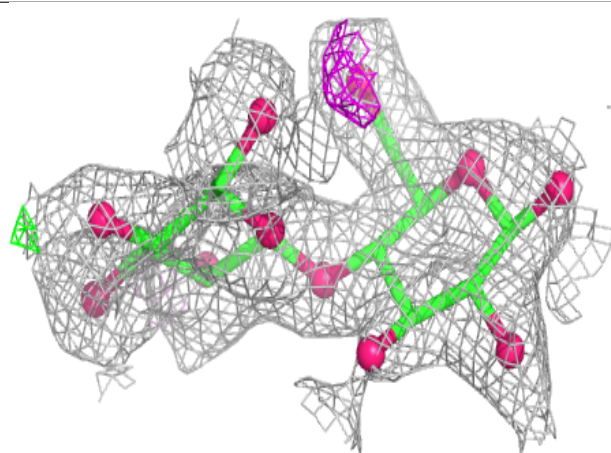
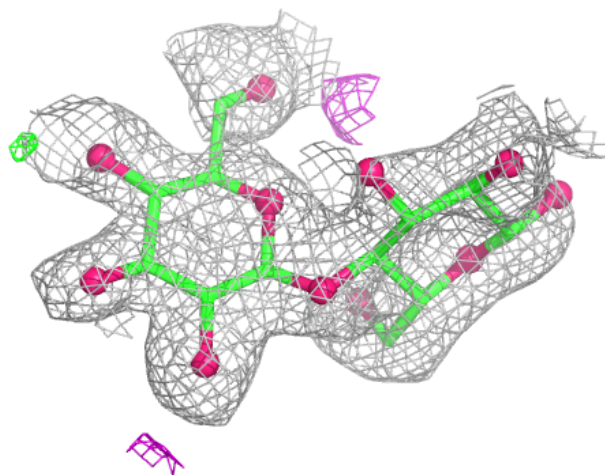
Electron density around Chain I:

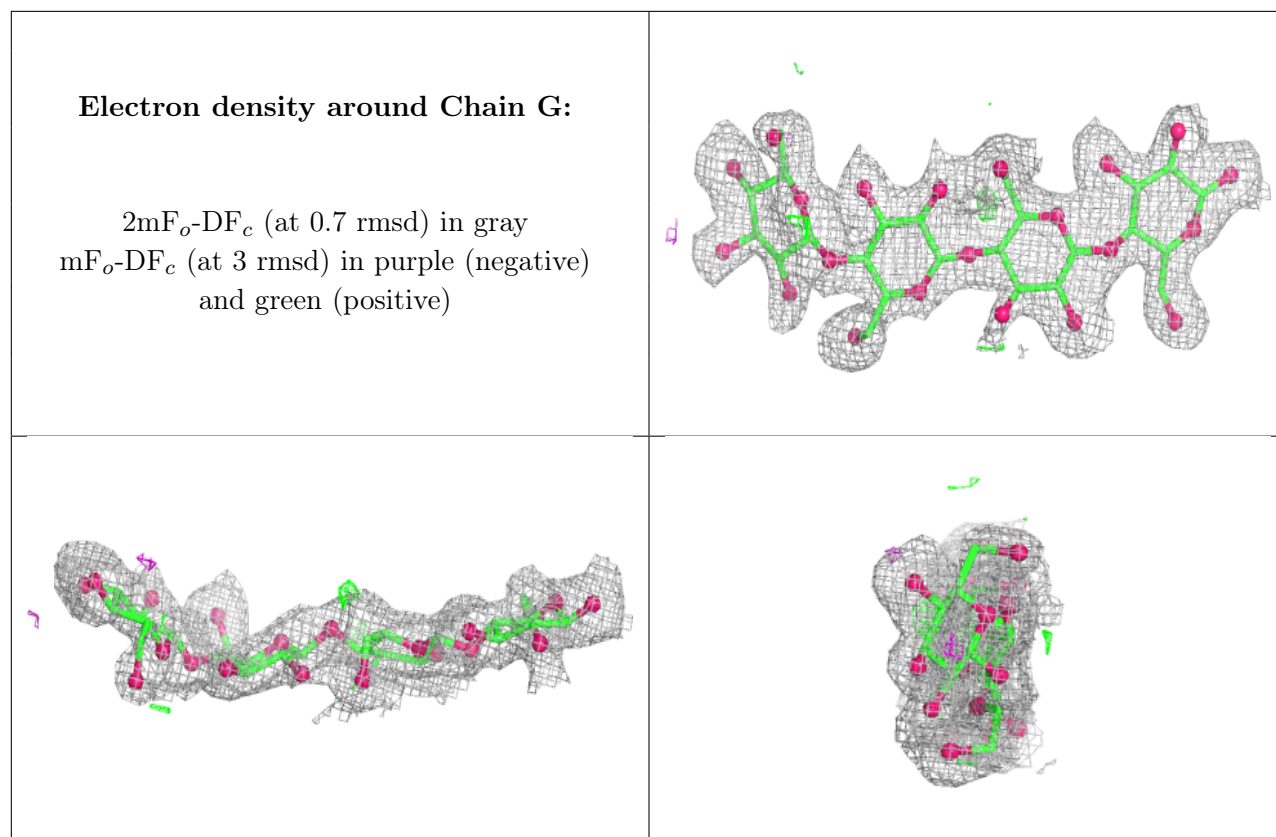
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain J:

$2mF_o-DF_c$ (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.