



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:10 PM BST

PDB ID : 3AIB
Title : Crystal Structure of Glucansucrase
Authors : Ito, K.; Ito, S.; Shimamura, T.; Iwata, S.
Deposited on : 2010-05-12
Resolution : 3.09 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

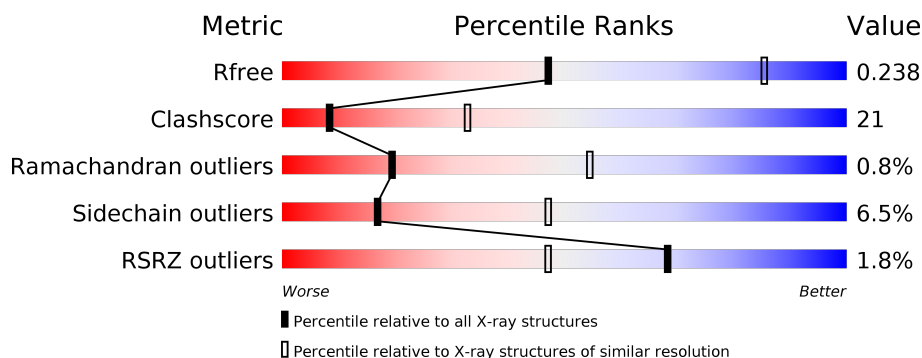
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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.





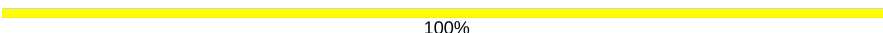
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on 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	844	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>•</div> </div> </div>
1	B	844	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>32%</div> <div>5%</div> <div>11%</div> </div> </div>
1	C	844	<div> <div></div> <div> <div></div> <div>73%</div> <div>24%</div> <div>•</div> </div> </div>
1	D	844	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>•</div> </div> </div>
1	E	844	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>•</div> </div> </div>
1	F	844	<div> <div></div> <div> <div></div> <div>60%</div> <div>36%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	844	
1	H	844	
2	I	2	

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
4	MES	B	5001	-	X	-	-
4	MES	D	5001	-	X	-	-
4	MES	F	5001	-	X	-	-
4	MES	H	5001	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 52615 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 Glucosyltransferase-SI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	0	0
			6643	4184	1141	1302	16			
1	B	749	Total	C	N	O	S	0	0	0
			5868	3692	1008	1154	14			
1	C	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	D	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	G	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	E	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	F	844	Total	C	N	O	S	0	0	0
			6660	4196	1143	1305	16			
1	H	808	Total	C	N	O	S	0	0	0
			6378	4022	1094	1246	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	597	ASP	ASN	SEE REMARK 999	UNP P13470
A	600	LYS	ARG	SEE REMARK 999	UNP P13470
A	727	ILE	THR	SEE REMARK 999	UNP P13470
A	734	VAL	ALA	SEE REMARK 999	UNP P13470
B	597	ASP	ASN	SEE REMARK 999	UNP P13470
B	600	LYS	ARG	SEE REMARK 999	UNP P13470
B	727	ILE	THR	SEE REMARK 999	UNP P13470
B	734	VAL	ALA	SEE REMARK 999	UNP P13470
C	597	ASP	ASN	SEE REMARK 999	UNP P13470
C	600	LYS	ARG	SEE REMARK 999	UNP P13470
C	727	ILE	THR	SEE REMARK 999	UNP P13470
C	734	VAL	ALA	SEE REMARK 999	UNP P13470
D	597	ASP	ASN	SEE REMARK 999	UNP P13470

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Chain	Residue	Modelled	Actual	Comment	Reference
D	600	LYS	ARG	SEE REMARK 999	UNP P13470
D	727	ILE	THR	SEE REMARK 999	UNP P13470
D	734	VAL	ALA	SEE REMARK 999	UNP P13470
G	597	ASP	ASN	SEE REMARK 999	UNP P13470
G	600	LYS	ARG	SEE REMARK 999	UNP P13470
G	727	ILE	THR	SEE REMARK 999	UNP P13470
G	734	VAL	ALA	SEE REMARK 999	UNP P13470
E	597	ASP	ASN	SEE REMARK 999	UNP P13470
E	600	LYS	ARG	SEE REMARK 999	UNP P13470
E	727	ILE	THR	SEE REMARK 999	UNP P13470
E	734	VAL	ALA	SEE REMARK 999	UNP P13470
F	597	ASP	ASN	SEE REMARK 999	UNP P13470
F	600	LYS	ARG	SEE REMARK 999	UNP P13470
F	727	ILE	THR	SEE REMARK 999	UNP P13470
F	734	VAL	ALA	SEE REMARK 999	UNP P13470
H	597	ASP	ASN	SEE REMARK 999	UNP P13470
H	600	LYS	ARG	SEE REMARK 999	UNP P13470
H	727	ILE	THR	SEE REMARK 999	UNP P13470
H	734	VAL	ALA	SEE REMARK 999	UNP P13470

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



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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

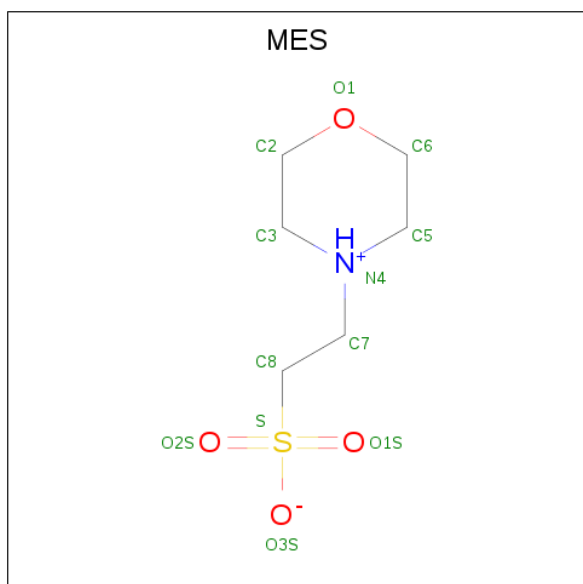
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

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

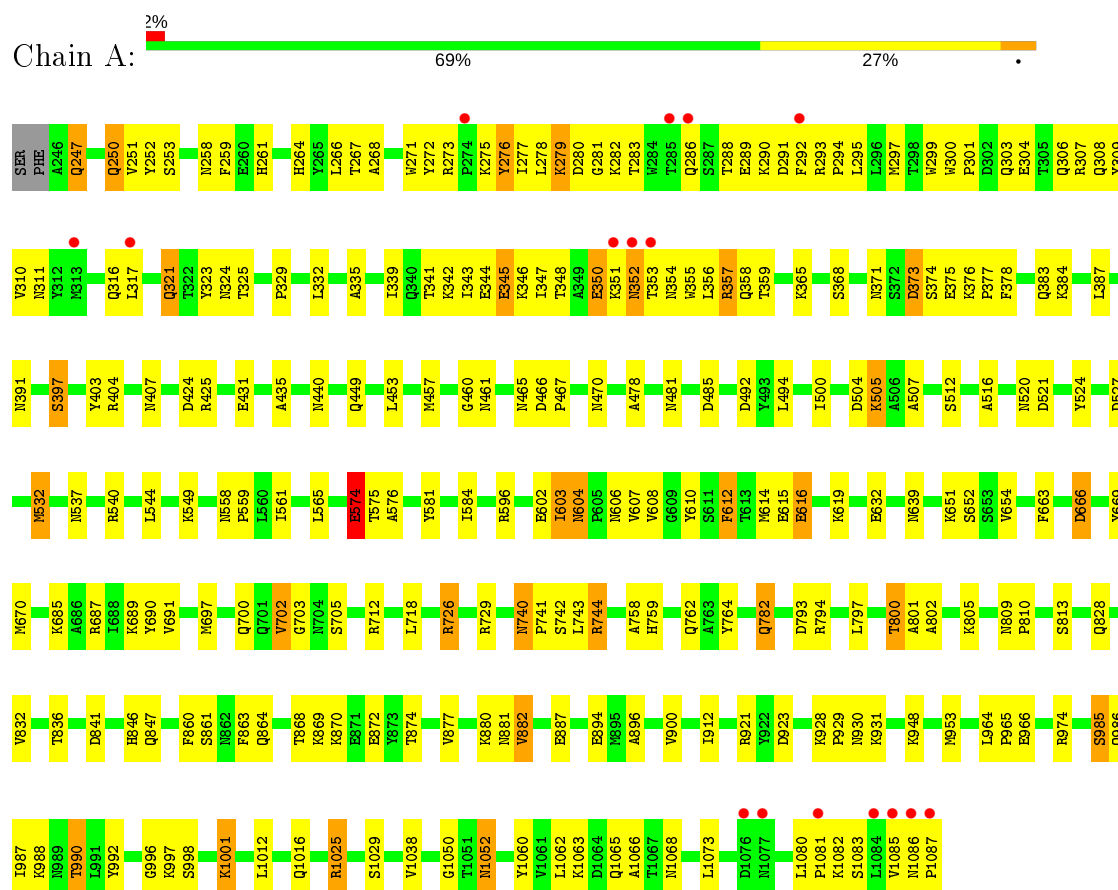
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	20	Total	O	0	0
			20	20		
5	C	59	Total	O	0	0
			59	59		
5	D	50	Total	O	0	0
			50	50		
5	G	46	Total	O	0	0
			46	46		
5	E	38	Total	O	0	0
			38	38		
5	F	23	Total	O	0	0
			23	23		
5	H	28	Total	O	0	0
			28	28		

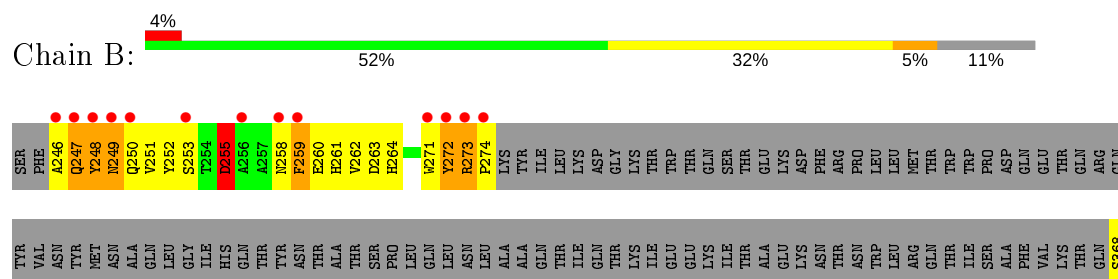
3 Residue-property plots

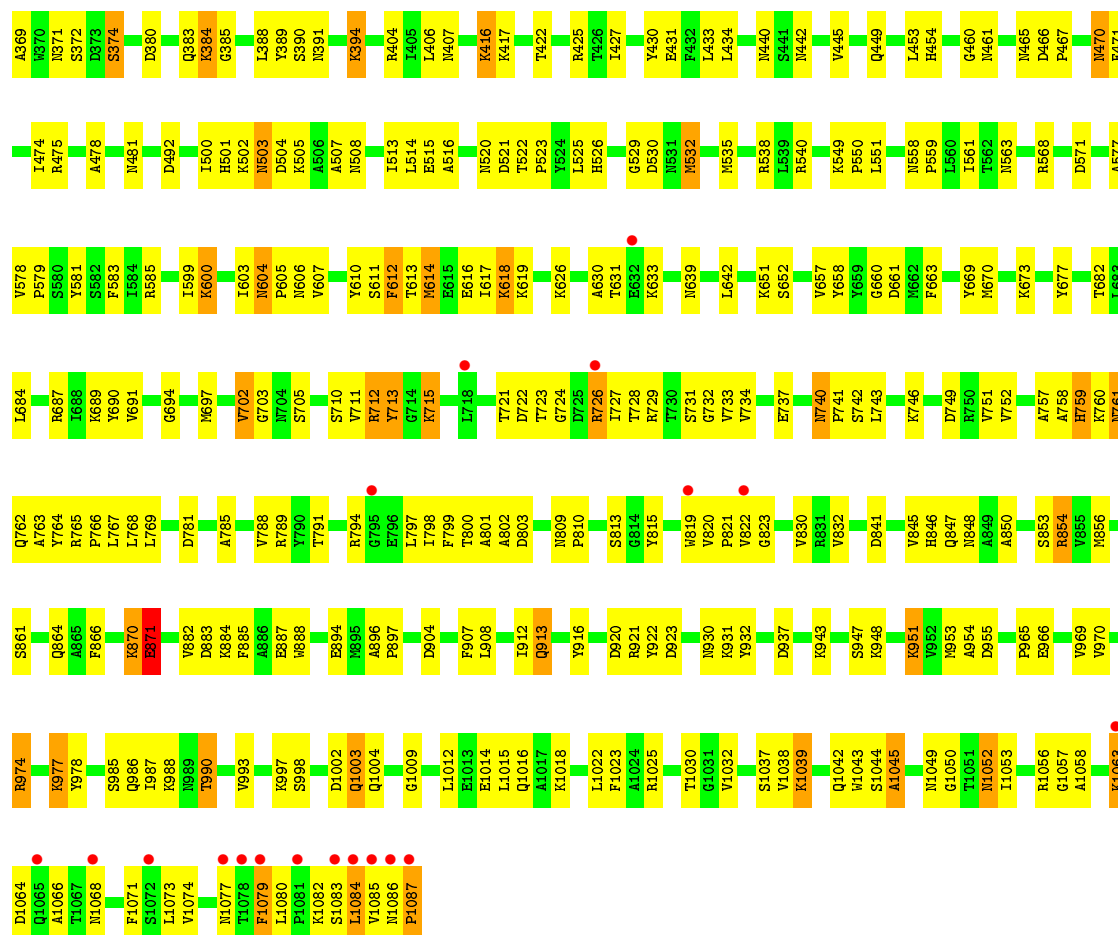
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glucosyltransferase-SI



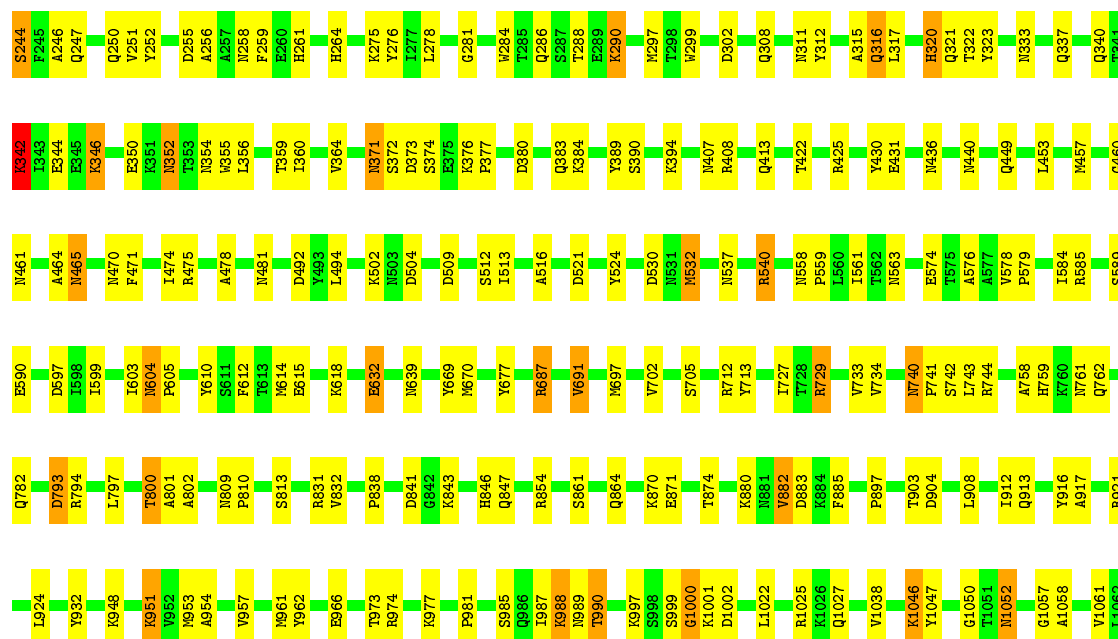
• Molecule 1: Glucosyltransferase-SI

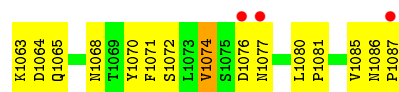




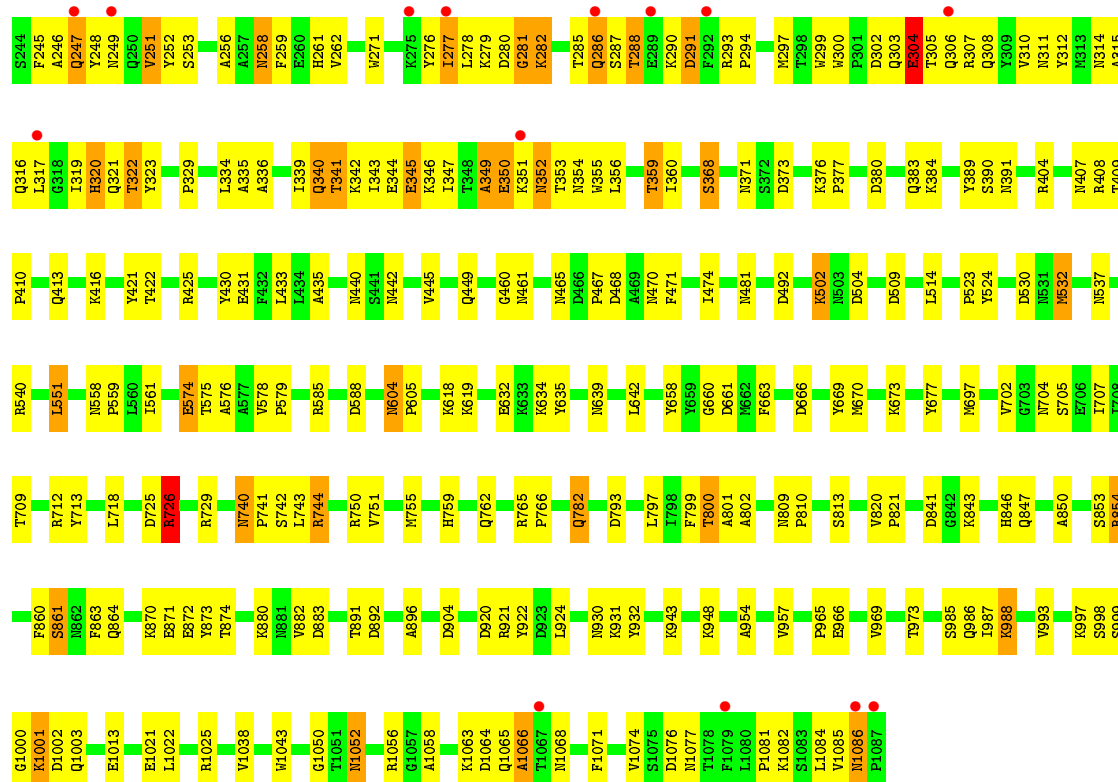
● Molecule 1: Glucosyltransferase-SI

Chain C: 73% 24% ●

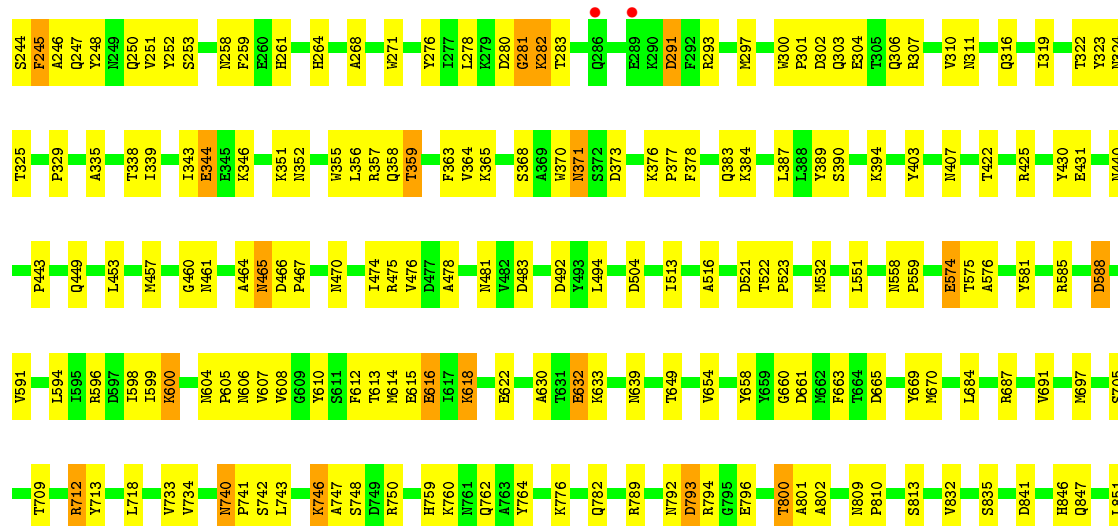


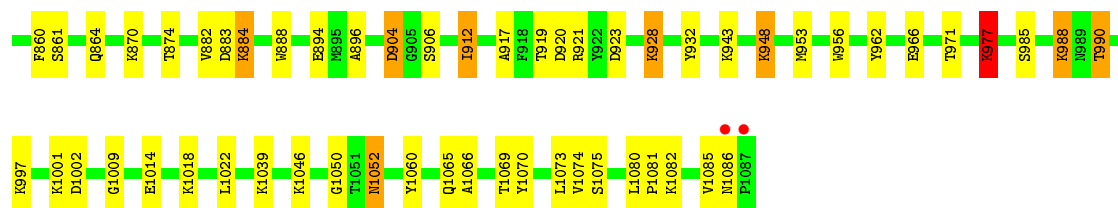


• Molecule 1: Glucosyltransferase-SI

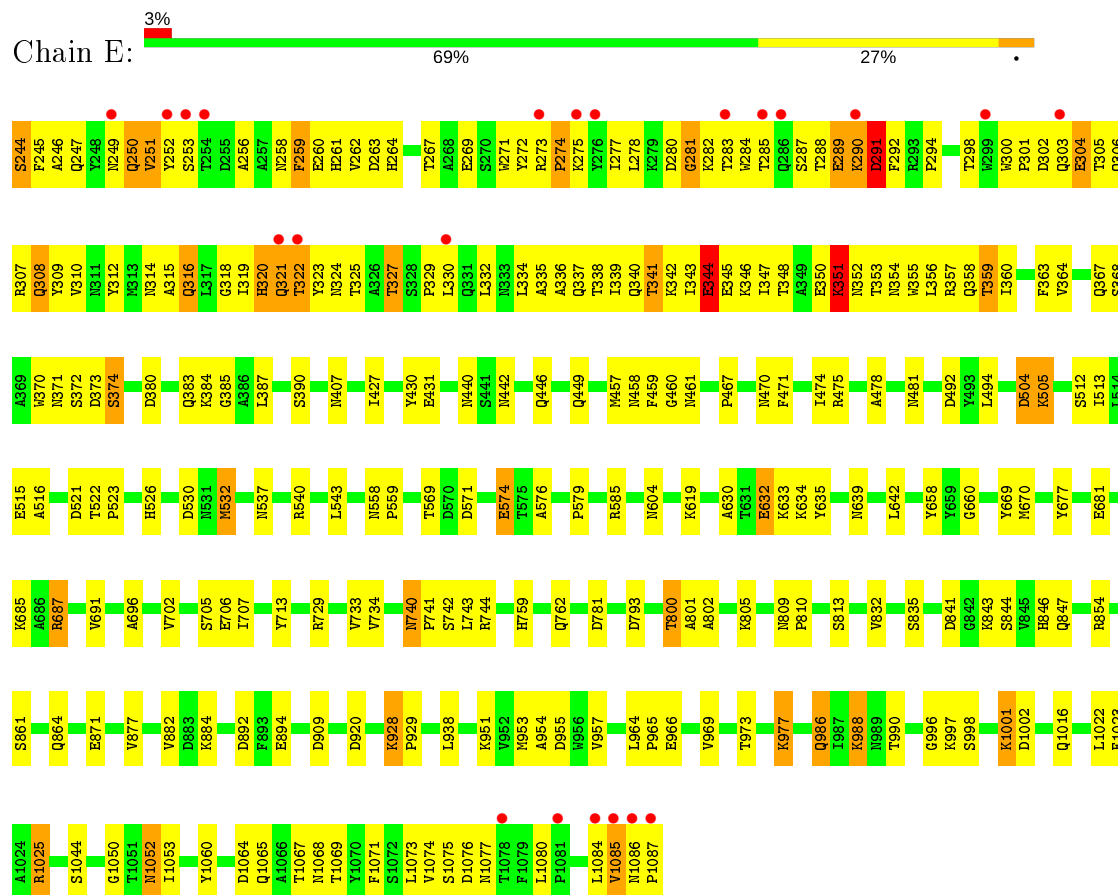


• Molecule 1: Glucosyltransferase-SI

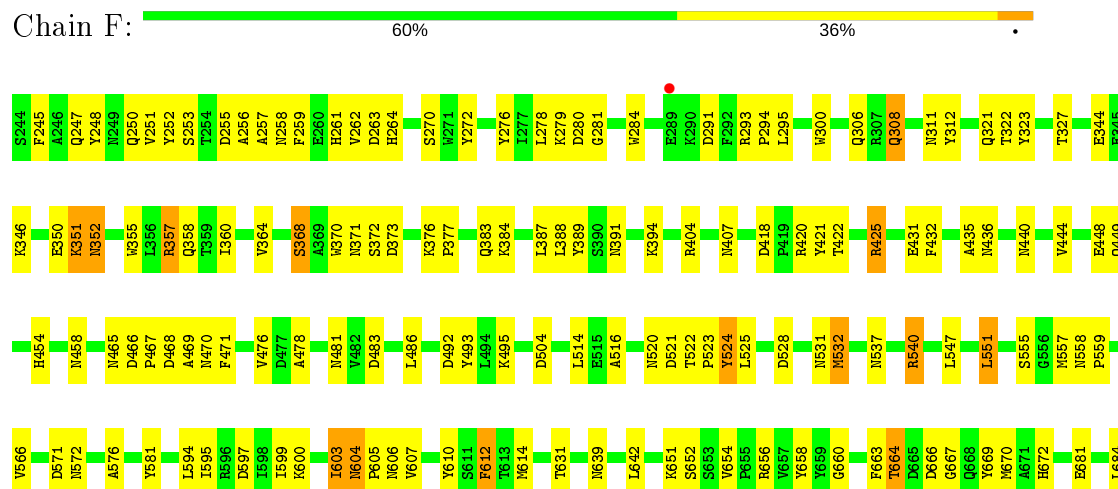


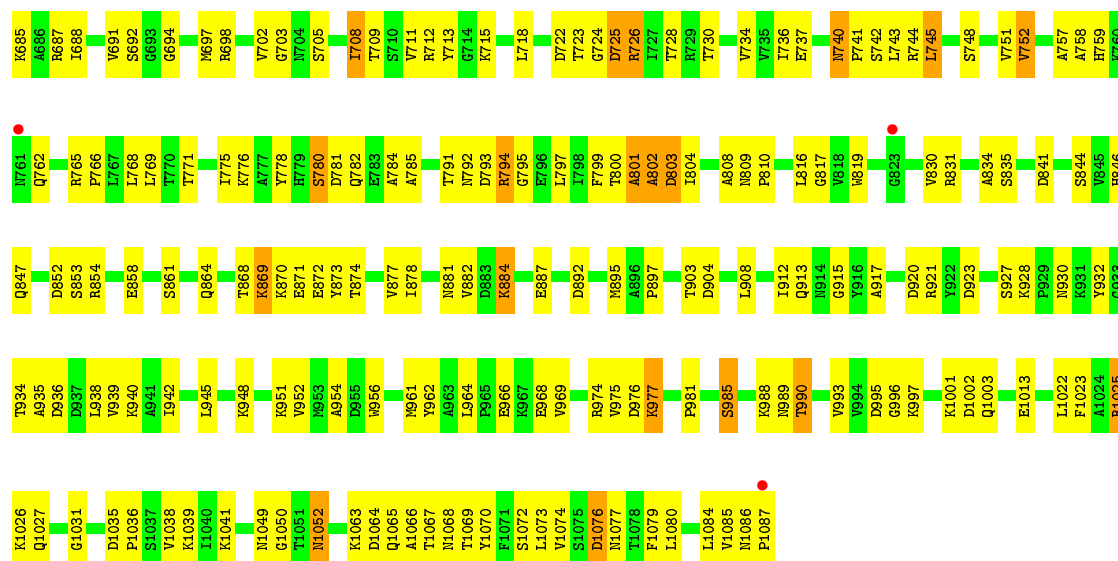


• Molecule 1: Glucosyltransferase-SI

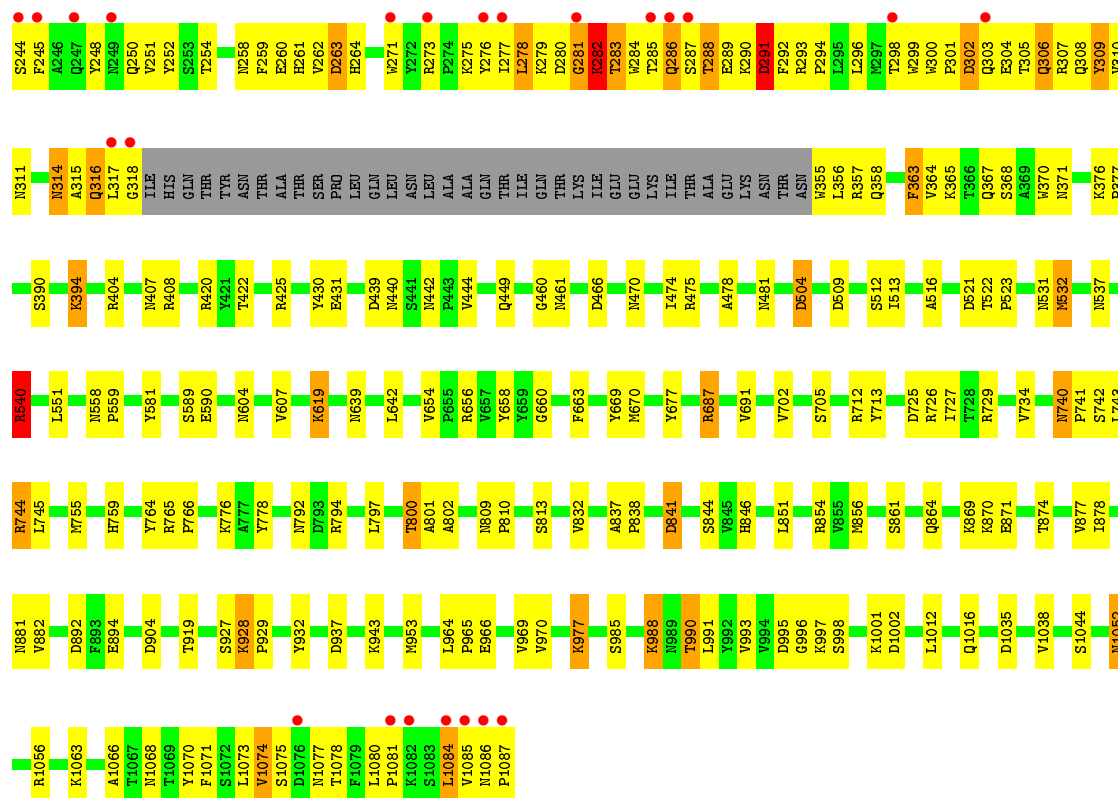


• Molecule 1: Glucosyltransferase-SI

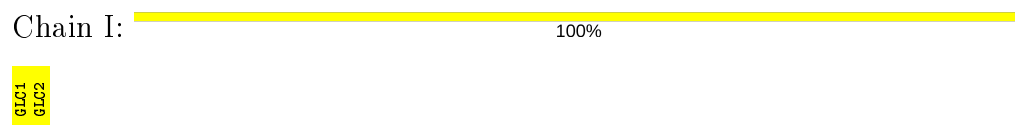




• Molecule 1: Glucosyltransferase-SI



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	295.42Å 213.94Å 220.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.67 – 3.09 50.67 – 3.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.67-3.09) 97.8 (50.67-3.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.211 , 0.241 0.207 , 0.238	Depositor DCC
R_{free} test set	12657 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	52615	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8896e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: CA, GLC, MES

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	1.07	9/6784 (0.1%)	0.97	5/9213 (0.1%)
1	B	0.95	6/5990 (0.1%)	0.96	6/8132 (0.1%)
1	C	1.10	11/6802 (0.2%)	0.98	18/9237 (0.2%)
1	D	1.06	9/6802 (0.1%)	0.97	10/9237 (0.1%)
1	E	1.07	6/6802 (0.1%)	0.96	10/9237 (0.1%)
1	F	0.87	2/6802 (0.0%)	0.88	6/9237 (0.1%)
1	G	1.10	15/6802 (0.2%)	0.99	15/9237 (0.2%)
1	H	0.96	3/6516 (0.0%)	0.95	19/8845 (0.2%)
All	All	1.03	61/53300 (0.1%)	0.96	89/72375 (0.1%)

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	244	SER	CB-OG	8.60	1.53	1.42
1	H	314	ASN	CG-ND2	-8.57	1.11	1.32
1	E	632	GLU	CG-CD	8.44	1.64	1.51
1	G	608	VAL	CB-CG1	7.45	1.68	1.52
1	E	574	GLU	CD-OE1	7.36	1.33	1.25
1	D	340	GLN	CA-CB	7.32	1.70	1.53
1	E	632	GLU	CD-OE2	7.30	1.33	1.25
1	G	632	GLU	CG-CD	7.07	1.62	1.51
1	D	1013	GLU	CD-OE1	7.06	1.33	1.25
1	A	726	ARG	CG-CD	6.96	1.69	1.51
1	G	615	GLU	CD-OE1	6.95	1.33	1.25
1	G	616	GLU	CD-OE1	6.70	1.33	1.25
1	C	632	GLU	CD-OE2	6.58	1.32	1.25
1	G	632	GLU	CD-OE1	6.46	1.32	1.25
1	D	340	GLN	CB-CG	-6.35	1.35	1.52
1	C	615	GLU	CD-OE1	6.24	1.32	1.25
1	B	1079	PHE	CG-CD2	6.19	1.48	1.38
1	D	632	GLU	CD-OE2	6.18	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1039	LYS	CB-CG	-6.02	1.36	1.52
1	G	750	ARG	CZ-NH1	6.01	1.40	1.33
1	A	507	ALA	CA-CB	-6.01	1.39	1.52
1	A	616	GLU	CD-OE1	6.00	1.32	1.25
1	C	691	VAL	CB-CG1	-5.95	1.40	1.52
1	C	615	GLU	CG-CD	5.92	1.60	1.51
1	F	1013	GLU	CD-OE1	5.86	1.32	1.25
1	A	505	LYS	CE-NZ	5.74	1.63	1.49
1	A	608	VAL	CB-CG1	5.66	1.64	1.52
1	A	616	GLU	CG-CD	5.64	1.60	1.51
1	E	632	GLU	CD-OE1	5.62	1.31	1.25
1	C	394	LYS	CD-CE	5.61	1.65	1.51
1	G	622	GLU	CG-CD	5.60	1.60	1.51
1	D	726	ARG	CG-CD	5.58	1.65	1.51
1	H	363	PHE	CG-CD1	-5.54	1.30	1.38
1	D	872	GLU	CG-CD	-5.50	1.43	1.51
1	B	1087	PRO	CB-CG	5.49	1.77	1.50
1	D	249	ASN	CG-ND2	5.45	1.46	1.32
1	G	610	TYR	CE2-CZ	5.43	1.45	1.38
1	A	612	PHE	CE2-CZ	5.38	1.47	1.37
1	E	344	GLU	CG-CD	5.35	1.59	1.51
1	G	615	GLU	CD-OE2	5.35	1.31	1.25
1	D	632	GLU	CG-CD	5.33	1.59	1.51
1	C	794	ARG	CZ-NH1	5.33	1.40	1.33
1	C	988	LYS	CD-CE	5.33	1.64	1.51
1	G	894	GLU	CD-OE1	5.32	1.31	1.25
1	G	618	LYS	CD-CE	5.30	1.64	1.51
1	C	632	GLU	CD-OE1	5.28	1.31	1.25
1	G	344	GLU	CG-CD	5.27	1.59	1.51
1	D	618	LYS	CD-CE	5.26	1.64	1.51
1	B	1079	PHE	CE1-CZ	5.24	1.47	1.37
1	G	358	GLN	CD-OE1	5.24	1.35	1.24
1	C	563	ASN	CB-CG	5.21	1.63	1.51
1	G	358	GLN	CG-CD	5.20	1.63	1.51
1	C	871	GLU	CG-CD	5.20	1.59	1.51
1	F	1002	ASP	CB-CG	-5.17	1.41	1.51
1	B	252	TYR	CG-CD1	5.13	1.45	1.39
1	B	871	GLU	CG-CD	5.11	1.59	1.51
1	A	574	GLU	CD-OE2	5.08	1.31	1.25
1	A	632	GLU	CD-OE2	5.04	1.31	1.25
1	E	706	GLU	CD-OE1	5.03	1.31	1.25
1	H	894	GLU	CD-OE1	5.01	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	632	GLU	CD-OE2	5.00	1.31	1.25

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	245	PHE	CB-CA-C	-10.38	89.64	110.40
1	F	1002	ASP	CB-CG-OD1	-8.53	110.63	118.30
1	B	1002	ASP	CB-CG-OD1	8.37	125.84	118.30
1	H	725	ASP	CB-CG-OD1	8.19	125.67	118.30
1	D	425	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	F	425	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	G	1002	ASP	CB-CG-OD1	7.53	125.08	118.30
1	D	750	ARG	NE-CZ-NH1	-7.01	116.79	120.30
1	D	712	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	G	712	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	E	687	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	D	509	ASP	CB-CG-OD1	-6.67	112.30	118.30
1	E	504	ASP	CB-CG-OD1	-6.54	112.41	118.30
1	E	1025	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	425	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	C	854	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	C	831	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	C	614	MET	CG-SD-CE	-6.16	90.35	100.20
1	G	750	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	793	ASP	CB-CG-OD1	-6.11	112.80	118.30
1	H	404	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	H	841	ASP	CB-CG-OD1	6.06	123.75	118.30
1	G	551	LEU	CB-CG-CD2	-6.05	100.72	111.00
1	H	404	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	729	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	H	363	PHE	CB-CG-CD1	-5.95	116.63	120.80
1	G	371	ASN	CB-CA-C	-5.93	98.53	110.40
1	H	687	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	E	585	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	H	540	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	712	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	H	420	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	373	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	D	509	ASP	CB-CG-OD2	5.82	123.54	118.30
1	C	854	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	371	ASN	CB-CA-C	-5.79	98.81	110.40
1	G	904	ASP	CB-CG-OD1	-5.75	113.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	291	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	C	540	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	425	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	H	245	PHE	N-CA-C	5.58	126.08	111.00
1	H	1035	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	E	320	HIS	N-CA-C	5.58	126.06	111.00
1	H	1002	ASP	CB-CG-OD1	5.55	123.30	118.30
1	E	344	GLU	CB-CA-C	-5.53	99.35	110.40
1	C	712	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	G	291	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	G	977	LYS	CD-CE-NZ	-5.49	99.08	111.70
1	C	597	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	H	509	ASP	CB-CG-OD1	-5.44	113.40	118.30
1	E	1025	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	C	904	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	G	608	VAL	CG1-CB-CG2	5.38	119.51	110.90
1	A	527	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	255	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	D	291	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	C	618	LYS	CD-CE-NZ	-5.29	99.52	111.70
1	C	342	LYS	CD-CE-NZ	-5.28	99.55	111.70
1	F	1026	LYS	CD-CE-NZ	-5.27	99.58	111.70
1	G	425	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	H	504	ASP	CB-CG-OD1	-5.26	113.57	118.30
1	B	538	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	F	1002	ASP	N-CA-CB	-5.25	101.15	110.60
1	C	509	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	C	687	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	E	781	ASP	CB-CG-OD1	5.22	123.00	118.30
1	D	755	MET	CG-SD-CE	5.21	108.54	100.20
1	G	665	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	E	505	LYS	CD-CE-NZ	-5.19	99.77	111.70
1	G	245	PHE	N-CA-C	-5.15	97.08	111.00
1	D	588	ASP	CB-CG-OD1	5.14	122.93	118.30
1	H	289	GLU	N-CA-C	-5.14	97.13	111.00
1	B	614	MET	CG-SD-CE	-5.14	91.98	100.20
1	H	1084	LEU	CA-CB-CG	-5.14	103.48	115.30
1	F	1002	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	937	ASP	CB-CG-OD1	5.12	122.91	118.30
1	G	793	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	C	425	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	B	977	LYS	CB-CA-C	-5.08	100.23	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	291	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	712	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	H	725	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	E	909	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	G	1002	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	C	585	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	666	ASP	C-N-CA	-5.04	111.71	122.30
1	H	841	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	H	712	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	D	744	ARG	NE-CZ-NH1	-5.01	117.80	120.30

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	6643	0	6475	243	0
1	B	5868	0	5704	333	0
1	C	6660	0	6489	181	0
1	D	6660	0	6489	261	0
1	E	6660	0	6489	314	0
1	F	6660	0	6489	349	0
1	G	6660	0	6489	209	0
1	H	6378	0	6201	272	0
2	I	23	0	21	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	12	0	12	4	0
4	B	12	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	12	0	12	1	0
4	D	12	0	12	1	0
4	E	12	0	12	1	0
4	F	12	0	12	1	0
4	G	12	0	12	2	0
4	H	12	0	12	1	0
5	A	35	0	0	1	0
5	B	20	0	0	0	0
5	C	59	0	0	5	0
5	D	50	0	0	2	0
5	E	38	0	0	0	0
5	F	23	0	0	2	0
5	G	46	0	0	1	0
5	H	28	0	0	0	0
All	All	52615	0	50942	2162	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 21.

All (2162) 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:B:1087:PRO:CG	1:B:1087:PRO:CB	1.77	1.54
1:E:271:TRP:CZ2	1:E:357:ARG:HD3	1.51	1.43
1:C:475:ARG:HB2	1:C:953:MET:CE	1.53	1.39
1:E:277:ILE:CD1	1:E:291:ASP:HB3	1.50	1.38
1:H:278:LEU:HD11	1:H:282:LYS:N	1.41	1.34
1:E:347:ILE:CD1	1:E:353:THR:HG22	1.57	1.33
1:D:277:ILE:CD1	1:D:291:ASP:HB3	1.61	1.30
1:G:475:ARG:HB2	1:G:953:MET:CE	1.71	1.19
1:E:352:ASN:ND2	1:E:354:ASN:HB2	1.57	1.17
1:E:1085:VAL:HG23	1:E:1086:ASN:N	1.56	1.17
1:E:278:LEU:O	1:E:344:GLU:HG3	1.45	1.17
1:E:277:ILE:HD11	1:E:291:ASP:HB3	1.23	1.17
1:D:252:TYR:HB3	1:D:258:ASN:HD21	1.04	1.16
1:F:350:GLU:HB3	1:F:352:ASN:ND2	1.61	1.15
1:E:271:TRP:CZ2	1:E:357:ARG:CD	2.30	1.15
1:E:475:ARG:HB2	1:E:953:MET:HE1	1.28	1.15
1:E:347:ILE:CG1	1:E:353:THR:HG22	1.77	1.14
1:H:278:LEU:CD1	1:H:282:LYS:H	1.57	1.14
4:G:5001:MES:H52	4:G:5001:MES:O3S	1.48	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:248:TYR:HB3	1:H:276:TYR:HB2	1.27	1.13
1:E:1085:VAL:CG2	1:E:1086:ASN:H	1.60	1.13
1:D:281:GLY:HA3	1:D:341:THR:CG2	1.79	1.12
1:E:513:ILE:HG12	1:E:953:MET:HE3	1.22	1.12
1:B:800:THR:HG22	1:B:802:ALA:N	1.63	1.12
1:E:475:ARG:HB2	1:E:953:MET:CE	1.80	1.12
1:D:277:ILE:HD13	1:D:291:ASP:HB3	1.30	1.11
1:G:475:ARG:HB2	1:G:953:MET:HE2	1.23	1.11
1:H:278:LEU:HD21	1:H:281:GLY:HA2	1.29	1.11
1:F:726:ARG:HH11	1:F:726:ARG:CG	1.63	1.11
1:E:277:ILE:HD12	1:E:291:ASP:HB3	1.24	1.11
1:B:712:ARG:HG3	1:B:712:ARG:HH11	1.01	1.10
1:E:273:ARG:HG3	1:E:292:PHE:CD2	1.86	1.10
1:H:513:ILE:HG12	1:H:953:MET:HE1	1.33	1.10
1:H:513:ILE:HG12	1:H:953:MET:CE	1.80	1.10
1:F:709:THR:HG22	1:F:736:ILE:HD13	1.34	1.09
1:D:336:ALA:HA	1:D:339:ILE:HD12	1.29	1.09
1:B:712:ARG:CG	1:B:712:ARG:HH11	1.64	1.09
1:F:726:ARG:HH11	1:F:726:ARG:HG2	1.14	1.09
1:G:800:THR:HG22	1:G:802:ALA:N	1.67	1.09
1:B:1074:VAL:CG1	1:B:1077:ASN:HB3	1.80	1.09
1:E:347:ILE:CD1	1:E:353:THR:CG2	2.31	1.08
1:H:669:TYR:HE2	1:H:670:MET:HE2	1.08	1.08
1:D:669:TYR:CE2	1:D:670:MET:HE2	1.87	1.08
1:H:394:LYS:HD3	1:H:394:LYS:N	1.63	1.08
1:A:251:VAL:HG21	1:A:259:PHE:CZ	1.89	1.08
1:D:726:ARG:HH11	1:D:726:ARG:HG2	1.13	1.07
1:H:800:THR:HG22	1:H:802:ALA:H	1.18	1.07
1:B:854:ARG:HG2	1:B:854:ARG:HH11	1.20	1.06
1:B:262:VAL:HG12	1:B:969:VAL:HG23	1.30	1.06
1:D:303:GLN:NE2	1:D:329:PRO:HG3	1.69	1.06
1:D:669:TYR:CE2	1:D:670:MET:CE	2.40	1.05
1:B:669:TYR:CE2	1:B:670:MET:CE	2.39	1.05
1:E:252:TYR:HB3	1:E:258:ASN:HD21	1.20	1.05
1:B:712:ARG:HG3	1:B:712:ARG:NH1	1.58	1.04
1:F:726:ARG:HG2	1:F:726:ARG:NH1	1.64	1.04
1:F:261:HIS:HD2	1:F:264:HIS:H	1.06	1.04
1:D:281:GLY:HA3	1:D:341:THR:HG23	1.37	1.04
1:E:329:PRO:HA	1:E:332:LEU:HD12	1.09	1.03
1:B:1003:GLN:OE1	1:B:1003:GLN:HA	1.56	1.03
1:H:669:TYR:HE2	1:H:670:MET:CE	1.71	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:ARG:HB2	1:C:953:MET:HE2	1.05	1.03
1:E:271:TRP:CE2	1:E:357:ARG:HD3	1.92	1.03
1:B:669:TYR:CE2	1:B:670:MET:HE2	1.93	1.03
1:F:745:LEU:HD13	1:F:801:ALA:HA	1.38	1.03
1:E:273:ARG:HG3	1:E:292:PHE:CE2	1.92	1.02
1:H:669:TYR:CE2	1:H:670:MET:HE2	1.94	1.02
1:F:713:TYR:O	1:F:759:HIS:HE1	1.41	1.02
1:E:347:ILE:HD11	1:E:353:THR:HG22	1.38	1.02
1:H:316:GLN:NE2	1:H:316:GLN:HA	1.68	1.02
1:H:316:GLN:HE21	1:H:316:GLN:HA	1.19	1.02
1:D:303:GLN:HE22	1:D:329:PRO:HG3	1.22	1.01
1:B:610:TYR:HA	1:B:612:PHE:CE2	1.95	1.01
1:F:669:TYR:HE2	1:F:670:MET:HE2	1.20	1.01
1:G:316:GLN:NE2	1:G:316:GLN:HA	1.71	1.01
1:B:513:ILE:HD13	1:B:856:MET:HE1	1.42	1.01
1:C:861:SER:H	1:C:864:GLN:NE2	1.60	1.00
1:H:1063:LYS:HE2	1:H:1068:ASN:ND2	1.75	1.00
1:B:861:SER:H	1:B:864:GLN:HE21	1.07	1.00
1:H:669:TYR:CE2	1:H:670:MET:CE	2.45	1.00
1:H:1085:VAL:HG23	1:H:1086:ASN:H	1.25	1.00
1:B:800:THR:CG2	1:B:802:ALA:H	1.73	0.99
1:E:262:VAL:HG12	1:E:969:VAL:HG23	1.43	0.99
1:C:475:ARG:CB	1:C:953:MET:HE2	1.92	0.99
1:E:316:GLN:HG2	1:E:359:THR:CG2	1.92	0.99
1:G:800:THR:HG22	1:G:802:ALA:H	0.83	0.99
1:B:974:ARG:HH11	1:B:974:ARG:HG3	1.21	0.99
1:E:330:LEU:O	1:E:330:LEU:HD12	1.62	0.99
1:C:440:ASN:HD21	1:C:449:GLN:HE21	1.11	0.99
1:A:300:TRP:CD2	1:A:306:GLN:HG3	1.98	0.99
1:D:278:LEU:HG	1:D:281:GLY:HA2	1.42	0.99
1:B:1052:ASN:HD22	1:B:1052:ASN:H	1.09	0.99
1:G:492:ASP:HB3	1:G:1022:LEU:HD22	1.46	0.98
1:D:281:GLY:CA	1:D:341:THR:HG23	1.94	0.98
1:E:513:ILE:HG12	1:E:953:MET:CE	1.92	0.98
1:F:669:TYR:CE2	1:F:670:MET:CE	2.46	0.98
1:G:513:ILE:HG12	1:G:953:MET:HE3	1.42	0.98
1:F:669:TYR:CE2	1:F:670:MET:HE2	1.97	0.98
1:A:278:LEU:HG	1:A:281:GLY:HA2	1.47	0.97
1:B:673:LYS:HE2	1:B:677:TYR:CE2	1.99	0.97
1:B:974:ARG:NH1	1:B:974:ARG:HG3	1.78	0.97
1:D:726:ARG:HH11	1:D:726:ARG:CG	1.78	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:350:GLU:HB3	1:F:352:ASN:HD21	1.29	0.97
1:E:347:ILE:HG12	1:E:353:THR:HG22	1.44	0.97
1:F:669:TYR:HE2	1:F:670:MET:CE	1.78	0.97
1:E:273:ARG:CD	1:E:292:PHE:HE2	1.77	0.97
1:B:416:LYS:HE2	1:F:551:LEU:CD1	1.94	0.96
1:E:861:SER:H	1:E:864:GLN:HE21	1.00	0.96
1:H:300:TRP:CD2	1:H:306:GLN:HG3	2.00	0.96
1:E:316:GLN:HG2	1:E:359:THR:HG21	1.45	0.96
1:H:466:ASP:OD2	1:H:943:LYS:HE3	1.64	0.96
1:G:800:THR:CG2	1:G:802:ALA:H	1.77	0.96
4:A:5001:MES:O2S	4:A:5001:MES:C5	2.14	0.96
1:D:639:ASN:HD21	1:D:813:SER:H	1.06	0.96
1:E:273:ARG:CG	1:E:292:PHE:CD2	2.49	0.96
1:E:639:ASN:HD21	1:E:813:SER:H	1.11	0.96
1:G:475:ARG:CB	1:G:953:MET:HE2	1.96	0.96
1:B:800:THR:HG22	1:B:802:ALA:H	0.81	0.95
1:C:475:ARG:CB	1:C:953:MET:CE	2.42	0.95
1:G:966:GLU:HB2	1:G:997:LYS:HB2	1.49	0.95
1:A:275:LYS:C	1:A:276:TYR:HD2	1.69	0.95
1:C:371:ASN:HB3	1:C:373:ASP:H	1.30	0.95
1:B:568:ARG:O	1:B:697:MET:HB2	1.67	0.95
1:E:273:ARG:HH11	1:E:289:GLU:HA	1.32	0.95
1:E:800:THR:HG22	1:E:802:ALA:H	1.28	0.95
1:G:335:ALA:O	1:G:339:ILE:HD12	1.65	0.95
1:C:861:SER:H	1:C:864:GLN:HE21	1.13	0.94
1:A:440:ASN:HD21	1:A:449:GLN:HE21	1.05	0.94
1:E:277:ILE:CD1	1:E:291:ASP:CB	2.45	0.94
1:D:861:SER:H	1:D:864:GLN:HE21	1.10	0.94
1:A:800:THR:HG22	1:A:802:ALA:H	1.33	0.94
1:B:871:GLU:N	1:B:871:GLU:OE1	2.00	0.94
1:G:861:SER:H	1:G:864:GLN:HE21	1.13	0.94
1:E:320:HIS:O	1:E:321:GLN:O	1.86	0.94
1:C:639:ASN:HD21	1:C:813:SER:H	1.15	0.93
1:B:1074:VAL:HG12	1:B:1077:ASN:HB3	1.48	0.93
1:B:394:LYS:CD	1:B:394:LYS:H	1.80	0.93
1:E:1085:VAL:HG23	1:E:1086:ASN:H	0.79	0.93
1:H:1085:VAL:HG23	1:H:1086:ASN:N	1.82	0.93
1:B:1003:GLN:CA	1:B:1003:GLN:OE1	2.14	0.93
1:D:355:TRP:CE3	1:D:359:THR:HG21	2.03	0.93
1:B:715:LYS:HG3	1:B:830:VAL:HB	1.50	0.93
1:G:440:ASN:HD21	1:G:449:GLN:HE21	1.12	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:745:LEU:HD12	1:F:745:LEU:H	1.33	0.93
1:B:713:TYR:O	1:B:732:GLY:HA3	1.69	0.92
1:G:740:ASN:ND2	1:G:742:SER:H	1.66	0.92
1:F:705:SER:HB3	1:F:743:LEU:HD13	1.49	0.92
1:F:311:ASN:HD21	1:F:323:TYR:H	1.18	0.92
1:H:440:ASN:HD21	1:H:449:GLN:HE21	1.13	0.92
1:A:460:GLY:H	1:A:470:ASN:HD22	1.16	0.92
1:G:316:GLN:HE21	1:G:316:GLN:HA	1.26	0.92
1:C:460:GLY:H	1:C:470:ASN:HD22	1.10	0.91
1:E:440:ASN:HD21	1:E:449:GLN:HE21	1.04	0.91
1:F:478:ALA:HB1	1:F:481:ASN:HD22	1.32	0.91
1:F:709:THR:HG22	1:F:736:ILE:CD1	2.00	0.91
1:F:809:ASN:HB2	1:F:810:PRO:HD2	1.50	0.91
1:E:347:ILE:HG12	1:E:353:THR:CG2	2.00	0.91
1:F:791:THR:HG21	1:F:795:GLY:HA2	1.52	0.91
1:G:303:GLN:OE1	1:G:329:PRO:HG3	1.71	0.91
1:F:724:GLY:H	1:F:758:ALA:HB2	1.33	0.91
1:H:993:VAL:HG12	1:H:1056:ARG:NH1	1.85	0.91
1:F:745:LEU:HD13	1:F:801:ALA:CA	2.01	0.90
4:A:5001:MES:O2S	4:A:5001:MES:H52	1.71	0.90
1:B:416:LYS:HE2	1:F:551:LEU:HD11	1.52	0.90
1:F:762:GLN:H	1:F:791:THR:HB	1.34	0.90
1:E:273:ARG:CD	1:E:292:PHE:CE2	2.55	0.90
1:B:504:ASP:OD1	1:B:846:HIS:HD2	1.55	0.90
1:A:273:ARG:HH21	1:A:288:THR:C	1.75	0.89
1:D:1052:ASN:H	1:D:1052:ASN:HD22	1.09	0.89
1:E:273:ARG:NE	1:E:292:PHE:HE2	1.70	0.89
1:H:861:SER:H	1:H:864:GLN:HE21	1.14	0.89
1:B:966:GLU:HB2	1:B:997:LYS:HB2	1.52	0.89
1:C:1052:ASN:HD22	1:C:1052:ASN:H	1.20	0.89
1:H:304:GLU:OE1	1:H:304:GLU:HA	1.70	0.89
1:B:394:LYS:H	1:B:394:LYS:CE	1.85	0.89
1:D:303:GLN:CD	1:D:329:PRO:HG3	1.92	0.89
1:E:277:ILE:HD12	1:E:291:ASP:CB	2.03	0.88
1:F:861:SER:H	1:F:864:GLN:HE21	1.16	0.88
1:D:252:TYR:HB3	1:D:258:ASN:ND2	1.89	0.88
1:B:951:LYS:N	1:B:951:LYS:HD3	1.86	0.88
1:D:726:ARG:NH1	1:D:726:ARG:HG2	1.83	0.88
1:E:273:ARG:CG	1:E:292:PHE:CE2	2.56	0.88
1:H:639:ASN:HD21	1:H:813:SER:H	1.20	0.87
1:G:251:VAL:HG21	1:G:259:PHE:CZ	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:572:ASN:O	1:F:718:LEU:HD13	1.74	0.87
1:E:281:GLY:HA3	1:E:341:THR:HG22	1.55	0.87
1:B:262:VAL:CG1	1:B:969:VAL:HG23	2.04	0.87
1:E:261:HIS:HD2	1:E:264:HIS:H	1.23	0.87
1:F:492:ASP:HB3	1:F:1022:LEU:CD2	2.05	0.87
1:B:639:ASN:HD21	1:B:813:SER:H	1.19	0.86
1:G:475:ARG:CB	1:G:953:MET:CE	2.52	0.86
1:H:278:LEU:HD11	1:H:282:LYS:H	0.88	0.86
1:H:278:LEU:CD2	1:H:281:GLY:HA2	2.04	0.86
1:F:791:THR:CG2	1:F:795:GLY:HA2	2.04	0.86
1:H:251:VAL:HG21	1:H:259:PHE:CZ	2.10	0.86
1:A:280:ASP:O	1:A:282:LYS:HG3	1.73	0.86
1:G:261:HIS:HD2	1:G:264:HIS:H	1.20	0.86
1:A:988:LYS:H	1:A:990:THR:CG2	1.87	0.86
1:E:288:THR:HG22	1:E:289:GLU:N	1.90	0.86
1:H:376:LYS:HB3	1:H:377:PRO:HA	1.56	0.86
1:B:752:VAL:HG22	1:B:798:ILE:HG12	1.57	0.86
1:C:261:HIS:CD2	1:C:264:HIS:H	1.94	0.86
1:G:252:TYR:HB3	1:G:258:ASN:HD21	1.40	0.86
1:D:281:GLY:HA3	1:D:341:THR:HG22	1.55	0.86
1:E:304:GLU:OE1	1:E:304:GLU:HA	1.74	0.86
1:B:466:ASP:OD2	1:B:943:LYS:HE3	1.76	0.86
1:D:303:GLN:OE1	1:D:329:PRO:HG3	1.75	0.85
1:D:339:ILE:O	1:D:343:ILE:HG13	1.75	0.85
1:B:394:LYS:H	1:B:394:LYS:HE2	1.40	0.85
1:F:740:ASN:ND2	1:F:742:SER:H	1.74	0.85
1:E:861:SER:H	1:E:864:GLN:NE2	1.72	0.85
1:C:261:HIS:HD2	1:C:264:HIS:H	1.20	0.85
1:E:252:TYR:HB3	1:E:258:ASN:ND2	1.90	0.85
1:F:357:ARG:HH11	1:F:357:ARG:HG2	1.42	0.85
1:H:250:GLN:HE21	1:H:275:LYS:HG3	1.39	0.85
1:C:252:TYR:HB3	1:C:258:ASN:HD21	1.42	0.84
1:D:800:THR:HG22	1:D:802:ALA:H	1.42	0.84
1:E:314:ASN:HB3	1:E:319:ILE:O	1.76	0.84
1:E:347:ILE:HD13	1:E:353:THR:CG2	2.06	0.84
1:F:492:ASP:HB3	1:F:1022:LEU:HD22	1.56	0.84
1:F:1052:ASN:H	1:F:1052:ASN:HD22	1.23	0.84
1:H:1052:ASN:HD22	1:H:1052:ASN:H	1.19	0.84
1:C:513:ILE:HG12	1:C:953:MET:HE3	1.58	0.84
1:B:440:ASN:HD21	1:B:449:GLN:HE21	1.23	0.84
1:B:669:TYR:CE2	1:B:670:MET:HE3	2.09	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:ILE:HD13	1:B:856:MET:CE	2.08	0.84
1:D:293:ARG:HB3	1:D:297:MET:HE2	1.60	0.84
1:G:513:ILE:HG12	1:G:953:MET:CE	2.07	0.84
1:B:724:GLY:HA3	1:B:728:THR:HB	1.59	0.84
1:B:854:ARG:HG2	1:B:854:ARG:NH1	1.90	0.84
1:F:261:HIS:CD2	1:F:264:HIS:H	1.94	0.84
1:F:726:ARG:CB	1:F:726:ARG:HH11	1.90	0.84
1:B:631:THR:HG23	1:B:809:ASN:CA	2.08	0.84
1:D:1065:GLN:HG3	1:D:1066:ALA:N	1.90	0.84
1:C:460:GLY:N	1:C:470:ASN:HD22	1.76	0.84
1:G:639:ASN:HD21	1:G:813:SER:H	1.24	0.84
1:A:639:ASN:HD21	1:A:813:SER:H	1.24	0.83
4:G:5001:MES:O3S	4:G:5001:MES:C5	2.25	0.83
1:B:705:SER:HB3	1:B:743:LEU:HD13	1.59	0.83
1:D:310:VAL:HG22	1:D:339:ILE:CD1	2.08	0.83
1:G:1085:VAL:HG23	1:G:1086:ASN:N	1.94	0.83
1:G:475:ARG:HB2	1:G:953:MET:HE1	1.59	0.83
1:B:800:THR:CG2	1:B:801:ALA:N	2.40	0.83
1:E:271:TRP:CD2	1:E:357:ARG:NH1	2.47	0.83
1:B:669:TYR:HE2	1:B:670:MET:HE3	1.39	0.83
1:D:492:ASP:HB3	1:D:1022:LEU:HD22	1.61	0.83
1:D:347:ILE:CD1	1:D:353:THR:HG22	2.08	0.83
1:E:740:ASN:HD22	1:E:742:SER:H	1.25	0.83
1:F:357:ARG:CG	1:F:357:ARG:HH11	1.92	0.83
1:B:669:TYR:HE2	1:B:670:MET:CE	1.84	0.82
1:E:277:ILE:HD11	1:E:291:ASP:CB	2.06	0.82
1:H:669:TYR:CD2	1:H:670:MET:HE3	2.14	0.82
1:D:356:LEU:HA	1:D:359:THR:HG23	1.59	0.82
1:F:861:SER:H	1:F:864:GLN:NE2	1.76	0.82
1:F:713:TYR:O	1:F:759:HIS:CE1	2.32	0.82
1:D:740:ASN:ND2	1:D:742:SER:H	1.77	0.82
1:D:460:GLY:H	1:D:470:ASN:HD22	1.27	0.81
1:D:277:ILE:HD13	1:D:291:ASP:CB	2.10	0.81
1:C:800:THR:HG22	1:C:802:ALA:H	1.45	0.81
1:E:281:GLY:HA3	1:E:341:THR:CG2	2.09	0.81
1:E:288:THR:HG22	1:E:289:GLU:H	1.44	0.81
1:D:303:GLN:HE22	1:D:329:PRO:CG	1.93	0.81
1:G:614:MET:HG3	1:G:618:LYS:HE3	1.61	0.81
1:F:1072:SER:OG	1:F:1074:VAL:HG12	1.81	0.81
1:A:604:ASN:HD21	1:A:607:VAL:HA	1.46	0.81
1:F:765:ARG:HD3	1:F:784:ALA:CB	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:877:VAL:HG12	1:F:881:ASN:HD22	1.44	0.81
1:B:1016:GLN:HE21	1:G:748:SER:HA	1.45	0.81
1:B:513:ILE:HG23	1:B:953:MET:HE1	1.60	0.81
1:E:740:ASN:ND2	1:E:742:SER:H	1.79	0.81
1:G:1052:ASN:HD22	1:G:1052:ASN:H	1.28	0.81
1:H:513:ILE:CG1	1:H:953:MET:HE1	2.09	0.81
1:B:394:LYS:H	1:B:394:LYS:HD3	1.45	0.81
1:D:861:SER:H	1:D:864:GLN:NE2	1.76	0.81
1:E:861:SER:N	1:E:864:GLN:HE21	1.77	0.80
1:G:251:VAL:HG21	1:G:259:PHE:HZ	1.47	0.80
1:H:1085:VAL:CG2	1:H:1086:ASN:H	1.93	0.80
1:H:466:ASP:OD2	1:H:943:LYS:CE	2.28	0.80
1:A:251:VAL:HG21	1:A:259:PHE:HZ	1.36	0.80
1:B:394:LYS:HD3	1:B:394:LYS:N	1.96	0.80
1:B:631:THR:HG23	1:B:809:ASN:HA	1.63	0.80
1:D:440:ASN:HD21	1:D:449:GLN:HE21	1.29	0.80
1:F:669:TYR:CE2	1:F:670:MET:HE3	2.16	0.80
1:H:966:GLU:HB2	1:H:997:LYS:HB2	1.61	0.80
1:F:1063:LYS:HE2	1:F:1068:ASN:HD21	1.44	0.80
1:H:394:LYS:H	1:H:394:LYS:HD3	1.40	0.80
1:B:1074:VAL:CG1	1:B:1077:ASN:CB	2.59	0.80
1:F:809:ASN:HB2	1:F:810:PRO:CD	2.11	0.80
1:H:278:LEU:CD1	1:H:283:THR:O	2.30	0.80
1:F:708:ILE:HD13	1:F:708:ILE:H	1.46	0.79
1:A:460:GLY:H	1:A:470:ASN:ND2	1.78	0.79
1:D:293:ARG:HB3	1:D:297:MET:CE	2.11	0.79
1:F:964:LEU:HD12	1:F:996:GLY:HA2	1.63	0.79
1:G:371:ASN:HB3	1:G:373:ASP:H	1.47	0.79
1:B:1083:SER:O	1:B:1087:PRO:HG3	1.81	0.79
1:A:278:LEU:O	1:A:344:GLU:HG3	1.82	0.79
1:B:1073:LEU:HD11	1:B:1080:LEU:HD21	1.64	0.79
1:B:466:ASP:OD2	1:B:943:LYS:CE	2.31	0.79
1:D:669:TYR:HE2	1:D:670:MET:CE	1.89	0.79
1:B:513:ILE:HG12	1:B:953:MET:HE2	1.65	0.79
1:H:669:TYR:CE2	1:H:670:MET:HE3	2.17	0.79
1:A:604:ASN:HD21	1:A:607:VAL:CA	1.94	0.79
1:C:861:SER:N	1:C:864:GLN:HE21	1.81	0.79
1:B:1052:ASN:HD22	1:B:1052:ASN:N	1.80	0.78
1:F:687:ARG:HA	1:F:691:VAL:HG23	1.64	0.78
1:G:460:GLY:H	1:G:470:ASN:HD22	1.31	0.78
1:F:1063:LYS:CE	1:F:1068:ASN:ND2	2.46	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1063:LYS:NZ	1:B:1068:ASN:HB3	1.99	0.78
1:F:551:LEU:HD12	1:F:551:LEU:O	1.84	0.78
1:G:311:ASN:HD21	1:G:323:TYR:H	1.30	0.78
1:H:513:ILE:HG12	1:H:953:MET:HE3	1.62	0.78
1:D:1065:GLN:HG3	1:D:1066:ALA:H	1.46	0.78
1:D:300:TRP:CG	1:D:306:GLN:HB2	2.18	0.78
1:G:639:ASN:ND2	1:G:813:SER:H	1.82	0.78
1:F:861:SER:N	1:F:864:GLN:HE21	1.81	0.78
1:H:861:SER:H	1:H:864:GLN:NE2	1.82	0.78
1:A:339:ILE:O	1:A:343:ILE:HG13	1.84	0.78
1:B:614:MET:O	1:B:618:LYS:HG3	1.83	0.78
1:E:256:ALA:HA	1:E:1073:LEU:HD13	1.65	0.78
1:F:440:ASN:HD21	1:F:449:GLN:HE21	1.28	0.78
1:G:346:LYS:HD3	1:G:355:TRP:CZ2	2.18	0.78
1:B:610:TYR:HA	1:B:612:PHE:HE2	1.44	0.78
1:D:277:ILE:HD12	1:D:291:ASP:HB3	1.66	0.78
1:H:740:ASN:ND2	1:H:742:SER:H	1.82	0.78
1:D:468:ASP:OD1	1:D:943:LYS:HG3	1.84	0.77
1:G:300:TRP:CD2	1:G:306:GLN:HG3	2.18	0.77
1:G:316:GLN:NE2	1:G:316:GLN:CA	2.38	0.77
1:A:861:SER:H	1:A:864:GLN:HE21	1.29	0.77
1:F:251:VAL:HG21	1:F:259:PHE:CZ	2.18	0.77
1:H:281:GLY:O	1:H:282:LYS:CG	2.32	0.77
1:H:316:GLN:NE2	1:H:316:GLN:CA	2.39	0.77
1:D:433:LEU:HD22	1:D:481:ASN:HD22	1.49	0.77
1:H:800:THR:HG22	1:H:802:ALA:N	1.96	0.77
1:A:460:GLY:N	1:A:470:ASN:ND2	2.33	0.77
1:B:374:SER:HA	1:B:986:GLN:NE2	1.99	0.77
1:E:475:ARG:HB2	1:E:953:MET:HE2	1.66	0.77
1:B:759:HIS:CD2	1:B:764:TYR:OH	2.38	0.77
1:G:504:ASP:OD1	1:G:846:HIS:HD2	1.66	0.77
1:H:300:TRP:CG	1:H:306:GLN:HG3	2.19	0.77
1:B:715:LYS:HD2	1:B:830:VAL:HA	1.66	0.77
1:A:740:ASN:HD22	1:A:740:ASN:C	1.88	0.77
1:E:339:ILE:HG22	1:E:343:ILE:HD11	1.66	0.76
1:F:1063:LYS:HE2	1:F:1068:ASN:ND2	1.99	0.76
1:G:492:ASP:HB3	1:G:1022:LEU:CD2	2.15	0.76
1:D:669:TYR:CD2	1:D:670:MET:HE3	2.20	0.76
1:G:740:ASN:HD22	1:G:742:SER:H	1.33	0.76
1:E:352:ASN:HD22	1:E:354:ASN:HB2	1.45	0.76
1:F:740:ASN:HD22	1:F:742:SER:H	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:HIS:HD2	1:B:264:HIS:H	1.34	0.76
1:D:639:ASN:ND2	1:D:813:SER:H	1.84	0.76
1:B:516:ALA:HB1	1:B:521:ASP:OD2	1.84	0.76
1:H:300:TRP:CD2	1:H:306:GLN:CG	2.68	0.76
1:D:311:ASN:HD21	1:D:323:TYR:H	1.32	0.76
1:A:278:LEU:HG	1:A:281:GLY:CA	2.15	0.76
1:H:248:TYR:HB2	1:H:284:TRP:CZ3	2.21	0.76
1:E:1052:ASN:H	1:E:1052:ASN:HD22	1.31	0.76
1:H:861:SER:N	1:H:864:GLN:HE21	1.84	0.76
1:E:261:HIS:CD2	1:E:264:HIS:H	2.04	0.75
1:F:882:VAL:HG22	1:F:948:LYS:HG3	1.69	0.75
1:H:277:ILE:HG13	1:H:291:ASP:HB3	1.67	0.75
1:H:740:ASN:HD22	1:H:740:ASN:C	1.90	0.75
1:B:513:ILE:HG12	1:B:953:MET:CE	2.16	0.75
1:F:516:ALA:HB1	1:F:521:ASP:OD2	1.86	0.75
1:G:740:ASN:C	1:G:740:ASN:HD22	1.90	0.75
1:E:271:TRP:CG	1:E:357:ARG:NH1	2.55	0.75
1:C:1063:LYS:HE2	1:C:1068:ASN:ND2	2.02	0.75
1:C:460:GLY:N	1:C:470:ASN:ND2	2.35	0.75
1:D:705:SER:HB3	1:D:743:LEU:HD13	1.68	0.75
1:A:604:ASN:ND2	1:A:607:VAL:HB	2.02	0.75
1:F:669:TYR:CD2	1:F:670:MET:HE3	2.21	0.75
1:H:317:LEU:O	1:H:318:GLY:C	2.25	0.75
1:A:1073:LEU:HD21	1:A:1080:LEU:HD21	1.67	0.74
1:G:261:HIS:CD2	1:G:264:HIS:H	2.04	0.74
1:F:1070:TYR:CD2	5:F:242:HOH:O	2.41	0.74
1:F:407:ASN:ND2	1:F:431:GLU:H	1.86	0.74
1:B:1063:LYS:NZ	1:B:1068:ASN:CB	2.49	0.74
1:H:302:ASP:O	1:H:305:THR:HG22	1.87	0.74
1:F:250:GLN:HB2	1:F:1084:LEU:O	1.87	0.74
1:H:252:TYR:HB3	1:H:258:ASN:HD21	1.51	0.74
1:E:288:THR:CG2	1:E:289:GLU:H	2.01	0.74
1:D:999:SER:O	1:D:1001:LYS:N	2.21	0.74
1:D:355:TRP:HE3	1:D:359:THR:HG21	1.52	0.74
1:F:350:GLU:HB3	1:F:352:ASN:HD22	1.49	0.74
1:A:861:SER:H	1:A:864:GLN:NE2	1.86	0.74
1:F:248:TYR:HB3	1:F:276:TYR:HB2	1.70	0.74
1:B:1074:VAL:HG11	1:B:1077:ASN:HB3	1.68	0.73
1:F:745:LEU:HD12	1:F:745:LEU:N	2.02	0.73
1:H:281:GLY:O	1:H:282:LYS:HG3	1.88	0.73
1:A:988:LYS:N	1:A:990:THR:CG2	2.51	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:SER:N	1:E:246:ALA:H	1.85	0.73
1:E:475:ARG:CB	1:E:953:MET:CE	2.62	0.73
1:F:1052:ASN:ND2	1:F:1052:ASN:H	1.85	0.73
1:H:440:ASN:HD21	1:H:449:GLN:NE2	1.86	0.73
1:A:1073:LEU:CD2	1:A:1080:LEU:HD21	2.19	0.73
1:G:861:SER:N	1:G:864:GLN:HE21	1.85	0.73
1:D:740:ASN:C	1:D:740:ASN:HD22	1.91	0.73
1:H:1085:VAL:CG2	1:H:1086:ASN:N	2.51	0.73
1:A:1052:ASN:H	1:A:1052:ASN:HD22	1.35	0.73
1:B:259:PHE:CD2	1:B:259:PHE:N	2.56	0.73
1:B:726:ARG:HG2	1:B:727:ILE:H	1.54	0.73
1:B:416:LYS:HE2	1:F:551:LEU:HD12	1.71	0.73
1:F:745:LEU:CD1	1:F:801:ALA:HA	2.17	0.73
1:D:1052:ASN:H	1:D:1052:ASN:ND2	1.82	0.73
1:D:740:ASN:HD22	1:D:742:SER:H	1.33	0.73
1:E:1001:LYS:O	1:E:1001:LYS:CG	2.37	0.73
1:G:478:ALA:HB1	1:G:481:ASN:HD22	1.54	0.73
1:A:252:TYR:HA	1:A:275:LYS:HG2	1.71	0.73
1:A:276:TYR:HD2	1:A:276:TYR:N	1.85	0.72
1:C:251:VAL:HG21	1:C:259:PHE:CZ	2.24	0.72
1:C:461:ASN:H	1:C:470:ASN:HD21	1.37	0.72
1:E:475:ARG:CA	1:E:953:MET:HE2	2.18	0.72
1:A:604:ASN:ND2	1:A:607:VAL:CA	2.52	0.72
1:D:782:GLN:HA	1:D:782:GLN:HE21	1.53	0.72
1:D:966:GLU:HB2	1:D:997:LYS:HB2	1.71	0.72
1:A:261:HIS:HD2	1:A:264:HIS:H	1.33	0.72
1:A:258:ASN:HD22	1:A:273:ARG:HB3	1.53	0.72
1:A:281:GLY:HA3	1:A:341:THR:HG23	1.71	0.72
1:A:440:ASN:ND2	1:A:449:GLN:HE21	1.84	0.72
1:D:861:SER:N	1:D:864:GLN:HE21	1.84	0.72
1:E:347:ILE:CG1	1:E:353:THR:CG2	2.55	0.72
1:F:278:LEU:HD23	1:F:281:GLY:HA2	1.71	0.72
1:H:740:ASN:HD22	1:H:742:SER:H	1.34	0.72
1:C:492:ASP:OD2	1:C:1025:ARG:NH1	2.22	0.72
1:E:1001:LYS:O	1:E:1001:LYS:HG2	1.89	0.72
1:E:965:PRO:HD2	1:E:997:LYS:O	1.88	0.72
1:F:383:GLN:O	1:F:384:LYS:HB2	1.89	0.72
1:B:848:ASN:OD1	1:B:850:ALA:HB3	1.89	0.72
1:F:252:TYR:HB3	1:F:258:ASN:HD21	1.55	0.72
1:A:966:GLU:HB2	1:A:997:LYS:HB2	1.72	0.72
1:B:871:GLU:CD	1:B:871:GLU:H	1.93	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LYS:C	1:A:276:TYR:CD2	2.60	0.71
1:A:273:ARG:HH21	1:A:289:GLU:N	1.86	0.71
1:C:999:SER:O	1:C:1001:LYS:N	2.23	0.71
1:G:614:MET:CG	1:G:618:LYS:HE3	2.21	0.71
1:A:494:LEU:HB3	1:A:500:ILE:HD13	1.72	0.71
1:A:740:ASN:HD22	1:A:741:PRO:N	1.88	0.71
1:E:245:PHE:O	1:E:249:ASN:HB2	1.90	0.71
1:F:278:LEU:CD2	1:F:281:GLY:HA2	2.20	0.71
1:D:841:ASP:OD1	1:D:846:HIS:HE1	1.73	0.71
1:D:504:ASP:OD1	1:D:846:HIS:HD2	1.73	0.71
1:E:475:ARG:N	1:E:953:MET:HE2	2.04	0.71
1:F:920:ASP:OD2	1:F:1003:GLN:HB2	1.91	0.71
1:H:300:TRP:CE3	1:H:306:GLN:HG3	2.26	0.71
1:H:315:ALA:O	1:H:318:GLY:N	2.23	0.71
1:A:252:TYR:CZ	1:A:273:ARG:NH1	2.59	0.71
1:D:288:THR:HG23	1:D:291:ASP:OD2	1.90	0.71
1:E:329:PRO:CA	1:E:332:LEU:HD12	2.04	0.71
1:E:271:TRP:CD2	1:E:357:ARG:CZ	2.73	0.71
1:A:460:GLY:N	1:A:470:ASN:HD22	1.89	0.71
1:C:504:ASP:OD1	1:C:846:HIS:HD2	1.73	0.71
1:F:1067:THR:HG22	1:F:1069:THR:OG1	1.91	0.71
1:B:526:HIS:HA	1:B:530:ASP:OD1	1.90	0.70
1:D:460:GLY:H	1:D:470:ASN:ND2	1.89	0.70
1:A:841:ASP:OD1	1:A:846:HIS:HE1	1.74	0.70
1:H:278:LEU:CD1	1:H:282:LYS:N	2.30	0.70
1:D:407:ASN:ND2	1:D:431:GLU:H	1.89	0.70
1:G:740:ASN:HD22	1:G:741:PRO:N	1.89	0.70
1:B:1063:LYS:HZ3	1:B:1068:ASN:CA	2.05	0.70
1:A:276:TYR:CD2	1:A:276:TYR:N	2.58	0.70
1:A:453:LEU:HD11	1:A:457:MET:HE1	1.73	0.70
1:E:273:ARG:CG	1:E:292:PHE:HD2	2.04	0.70
1:D:352:ASN:OD1	1:D:354:ASN:HB2	1.92	0.70
1:H:1063:LYS:HE2	1:H:1068:ASN:HD21	1.56	0.70
1:A:604:ASN:HD22	1:A:607:VAL:HB	1.55	0.69
1:B:407:ASN:ND2	1:B:431:GLU:H	1.89	0.69
1:D:669:TYR:HE2	1:D:670:MET:HE2	1.43	0.69
1:E:475:ARG:CB	1:E:953:MET:HE2	2.22	0.69
1:D:256:ALA:HB1	1:D:261:HIS:CE1	2.27	0.69
1:E:288:THR:CG2	1:E:289:GLU:N	2.56	0.69
1:E:339:ILE:O	1:E:343:ILE:HG13	1.91	0.69
1:F:360:ILE:O	1:F:364:VAL:HG23	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:LEU:HA	1:D:359:THR:CG2	2.23	0.69
1:E:319:ILE:HD11	1:E:342:LYS:HE2	1.73	0.69
1:E:337:GLN:O	1:E:340:GLN:N	2.24	0.69
1:B:383:GLN:O	1:B:384:LYS:HB2	1.92	0.69
1:D:759:HIS:HD2	1:D:762:GLN:OE1	1.75	0.69
1:C:669:TYR:HE2	1:C:670:MET:HE3	1.58	0.69
1:B:731:SER:O	1:B:821:PRO:HG3	1.92	0.69
1:A:376:LYS:HB3	1:A:377:PRO:HA	1.75	0.69
1:A:740:ASN:ND2	1:A:742:SER:H	1.91	0.69
1:H:1052:ASN:ND2	1:H:1052:ASN:H	1.90	0.68
1:D:271:TRP:CD1	1:D:294:PRO:HA	2.28	0.68
1:D:347:ILE:HG12	1:D:353:THR:HG22	1.74	0.68
1:F:1067:THR:CG2	1:F:1069:THR:OG1	2.41	0.68
1:G:247:GLN:O	1:G:250:GLN:HG2	1.92	0.68
1:D:1052:ASN:N	1:D:1052:ASN:HD22	1.89	0.68
1:H:304:GLU:CA	1:H:304:GLU:OE1	2.37	0.68
1:E:1068:ASN:O	1:E:1068:ASN:CG	2.32	0.68
1:F:261:HIS:HD2	1:F:264:HIS:N	1.87	0.68
1:A:278:LEU:CG	1:A:281:GLY:HA2	2.22	0.68
1:C:440:ASN:HD21	1:C:449:GLN:NE2	1.88	0.68
1:E:272:TYR:HD1	1:E:273:ARG:N	1.92	0.68
1:E:740:ASN:C	1:E:740:ASN:HD22	1.95	0.68
1:D:461:ASN:OD1	1:D:467:PRO:HA	1.94	0.68
1:D:303:GLN:OE1	1:D:329:PRO:CG	2.42	0.68
1:H:301:PRO:HG2	1:H:305:THR:HG21	1.76	0.68
1:B:920:ASP:OD2	1:B:923:ASP:HB2	1.93	0.68
1:F:255:ASP:O	1:F:258:ASN:HB2	1.94	0.68
1:H:278:LEU:HD13	1:H:283:THR:O	1.94	0.67
1:E:272:TYR:CE1	1:E:274:PRO:HG3	2.29	0.67
1:E:271:TRP:CH2	1:E:357:ARG:HG2	2.29	0.67
1:B:724:GLY:HA3	1:B:728:THR:CB	2.24	0.67
1:D:347:ILE:HD13	1:D:353:THR:HG22	1.77	0.67
1:F:658:TYR:CE2	1:F:660:GLY:HA3	2.28	0.67
1:F:711:VAL:HG22	1:F:734:VAL:HG23	1.77	0.67
1:F:740:ASN:ND2	1:F:741:PRO:HD2	2.09	0.67
1:D:347:ILE:CG1	1:D:353:THR:HG22	2.24	0.67
1:E:320:HIS:O	1:E:321:GLN:C	2.33	0.67
1:E:513:ILE:CG1	1:E:953:MET:CE	2.72	0.67
1:H:656:ARG:HG3	1:H:856:MET:HB3	1.76	0.67
1:E:272:TYR:CD1	1:E:273:ARG:N	2.63	0.67
1:C:311:ASN:HD21	1:C:323:TYR:H	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:VAL:HG22	1:D:339:ILE:HD11	1.76	0.67
1:A:1063:LYS:HE2	1:A:1068:ASN:ND2	2.10	0.67
1:A:440:ASN:HD21	1:A:449:GLN:NE2	1.85	0.67
1:E:1073:LEU:HD21	1:E:1080:LEU:HD21	1.75	0.67
1:E:262:VAL:CG1	1:E:969:VAL:HG23	2.22	0.66
1:B:535:MET:HE2	1:B:583:PHE:CE2	2.31	0.66
1:B:651:LYS:O	1:B:652:SER:HB2	1.94	0.66
1:C:513:ILE:HG12	1:C:953:MET:CE	2.25	0.66
1:D:634:LYS:O	1:D:634:LYS:HG2	1.95	0.66
1:E:273:ARG:NE	1:E:292:PHE:CE2	2.60	0.66
1:F:346:LYS:HB3	1:F:355:TRP:CZ2	2.31	0.66
1:C:687:ARG:HA	1:C:691:VAL:CG2	2.25	0.66
1:D:293:ARG:CB	1:D:297:MET:HE2	2.25	0.66
1:H:262:VAL:HG12	1:H:969:VAL:HG23	1.75	0.66
1:H:440:ASN:ND2	1:H:449:GLN:HE21	1.91	0.66
1:G:281:GLY:H	1:G:344:GLU:HB3	1.61	0.66
1:H:993:VAL:HG12	1:H:1056:ARG:HH12	1.61	0.66
1:A:376:LYS:HE2	1:A:378:PHE:CE1	2.30	0.66
1:A:928:LYS:HB2	1:A:929:PRO:CD	2.25	0.66
1:C:800:THR:CG2	1:C:801:ALA:N	2.58	0.66
1:D:460:GLY:N	1:D:470:ASN:ND2	2.44	0.66
1:E:339:ILE:HG22	1:E:343:ILE:CD1	2.25	0.66
1:B:998:SER:OG	1:B:1043:TRP:N	2.29	0.66
1:C:669:TYR:CE2	1:C:670:MET:HE3	2.30	0.66
1:F:966:GLU:HB2	1:F:997:LYS:HB2	1.77	0.66
1:A:800:THR:HG22	1:A:802:ALA:N	2.08	0.66
1:G:355:TRP:CD2	1:G:356:LEU:N	2.64	0.66
1:B:682:THR:HG22	1:B:767:LEU:HD11	1.77	0.65
1:H:300:TRP:CG	1:H:306:GLN:CG	2.78	0.65
1:D:302:ASP:OD1	1:D:304:GLU:HB3	1.96	0.65
1:E:247:GLN:O	1:E:250:GLN:HG2	1.95	0.65
1:A:277:ILE:HD12	1:A:293:ARG:CZ	2.26	0.65
1:B:500:ILE:HG22	1:B:507:ALA:HA	1.77	0.65
1:B:684:LEU:HD13	1:B:888:TRP:HB3	1.78	0.65
1:H:261:HIS:HD2	1:H:264:HIS:H	1.44	0.65
1:B:740:ASN:ND2	1:B:742:SER:H	1.95	0.65
1:B:951:LYS:N	1:B:951:LYS:CD	2.58	0.65
1:C:250:GLN:HE21	1:C:275:LYS:NZ	1.95	0.65
1:H:1071:PHE:CD1	1:H:1081:PRO:HD3	2.31	0.65
1:H:278:LEU:HD12	1:H:283:THR:O	1.96	0.65
1:H:304:GLU:O	1:H:307:ARG:HB3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:HB2	1:A:352:ASN:HD22	1.62	0.65
1:F:800:THR:O	1:F:802:ALA:N	2.30	0.65
1:A:281:GLY:HA3	1:A:341:THR:CG2	2.27	0.65
1:B:759:HIS:HD2	1:B:764:TYR:OH	1.79	0.65
1:B:854:ARG:HH11	1:B:854:ARG:CG	2.05	0.65
1:H:474:ILE:C	1:H:953:MET:HE2	2.17	0.65
1:E:1064:ASP:HB2	1:E:1071:PHE:CE1	2.31	0.65
1:C:492:ASP:OD1	1:C:1025:ARG:NH1	2.29	0.65
1:F:669:TYR:O	1:F:670:MET:HB2	1.96	0.65
1:B:897:PRO:HG3	1:B:916:TYR:CE1	2.31	0.65
1:D:800:THR:HG22	1:D:802:ALA:N	2.12	0.65
1:E:271:TRP:CE2	1:E:357:ARG:NH1	2.64	0.65
1:E:273:ARG:HD3	1:E:292:PHE:CE2	2.32	0.65
1:G:383:GLN:O	1:G:384:LYS:HB2	1.96	0.65
1:H:713:TYR:O	1:H:759:HIS:HE1	1.78	0.65
1:H:993:VAL:HG12	1:H:1056:ARG:HH11	1.62	0.65
1:G:861:SER:H	1:G:864:GLN:NE2	1.90	0.65
1:B:740:ASN:HD22	1:B:741:PRO:N	1.95	0.64
1:D:293:ARG:CB	1:D:297:MET:CE	2.75	0.64
1:F:801:ALA:O	1:F:803:ASP:N	2.30	0.64
1:F:469:ALA:CB	1:F:939:VAL:HG13	2.27	0.64
1:A:861:SER:N	1:A:864:GLN:HE21	1.95	0.64
1:D:800:THR:CG2	1:D:802:ALA:H	2.11	0.64
1:E:759:HIS:HD2	1:E:762:GLN:OE1	1.79	0.64
1:F:557:MET:HE2	1:F:708:ILE:HD12	1.79	0.64
1:G:1085:VAL:CG2	1:G:1086:ASN:N	2.60	0.64
1:H:740:ASN:HD22	1:H:741:PRO:N	1.95	0.64
1:A:272:TYR:CD2	1:A:295:LEU:HD23	2.31	0.64
1:C:966:GLU:HB2	1:C:997:LYS:HB2	1.79	0.64
1:E:383:GLN:O	1:E:384:LYS:HB2	1.97	0.64
1:H:475:ARG:HB2	1:H:953:MET:CE	2.26	0.64
1:A:280:ASP:OD1	1:A:348:THR:CB	2.45	0.64
1:B:440:ASN:HD21	1:B:449:GLN:NE2	1.93	0.64
1:B:504:ASP:OD1	1:B:846:HIS:CD2	2.46	0.64
1:C:352:ASN:OD1	1:C:354:ASN:HB2	1.97	0.64
1:C:861:SER:N	1:C:864:GLN:NE2	2.39	0.64
1:E:271:TRP:CH2	1:E:357:ARG:CD	2.80	0.64
1:D:355:TRP:CZ3	1:D:359:THR:HG21	2.31	0.64
1:F:612:PHE:CD2	1:F:612:PHE:N	2.64	0.64
1:F:791:THR:HG22	1:F:792:ASN:N	2.11	0.64
1:A:782:GLN:HA	1:A:782:GLN:HE21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ASP:O	1:E:282:LYS:N	2.31	0.64
1:A:355:TRP:CD2	1:A:356:LEU:N	2.66	0.64
1:C:460:GLY:H	1:C:470:ASN:ND2	1.88	0.64
1:G:475:ARG:CA	1:G:953:MET:HE2	2.26	0.64
1:C:475:ARG:HB2	1:C:953:MET:HE1	1.68	0.64
1:A:304:GLU:HA	1:A:304:GLU:OE1	1.97	0.64
1:D:293:ARG:HG3	1:D:297:MET:HE1	1.80	0.64
1:G:1009:GLY:HA3	1:G:1039:LYS:HG2	1.80	0.64
1:H:250:GLN:HB2	1:H:1084:LEU:O	1.97	0.64
1:A:729:ARG:HD2	1:A:758:ALA:O	1.97	0.64
1:F:800:THR:O	1:F:801:ALA:C	2.34	0.64
1:G:988:LYS:H	1:G:990:THR:CG2	2.11	0.64
1:A:271:TRP:CE2	1:A:294:PRO:HG3	2.32	0.63
1:B:272:TYR:C	1:B:272:TYR:CD1	2.71	0.63
1:H:271:TRP:CD1	1:H:294:PRO:HA	2.33	0.63
1:H:460:GLY:H	1:H:470:ASN:HD22	1.47	0.63
1:A:273:ARG:HH21	1:A:288:THR:CA	2.10	0.63
1:B:585:ARG:HD3	1:B:661:ASP:OD1	1.98	0.63
1:E:352:ASN:HD21	1:E:354:ASN:HB2	1.54	0.63
1:E:335:ALA:O	1:E:339:ILE:HG13	1.98	0.63
1:E:346:LYS:O	1:E:350:GLU:CG	2.46	0.63
1:F:897:PRO:HG2	1:F:915:GLY:HA3	1.81	0.63
1:G:576:ALA:HB3	1:G:847:GLN:HB3	1.79	0.63
1:A:350:GLU:HB2	1:A:352:ASN:ND2	2.13	0.63
1:C:639:ASN:ND2	1:C:813:SER:H	1.93	0.63
1:B:610:TYR:CA	1:B:612:PHE:CE2	2.78	0.63
1:E:316:GLN:OE1	1:E:316:GLN:HA	1.96	0.63
1:F:877:VAL:HG12	1:F:881:ASN:ND2	2.12	0.63
1:F:350:GLU:CB	1:F:352:ASN:ND2	2.51	0.63
1:F:800:THR:N	1:F:803:ASP:OD2	2.30	0.63
1:E:669:TYR:HE2	1:E:670:MET:HE2	1.64	0.63
1:C:1052:ASN:ND2	1:C:1052:ASN:H	1.95	0.63
1:D:305:THR:O	1:D:308:GLN:HB2	1.98	0.63
1:H:288:THR:OG1	1:H:290:LYS:HB2	1.99	0.63
1:A:689:LYS:HG2	1:A:690:TYR:CE1	2.34	0.62
1:C:383:GLN:O	1:C:384:LYS:HB2	1.99	0.62
1:D:920:ASP:OD2	1:D:1002:ASP:HB2	1.99	0.62
1:E:272:TYR:CD1	1:E:272:TYR:C	2.73	0.62
1:F:664:THR:OG1	1:F:672:HIS:HB2	1.99	0.62
1:G:988:LYS:H	1:G:990:THR:HG23	1.64	0.62
1:H:1012:LEU:O	1:H:1016:GLN:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:ASN:ND2	1:A:813:SER:H	1.96	0.62
1:C:670:MET:HE1	1:C:885:PHE:HZ	1.64	0.62
1:F:642:LEU:HD12	1:F:642:LEU:N	2.15	0.62
1:F:794:ARG:HG2	1:F:794:ARG:NH1	2.13	0.62
1:A:299:TRP:CH2	1:A:301:PRO:HA	2.34	0.62
1:B:251:VAL:HG22	1:B:253:SER:H	1.64	0.62
1:E:492:ASP:HB3	1:E:1022:LEU:HD22	1.81	0.62
1:H:285:THR:O	1:H:286:GLN:C	2.37	0.62
1:H:363:PHE:C	1:H:365:LYS:N	2.49	0.62
1:A:882:VAL:HG13	1:A:948:LYS:HG3	1.80	0.62
1:F:350:GLU:CB	1:F:352:ASN:HD21	2.08	0.62
1:F:639:ASN:ND2	1:F:642:LEU:HD22	2.14	0.62
1:B:800:THR:HG23	1:B:801:ALA:N	2.13	0.62
1:C:687:ARG:HA	1:C:691:VAL:HG23	1.81	0.62
1:B:262:VAL:HG12	1:B:969:VAL:CG2	2.19	0.62
1:E:669:TYR:CE2	1:E:670:MET:CE	2.83	0.62
1:F:321:GLN:HG3	1:F:322:THR:N	2.15	0.62
1:G:800:THR:CG2	1:G:801:ALA:N	2.63	0.62
1:H:776:LYS:HG2	1:H:778:TYR:CZ	2.35	0.62
1:D:740:ASN:HD22	1:D:741:PRO:N	1.98	0.62
1:F:847:GLN:NE2	1:F:852:ASP:OD1	2.30	0.62
1:G:440:ASN:HD21	1:G:449:GLN:NE2	1.91	0.62
1:G:658:TYR:CE2	1:G:660:GLY:HA3	2.35	0.62
1:E:367:GLN:O	1:E:370:TRP:N	2.26	0.62
1:A:281:GLY:CA	1:A:341:THR:HG23	2.29	0.62
1:A:504:ASP:OD1	1:A:846:HIS:HD2	1.82	0.62
1:D:271:TRP:NE1	1:D:294:PRO:HB3	2.14	0.62
1:E:1052:ASN:ND2	1:E:1052:ASN:H	1.97	0.62
1:B:604:ASN:C	1:B:604:ASN:OD1	2.38	0.62
1:G:461:ASN:H	1:G:470:ASN:HD21	1.45	0.62
1:H:300:TRP:CD1	1:H:306:GLN:HA	2.35	0.62
1:A:347:ILE:HD13	1:A:353:THR:HG22	1.82	0.61
1:B:809:ASN:HB2	1:B:810:PRO:HD2	1.82	0.61
1:H:355:TRP:O	1:H:358:GLN:N	2.30	0.61
4:A:5001:MES:O2S	4:A:5001:MES:N4	2.32	0.61
1:B:715:LYS:CG	1:B:830:VAL:HB	2.28	0.61
1:C:457:MET:HE1	1:C:494:LEU:HD21	1.83	0.61
1:F:595:ILE:HG22	1:F:599:ILE:HD12	1.80	0.61
1:A:604:ASN:ND2	1:A:607:VAL:HA	2.13	0.61
1:D:355:TRP:CE3	1:D:359:THR:CG2	2.81	0.61
1:D:460:GLY:N	1:D:470:ASN:HD22	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:ARG:HH11	1:E:289:GLU:CA	2.10	0.61
1:E:271:TRP:CZ2	1:E:357:ARG:CG	2.84	0.61
1:E:281:GLY:CA	1:E:341:THR:HG23	2.30	0.61
1:F:557:MET:CE	1:F:708:ILE:HD12	2.31	0.61
1:G:278:LEU:O	1:G:344:GLU:HG3	1.99	0.61
1:B:259:PHE:N	1:B:259:PHE:HD2	1.97	0.61
1:E:346:LYS:O	1:E:350:GLU:HG2	2.00	0.61
1:F:262:VAL:HG12	1:F:969:VAL:HG23	1.83	0.61
1:F:520:ASN:O	1:F:523:PRO:HG2	2.01	0.61
1:A:604:ASN:ND2	1:A:607:VAL:CB	2.64	0.61
1:B:374:SER:HA	1:B:986:GLN:HE21	1.65	0.61
1:G:475:ARG:CA	1:G:953:MET:CE	2.78	0.61
1:G:669:TYR:CE1	1:G:874:THR:HG23	2.36	0.61
1:B:760:LYS:O	1:B:762:GLN:N	2.34	0.61
1:B:850:ALA:O	1:B:853:SER:HB2	2.00	0.61
1:C:740:ASN:C	1:C:740:ASN:HD22	2.02	0.61
1:B:762:GLN:HG3	1:B:763:ALA:N	2.16	0.61
1:B:800:THR:N	1:B:803:ASP:OD2	2.30	0.61
1:D:245:PHE:O	1:D:246:ALA:C	2.37	0.61
1:D:344:GLU:O	1:D:347:ILE:N	2.27	0.61
1:D:634:LYS:HD3	1:D:635:TYR:CE2	2.36	0.61
1:E:316:GLN:OE1	1:E:316:GLN:CA	2.46	0.61
1:A:403:TYR:O	1:A:404:ARG:HB2	2.01	0.60
1:B:1052:ASN:ND2	1:B:1052:ASN:N	2.45	0.60
1:B:726:ARG:HG2	1:B:727:ILE:N	2.16	0.60
1:D:537:ASN:OD1	1:D:540:ARG:NH1	2.33	0.60
1:H:302:ASP:O	1:H:302:ASP:OD1	2.17	0.60
1:H:475:ARG:N	1:H:953:MET:HE2	2.15	0.60
1:H:965:PRO:HD2	1:H:998:SER:HA	1.83	0.60
1:A:356:LEU:O	1:A:358:GLN:N	2.35	0.60
1:C:1071:PHE:CD1	1:C:1081:PRO:HD3	2.36	0.60
1:C:669:TYR:HE2	1:C:670:MET:CE	2.14	0.60
1:D:368:SER:O	1:D:371:ASN:HB2	2.01	0.60
1:E:460:GLY:H	1:E:470:ASN:HD22	1.49	0.60
1:F:687:ARG:HA	1:F:691:VAL:CG2	2.31	0.60
1:H:639:ASN:ND2	1:H:813:SER:H	1.97	0.60
1:A:424:ASP:HB3	1:A:520:ASN:ND2	2.17	0.60
1:D:344:GLU:O	1:D:345:GLU:C	2.40	0.60
1:F:256:ALA:C	1:F:258:ASN:H	2.02	0.60
1:C:1076:ASP:OD2	1:C:1077:ASN:HB2	2.02	0.60
1:D:293:ARG:CG	1:D:297:MET:HE1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:LEU:HD22	1:B:431:GLU:HG2	1.84	0.60
1:D:461:ASN:H	1:D:470:ASN:HD21	1.50	0.60
1:F:801:ALA:O	1:F:804:ILE:N	2.34	0.60
1:G:460:GLY:N	1:G:470:ASN:HD22	1.98	0.60
1:A:352:ASN:OD1	1:A:354:ASN:HB2	2.02	0.60
1:B:251:VAL:HG13	1:B:251:VAL:O	2.01	0.60
1:B:394:LYS:HE2	1:B:394:LYS:N	2.13	0.60
1:B:514:LEU:HD21	1:B:532:MET:HG3	1.82	0.60
1:B:612:PHE:N	1:B:612:PHE:CD2	2.68	0.60
1:B:722:ASP:O	1:B:757:ALA:HB3	2.02	0.60
1:C:1052:ASN:N	1:C:1052:ASN:HD22	1.94	0.60
1:F:708:ILE:HD11	1:F:737:GLU:HB2	1.81	0.60
1:G:669:TYR:CD1	1:G:874:THR:HG23	2.36	0.60
1:D:471:PHE:CG	1:D:954:ALA:HB2	2.37	0.60
1:D:669:TYR:CD2	1:D:670:MET:CE	2.79	0.60
1:E:809:ASN:HB2	1:E:810:PRO:CD	2.31	0.60
1:F:387:LEU:O	1:F:1050:GLY:HA3	2.02	0.60
1:G:904:ASP:OD2	1:G:906:SER:HB3	2.02	0.60
1:A:278:LEU:HD12	1:A:283:THR:N	2.16	0.60
1:B:1063:LYS:HZ1	1:B:1068:ASN:HB3	1.63	0.60
1:D:433:LEU:HD13	1:D:481:ASN:ND2	2.16	0.60
1:E:316:GLN:HG2	1:E:359:THR:HG23	1.81	0.60
1:E:461:ASN:H	1:E:470:ASN:HD21	1.49	0.60
1:A:317:LEU:HD13	1:A:342:LYS:HB3	1.84	0.60
1:A:321:GLN:OE1	1:A:321:GLN:HA	2.02	0.60
1:B:559:PRO:HB3	1:B:563:ASN:ND2	2.17	0.60
1:B:613:THR:OG1	1:B:616:GLU:HG3	2.02	0.60
1:E:281:GLY:CA	1:E:341:THR:CG2	2.80	0.60
1:H:475:ARG:HB2	1:H:953:MET:HE1	1.82	0.60
1:A:316:GLN:HA	1:A:316:GLN:OE1	2.01	0.59
1:A:461:ASN:H	1:A:470:ASN:HD21	1.48	0.59
1:E:871:GLU:OE1	1:E:871:GLU:N	2.33	0.59
1:F:1085:VAL:HG23	1:F:1086:ASN:N	2.16	0.59
1:E:310:VAL:HG22	1:E:339:ILE:HD11	1.83	0.59
1:E:347:ILE:HD11	1:E:353:THR:CG2	2.15	0.59
1:E:670:MET:HE3	1:E:877:VAL:HG12	1.84	0.59
1:F:514:LEU:HD21	1:F:532:MET:HG3	1.84	0.59
1:G:440:ASN:ND2	1:G:449:GLN:HE21	1.93	0.59
1:H:307:ARG:O	1:H:310:VAL:HB	2.02	0.59
1:B:551:LEU:O	1:B:551:LEU:HD12	2.03	0.59
1:D:277:ILE:HD11	1:D:291:ASP:HB3	1.77	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:759:HIS:CD2	1:D:762:GLN:OE1	2.56	0.59
1:D:924:LEU:N	1:D:924:LEU:HD12	2.16	0.59
1:E:245:PHE:CD2	1:E:337:GLN:HG2	2.38	0.59
1:F:421:TYR:CD1	1:F:523:PRO:HB2	2.37	0.59
1:H:475:ARG:CA	1:H:953:MET:HE2	2.32	0.59
1:B:385:GLY:HA3	1:B:974:ARG:NH2	2.17	0.59
1:B:758:ALA:HB3	1:B:759:HIS:CE1	2.38	0.59
1:C:276:TYR:CE1	1:C:286:GLN:HG3	2.37	0.59
1:D:280:ASP:O	1:D:282:LYS:N	2.34	0.59
1:E:670:MET:CE	1:E:877:VAL:HG12	2.32	0.59
1:G:464:ALA:O	1:G:465:ASN:CB	2.50	0.59
1:A:251:VAL:CG2	1:A:259:PHE:CZ	2.78	0.59
1:E:280:ASP:OD1	1:E:348:THR:CB	2.50	0.59
1:E:513:ILE:HD11	1:E:953:MET:HE1	1.84	0.59
1:F:765:ARG:HD3	1:F:784:ALA:HB2	1.84	0.59
1:H:537:ASN:OD1	1:H:540:ARG:NH1	2.32	0.59
1:D:280:ASP:C	1:D:282:LYS:N	2.55	0.59
1:G:1052:ASN:ND2	1:G:1052:ASN:H	1.98	0.59
1:B:713:TYR:O	1:B:732:GLY:CA	2.48	0.59
1:F:1063:LYS:HE3	1:F:1068:ASN:ND2	2.17	0.59
1:F:407:ASN:HD22	1:F:431:GLU:N	2.00	0.59
1:F:917:ALA:HA	1:F:962:TYR:CD1	2.37	0.59
1:G:904:ASP:OD2	1:G:906:SER:CB	2.50	0.59
1:H:355:TRP:CD2	1:H:356:LEU:N	2.71	0.59
1:A:311:ASN:HD21	1:A:323:TYR:H	1.48	0.59
1:B:440:ASN:ND2	1:B:449:GLN:HE21	1.98	0.59
1:C:740:ASN:HD22	1:C:741:PRO:N	2.00	0.59
1:E:280:ASP:OD1	1:E:348:THR:HB	2.02	0.59
1:F:435:ALA:HA	1:F:1052:ASN:ND2	2.17	0.59
1:G:705:SER:HB3	1:G:743:LEU:HD13	1.84	0.59
1:B:800:THR:HG22	1:B:801:ALA:N	2.08	0.59
1:E:407:ASN:ND2	1:E:431:GLU:H	2.01	0.59
1:F:801:ALA:O	1:F:802:ALA:C	2.41	0.59
1:H:260:GLU:HG3	1:H:271:TRP:O	2.03	0.59
1:H:303:GLN:O	1:H:304:GLU:C	2.40	0.59
1:H:278:LEU:HA	1:H:283:THR:O	2.03	0.58
1:H:356:LEU:O	1:H:357:ARG:C	2.41	0.58
1:H:461:ASN:H	1:H:470:ASN:HD21	1.51	0.58
1:E:330:LEU:C	1:E:330:LEU:HD12	2.21	0.58
1:F:740:ASN:HD22	1:F:741:PRO:N	2.00	0.58
1:E:306:GLN:O	1:E:309:TYR:HB3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:304:GLU:HA	1:G:304:GLU:OE1	2.02	0.58
1:A:300:TRP:CG	1:A:306:GLN:HG3	2.38	0.58
1:A:356:LEU:C	1:A:358:GLN:H	2.06	0.58
1:C:1046:LYS:HE3	1:C:1047:TYR:CZ	2.39	0.58
1:E:272:TYR:HE1	1:E:274:PRO:CB	2.17	0.58
1:C:380:ASP:OD1	1:C:977:LYS:HE3	2.03	0.58
1:F:376:LYS:HB3	1:F:377:PRO:HA	1.85	0.58
1:G:574:GLU:HG3	1:G:575:THR:N	2.14	0.58
1:H:874:THR:HG22	1:H:878:ILE:HD12	1.86	0.58
1:C:882:VAL:HG13	1:C:948:LYS:HG3	1.85	0.58
1:G:355:TRP:CE3	1:G:356:LEU:N	2.72	0.58
1:H:278:LEU:HD11	1:H:281:GLY:C	2.21	0.58
1:C:1072:SER:OG	1:C:1074:VAL:HG12	2.03	0.58
1:C:1085:VAL:HG23	1:C:1086:ASN:N	2.19	0.58
1:G:600:LYS:HG2	1:G:607:VAL:HG12	1.86	0.58
1:A:584:ILE:HG13	1:A:584:ILE:O	2.02	0.58
1:A:964:LEU:HD12	1:A:996:GLY:HA2	1.86	0.58
1:B:514:LEU:CD2	1:B:532:MET:HG3	2.34	0.58
1:B:861:SER:H	1:B:864:GLN:NE2	1.90	0.58
1:E:319:ILE:HD11	1:E:342:LYS:CE	2.33	0.58
1:E:427:ILE:HG12	4:E:5001:MES:O3S	2.04	0.58
1:E:861:SER:HB3	1:E:864:GLN:HG3	1.85	0.58
1:G:407:ASN:ND2	1:G:431:GLU:H	2.00	0.58
1:A:300:TRP:CE3	1:A:306:GLN:HG3	2.38	0.58
1:A:987:ILE:HA	1:A:990:THR:HG21	1.86	0.58
1:A:1085:VAL:HG23	1:A:1086:ASN:N	2.19	0.58
1:A:272:TYR:CE2	1:A:295:LEU:HD23	2.39	0.58
1:E:669:TYR:CE2	1:E:670:MET:HE3	2.39	0.58
1:E:841:ASP:OD1	1:E:846:HIS:HE1	1.87	0.58
1:F:791:THR:CG2	1:F:792:ASN:N	2.66	0.58
1:A:261:HIS:CD2	1:A:264:HIS:H	2.19	0.57
1:D:841:ASP:HB2	5:D:101:HOH:O	2.03	0.57
1:E:251:VAL:HG21	1:E:259:PHE:CZ	2.39	0.57
1:E:272:TYR:CE1	1:E:274:PRO:CG	2.87	0.57
1:E:966:GLU:HB2	1:E:997:LYS:HB2	1.86	0.57
1:G:1065:GLN:HG3	1:G:1066:ALA:H	1.69	0.57
1:A:574:GLU:HG3	1:A:575:THR:N	2.18	0.57
1:E:271:TRP:CD1	1:E:357:ARG:NH1	2.72	0.57
1:G:792:ASN:HD21	1:G:796:GLU:HB2	1.70	0.57
1:A:310:VAL:HG21	1:A:335:ALA:HB3	1.86	0.57
1:D:854:ARG:HD3	1:D:892:ASP:OD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:HIS:CD2	1:F:264:HIS:N	2.67	0.57
1:H:298:THR:O	1:H:300:TRP:CZ3	2.57	0.57
1:B:248:TYR:CD2	1:B:248:TYR:N	2.73	0.57
1:B:614:MET:O	1:B:618:LYS:CG	2.51	0.57
1:D:356:LEU:HD12	1:D:360:ILE:HG12	1.85	0.57
1:E:639:ASN:ND2	1:E:813:SER:H	1.92	0.57
1:F:1076:ASP:C	1:F:1076:ASP:OD2	2.42	0.57
1:H:765:ARG:HB2	1:H:766:PRO:HD2	1.87	0.57
1:B:1063:LYS:HZ3	1:B:1068:ASN:HA	1.70	0.57
1:B:535:MET:CE	1:B:583:PHE:CE2	2.86	0.57
1:C:261:HIS:CD2	1:C:264:HIS:N	2.69	0.57
1:C:430:TYR:O	1:C:481:ASN:HA	2.05	0.57
1:D:639:ASN:HD21	1:D:813:SER:N	1.90	0.57
1:E:272:TYR:CD1	1:E:273:ARG:C	2.77	0.57
1:E:272:TYR:HD1	1:E:273:ARG:C	2.07	0.57
1:F:458:ASN:HA	1:F:470:ASN:OD1	2.05	0.57
1:B:1003:GLN:N	1:B:1003:GLN:OE1	2.37	0.57
1:B:1063:LYS:HZ3	1:B:1068:ASN:CB	2.18	0.57
1:C:252:TYR:HB3	1:C:258:ASN:ND2	2.17	0.57
1:H:262:VAL:CG1	1:H:969:VAL:HG23	2.35	0.57
1:H:305:THR:HG23	1:H:306:GLN:N	2.20	0.57
1:A:281:GLY:H	1:A:344:GLU:HB2	1.69	0.57
1:A:449:GLN:HA	1:A:449:GLN:OE1	2.05	0.57
1:D:344:GLU:O	1:D:346:LYS:N	2.38	0.57
1:G:585:ARG:NH2	1:G:591:VAL:HG22	2.20	0.57
1:H:800:THR:CG2	1:H:801:ALA:N	2.67	0.57
1:E:291:ASP:N	1:E:291:ASP:OD1	2.38	0.57
1:G:390:SER:HB2	1:G:971:THR:HB	1.86	0.57
1:A:616:GLU:O	1:A:619:LYS:HB3	2.04	0.57
1:B:1086:ASN:N	1:B:1087:PRO:HD3	2.18	0.57
1:B:974:ARG:HH11	1:B:974:ARG:CG	2.04	0.57
1:G:356:LEU:HA	1:G:359:THR:HG23	1.87	0.57
1:H:355:TRP:CG	1:H:356:LEU:N	2.64	0.57
1:A:782:GLN:HA	1:A:782:GLN:NE2	2.18	0.56
1:A:1052:ASN:H	1:A:1052:ASN:ND2	2.03	0.56
1:C:346:LYS:HE2	1:C:355:TRP:CD2	2.40	0.56
1:D:639:ASN:HB3	1:D:642:LEU:HB2	1.87	0.56
1:E:278:LEU:O	1:E:344:GLU:CG	2.37	0.56
1:E:288:THR:H	1:E:291:ASP:CG	2.08	0.56
1:E:471:PHE:CG	1:E:954:ALA:HB2	2.40	0.56
1:A:247:GLN:O	1:A:250:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:ASP:CG	1:C:1025:ARG:NH1	2.58	0.56
1:B:1052:ASN:H	1:B:1052:ASN:ND2	1.86	0.56
1:D:356:LEU:CA	1:D:359:THR:HG23	2.33	0.56
1:E:322:THR:CG2	1:E:323:TYR:N	2.69	0.56
1:G:280:ASP:O	1:G:282:LYS:N	2.39	0.56
1:A:310:VAL:HG21	1:A:335:ALA:CB	2.36	0.56
1:A:928:LYS:HB2	1:A:929:PRO:HD2	1.87	0.56
1:A:988:LYS:H	1:A:990:THR:HG22	1.70	0.56
1:D:355:TRP:HE3	1:D:359:THR:CG2	2.19	0.56
1:G:339:ILE:O	1:G:343:ILE:HG13	2.04	0.56
1:G:475:ARG:N	1:G:953:MET:HE2	2.21	0.56
1:H:280:ASP:O	1:H:281:GLY:C	2.44	0.56
1:C:1000:GLY:HA3	5:C:171:HOH:O	2.04	0.56
1:C:492:ASP:CG	1:C:1025:ARG:HH11	2.07	0.56
1:C:250:GLN:NE2	1:C:275:LYS:NZ	2.53	0.56
1:E:669:TYR:HE2	1:E:670:MET:CE	2.18	0.56
1:G:988:LYS:N	1:G:990:THR:HG23	2.20	0.56
1:H:277:ILE:HG13	1:H:291:ASP:CB	2.33	0.56
1:H:669:TYR:HD2	1:H:670:MET:HE3	1.66	0.56
1:A:316:GLN:CA	1:A:316:GLN:OE1	2.52	0.56
1:F:745:LEU:HD13	1:F:801:ALA:CB	2.34	0.56
1:G:244:SER:C	1:G:246:ALA:H	2.05	0.56
1:A:281:GLY:O	1:A:341:THR:HG23	2.05	0.56
1:B:920:ASP:OD2	1:B:1003:GLN:HB2	2.06	0.56
1:C:800:THR:HG23	1:C:801:ALA:N	2.21	0.56
1:E:669:TYR:CD2	1:E:670:MET:HE3	2.41	0.56
1:A:300:TRP:HB2	1:A:306:GLN:HB2	1.87	0.56
1:A:347:ILE:CD1	1:A:353:THR:HG22	2.36	0.56
1:B:689:LYS:HG2	1:B:690:TYR:CE1	2.41	0.56
1:B:922:TYR:HB2	1:B:1003:GLN:HB3	1.87	0.56
1:D:551:LEU:O	1:D:551:LEU:HD12	2.05	0.56
1:F:261:HIS:CD2	1:F:264:HIS:HA	2.41	0.56
1:F:740:ASN:C	1:F:740:ASN:HD22	2.09	0.56
1:A:253:SER:HB3	1:A:258:ASN:OD1	2.06	0.56
1:A:356:LEU:C	1:A:358:GLN:N	2.58	0.56
1:A:868:THR:HG22	1:A:868:THR:O	2.05	0.56
1:F:576:ALA:HB3	1:F:847:GLN:HB3	1.88	0.56
1:H:504:ASP:OD1	1:H:846:HIS:HD2	1.89	0.56
1:B:670:MET:HE1	1:B:885:PHE:HZ	1.71	0.56
1:C:320:HIS:N	1:C:320:HIS:ND1	2.52	0.56
1:H:300:TRP:HB3	1:H:305:THR:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:LEU:HD12	1:B:642:LEU:N	2.21	0.55
1:B:673:LYS:HE2	1:B:677:TYR:CZ	2.39	0.55
1:B:712:ARG:HB2	1:B:733:VAL:HG12	1.88	0.55
1:C:669:TYR:CE2	1:C:670:MET:CE	2.87	0.55
1:D:1071:PHE:CD1	1:D:1081:PRO:HD3	2.42	0.55
1:D:999:SER:OG	1:D:999:SER:O	2.24	0.55
1:F:454:HIS:ND1	1:F:493:TYR:OH	2.31	0.55
1:F:917:ALA:HA	1:F:962:TYR:CE1	2.41	0.55
1:H:263:ASP:O	1:H:264:HIS:HB2	2.04	0.55
1:H:301:PRO:HD2	1:H:305:THR:HG21	1.88	0.55
1:C:460:GLY:CA	1:C:470:ASN:ND2	2.69	0.55
1:C:841:ASP:OD1	1:C:846:HIS:HE1	1.89	0.55
1:D:705:SER:HB3	1:D:743:LEU:CD1	2.36	0.55
1:D:346:LYS:HA	1:D:349:ALA:HB3	1.88	0.55
1:E:339:ILE:CG2	1:E:343:ILE:HD11	2.33	0.55
1:E:475:ARG:CA	1:E:953:MET:CE	2.84	0.55
1:A:304:GLU:OE2	1:A:307:ARG:NH1	2.40	0.55
1:B:1085:VAL:HG23	1:B:1086:ASN:N	2.21	0.55
1:B:715:LYS:HD2	1:B:830:VAL:CA	2.35	0.55
1:E:307:ARG:HD2	1:E:324:ASN:O	2.07	0.55
1:F:726:ARG:NH1	1:F:726:ARG:CG	2.31	0.55
1:H:271:TRP:CZ2	1:H:294:PRO:HG3	2.41	0.55
1:H:794:ARG:HH11	1:H:794:ARG:HG2	1.72	0.55
1:A:602:GLU:C	1:A:603:ILE:HG13	2.26	0.55
1:C:1063:LYS:HE2	1:C:1068:ASN:CG	2.26	0.55
1:C:278:LEU:O	1:C:344:GLU:HG3	2.07	0.55
1:F:752:VAL:HG12	1:F:752:VAL:O	2.07	0.55
1:A:740:ASN:ND2	1:A:740:ASN:C	2.57	0.55
1:B:513:ILE:CD1	1:B:856:MET:HE1	2.26	0.55
1:D:355:TRP:O	1:D:359:THR:HG22	2.07	0.55
1:F:407:ASN:ND2	1:F:431:GLU:N	2.53	0.55
1:F:469:ALA:HB2	1:F:939:VAL:HG13	1.88	0.55
1:H:792:ASN:OD1	1:H:792:ASN:C	2.45	0.55
1:A:485:ASP:OD2	1:A:1029:SER:OG	2.22	0.55
1:F:765:ARG:HD3	1:F:784:ALA:HB3	1.87	0.55
1:G:457:MET:HE1	1:G:494:LEU:HD21	1.88	0.55
1:B:492:ASP:HB3	1:B:1022:LEU:CD2	2.37	0.55
1:B:260:GLU:HG3	1:B:271:TRP:O	2.07	0.55
1:D:666:ASP:HA	1:D:863:PHE:O	2.06	0.55
1:E:310:VAL:HG22	1:E:339:ILE:CD1	2.36	0.55
1:F:558:ASN:N	1:F:559:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:310:VAL:HG11	1:G:335:ALA:HB1	1.89	0.55
1:H:301:PRO:CD	1:H:305:THR:HG21	2.37	0.55
1:D:251:VAL:HG21	1:D:259:PHE:HZ	1.72	0.55
1:E:669:TYR:CE2	1:E:670:MET:HE2	2.42	0.55
1:F:794:ARG:CG	1:F:794:ARG:HH11	2.20	0.55
1:G:311:ASN:ND2	1:G:323:TYR:H	2.03	0.55
1:A:271:TRP:HZ2	1:A:357:ARG:HA	1.72	0.54
1:A:492:ASP:OD2	1:A:1025:ARG:HD2	2.08	0.54
1:C:261:HIS:HD2	1:C:264:HIS:N	1.96	0.54
1:C:461:ASN:N	1:C:470:ASN:HD21	2.04	0.54
1:D:281:GLY:CA	1:D:341:THR:CG2	2.62	0.54
1:F:1067:THR:O	1:F:1067:THR:HG22	2.06	0.54
1:F:245:PHE:O	1:F:247:GLN:N	2.40	0.54
1:H:288:THR:C	1:H:290:LYS:H	2.09	0.54
1:D:253:SER:H	1:D:258:ASN:ND2	2.04	0.54
1:F:691:VAL:CG1	1:F:712:ARG:NH1	2.70	0.54
1:C:800:THR:HG22	1:C:802:ALA:N	2.17	0.54
1:C:436:ASN:HB2	1:C:961:MET:O	2.08	0.54
1:F:651:LYS:O	1:F:652:SER:HB2	2.07	0.54
1:G:293:ARG:HB3	1:G:297:MET:CE	2.37	0.54
1:H:1087:PRO:OXT	1:H:1087:PRO:HD2	2.08	0.54
1:A:280:ASP:OD1	1:A:348:THR:HB	2.06	0.54
1:C:669:TYR:CD2	1:C:670:MET:HG3	2.40	0.54
1:D:809:ASN:HB2	1:D:810:PRO:CD	2.37	0.54
1:A:292:PHE:O	1:A:293:ARG:HD3	2.07	0.54
1:B:604:ASN:OD1	1:B:606:ASN:N	2.40	0.54
1:B:884:LYS:HE3	1:B:887:GLU:OE1	2.08	0.54
1:C:407:ASN:ND2	1:C:431:GLU:H	2.06	0.54
1:C:861:SER:HB3	1:C:864:GLN:HG3	1.89	0.54
1:D:433:LEU:HD22	1:D:481:ASN:ND2	2.21	0.54
1:D:673:LYS:HE2	1:D:677:TYR:CZ	2.43	0.54
1:F:751:VAL:HB	1:F:799:PHE:HB2	1.88	0.54
1:F:799:PHE:HE1	1:F:819:TRP:CH2	2.25	0.54
1:H:407:ASN:ND2	1:H:431:GLU:H	2.06	0.54
1:E:256:ALA:HB1	1:E:261:HIS:CE1	2.42	0.54
1:F:882:VAL:HG22	1:F:948:LYS:CG	2.37	0.54
1:A:988:LYS:H	1:A:990:THR:HG21	1.72	0.54
1:C:999:SER:C	1:C:1001:LYS:H	2.10	0.54
1:E:1073:LEU:CD2	1:E:1080:LEU:HD21	2.36	0.54
1:H:363:PHE:O	1:H:365:LYS:N	2.41	0.54
1:H:809:ASN:HB2	1:H:810:PRO:CD	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LYS:O	1:A:352:ASN:HB3	2.07	0.54
1:G:251:VAL:CG2	1:G:259:PHE:CZ	2.89	0.54
1:G:304:GLU:O	1:G:307:ARG:HB3	2.08	0.54
1:H:363:PHE:C	1:H:365:LYS:H	2.10	0.54
1:A:558:ASN:N	1:A:559:PRO:CD	2.71	0.54
1:A:877:VAL:O	1:A:881:ASN:ND2	2.41	0.54
1:B:258:ASN:C	1:B:259:PHE:CD2	2.82	0.54
1:B:639:ASN:HD21	1:B:813:SER:N	1.98	0.54
1:D:658:TYR:CE2	1:D:660:GLY:HA3	2.43	0.54
1:F:841:ASP:OD1	1:F:846:HIS:HE1	1.90	0.54
1:F:988:LYS:O	1:F:989:ASN:HB2	2.07	0.54
1:B:896:ALA:CB	1:B:932:TYR:CE2	2.91	0.54
1:C:740:ASN:ND2	1:C:742:SER:H	2.06	0.54
1:E:337:GLN:O	1:E:340:GLN:HB3	2.07	0.54
1:G:244:SER:C	1:G:246:ALA:N	2.59	0.54
1:H:363:PHE:O	1:H:364:VAL:C	2.42	0.54
1:H:705:SER:HB3	1:H:743:LEU:HD13	1.90	0.54
1:A:355:TRP:CG	1:A:356:LEU:N	2.76	0.53
1:B:388:LEU:HD12	1:B:1049:ASN:O	2.08	0.53
1:B:427:ILE:HG12	4:B:5001:MES:O3S	2.08	0.53
1:B:610:TYR:O	1:B:612:PHE:N	2.38	0.53
1:B:474:ILE:O	1:B:953:MET:HE3	2.07	0.53
1:E:250:GLN:HB2	1:E:1084:LEU:O	2.08	0.53
1:E:273:ARG:HD3	1:E:292:PHE:HE2	1.67	0.53
1:E:515:GLU:O	1:E:515:GLU:HG2	2.07	0.53
1:F:698:ARG:HB2	1:F:709:THR:OG1	2.08	0.53
1:G:713:TYR:O	1:G:759:HIS:HE1	1.91	0.53
1:B:478:ALA:HB1	1:B:481:ASN:HD22	1.73	0.53
1:C:457:MET:HE1	1:C:494:LEU:CD2	2.38	0.53
1:F:531:ASN:ND2	1:F:844:SER:OG	2.42	0.53
1:H:740:ASN:C	1:H:740:ASN:ND2	2.61	0.53
1:A:288:THR:C	1:A:290:LYS:H	2.12	0.53
1:A:304:GLU:CA	1:A:304:GLU:OE1	2.53	0.53
1:B:1012:LEU:O	1:B:1016:GLN:HB2	2.09	0.53
1:B:407:ASN:ND2	1:B:431:GLU:N	2.55	0.53
1:D:248:TYR:HB3	1:D:276:TYR:HB2	1.90	0.53
1:E:759:HIS:CD2	1:E:762:GLN:OE1	2.61	0.53
1:F:522:THR:N	1:F:523:PRO:HD2	2.23	0.53
1:A:537:ASN:OD1	1:A:540:ARG:NH1	2.39	0.53
1:B:272:TYR:CE1	1:B:274:PRO:HD3	2.43	0.53
1:B:535:MET:CE	1:B:583:PHE:HE2	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:THR:HG23	1:B:801:ALA:H	1.72	0.53
1:D:751:VAL:HB	1:D:799:PHE:HB2	1.91	0.53
1:E:250:GLN:HE21	1:E:275:LYS:HE2	1.73	0.53
1:E:334:LEU:HD23	1:E:337:GLN:OE1	2.09	0.53
1:E:512:SER:O	1:E:532:MET:HB2	2.08	0.53
1:B:535:MET:HE2	1:B:583:PHE:HE2	1.71	0.53
1:E:630:ALA:O	1:E:633:LYS:NZ	2.41	0.53
1:F:259:PHE:N	1:F:259:PHE:CD2	2.76	0.53
1:F:311:ASN:ND2	1:F:323:TYR:H	1.97	0.53
1:G:268:ALA:HB2	1:G:370:TRP:CE2	2.44	0.53
1:A:1085:VAL:HG23	1:A:1086:ASN:H	1.74	0.53
1:A:342:LYS:HA	1:A:345:GLU:OE1	2.08	0.53
1:B:558:ASN:HB3	1:B:559:PRO:HD3	1.89	0.53
1:E:537:ASN:OD1	1:E:540:ARG:NH1	2.34	0.53
1:F:831:ARG:HB3	1:F:853:SER:HB3	1.91	0.53
1:H:1087:PRO:CD	1:H:1087:PRO:OXT	2.56	0.53
1:C:261:HIS:CD2	1:C:264:HIS:HA	2.44	0.53
1:E:271:TRP:CE3	1:E:357:ARG:CZ	2.91	0.53
1:E:374:SER:HA	1:E:986:GLN:NE2	2.24	0.53
1:F:250:GLN:OE1	1:F:1087:PRO:HG3	2.08	0.53
1:G:581:TYR:HA	1:G:654:VAL:O	2.08	0.53
1:H:278:LEU:CD1	1:H:283:THR:N	2.71	0.53
1:H:513:ILE:HD13	1:H:856:MET:HE2	1.91	0.53
1:A:782:GLN:NE2	1:A:782:GLN:CA	2.72	0.53
1:B:407:ASN:HD21	1:B:431:GLU:H	1.57	0.53
1:E:347:ILE:HG13	1:E:355:TRP:HE1	1.73	0.53
1:F:639:ASN:HD22	1:F:642:LEU:HD13	1.73	0.53
1:G:759:HIS:HD2	1:G:762:GLN:OE1	1.92	0.53
1:G:861:SER:HB3	1:G:864:GLN:HG3	1.91	0.53
1:B:762:GLN:CG	1:B:763:ALA:N	2.72	0.53
1:D:304:GLU:OE1	1:D:307:ARG:NH1	2.41	0.53
1:D:604:ASN:OD1	1:D:604:ASN:C	2.47	0.53
1:A:868:THR:HB	1:A:872:GLU:OE1	2.08	0.53
1:B:930:ASN:O	1:B:931:LYS:C	2.46	0.53
1:D:987:ILE:HG22	1:D:987:ILE:O	2.08	0.53
1:E:329:PRO:O	1:E:332:LEU:HB2	2.09	0.53
1:F:492:ASP:CB	1:F:1022:LEU:HD22	2.34	0.53
1:F:685:LYS:NZ	1:F:887:GLU:OE2	2.42	0.53
1:H:301:PRO:CG	1:H:305:THR:HG21	2.38	0.53
1:A:271:TRP:CZ2	1:A:294:PRO:HG3	2.44	0.52
1:A:800:THR:CG2	1:A:801:ALA:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:GLN:HG3	1:B:763:ALA:H	1.74	0.52
1:D:280:ASP:C	1:D:282:LYS:H	2.13	0.52
1:D:355:TRP:CG	1:D:356:LEU:N	2.77	0.52
1:D:407:ASN:ND2	1:D:431:GLU:N	2.55	0.52
1:E:271:TRP:CE2	1:E:357:ARG:CD	2.77	0.52
1:E:336:ALA:HA	1:E:339:ILE:HD12	1.91	0.52
1:F:566:VAL:HG21	1:F:652:SER:HB3	1.91	0.52
1:A:273:ARG:NH2	1:A:288:THR:HA	2.24	0.52
1:E:558:ASN:N	1:E:559:PRO:CD	2.73	0.52
1:D:1052:ASN:N	1:D:1052:ASN:ND2	2.48	0.52
1:F:357:ARG:CG	1:F:357:ARG:NH1	2.60	0.52
1:F:691:VAL:HG12	1:F:712:ARG:NH1	2.25	0.52
1:B:920:ASP:HB3	1:B:923:ASP:HB3	1.91	0.52
1:D:300:TRP:CB	1:D:306:GLN:HB2	2.40	0.52
1:E:259:PHE:CD2	1:E:259:PHE:N	2.77	0.52
1:F:688:ILE:O	1:F:830:VAL:HG22	2.09	0.52
1:A:277:ILE:HG13	1:A:291:ASP:HB3	1.92	0.52
1:D:932:TYR:HA	5:D:1090:HOH:O	2.09	0.52
1:F:322:THR:HG22	1:F:323:TYR:N	2.24	0.52
1:H:522:THR:N	1:H:523:PRO:HD2	2.24	0.52
1:A:273:ARG:NH2	1:A:288:THR:CA	2.72	0.52
1:A:352:ASN:OD1	1:A:354:ASN:N	2.43	0.52
1:C:516:ALA:HB1	1:C:521:ASP:OD2	2.08	0.52
1:D:304:GLU:O	1:D:307:ARG:HB3	2.09	0.52
1:G:346:LYS:HD3	1:G:355:TRP:CH2	2.45	0.52
1:H:1071:PHE:CE1	1:H:1081:PRO:HD3	2.43	0.52
1:B:1063:LYS:NZ	1:B:1068:ASN:OD1	2.40	0.52
1:B:585:ARG:CD	1:B:661:ASP:OD1	2.57	0.52
1:D:973:THR:HG23	1:D:988:LYS:HA	1.92	0.52
1:F:694:GLY:HA3	1:F:718:LEU:O	2.08	0.52
1:F:631:THR:HG21	1:F:808:ALA:O	2.10	0.52
1:H:278:LEU:HG	1:H:278:LEU:O	2.09	0.52
1:A:278:LEU:O	1:A:344:GLU:CG	2.57	0.52
1:B:785:ALA:O	1:B:788:VAL:HG23	2.09	0.52
1:B:866:PHE:CZ	1:B:913:GLN:HG3	2.45	0.52
1:D:1064:ASP:O	1:D:1068:ASN:N	2.43	0.52
1:F:765:ARG:HB2	1:F:784:ALA:HB1	1.92	0.52
1:G:319:ILE:HD13	1:G:338:THR:HG22	1.90	0.52
1:F:874:THR:O	1:F:878:ILE:HG13	2.10	0.52
1:B:248:TYR:C	1:B:250:GLN:H	2.12	0.52
1:C:561:ILE:HG12	1:C:697:MET:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:504:ASP:OD1	1:D:846:HIS:CD2	2.59	0.52
1:D:957:VAL:HG12	1:D:957:VAL:O	2.09	0.52
1:E:319:ILE:HD11	1:E:342:LYS:HD2	1.90	0.52
1:F:794:ARG:CG	1:F:794:ARG:NH1	2.73	0.52
1:G:278:LEU:HG	1:G:281:GLY:HA2	1.92	0.52
1:G:697:MET:HA	1:G:709:THR:O	2.10	0.52
1:F:604:ASN:OD1	1:F:606:ASN:HB2	2.10	0.51
1:F:776:LYS:HE3	1:F:778:TYR:CE1	2.44	0.51
1:G:740:ASN:C	1:G:740:ASN:ND2	2.63	0.51
1:A:317:LEU:CD1	1:A:339:ILE:HG23	2.40	0.51
1:B:687:ARG:HA	1:B:691:VAL:CG2	2.39	0.51
1:D:334:LEU:O	1:D:335:ALA:C	2.47	0.51
1:D:371:ASN:HB3	1:D:373:ASP:H	1.73	0.51
1:D:442:ASN:HB3	1:D:445:VAL:HG23	1.93	0.51
1:F:877:VAL:CG1	1:F:881:ASN:ND2	2.74	0.51
1:H:356:LEU:C	1:H:358:GLN:N	2.62	0.51
1:A:1012:LEU:O	1:A:1016:GLN:HG3	2.11	0.51
1:B:579:PRO:HA	1:B:847:GLN:OE1	2.10	0.51
1:B:639:ASN:HB3	1:B:642:LEU:HB2	1.92	0.51
1:D:574:GLU:HG3	1:D:575:THR:N	2.26	0.51
1:F:256:ALA:HA	1:F:1073:LEU:HD13	1.92	0.51
1:B:246:ALA:O	1:B:249:ASN:HB2	2.10	0.51
1:E:385:GLY:HA3	1:E:1053:ILE:HD13	1.92	0.51
1:E:522:THR:N	1:E:523:PRO:HD2	2.25	0.51
1:F:444:VAL:HG11	1:F:1038:VAL:HG22	1.92	0.51
1:F:869:LYS:HD2	1:F:871:GLU:OE1	2.10	0.51
1:H:278:LEU:HD21	1:H:281:GLY:CA	2.20	0.51
1:H:995:ASP:OD1	1:H:1056:ARG:NH2	2.41	0.51
1:A:258:ASN:ND2	1:A:273:ARG:HB3	2.25	0.51
1:A:596:ARG:HB2	1:A:612:PHE:HZ	1.74	0.51
1:B:246:ALA:O	1:B:249:ASN:N	2.30	0.51
1:C:492:ASP:HB3	1:C:1022:LEU:CD2	2.41	0.51
1:C:321:GLN:HG2	1:C:322:THR:H	1.76	0.51
1:C:743:LEU:O	1:C:744:ARG:NH1	2.39	0.51
1:E:273:ARG:HG2	1:E:292:PHE:HD2	1.73	0.51
1:E:478:ALA:HB1	1:E:481:ASN:HD22	1.75	0.51
1:H:407:ASN:HD21	1:H:431:GLU:H	1.57	0.51
1:A:277:ILE:CG1	1:A:291:ASP:HB3	2.40	0.51
1:A:512:SER:O	1:A:532:MET:HB2	2.11	0.51
1:B:407:ASN:ND2	1:B:431:GLU:HB2	2.26	0.51
1:D:355:TRP:CD2	1:D:356:LEU:N	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:860:PHE:CG	1:D:896:ALA:HB2	2.45	0.51
1:H:302:ASP:O	1:H:303:GLN:C	2.48	0.51
1:B:809:ASN:HB2	1:B:810:PRO:CD	2.40	0.51
1:B:866:PHE:HZ	1:B:913:GLN:HG3	1.76	0.51
1:D:312:TYR:O	1:D:315:ALA:HB3	2.10	0.51
1:D:421:TYR:CD1	1:D:523:PRO:HB2	2.46	0.51
1:E:440:ASN:ND2	1:E:449:GLN:HE21	1.88	0.51
1:F:816:LEU:HD12	1:F:817:GLY:N	2.26	0.51
1:A:435:ALA:HA	1:A:1052:ASN:ND2	2.24	0.51
1:C:278:LEU:HD13	1:C:284:TRP:CE2	2.45	0.51
1:E:928:LYS:HB2	1:E:929:PRO:HD2	1.92	0.51
1:F:1064:ASP:O	1:F:1068:ASN:N	2.43	0.51
1:B:740:ASN:C	1:B:740:ASN:HD22	2.14	0.51
1:C:1000:GLY:CA	5:C:171:HOH:O	2.59	0.51
1:C:299:TRP:NE1	1:C:1081:PRO:HB3	2.26	0.51
1:C:800:THR:HG23	1:C:801:ALA:H	1.76	0.51
1:E:271:TRP:CH2	1:E:357:ARG:CG	2.94	0.51
1:F:606:ASN:O	1:F:607:VAL:C	2.49	0.51
1:B:729:ARG:HD2	1:B:758:ALA:O	2.11	0.51
1:B:639:ASN:ND2	1:B:813:SER:H	1.99	0.51
1:D:293:ARG:CB	1:D:297:MET:HE1	2.41	0.51
1:G:355:TRP:CG	1:G:356:LEU:N	2.76	0.51
1:G:504:ASP:OD1	1:G:846:HIS:CD2	2.56	0.51
1:B:504:ASP:O	1:B:508:ASN:HB2	2.11	0.50
1:C:537:ASN:OD1	1:C:540:ARG:NH1	2.41	0.50
1:E:337:GLN:O	1:E:340:GLN:CB	2.59	0.50
1:E:457:MET:HE1	1:E:494:LEU:HD21	1.93	0.50
1:G:363:PHE:O	1:G:364:VAL:C	2.48	0.50
1:G:558:ASN:N	1:G:559:PRO:CD	2.73	0.50
1:B:781:ASP:OD2	1:B:822:VAL:HG13	2.11	0.50
1:B:513:ILE:HG21	1:B:856:MET:CE	2.41	0.50
1:F:256:ALA:C	1:F:258:ASN:N	2.65	0.50
1:F:256:ALA:O	1:F:258:ASN:N	2.44	0.50
1:F:391:ASN:OD1	1:F:404:ARG:HD2	2.12	0.50
1:B:820:VAL:HB	1:B:821:PRO:HD2	1.92	0.50
1:D:299:TRP:NE1	1:D:1081:PRO:HB3	2.26	0.50
1:E:964:LEU:HD12	1:E:996:GLY:HA2	1.92	0.50
1:F:1074:VAL:HG13	1:F:1077:ASN:HB3	1.93	0.50
1:F:440:ASN:HD21	1:F:449:GLN:NE2	2.03	0.50
1:G:248:TYR:HB3	1:G:276:TYR:HB2	1.94	0.50
1:H:308:GLN:NE2	1:H:367:GLN:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1030:THR:HB	1:B:1032:VAL:HG22	1.94	0.50
1:B:631:THR:HG23	1:B:809:ASN:C	2.31	0.50
1:G:457:MET:HE1	1:G:494:LEU:CD2	2.41	0.50
1:H:376:LYS:HB3	1:H:377:PRO:CA	2.36	0.50
1:B:454:HIS:ND1	1:B:1015:LEU:HD21	2.27	0.50
1:B:522:THR:N	1:B:523:PRO:HD2	2.26	0.50
1:D:271:TRP:CG	1:D:294:PRO:HA	2.46	0.50
1:D:321:GLN:HG2	1:D:322:THR:H	1.77	0.50
1:E:530:ASP:O	1:E:844:SER:HB2	2.11	0.50
1:F:1052:ASN:ND2	1:F:1052:ASN:N	2.54	0.50
1:F:346:LYS:HE2	1:F:355:TRP:CE3	2.46	0.50
1:F:436:ASN:HB2	1:F:961:MET:O	2.10	0.50
1:G:1052:ASN:ND2	1:G:1052:ASN:N	2.58	0.50
1:H:1052:ASN:ND2	1:H:1052:ASN:N	2.60	0.50
1:A:604:ASN:HD21	1:A:607:VAL:N	2.10	0.50
1:D:965:PRO:HD2	1:D:997:LYS:O	2.12	0.50
1:E:350:GLU:C	1:E:352:ASN:H	2.13	0.50
1:H:928:LYS:HE2	1:H:929:PRO:O	2.12	0.50
1:D:800:THR:CG2	1:D:801:ALA:N	2.74	0.50
1:G:344:GLU:HA	1:G:344:GLU:OE1	2.12	0.50
1:G:663:PHE:CZ	1:G:670:MET:HG2	2.46	0.50
1:H:287:SER:HA	1:H:291:ASP:OD2	2.11	0.50
1:H:965:PRO:HD2	1:H:997:LYS:O	2.11	0.50
1:B:1085:VAL:C	1:B:1087:PRO:HD3	2.32	0.50
1:D:303:GLN:HE22	1:D:329:PRO:CD	2.24	0.50
1:D:310:VAL:HG11	1:D:335:ALA:HB1	1.94	0.50
1:E:713:TYR:O	1:E:759:HIS:HE1	1.94	0.50
1:E:474:ILE:C	1:E:953:MET:HE2	2.32	0.50
1:F:745:LEU:HD11	1:F:804:ILE:O	2.12	0.50
1:H:251:VAL:HG21	1:H:259:PHE:HZ	1.72	0.50
1:C:250:GLN:HE21	1:C:275:LYS:CE	2.25	0.49
1:C:999:SER:OG	1:C:999:SER:O	2.29	0.49
1:F:765:ARG:HG2	1:F:781:ASP:OD1	2.12	0.49
1:G:1080:LEU:HB3	1:G:1081:PRO:CD	2.42	0.49
1:G:271:TRP:HZ2	1:G:357:ARG:HA	1.77	0.49
1:H:278:LEU:CG	1:H:281:GLY:HA2	2.42	0.49
1:A:700:GLN:HE21	1:A:702:VAL:HG13	1.76	0.49
1:C:251:VAL:O	1:C:275:LYS:HE3	2.12	0.49
1:C:759:HIS:HD2	1:C:762:GLN:OE1	1.94	0.49
1:D:634:LYS:HD3	1:D:635:TYR:CZ	2.48	0.49
1:E:407:ASN:ND2	1:E:431:GLU:N	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:993:VAL:O	1:H:1056:ARG:NH1	2.45	0.49
1:H:407:ASN:ND2	1:H:431:GLU:N	2.60	0.49
1:A:516:ALA:HB1	1:A:521:ASP:OD2	2.12	0.49
1:C:346:LYS:HB3	1:C:355:TRP:CZ2	2.47	0.49
1:C:478:ALA:HB1	1:C:481:ASN:HD22	1.76	0.49
1:D:965:PRO:HD2	1:D:998:SER:HA	1.94	0.49
1:E:271:TRP:CZ2	1:E:357:ARG:HG2	2.47	0.49
1:E:513:ILE:CD1	1:E:953:MET:HE1	2.42	0.49
1:F:1067:THR:HG21	1:F:1069:THR:OG1	2.12	0.49
1:F:537:ASN:OD1	1:F:540:ARG:NH1	2.44	0.49
1:G:596:ARG:HB2	1:G:612:PHE:HZ	1.76	0.49
1:G:917:ALA:HA	1:G:962:TYR:CD1	2.47	0.49
1:H:512:SER:O	1:H:532:MET:HB2	2.12	0.49
1:A:666:ASP:HA	1:A:863:PHE:O	2.12	0.49
1:B:993:VAL:O	1:B:1056:ARG:NH1	2.44	0.49
1:C:713:TYR:O	1:C:759:HIS:HE1	1.94	0.49
1:D:663:PHE:CZ	1:D:670:MET:HG2	2.48	0.49
1:E:280:ASP:C	1:E:282:LYS:N	2.65	0.49
1:E:273:ARG:HD3	1:E:289:GLU:HA	1.94	0.49
1:E:407:ASN:HD21	1:E:431:GLU:H	1.58	0.49
1:F:1069:THR:HB	1:F:1079:PHE:HE2	1.77	0.49
1:F:1085:VAL:CG2	1:F:1086:ASN:N	2.75	0.49
1:F:421:TYR:CE1	1:F:523:PRO:HB2	2.47	0.49
1:F:669:TYR:CD1	1:F:874:THR:HG23	2.47	0.49
1:G:860:PHE:CG	1:G:896:ALA:HB2	2.47	0.49
1:B:988:LYS:N	1:B:990:THR:HG23	2.27	0.49
1:E:269:GLU:HG3	1:E:364:VAL:HG21	1.94	0.49
1:E:355:TRP:CG	1:E:356:LEU:N	2.80	0.49
1:E:530:ASP:HB2	1:E:843:LYS:HB3	1.94	0.49
1:F:927:SER:OG	1:F:928:LYS:HG2	2.12	0.49
1:B:694:GLY:O	1:B:712:ARG:HD2	2.12	0.49
1:D:740:ASN:ND2	1:D:740:ASN:C	2.61	0.49
1:A:294:PRO:HG2	1:A:356:LEU:HD21	1.94	0.49
1:A:453:LEU:HD11	1:A:457:MET:CE	2.42	0.49
1:B:260:GLU:OE1	1:B:271:TRP:HB2	2.13	0.49
1:D:251:VAL:O	1:D:251:VAL:HG12	2.12	0.49
1:E:300:TRP:CD1	1:E:306:GLN:HA	2.48	0.49
1:E:371:ASN:HB3	1:E:373:ASP:H	1.78	0.49
1:F:368:SER:O	1:F:371:ASN:HB2	2.12	0.49
1:F:975:VAL:HG12	1:F:981:PRO:HA	1.95	0.49
1:G:324:ASN:OD1	1:G:324:ASN:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:581:TYR:HA	1:H:654:VAL:O	2.13	0.49
1:H:474:ILE:O	1:H:953:MET:HE2	2.13	0.49
1:A:252:TYR:CE2	1:A:273:ARG:NH1	2.78	0.49
1:A:868:THR:CG2	1:A:868:THR:O	2.61	0.49
1:G:376:LYS:HE2	1:G:378:PHE:CE1	2.47	0.49
1:G:516:ALA:HB1	1:G:521:ASP:OD2	2.13	0.49
1:B:369:ALA:O	1:B:1057:GLY:HA3	2.12	0.49
1:B:689:LYS:HD2	1:B:690:TYR:CE1	2.48	0.49
1:D:1074:VAL:CG2	1:D:1077:ASN:HB2	2.42	0.49
1:D:1085:VAL:HG23	1:D:1086:ASN:N	2.27	0.49
1:D:278:LEU:O	1:D:344:GLU:HG3	2.12	0.49
1:F:816:LEU:HD12	1:F:817:GLY:H	1.78	0.49
1:H:288:THR:C	1:H:290:LYS:N	2.63	0.49
1:A:271:TRP:CZ2	1:A:357:ARG:HA	2.46	0.49
1:A:809:ASN:HB2	1:A:810:PRO:CD	2.43	0.49
1:F:279:LYS:O	1:F:280:ASP:HB3	2.12	0.49
1:G:387:LEU:O	1:G:1050:GLY:HA3	2.13	0.49
1:H:248:TYR:HD1	1:H:276:TYR:CD2	2.31	0.49
1:H:531:ASN:ND2	1:H:844:SER:OG	2.45	0.49
1:H:869:LYS:HG3	1:H:871:GLU:OE1	2.13	0.49
1:B:1071:PHE:HA	1:B:1079:PHE:HD1	1.78	0.48
1:B:513:ILE:HG12	1:B:953:MET:HE1	1.94	0.48
1:C:281:GLY:H	1:C:344:GLU:HB3	1.77	0.48
1:C:903:THR:HG22	1:C:913:GLN:NE2	2.27	0.48
1:F:711:VAL:CG2	1:F:734:VAL:HG23	2.42	0.48
1:A:275:LYS:O	1:A:276:TYR:CD2	2.66	0.48
1:B:689:LYS:O	1:B:830:VAL:HG13	2.13	0.48
1:B:920:ASP:HB3	1:B:923:ASP:CB	2.43	0.48
1:C:987:ILE:HG12	1:C:1058:ALA:HB2	1.94	0.48
1:H:280:ASP:O	1:H:281:GLY:O	2.30	0.48
1:H:687:ARG:HA	1:H:691:VAL:HG23	1.94	0.48
1:A:317:LEU:HD11	1:A:339:ILE:HG23	1.95	0.48
1:D:514:LEU:HD21	1:D:532:MET:HG3	1.94	0.48
1:D:262:VAL:HG12	1:D:969:VAL:HG23	1.94	0.48
1:E:347:ILE:O	1:E:351:LYS:N	2.46	0.48
1:E:516:ALA:HB1	1:E:521:ASP:OD2	2.13	0.48
1:F:1065:GLN:HG3	1:F:1066:ALA:H	1.78	0.48
1:G:280:ASP:C	1:G:282:LYS:N	2.66	0.48
1:A:1065:GLN:HG3	1:A:1066:ALA:N	2.28	0.48
1:A:397:SER:HB3	5:A:1093:HOH:O	2.14	0.48
1:D:987:ILE:HG12	1:D:1058:ALA:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:ASP:C	1:E:380:ASP:OD1	2.51	0.48
1:F:514:LEU:HD11	1:F:525:LEU:HD13	1.95	0.48
1:F:726:ARG:H	1:F:726:ARG:HD3	1.79	0.48
1:G:376:LYS:HA	1:G:377:PRO:C	2.33	0.48
4:H:5001:MES:H82	4:H:5001:MES:H52	1.21	0.48
1:A:387:LEU:O	1:A:1050:GLY:HA3	2.13	0.48
1:A:705:SER:HB3	1:A:743:LEU:HD13	1.95	0.48
1:E:1068:ASN:OD1	1:E:1068:ASN:O	2.30	0.48
1:E:634:LYS:HD3	1:E:635:TYR:CE2	2.49	0.48
1:F:930:ASN:C	1:F:930:ASN:OD1	2.51	0.48
1:G:301:PRO:O	1:G:302:ASP:HB3	2.14	0.48
1:H:248:TYR:HB3	1:H:276:TYR:CB	2.20	0.48
1:H:874:THR:HB	1:H:932:TYR:HB3	1.95	0.48
1:A:948:LYS:HE2	1:A:948:LYS:HA	1.96	0.48
1:B:768:LEU:O	1:B:769:LEU:HD23	2.13	0.48
1:D:294:PRO:HG2	1:D:297:MET:HB2	1.94	0.48
1:D:407:ASN:HD21	1:D:431:GLU:H	1.61	0.48
1:E:387:LEU:O	1:E:1050:GLY:HA3	2.13	0.48
1:F:1023:PHE:CD1	1:F:1036:PRO:HG3	2.48	0.48
1:F:483:ASP:C	1:F:483:ASP:OD1	2.50	0.48
1:H:841:ASP:OD1	1:H:846:HIS:HE1	1.97	0.48
1:B:1063:LYS:NZ	1:B:1068:ASN:CA	2.76	0.48
1:E:460:GLY:H	1:E:470:ASN:ND2	2.12	0.48
1:E:639:ASN:HB3	1:E:642:LEU:HB2	1.95	0.48
1:F:800:THR:O	1:F:803:ASP:OD2	2.30	0.48
1:F:974:ARG:HB2	1:F:985:SER:OG	2.14	0.48
1:G:453:LEU:CD1	1:G:474:ILE:HG21	2.44	0.48
1:A:355:TRP:CE3	1:A:356:LEU:N	2.81	0.48
1:C:1085:VAL:CG2	1:C:1086:ASN:N	2.77	0.48
1:D:713:TYR:O	1:D:759:HIS:HE1	1.96	0.48
1:F:766:PRO:HA	1:F:819:TRP:CD1	2.49	0.48
1:G:389:TYR:CZ	1:G:1050:GLY:HA2	2.49	0.48
1:G:464:ALA:O	1:G:465:ASN:HB2	2.13	0.48
1:H:996:GLY:O	1:H:1044:SER:HA	2.13	0.48
1:A:700:GLN:HE21	1:A:702:VAL:CG1	2.27	0.48
1:G:293:ARG:HB3	1:G:297:MET:HE2	1.95	0.48
1:H:364:VAL:HG13	1:H:370:TRP:CE3	2.49	0.48
1:H:513:ILE:HD13	1:H:856:MET:CE	2.44	0.48
1:C:356:LEU:HA	1:C:359:THR:HG22	1.96	0.48
1:C:475:ARG:CA	1:C:953:MET:CE	2.92	0.48
1:D:585:ARG:HD3	1:D:661:ASP:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:917:ALA:HB1	1:F:962:TYR:CD1	2.49	0.48
1:H:285:THR:O	1:H:286:GLN:O	2.32	0.48
1:B:571:ASP:OD2	1:B:651:LYS:HG2	2.14	0.47
1:D:304:GLU:O	1:D:307:ARG:CB	2.62	0.47
1:G:809:ASN:HB2	1:G:810:PRO:CD	2.44	0.47
1:H:309:TYR:C	1:H:309:TYR:CD2	2.88	0.47
1:A:280:ASP:OD1	1:A:348:THR:OG1	2.31	0.47
1:A:985:SER:OG	1:A:986:GLN:N	2.46	0.47
1:B:558:ASN:N	1:B:559:PRO:CD	2.77	0.47
1:C:599:ILE:HA	1:C:603:ILE:HB	1.96	0.47
1:D:502:LYS:HA	1:D:502:LYS:HD2	1.49	0.47
1:E:263:ASP:O	1:E:264:HIS:HB2	2.13	0.47
1:E:658:TYR:CE2	1:E:660:GLY:HA3	2.49	0.47
1:E:800:THR:CG2	1:E:801:ALA:N	2.76	0.47
1:F:708:ILE:CD1	1:F:708:ILE:H	2.21	0.47
1:H:261:HIS:HD2	1:H:264:HIS:N	2.09	0.47
1:A:407:ASN:ND2	1:A:431:GLU:H	2.12	0.47
1:B:530:ASP:O	1:B:845:VAL:HG23	2.14	0.47
1:E:733:VAL:HG22	1:E:734:VAL:N	2.29	0.47
1:F:471:PHE:CG	1:F:954:ALA:HB2	2.49	0.47
1:F:571:ASP:OD2	1:F:651:LYS:HG2	2.15	0.47
1:G:356:LEU:HA	1:G:359:THR:CG2	2.44	0.47
1:H:291:ASP:N	1:H:291:ASP:OD1	2.47	0.47
1:H:743:LEU:O	1:H:744:ARG:HD3	2.14	0.47
1:H:874:THR:HG22	1:H:878:ILE:CD1	2.43	0.47
1:C:346:LYS:HE2	1:C:355:TRP:CE3	2.49	0.47
1:C:407:ASN:ND2	1:C:431:GLU:N	2.62	0.47
1:D:442:ASN:HB3	1:D:445:VAL:CG2	2.44	0.47
1:E:319:ILE:CD1	1:E:342:LYS:HE2	2.43	0.47
1:B:896:ALA:HB1	1:B:932:TYR:CE2	2.50	0.47
1:B:920:ASP:CG	1:B:923:ASP:HB2	2.34	0.47
1:C:610:TYR:HD2	1:C:612:PHE:HZ	1.62	0.47
1:C:874:THR:HB	1:C:932:TYR:HB3	1.97	0.47
1:D:576:ALA:HB3	1:D:847:GLN:HB3	1.96	0.47
1:E:504:ASP:OD1	1:E:846:HIS:HD2	1.96	0.47
1:H:356:LEU:O	1:H:358:GLN:N	2.47	0.47
1:B:1064:ASP:HB2	1:B:1071:PHE:CZ	2.48	0.47
1:B:246:ALA:O	1:B:247:GLN:C	2.51	0.47
1:B:822:VAL:HG12	1:B:823:GLY:N	2.30	0.47
1:D:276:TYR:HA	1:D:285:THR:O	2.14	0.47
1:E:273:ARG:NH1	1:E:289:GLU:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:457:MET:HE3	1:G:494:LEU:HD23	1.96	0.47
1:G:883:ASP:OD1	1:G:948:LYS:HE3	2.15	0.47
1:H:639:ASN:HD22	1:H:642:LEU:HD13	1.79	0.47
1:B:740:ASN:HD22	1:B:742:SER:H	1.62	0.47
1:B:841:ASP:OD1	1:B:846:HIS:HE1	1.97	0.47
1:C:729:ARG:HD2	1:C:758:ALA:O	2.14	0.47
1:F:917:ALA:CB	1:F:962:TYR:CE1	2.98	0.47
1:B:603:ILE:HG22	1:B:604:ASN:N	2.30	0.47
1:C:727:ILE:HG23	1:C:727:ILE:HD12	1.60	0.47
1:E:920:ASP:OD2	1:E:1002:ASP:HB2	2.14	0.47
1:F:801:ALA:HA	1:F:804:ILE:O	2.14	0.47
1:F:964:LEU:CD1	1:F:996:GLY:HA2	2.41	0.47
1:A:252:TYR:HD2	1:A:258:ASN:HD21	1.61	0.47
1:B:407:ASN:HD22	1:B:431:GLU:N	2.13	0.47
1:B:789:ARG:NH2	1:B:798:ILE:O	2.40	0.47
1:C:1071:PHE:CE1	1:C:1081:PRO:HD3	2.49	0.47
1:D:922:TYR:HB2	1:D:1003:GLN:HB3	1.97	0.47
1:E:346:LYS:HG2	1:E:355:TRP:CE2	2.49	0.47
1:E:385:GLY:C	1:E:1053:ILE:HG23	2.35	0.47
1:E:854:ARG:NH1	1:E:892:ASP:OD2	2.44	0.47
1:F:724:GLY:HA3	1:F:728:THR:OG1	2.15	0.47
1:H:252:TYR:HB3	1:H:258:ASN:ND2	2.26	0.47
1:C:584:ILE:HG13	1:C:584:ILE:O	2.13	0.47
1:C:576:ALA:HB3	1:C:847:GLN:HB3	1.97	0.47
1:F:1027:GLN:O	1:F:1031:GLY:N	2.46	0.47
1:F:751:VAL:HG12	1:F:751:VAL:O	2.13	0.47
1:G:718:LEU:HA	1:G:718:LEU:HD23	1.65	0.47
1:A:988:LYS:C	1:A:990:THR:HG22	2.35	0.47
1:B:578:VAL:HG13	1:B:579:PRO:HD2	1.98	0.47
1:B:471:PHE:CG	1:B:954:ALA:HB2	2.49	0.47
1:C:782:GLN:NE2	1:C:782:GLN:HA	2.30	0.47
1:C:973:THR:HB	5:C:1091:HOH:O	2.14	0.47
1:D:286:GLN:O	1:D:287:SER:C	2.52	0.47
1:F:1035:ASP:OD1	1:F:1035:ASP:C	2.53	0.47
1:F:263:ASP:OD2	1:F:968:GLU:HA	2.15	0.47
1:G:483:ASP:C	1:G:483:ASP:OD1	2.53	0.47
1:G:733:VAL:HG22	1:G:734:VAL:N	2.30	0.47
1:B:669:TYR:CZ	1:B:670:MET:HE2	2.47	0.46
1:C:321:GLN:HG2	1:C:322:THR:N	2.30	0.46
1:E:290:LYS:HE2	1:E:290:LYS:HB2	1.54	0.46
1:F:663:PHE:O	1:F:664:THR:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:687:ARG:HA	1:G:691:VAL:HG23	1.97	0.46
1:H:356:LEU:HD12	1:H:356:LEU:HA	1.76	0.46
1:H:871:GLU:N	1:H:871:GLU:OE1	2.31	0.46
1:A:299:TRP:CZ2	1:A:301:PRO:HA	2.50	0.46
1:A:347:ILE:HG12	1:A:352:ASN:O	2.15	0.46
1:B:658:TYR:CE2	1:B:660:GLY:HA3	2.50	0.46
1:B:721:THR:O	1:B:757:ALA:CB	2.63	0.46
1:C:1080:LEU:HB2	1:C:1085:VAL:HG11	1.96	0.46
1:E:687:ARG:HA	1:E:691:VAL:HG23	1.98	0.46
1:F:642:LEU:N	1:F:642:LEU:CD1	2.77	0.46
1:F:476:VAL:HG22	1:F:956:TRP:HE3	1.80	0.46
1:H:367:GLN:O	1:H:371:ASN:HB2	2.15	0.46
1:A:988:LYS:O	1:A:990:THR:HG22	2.15	0.46
1:C:974:ARG:HG2	1:C:987:ILE:HB	1.96	0.46
1:E:325:THR:C	1:E:327:THR:H	2.18	0.46
1:E:973:THR:HG23	1:E:988:LYS:HA	1.97	0.46
1:H:607:VAL:HG13	1:H:607:VAL:O	2.15	0.46
1:B:728:THR:HG22	1:B:758:ALA:CB	2.45	0.46
1:B:731:SER:O	1:B:821:PRO:CG	2.61	0.46
1:C:604:ASN:C	1:C:604:ASN:OD1	2.53	0.46
1:E:461:ASN:OD1	1:E:467:PRO:HA	2.15	0.46
1:E:677:TYR:CD2	1:E:677:TYR:C	2.88	0.46
1:F:581:TYR:HA	1:F:654:VAL:O	2.16	0.46
1:F:712:ARG:HG3	1:F:712:ARG:HH11	1.81	0.46
1:F:740:ASN:ND2	1:F:741:PRO:CD	2.78	0.46
1:F:884:LYS:HD3	1:F:884:LYS:HA	1.61	0.46
1:A:561:ILE:HG12	1:A:697:MET:HB3	1.96	0.46
1:B:417:LYS:HE3	1:F:555:SER:HB3	1.96	0.46
1:B:987:ILE:O	1:B:987:ILE:HG22	2.14	0.46
1:C:350:GLU:O	1:C:352:ASN:N	2.48	0.46
1:D:578:VAL:HG13	1:D:579:PRO:HD2	1.98	0.46
1:E:303:GLN:O	1:E:304:GLU:C	2.52	0.46
1:E:707:ILE:HD12	1:E:707:ILE:C	2.35	0.46
1:F:724:GLY:HA3	1:F:728:THR:CB	2.46	0.46
1:A:565:LEU:HD23	1:A:565:LEU:HA	1.66	0.46
1:B:1009:GLY:HA3	1:B:1039:LYS:HB2	1.98	0.46
1:C:512:SER:O	1:C:532:MET:HB2	2.15	0.46
1:C:973:THR:CB	5:C:1091:HOH:O	2.64	0.46
1:D:339:ILE:HG22	1:D:339:ILE:O	2.14	0.46
1:D:726:ARG:CG	1:D:726:ARG:NH1	2.52	0.46
1:F:664:THR:HB	1:F:667:GLY:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:692:SER:OG	1:F:715:LYS:HA	2.15	0.46
1:G:800:THR:HG23	1:G:801:ALA:N	2.31	0.46
1:H:797:LEU:HD23	1:H:797:LEU:HA	1.62	0.46
1:B:461:ASN:OD1	1:B:467:PRO:HB3	2.16	0.46
1:B:630:ALA:O	1:B:633:LYS:NZ	2.48	0.46
1:B:907:PHE:CG	1:B:908:LEU:N	2.82	0.46
1:C:255:ASP:O	1:C:258:ASN:HB2	2.15	0.46
1:D:492:ASP:HB3	1:D:1022:LEU:CD2	2.38	0.46
1:D:765:ARG:HB2	1:D:766:PRO:HD2	1.97	0.46
1:E:273:ARG:HH12	1:E:289:GLU:HG2	1.81	0.46
1:E:569:THR:O	1:E:696:ALA:HA	2.15	0.46
1:E:740:ASN:C	1:E:740:ASN:ND2	2.68	0.46
1:E:705:SER:HB3	1:E:743:LEU:HD13	1.97	0.46
1:G:316:GLN:HE21	1:G:316:GLN:CA	1.97	0.46
1:G:684:LEU:HD13	1:G:888:TRP:HB3	1.97	0.46
1:G:919:THR:O	1:G:919:THR:HG22	2.16	0.46
1:H:516:ALA:HB1	1:H:521:ASP:OD2	2.15	0.46
1:A:466:ASP:HA	1:A:467:PRO:HD2	1.75	0.46
1:B:520:ASN:O	1:B:523:PRO:HG2	2.15	0.46
1:C:558:ASN:N	1:C:559:PRO:CD	2.79	0.46
1:D:344:GLU:C	1:D:346:LYS:N	2.68	0.46
1:E:988:LYS:O	1:E:990:THR:HG23	2.15	0.46
1:F:250:GLN:OE1	1:F:1087:PRO:CG	2.64	0.46
1:F:524:TYR:C	1:F:524:TYR:CD2	2.89	0.46
1:F:551:LEU:CD2	1:F:741:PRO:HG2	2.45	0.46
1:G:280:ASP:OD2	1:G:282:LYS:NZ	2.48	0.46
1:G:453:LEU:HD11	1:G:474:ILE:HG21	1.98	0.46
1:A:356:LEU:O	1:A:357:ARG:C	2.52	0.46
1:B:272:TYR:CD1	1:B:273:ARG:N	2.84	0.46
1:C:1027:GLN:OE1	1:C:1027:GLN:HA	2.16	0.46
1:C:797:LEU:HD23	1:C:797:LEU:HA	1.86	0.46
1:F:525:LEU:O	1:F:528:ASP:HB3	2.16	0.46
1:F:594:LEU:O	1:F:597:ASP:HB2	2.15	0.46
1:F:669:TYR:CG	1:F:874:THR:HG23	2.50	0.46
1:F:725:ASP:OD1	1:F:725:ASP:C	2.54	0.46
1:G:928:LYS:HE3	1:G:928:LYS:HB2	1.70	0.46
1:B:600:LYS:HG3	1:B:607:VAL:HG12	1.98	0.46
1:B:930:ASN:O	1:B:932:TYR:N	2.49	0.46
1:B:430:TYR:HB3	1:B:978:TYR:CE1	2.51	0.46
1:C:360:ILE:O	1:C:364:VAL:HG23	2.16	0.46
1:C:502:LYS:HE2	5:C:165:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:GLN:HG2	1:D:322:THR:N	2.31	0.46
1:D:376:LYS:HB3	1:D:377:PRO:HA	1.98	0.46
1:E:339:ILE:O	1:E:343:ILE:CG1	2.63	0.46
1:E:471:PHE:CD1	1:E:954:ALA:HB2	2.51	0.46
1:F:708:ILE:CD1	1:F:708:ILE:N	2.78	0.46
1:F:769:LEU:HD21	1:F:819:TRP:CZ2	2.51	0.46
1:G:977:LYS:HE2	1:G:977:LYS:HB2	1.59	0.46
1:A:288:THR:OG1	1:A:290:LYS:HB2	2.15	0.45
1:A:604:ASN:ND2	1:A:607:VAL:N	2.64	0.45
4:C:5001:MES:H82	4:C:5001:MES:H51	1.43	0.45
1:C:957:VAL:O	1:C:957:VAL:HG12	2.16	0.45
1:D:873:TYR:O	1:D:874:THR:C	2.54	0.45
1:E:301:PRO:O	1:E:1065:GLN:CG	2.64	0.45
1:G:794:ARG:HH11	1:G:794:ARG:HG2	1.81	0.45
1:H:271:TRP:CE2	1:H:294:PRO:HG3	2.51	0.45
1:H:305:THR:CG2	1:H:306:GLN:N	2.79	0.45
1:A:252:TYR:HA	1:A:275:LYS:CG	2.43	0.45
1:A:576:ALA:HB3	1:A:847:GLN:HB3	1.98	0.45
1:B:1073:LEU:CD1	1:B:1080:LEU:HD21	2.42	0.45
1:B:515:GLU:HG2	1:B:515:GLU:O	2.16	0.45
1:C:297:MET:SD	1:C:340:GLN:HG3	2.55	0.45
1:E:320:HIS:C	1:E:321:GLN:O	2.54	0.45
1:E:346:LYS:HG2	1:E:355:TRP:CZ2	2.51	0.45
1:H:993:VAL:CG1	1:H:1056:ARG:NH1	2.71	0.45
1:H:460:GLY:H	1:H:470:ASN:ND2	2.13	0.45
1:H:870:LYS:NZ	1:H:937:ASP:OD2	2.49	0.45
1:H:988:LYS:H	1:H:990:THR:CG2	2.29	0.45
1:A:407:ASN:ND2	1:A:431:GLU:N	2.64	0.45
1:D:407:ASN:HD22	1:D:431:GLU:N	2.14	0.45
1:D:704:ASN:OD1	1:D:704:ASN:N	2.42	0.45
1:D:871:GLU:CD	1:D:871:GLU:H	2.18	0.45
1:E:743:LEU:O	1:E:744:ARG:NH1	2.47	0.45
1:F:440:ASN:ND2	1:F:449:GLN:HE21	2.06	0.45
1:F:920:ASP:HB3	1:F:923:ASP:HB2	1.98	0.45
1:G:319:ILE:CD1	1:G:338:THR:HG22	2.45	0.45
1:H:871:GLU:H	1:H:871:GLU:CD	2.16	0.45
1:A:294:PRO:O	1:A:297:MET:HB3	2.16	0.45
1:A:651:LYS:O	1:A:652:SER:HB2	2.17	0.45
1:A:900:VAL:HG23	1:A:923:ASP:O	2.16	0.45
1:B:442:ASN:HB3	1:B:445:VAL:HB	1.99	0.45
1:D:317:LEU:HD13	1:D:342:LYS:HB3	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:LEU:HD13	1:D:481:ASN:HD21	1.79	0.45
1:D:850:ALA:O	1:D:853:SER:HB2	2.16	0.45
1:D:930:ASN:O	1:D:931:LYS:C	2.54	0.45
1:F:251:VAL:HG21	1:F:259:PHE:HZ	1.76	0.45
1:F:663:PHE:CZ	1:F:670:MET:HG2	2.52	0.45
1:H:298:THR:C	1:H:300:TRP:CZ3	2.90	0.45
1:H:300:TRP:N	1:H:300:TRP:CE3	2.85	0.45
1:H:408:ARG:HD3	1:H:408:ARG:HA	1.74	0.45
1:A:759:HIS:HD2	1:A:762:GLN:OE1	2.00	0.45
1:B:1014:GLU:CG	1:B:1018:LYS:HE3	2.47	0.45
1:B:1074:VAL:HG11	1:B:1077:ASN:CB	2.39	0.45
1:B:687:ARG:HA	1:B:691:VAL:HG23	1.97	0.45
1:C:317:LEU:HD13	1:C:342:LYS:HB3	1.98	0.45
1:C:376:LYS:HB3	1:C:377:PRO:HA	1.96	0.45
1:E:301:PRO:O	1:E:1065:GLN:HG3	2.16	0.45
1:E:280:ASP:OD1	1:E:348:THR:HG21	2.16	0.45
1:E:347:ILE:HG12	1:E:353:THR:HG23	1.93	0.45
1:E:355:TRP:O	1:E:358:GLN:HB3	2.16	0.45
1:E:356:LEU:HD11	1:E:360:ILE:HD11	1.97	0.45
1:F:308:GLN:HE21	1:F:308:GLN:HB3	1.55	0.45
1:F:610:TYR:O	1:F:908:LEU:HB2	2.16	0.45
1:G:1052:ASN:HD22	1:G:1052:ASN:N	2.03	0.45
1:G:776:LYS:HD2	5:G:80:HOH:O	2.16	0.45
1:A:279:LYS:HB3	1:A:279:LYS:HE2	1.78	0.45
1:A:273:ARG:NH2	1:A:288:THR:C	2.57	0.45
1:C:407:ASN:HD21	1:C:431:GLU:H	1.64	0.45
1:E:513:ILE:CG1	1:E:953:MET:HE1	2.45	0.45
1:C:740:ASN:C	1:C:740:ASN:ND2	2.69	0.45
1:E:308:GLN:HE21	1:E:308:GLN:HB3	1.54	0.45
1:F:1041:LYS:HD2	1:F:1041:LYS:HA	1.69	0.45
1:F:1070:TYR:HD2	5:F:242:HOH:O	1.89	0.45
1:F:656:ARG:HD2	1:F:858:GLU:HB2	1.98	0.45
1:F:681:GLU:HG2	1:F:685:LYS:HD2	1.99	0.45
1:G:245:PHE:O	1:G:246:ALA:C	2.55	0.45
1:H:315:ALA:O	1:H:318:GLY:CA	2.65	0.45
1:H:928:LYS:HE3	1:H:928:LYS:HB2	1.75	0.45
1:B:689:LYS:HG2	1:B:690:TYR:CD1	2.51	0.45
1:C:389:TYR:CE1	1:C:1050:GLY:HA2	2.51	0.45
1:D:642:LEU:HD12	1:D:642:LEU:N	2.32	0.45
1:D:924:LEU:CD1	1:D:924:LEU:N	2.80	0.45
1:E:281:GLY:H	1:E:344:GLU:HB2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:457:MET:CE	1:G:494:LEU:HD23	2.46	0.45
1:G:912:ILE:HA	1:G:912:ILE:HD12	1.51	0.45
1:H:513:ILE:CD1	1:H:953:MET:HE1	2.47	0.45
1:A:800:THR:CG2	1:A:802:ALA:H	2.15	0.45
1:B:442:ASN:HB3	1:B:445:VAL:CG2	2.46	0.45
1:D:800:THR:HG23	1:D:801:ALA:N	2.32	0.45
1:D:841:ASP:OD1	1:D:846:HIS:CE1	2.63	0.45
1:F:769:LEU:HD12	1:F:778:TYR:HE2	1.82	0.45
1:F:895:MET:HE2	1:F:895:MET:HB3	1.74	0.45
1:H:299:TRP:HA	1:H:300:TRP:CE3	2.52	0.45
1:H:310:VAL:HG12	1:H:311:ASN:N	2.31	0.45
1:H:394:LYS:CD	1:H:394:LYS:N	2.55	0.45
1:A:332:LEU:HA	1:A:332:LEU:HD23	1.67	0.45
1:A:376:LYS:HE2	1:A:378:PHE:CZ	2.52	0.45
1:D:280:ASP:O	1:D:281:GLY:C	2.54	0.45
1:E:1085:VAL:CG2	1:E:1086:ASN:N	2.31	0.45
1:E:271:TRP:NE1	1:E:294:PRO:HB3	2.32	0.45
1:F:278:LEU:HB3	1:F:344:GLU:HG3	1.99	0.45
1:F:791:THR:CG2	1:F:795:GLY:CA	2.87	0.45
1:G:310:VAL:CG1	1:G:335:ALA:HB1	2.47	0.45
1:G:792:ASN:ND2	1:G:796:GLU:HB2	2.32	0.45
1:A:383:GLN:O	1:A:384:LYS:HB2	2.18	0.44
1:B:1074:VAL:HG13	1:B:1077:ASN:H	1.82	0.44
1:B:434:LEU:HD23	1:B:434:LEU:HA	1.79	0.44
1:B:603:ILE:HD11	1:B:619:LYS:HG3	1.99	0.44
1:C:312:TYR:CD2	1:C:312:TYR:C	2.90	0.44
1:E:460:GLY:N	1:E:470:ASN:ND2	2.65	0.44
1:F:1025:ARG:HG2	1:F:1027:GLN:NE2	2.32	0.44
1:F:467:PRO:HA	1:F:470:ASN:ND2	2.32	0.44
1:F:604:ASN:C	1:F:606:ASN:H	2.21	0.44
1:F:722:ASP:O	1:F:757:ALA:HB3	2.17	0.44
1:F:964:LEU:O	1:F:995:ASP:HB3	2.17	0.44
1:G:599:ILE:O	1:G:600:LYS:C	2.56	0.44
1:H:364:VAL:HG12	1:H:370:TRP:HB3	1.98	0.44
1:H:851:LEU:HD12	1:H:851:LEU:HA	1.87	0.44
1:B:406:LEU:CD2	1:B:431:GLU:HG2	2.47	0.44
1:B:549:LYS:HB3	1:B:550:PRO:HD2	1.99	0.44
1:E:319:ILE:HD11	1:E:342:LYS:CD	2.47	0.44
1:E:988:LYS:HB2	1:E:988:LYS:HE2	1.78	0.44
1:F:697:MET:HA	1:F:709:THR:O	2.16	0.44
1:F:868:THR:HB	1:F:872:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:492:ASP:CB	1:G:1022:LEU:HD22	2.33	0.44
1:H:745:LEU:N	1:H:745:LEU:HD12	2.33	0.44
1:H:861:SER:HB3	1:H:864:GLN:HG3	1.99	0.44
1:A:860:PHE:CG	1:A:896:ALA:HB2	2.51	0.44
4:D:5001:MES:H52	4:D:5001:MES:H82	1.18	0.44
1:D:578:VAL:CG1	1:D:579:PRO:HD2	2.48	0.44
1:E:347:ILE:HG12	1:E:352:ASN:O	2.17	0.44
1:F:458:ASN:C	1:F:470:ASN:OD1	2.55	0.44
1:F:514:LEU:CD2	1:F:532:MET:HG3	2.47	0.44
1:G:244:SER:N	1:G:246:ALA:H	2.16	0.44
1:H:303:GLN:O	1:H:307:ARG:N	2.50	0.44
1:B:746:LYS:HB2	1:B:749:ASP:CG	2.38	0.44
1:C:471:PHE:CG	1:C:954:ALA:HB2	2.52	0.44
1:D:809:ASN:HB2	1:D:810:PRO:HD2	1.99	0.44
1:D:530:ASP:HB2	1:D:843:LYS:HB3	1.98	0.44
1:E:271:TRP:CE2	1:E:357:ARG:CZ	3.01	0.44
1:E:335:ALA:O	1:E:339:ILE:CG1	2.65	0.44
1:F:466:ASP:C	1:F:468:ASP:H	2.21	0.44
1:F:558:ASN:N	1:F:559:PRO:CD	2.81	0.44
1:F:740:ASN:HD22	1:F:742:SER:N	2.08	0.44
1:G:389:TYR:CE1	1:G:1050:GLY:HA2	2.52	0.44
1:H:478:ALA:HB1	1:H:481:ASN:HD22	1.81	0.44
1:H:856:MET:HG3	1:H:892:ASP:HB2	1.99	0.44
1:A:1001:LYS:HE2	1:A:1001:LYS:HB2	1.69	0.44
1:A:303:GLN:OE1	1:A:329:PRO:HG3	2.17	0.44
1:A:988:LYS:N	1:A:990:THR:HG23	2.31	0.44
1:E:303:GLN:OE1	1:E:332:LEU:HD13	2.16	0.44
1:E:356:LEU:O	1:E:360:ILE:HG12	2.18	0.44
1:F:752:VAL:CG1	1:F:752:VAL:O	2.65	0.44
1:F:797:LEU:HD23	1:F:797:LEU:HA	1.74	0.44
1:G:740:ASN:HD22	1:G:741:PRO:CD	2.30	0.44
1:B:599:ILE:HA	1:B:603:ILE:HB	1.99	0.44
1:E:280:ASP:C	1:E:282:LYS:H	2.21	0.44
1:E:579:PRO:HA	1:E:847:GLN:OE1	2.18	0.44
1:F:351:LYS:HE3	1:F:351:LYS:HB3	1.33	0.44
1:F:780:SER:OG	1:F:782:GLN:HB3	2.18	0.44
1:G:613:THR:OG1	1:G:616:GLU:HG3	2.17	0.44
1:A:300:TRP:CD2	1:A:300:TRP:N	2.85	0.44
1:B:721:THR:O	1:B:757:ALA:HB2	2.18	0.44
1:C:244:SER:C	1:C:246:ALA:H	2.21	0.44
1:C:333:ASN:O	1:C:337:GLN:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:ILE:N	1:D:285:THR:O	2.49	0.44
1:E:340:GLN:HA	1:E:343:ILE:HD12	1.99	0.44
1:F:658:TYR:CE2	1:F:660:GLY:CA	2.98	0.44
1:H:250:GLN:HB3	1:H:1087:PRO:HG3	1.99	0.44
1:H:558:ASN:N	1:H:559:PRO:CD	2.81	0.44
1:H:809:ASN:HB2	1:H:810:PRO:HD2	1.98	0.44
1:A:268:ALA:HA	1:A:1062:LEU:HD11	2.00	0.44
1:A:1083:SER:O	1:A:1087:PRO:HG3	2.18	0.44
1:B:272:TYR:HD1	1:B:273:ARG:N	2.16	0.44
1:B:751:VAL:HB	1:B:799:PHE:HB2	1.99	0.44
1:C:759:HIS:CD2	1:C:762:GLN:OE1	2.71	0.44
1:C:974:ARG:O	1:C:981:PRO:HA	2.18	0.44
1:D:277:ILE:CD1	1:D:291:ASP:CB	2.57	0.44
1:D:356:LEU:CD1	1:D:360:ILE:HG12	2.47	0.44
1:D:782:GLN:NE2	1:D:782:GLN:CA	2.81	0.44
1:D:988:LYS:O	1:D:988:LYS:HG3	2.16	0.44
1:E:271:TRP:CH2	1:E:357:ARG:NE	2.86	0.44
1:G:461:ASN:OD1	1:G:467:PRO:HA	2.18	0.44
1:G:841:ASP:OD1	1:G:846:HIS:HE1	2.01	0.44
1:H:305:THR:C	1:H:307:ARG:N	2.71	0.44
1:H:759:HIS:CD2	1:H:764:TYR:OH	2.71	0.44
1:B:737:GLU:HA	1:B:815:TYR:O	2.18	0.44
1:C:453:LEU:CD1	1:C:474:ILE:HG21	2.48	0.44
1:D:1081:PRO:O	1:D:1082:LYS:C	2.55	0.44
1:D:524:TYR:CD2	1:D:524:TYR:C	2.91	0.44
1:D:797:LEU:HA	1:D:797:LEU:HD23	1.84	0.44
1:D:948:LYS:HA	1:D:948:LYS:HD3	1.75	0.44
1:E:250:GLN:NE2	1:E:275:LYS:HE2	2.32	0.44
1:E:347:ILE:HD13	1:E:353:THR:HG21	1.94	0.44
1:F:279:LYS:O	1:F:280:ASP:CB	2.66	0.44
1:F:388:LEU:HD12	1:F:1049:ASN:O	2.18	0.44
1:F:547:LEU:O	1:F:639:ASN:HB2	2.17	0.44
1:G:759:HIS:CD2	1:G:764:TYR:OH	2.71	0.44
1:H:988:LYS:N	1:H:990:THR:CG2	2.81	0.44
1:A:300:TRP:CB	1:A:306:GLN:HB2	2.48	0.43
1:A:309:TYR:CD2	1:A:309:TYR:C	2.91	0.43
1:A:797:LEU:HA	1:A:797:LEU:HD23	1.74	0.43
1:A:800:THR:HG23	1:A:801:ALA:N	2.32	0.43
1:B:614:MET:CE	1:B:618:LYS:HD2	2.48	0.43
1:B:689:LYS:CG	1:B:690:TYR:CE1	3.01	0.43
1:B:760:LYS:O	1:B:761:ASN:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:670:MET:HE1	1:C:885:PHE:CZ	2.48	0.43
1:D:310:VAL:HG13	1:D:339:ILE:HD11	2.00	0.43
1:D:413:GLN:O	1:D:413:GLN:HG2	2.17	0.43
1:F:492:ASP:HB3	1:F:1022:LEU:HD21	1.95	0.43
1:F:740:ASN:HA	1:F:741:PRO:HD3	1.91	0.43
1:H:260:GLU:OE2	1:H:357:ARG:NH2	2.37	0.43
1:H:460:GLY:N	1:H:470:ASN:ND2	2.66	0.43
1:B:249:ASN:O	1:B:1084:LEU:HD22	2.18	0.43
1:B:253:SER:C	1:B:255:ASP:H	2.20	0.43
1:C:475:ARG:CA	1:C:953:MET:HE3	2.48	0.43
1:C:530:ASP:HB2	1:C:843:LYS:HB3	2.00	0.43
1:D:310:VAL:HG22	1:D:339:ILE:HD12	1.97	0.43
1:D:440:ASN:ND2	1:D:449:GLN:HE21	2.07	0.43
1:D:782:GLN:HE21	1:D:782:GLN:CA	2.19	0.43
1:E:283:THR:HG22	1:E:284:TRP:O	2.18	0.43
1:F:270:SER:HB2	1:F:295:LEU:HD12	1.99	0.43
1:F:708:ILE:HD13	1:F:708:ILE:N	2.16	0.43
1:F:745:LEU:CD1	1:F:745:LEU:H	2.18	0.43
1:H:310:VAL:O	1:H:311:ASN:C	2.56	0.43
1:B:433:LEU:HG	1:B:434:LEU:HG	2.00	0.43
1:E:287:SER:HB3	1:E:291:ASP:HB2	1.99	0.43
1:E:965:PRO:HD2	1:E:998:SER:HA	1.99	0.43
1:F:389:TYR:CE1	1:F:1050:GLY:HA2	2.53	0.43
1:F:469:ALA:HA	1:F:942:ILE:HG22	2.00	0.43
1:F:740:ASN:HD22	1:F:741:PRO:CD	2.30	0.43
1:F:948:LYS:HD3	1:F:948:LYS:HA	1.68	0.43
1:G:449:GLN:HA	1:G:449:GLN:OE1	2.18	0.43
1:H:301:PRO:O	1:H:302:ASP:HB3	2.18	0.43
1:B:380:ASP:C	1:B:380:ASP:OD1	2.56	0.43
1:B:453:LEU:CD1	1:B:474:ILE:HG21	2.48	0.43
1:C:809:ASN:HB2	1:C:810:PRO:CD	2.48	0.43
1:D:435:ALA:HA	1:D:1052:ASN:ND2	2.33	0.43
1:E:350:GLU:O	1:E:352:ASN:N	2.52	0.43
1:F:492:ASP:OD2	1:F:1025:ARG:HD2	2.19	0.43
1:F:712:ARG:NH1	1:F:712:ARG:HG3	2.32	0.43
1:F:669:TYR:CE1	1:F:874:THR:HG23	2.53	0.43
1:F:969:VAL:HG22	1:F:993:VAL:HG22	1.99	0.43
1:H:988:LYS:N	1:H:990:THR:HG23	2.33	0.43
1:A:278:LEU:CD2	1:A:281:GLY:HA2	2.49	0.43
1:B:631:THR:CG2	1:B:809:ASN:HA	2.41	0.43
1:D:1071:PHE:CE1	1:D:1081:PRO:HD3	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1085:VAL:O	1:E:1087:PRO:HD3	2.18	0.43
1:A:894:GLU:HA	1:A:953:MET:HB3	2.00	0.43
1:B:530:ASP:OD2	1:B:579:PRO:HD3	2.17	0.43
1:B:765:ARG:HB2	1:B:766:PRO:HD2	2.01	0.43
1:B:908:LEU:HD12	1:B:908:LEU:O	2.18	0.43
1:C:475:ARG:CB	1:C:953:MET:HE3	2.45	0.43
1:C:917:ALA:HB1	1:C:962:TYR:CG	2.54	0.43
1:C:883:ASP:OD1	1:C:948:LYS:HE3	2.18	0.43
1:C:987:ILE:CG1	1:C:1058:ALA:HB2	2.48	0.43
1:D:281:GLY:HA2	1:D:341:THR:HG23	1.93	0.43
1:D:340:GLN:O	1:D:343:ILE:HB	2.19	0.43
1:D:820:VAL:HB	1:D:821:PRO:HD2	2.01	0.43
1:E:1067:THR:OG1	1:E:1069:THR:HB	2.18	0.43
1:G:371:ASN:HB3	1:G:373:ASP:N	2.25	0.43
1:H:677:TYR:C	1:H:677:TYR:CD2	2.92	0.43
1:A:346:LYS:HE2	1:A:355:TRP:CD2	2.53	0.43
1:A:687:ARG:HA	1:A:691:VAL:CG2	2.48	0.43
1:A:974:ARG:HG2	1:A:987:ILE:HB	1.99	0.43
1:C:733:VAL:HG22	1:C:734:VAL:N	2.33	0.43
1:C:908:LEU:O	1:C:912:ILE:HG13	2.19	0.43
1:C:951:LYS:HA	1:C:951:LYS:HD3	1.53	0.43
1:E:272:TYR:HE1	1:E:274:PRO:CA	2.32	0.43
1:E:604:ASN:C	1:E:604:ASN:OD1	2.56	0.43
1:F:364:VAL:HG13	1:F:370:TRP:CE3	2.53	0.43
1:G:356:LEU:O	1:G:357:ARG:C	2.56	0.43
1:G:594:LEU:O	1:G:598:ILE:HG13	2.19	0.43
1:B:272:TYR:CE1	1:B:274:PRO:CD	3.01	0.43
1:B:502:LYS:C	1:B:503:ASN:HD22	2.22	0.43
1:B:535:MET:CE	1:B:583:PHE:CZ	3.02	0.43
1:B:726:ARG:NE	1:B:726:ARG:H	2.17	0.43
1:E:261:HIS:CD2	1:E:264:HIS:N	2.79	0.43
1:F:854:ARG:NH1	1:F:892:ASP:OD2	2.48	0.43
1:H:1073:LEU:HD21	1:H:1080:LEU:HD21	2.00	0.43
1:H:444:VAL:CG1	1:H:1038:VAL:HG22	2.48	0.43
1:A:267:THR:HB	1:A:1060:TYR:CE2	2.54	0.43
1:A:663:PHE:CZ	1:A:670:MET:HG2	2.54	0.43
1:A:689:LYS:HG2	1:A:690:TYR:CD1	2.54	0.43
1:B:391:ASN:OD1	1:B:404:ARG:HD2	2.18	0.43
1:B:389:TYR:CE1	1:B:970:VAL:HG21	2.54	0.43
1:E:244:SER:C	1:E:246:ALA:H	2.20	0.43
1:E:337:GLN:O	1:E:338:THR:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:861:SER:N	1:F:864:GLN:NE2	2.52	0.43
1:G:585:ARG:HD3	1:G:661:ASP:OD1	2.19	0.43
1:H:288:THR:H	1:H:291:ASP:CG	2.21	0.43
1:H:303:GLN:HE21	1:H:303:GLN:HB3	1.23	0.43
1:H:316:GLN:HE21	1:H:316:GLN:CA	1.97	0.43
1:B:261:HIS:CD2	1:B:264:HIS:HD2	2.37	0.43
1:B:475:ARG:HD3	1:B:955:ASP:OD1	2.19	0.43
1:B:577:ALA:C	1:B:578:VAL:HG23	2.39	0.43
1:C:1002:ASP:OD1	1:C:1002:ASP:N	2.33	0.43
1:C:464:ALA:O	1:C:465:ASN:HB2	2.19	0.43
1:D:320:HIS:N	1:D:320:HIS:ND1	2.63	0.43
1:D:350:GLU:O	1:D:352:ASN:N	2.52	0.43
1:H:300:TRP:CD2	1:H:306:GLN:HG2	2.51	0.43
1:H:551:LEU:HD12	1:H:551:LEU:O	2.19	0.43
1:H:604:ASN:OD1	1:H:604:ASN:C	2.57	0.43
1:H:658:TYR:CE2	1:H:660:GLY:HA3	2.54	0.43
1:A:321:GLN:OE1	1:A:321:GLN:CA	2.66	0.42
1:A:524:TYR:CD2	1:A:524:TYR:C	2.92	0.42
1:A:718:LEU:HA	1:A:718:LEU:HD23	1.79	0.42
1:A:759:HIS:CD2	1:A:764:TYR:OH	2.72	0.42
1:B:689:LYS:CD	1:B:690:TYR:CE1	3.02	0.42
1:E:1086:ASN:HA	1:E:1087:PRO:HD3	1.71	0.42
1:E:322:THR:HG23	1:E:323:TYR:N	2.35	0.42
1:F:1063:LYS:HE3	1:F:1068:ASN:CG	2.39	0.42
1:F:1067:THR:O	1:F:1067:THR:CG2	2.67	0.42
1:B:416:LYS:CE	1:F:551:LEU:HD11	2.37	0.42
1:F:794:ARG:HG2	1:F:794:ARG:HH11	1.76	0.42
1:F:884:LYS:HE2	1:F:887:GLU:OE1	2.19	0.42
1:F:976:ASP:C	1:F:976:ASP:OD1	2.57	0.42
1:G:307:ARG:CZ	1:G:325:THR:HG22	2.48	0.42
1:G:588:ASP:OD1	1:G:588:ASP:N	2.39	0.42
1:G:513:ILE:CG1	1:G:953:MET:CE	2.88	0.42
1:H:278:LEU:HD13	1:H:283:THR:N	2.35	0.42
1:H:744:ARG:HA	1:H:744:ARG:HD3	1.86	0.42
1:A:371:ASN:OD1	1:A:373:ASP:HB2	2.19	0.42
1:C:389:TYR:CZ	1:C:1050:GLY:HA2	2.54	0.42
1:C:988:LYS:O	1:C:989:ASN:HB2	2.19	0.42
1:D:259:PHE:CD2	1:D:259:PHE:N	2.87	0.42
1:F:599:ILE:HG22	1:F:600:LYS:N	2.35	0.42
1:G:1065:GLN:HG3	1:G:1066:ALA:N	2.34	0.42
1:G:430:TYR:CZ	1:G:977:LYS:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:TYR:HA	1:A:654:VAL:O	2.18	0.42
1:B:657:VAL:HG12	1:B:658:TYR:N	2.33	0.42
1:B:711:VAL:HG22	1:B:734:VAL:HG23	2.01	0.42
1:C:250:GLN:OE1	1:C:1087:PRO:CG	2.67	0.42
1:E:273:ARG:HA	1:E:274:PRO:HD3	1.70	0.42
1:E:312:TYR:O	1:E:315:ALA:HB3	2.18	0.42
1:E:460:GLY:N	1:E:470:ASN:HD22	2.15	0.42
1:F:1073:LEU:HD21	1:F:1080:LEU:HD21	2.01	0.42
1:F:323:TYR:CD1	1:F:327:THR:HG21	2.55	0.42
1:F:358:GLN:HG2	1:F:358:GLN:O	2.18	0.42
1:F:912:ILE:HD12	1:F:912:ILE:HA	1.80	0.42
1:F:874:THR:HB	1:F:932:TYR:HB3	2.00	0.42
1:F:935:ALA:O	1:F:938:LEU:HB3	2.18	0.42
1:G:281:GLY:H	1:G:344:GLU:CB	2.30	0.42
1:H:262:VAL:O	1:H:263:ASP:C	2.55	0.42
1:H:919:THR:HG22	1:H:919:THR:O	2.19	0.42
1:A:610:TYR:O	1:A:612:PHE:N	2.52	0.42
1:A:703:GLY:HA3	1:A:744:ARG:O	2.19	0.42
1:B:389:TYR:CZ	1:B:1050:GLY:HA2	2.55	0.42
1:B:673:LYS:HE2	1:B:677:TYR:CD2	2.50	0.42
1:B:740:ASN:HA	1:B:741:PRO:HD2	1.74	0.42
1:D:346:LYS:CG	1:D:346:LYS:O	2.67	0.42
1:E:360:ILE:O	1:E:363:PHE:N	2.53	0.42
1:F:418:ASP:OD2	1:F:420:ARG:NH2	2.43	0.42
1:G:293:ARG:CG	1:G:297:MET:HE1	2.49	0.42
1:H:273:ARG:NE	1:H:288:THR:O	2.52	0.42
1:H:365:LYS:HD3	1:H:365:LYS:HA	1.96	0.42
1:A:391:ASN:OD1	1:A:404:ARG:HD2	2.20	0.42
1:B:368:SER:HA	1:B:371:ASN:CB	2.49	0.42
1:C:578:VAL:CG1	1:C:579:PRO:HD2	2.50	0.42
1:D:430:TYR:O	1:D:481:ASN:HA	2.20	0.42
1:F:293:ARG:HB3	1:F:294:PRO:CD	2.49	0.42
1:F:903:THR:HG22	1:F:913:GLN:NE2	2.35	0.42
1:G:522:THR:N	1:G:523:PRO:HD2	2.35	0.42
1:G:920:ASP:OD2	1:G:923:ASP:HB2	2.20	0.42
1:H:460:GLY:N	1:H:470:ASN:HD22	2.14	0.42
1:A:793:ASP:OD2	1:G:746:LYS:HE3	2.18	0.42
1:B:1023:PHE:HB3	1:G:747:ALA:HB3	2.01	0.42
1:B:417:LYS:CE	1:F:555:SER:HB3	2.49	0.42
1:C:705:SER:HB3	1:C:743:LEU:HD13	2.02	0.42
1:D:278:LEU:HG	1:D:281:GLY:CA	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:ASN:N	1:D:559:PRO:CD	2.83	0.42
1:D:697:MET:HA	1:D:709:THR:O	2.20	0.42
1:D:718:LEU:HD23	1:D:718:LEU:HA	1.90	0.42
1:E:440:ASN:HD21	1:E:449:GLN:NE2	1.89	0.42
1:F:681:GLU:OE2	1:F:884:LYS:NZ	2.43	0.42
1:F:702:VAL:O	1:F:703:GLY:C	2.57	0.42
1:G:792:ASN:OD1	1:G:794:ARG:N	2.48	0.42
1:G:851:LEU:HD12	1:G:851:LEU:HA	1.90	0.42
1:H:290:LYS:O	1:H:292:PHE:N	2.46	0.42
1:H:466:ASP:OD2	1:H:943:LYS:HE2	2.14	0.42
1:H:991:LEU:HG	1:H:1070:TYR:CE2	2.54	0.42
1:A:281:GLY:N	1:A:344:GLU:HB2	2.34	0.42
1:B:740:ASN:HD22	1:B:741:PRO:CD	2.32	0.42
1:C:1052:ASN:N	1:C:1052:ASN:ND2	2.58	0.42
1:C:589:SER:O	1:C:590:GLU:HB2	2.19	0.42
1:C:610:TYR:HA	1:C:612:PHE:CE2	2.54	0.42
1:D:993:VAL:O	1:D:1056:ARG:NH1	2.53	0.42
1:D:408:ARG:HA	1:D:408:ARG:HD3	1.68	0.42
1:D:561:ILE:HG12	1:D:697:MET:HB3	2.02	0.42
1:E:277:ILE:HD12	1:E:291:ASP:CG	2.39	0.42
1:F:603:ILE:HG22	1:F:604:ASN:N	2.34	0.42
1:F:711:VAL:HG22	1:F:734:VAL:CG2	2.48	0.42
1:F:951:LYS:HA	1:F:951:LYS:HD3	1.79	0.42
1:G:794:ARG:NH1	1:G:794:ARG:HG2	2.34	0.42
1:H:800:THR:HG23	1:H:801:ALA:N	2.34	0.42
1:C:464:ALA:O	1:C:465:ASN:CB	2.67	0.42
1:D:1022:LEU:HD23	1:D:1022:LEU:N	2.35	0.42
1:E:670:MET:HE3	1:E:877:VAL:CG1	2.49	0.42
1:F:300:TRP:CD2	1:F:306:GLN:HG3	2.54	0.42
1:G:293:ARG:CB	1:G:297:MET:HE1	2.50	0.42
1:G:630:ALA:O	1:G:633:LYS:NZ	2.51	0.42
1:A:300:TRP:HB3	1:A:301:PRO:HD2	2.02	0.42
1:B:466:ASP:HA	1:B:467:PRO:HD3	1.75	0.42
1:B:551:LEU:HD22	1:B:741:PRO:HG3	2.02	0.42
1:B:733:VAL:HG22	1:B:734:VAL:N	2.35	0.42
1:B:797:LEU:HA	1:B:797:LEU:HD23	1.52	0.42
1:B:870:LYS:HB3	1:B:871:GLU:OE1	2.20	0.42
1:B:513:ILE:CG2	1:B:953:MET:HE1	2.40	0.42
1:C:288:THR:C	1:C:290:LYS:N	2.73	0.42
1:D:383:GLN:O	1:D:384:LYS:HB2	2.19	0.42
1:E:951:LYS:HA	1:E:951:LYS:HD3	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:684:LEU:HD23	1:F:684:LEU:HA	1.88	0.42
1:G:403:TYR:CE2	1:G:443:PRO:HD2	2.55	0.42
1:H:394:LYS:CD	1:H:394:LYS:H	2.21	0.42
1:H:442:ASN:OD1	1:H:442:ASN:C	2.57	0.42
1:H:794:ARG:NH1	1:H:794:ARG:HG2	2.34	0.42
1:C:492:ASP:HB3	1:C:1022:LEU:HD23	2.02	0.42
1:C:924:LEU:HD12	1:C:924:LEU:N	2.35	0.42
1:D:409:THR:O	1:D:410:PRO:C	2.58	0.42
1:D:449:GLN:HA	1:D:449:GLN:OE1	2.19	0.42
1:E:681:GLU:OE2	1:E:884:LYS:NZ	2.53	0.42
1:E:740:ASN:HD22	1:E:741:PRO:N	2.18	0.42
1:F:312:TYR:C	1:F:312:TYR:CD2	2.93	0.42
1:F:344:GLU:HA	1:F:344:GLU:OE1	2.19	0.42
1:F:432:PHE:HB2	1:F:977:LYS:HA	2.00	0.42
1:F:571:ASP:OD1	1:F:571:ASP:C	2.58	0.42
1:G:740:ASN:ND2	1:G:741:PRO:HD2	2.35	0.42
1:G:760:LYS:HG2	1:G:793:ASP:O	2.20	0.42
1:H:293:ARG:HB3	1:H:294:PRO:CD	2.50	0.42
1:H:305:THR:O	1:H:307:ARG:N	2.53	0.42
1:H:734:VAL:HB	1:H:755:MET:CE	2.50	0.42
1:B:617:ILE:CG2	1:B:617:ILE:O	2.66	0.41
1:B:561:ILE:HG12	1:B:697:MET:HB3	2.01	0.41
1:D:308:GLN:HE21	1:D:308:GLN:HB3	1.46	0.41
1:D:782:GLN:HA	1:D:782:GLN:NE2	2.29	0.41
1:E:271:TRP:CD1	1:E:294:PRO:HA	2.55	0.41
1:E:729:ARG:NH2	1:E:762:GLN:HB2	2.35	0.41
1:E:576:ALA:HB3	1:E:847:GLN:HB3	2.01	0.41
1:F:448:GLU:OE1	1:F:448:GLU:HA	2.20	0.41
1:F:610:TYR:HA	1:F:612:PHE:CE2	2.55	0.41
1:F:988:LYS:O	1:F:990:THR:HG22	2.19	0.41
1:G:407:ASN:ND2	1:G:431:GLU:N	2.67	0.41
1:G:649:THR:O	1:G:712:ARG:HD3	2.20	0.41
1:H:964:LEU:HD12	1:H:996:GLY:HA2	2.02	0.41
1:A:407:ASN:HD21	1:A:431:GLU:H	1.67	0.41
1:A:930:ASN:O	1:A:931:LYS:C	2.57	0.41
1:B:529:GLY:O	1:B:530:ASP:C	2.57	0.41
1:B:702:VAL:O	1:B:703:GLY:C	2.58	0.41
1:B:759:HIS:N	1:B:759:HIS:ND1	2.68	0.41
1:C:371:ASN:O	1:C:1057:GLY:HA2	2.21	0.41
1:D:311:ASN:ND2	1:D:323:TYR:H	2.09	0.41
1:D:725:ASP:OD1	1:D:725:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:GLU:HA	1:E:344:GLU:OE1	2.19	0.41
4:F:5001:MES:H52	4:F:5001:MES:H82	1.15	0.41
1:F:664:THR:HG22	1:F:666:ASP:OD1	2.20	0.41
1:F:930:ASN:OD1	1:F:932:TYR:N	2.46	0.41
1:F:934:THR:O	1:F:935:ALA:C	2.59	0.41
1:G:1014:GLU:HG3	1:G:1018:LYS:HE3	2.01	0.41
1:H:296:LEU:HA	1:H:296:LEU:HD23	1.78	0.41
1:H:302:ASP:OD1	1:H:305:THR:HG22	2.20	0.41
4:A:5001:MES:H81	4:A:5001:MES:H51	1.34	0.41
1:B:660:GLY:HA2	1:B:663:PHE:O	2.19	0.41
1:D:314:ASN:O	1:D:319:ILE:N	2.53	0.41
1:E:271:TRP:CZ2	1:E:357:ARG:NE	2.87	0.41
1:E:272:TYR:CE1	1:E:274:PRO:CB	3.00	0.41
1:E:571:ASP:OD1	1:E:571:ASP:C	2.58	0.41
1:E:809:ASN:CB	1:E:810:PRO:CD	2.98	0.41
1:F:372:SER:O	1:F:373:ASP:C	2.58	0.41
1:F:458:ASN:CA	1:F:470:ASN:OD1	2.68	0.41
1:F:799:PHE:CD2	1:F:799:PHE:N	2.88	0.41
1:G:466:ASP:HA	1:G:467:PRO:HD2	1.87	0.41
1:G:759:HIS:CD2	1:G:762:GLN:OE1	2.71	0.41
1:H:1074:VAL:CG2	1:H:1077:ASN:HB2	2.49	0.41
1:A:324:ASN:C	1:A:324:ASN:OD1	2.58	0.41
1:A:685:LYS:NZ	1:A:887:GLU:OE2	2.41	0.41
1:B:530:ASP:OD2	1:B:579:PRO:CD	2.68	0.41
1:B:965:PRO:HD2	1:B:997:LYS:O	2.21	0.41
1:D:1063:LYS:CE	1:D:1068:ASN:ND2	2.83	0.41
1:D:389:TYR:CZ	1:D:1050:GLY:HA2	2.55	0.41
1:E:894:GLU:HA	1:E:953:MET:HB3	2.01	0.41
1:F:571:ASP:OD1	1:F:651:LYS:NZ	2.53	0.41
1:F:669:TYR:CD2	1:F:874:THR:HG23	2.55	0.41
1:F:768:LEU:HD22	1:F:775:ILE:CG2	2.50	0.41
1:F:504:ASP:HB3	1:F:834:ALA:HB1	2.02	0.41
1:F:917:ALA:CB	1:F:962:TYR:CD1	3.03	0.41
1:F:977:LYS:H	1:F:977:LYS:HG3	1.47	0.41
1:G:370:TRP:CD1	1:G:1060:TYR:HA	2.55	0.41
1:H:425:ARG:HD3	1:H:425:ARG:HH11	1.72	0.41
1:A:375:GLU:OE2	1:A:992:TYR:OH	2.24	0.41
1:A:689:LYS:HD3	1:A:828:GLN:HB3	2.02	0.41
1:B:460:GLY:C	1:B:466:ASP:O	2.59	0.41
1:C:988:LYS:N	1:C:990:THR:HG23	2.35	0.41
1:D:997:LYS:HA	1:D:1043:TRP:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:854:ARG:HB3	1:D:891:THR:OG1	2.20	0.41
1:E:267:THR:HB	1:E:1060:TYR:CE2	2.55	0.41
1:E:526:HIS:HA	1:E:530:ASP:OD1	2.20	0.41
1:F:251:VAL:HG23	1:F:272:TYR:HD1	1.86	0.41
1:F:346:LYS:HD3	1:F:355:TRP:CH2	2.56	0.41
1:G:884:LYS:HD3	1:G:884:LYS:HA	1.74	0.41
1:H:311:ASN:O	1:H:314:ASN:HB2	2.21	0.41
1:H:970:VAL:O	1:H:991:LEU:HA	2.20	0.41
1:A:266:LEU:HD13	1:A:295:LEU:HD11	2.02	0.41
1:A:912:ILE:H	1:A:912:ILE:HG13	1.51	0.41
1:B:1003:GLN:O	1:B:1004:GLN:C	2.57	0.41
1:B:404:ARG:NH2	1:B:1045:ALA:O	2.54	0.41
1:B:894:GLU:HA	1:B:953:MET:HB3	2.01	0.41
1:C:897:PRO:HG3	1:C:916:TYR:CE2	2.55	0.41
1:D:312:TYR:O	1:D:316:GLN:HG2	2.21	0.41
1:G:884:LYS:HD2	1:G:888:TRP:CZ2	2.56	0.41
1:H:1084:LEU:HA	1:H:1084:LEU:HD23	1.56	0.41
1:H:305:THR:CG2	1:H:306:GLN:H	2.34	0.41
1:H:355:TRP:O	1:H:356:LEU:C	2.59	0.41
1:B:251:VAL:O	1:B:251:VAL:CG1	2.68	0.41
1:B:513:ILE:HB	1:B:581:TYR:CE2	2.55	0.41
1:B:769:LEU:HD21	1:B:819:TRP:CZ2	2.56	0.41
1:B:987:ILE:CG1	1:B:1058:ALA:HB2	2.51	0.41
1:C:524:TYR:CD2	1:C:524:TYR:C	2.94	0.41
1:C:677:TYR:CD2	1:C:677:TYR:C	2.94	0.41
1:D:883:ASP:OD1	1:D:948:LYS:HE3	2.21	0.41
1:E:513:ILE:CD1	1:E:953:MET:CE	2.98	0.41
1:F:945:LEU:HD13	1:F:952:VAL:HG22	2.02	0.41
1:G:1073:LEU:HD21	1:G:1080:LEU:HD21	2.03	0.41
1:H:589:SER:O	1:H:590:GLU:HB2	2.21	0.41
1:A:921:ARG:HD3	1:A:921:ARG:HH11	1.74	0.41
1:B:883:ASP:OD1	1:B:948:LYS:HE3	2.21	0.41
1:D:251:VAL:HG21	1:D:259:PHE:CZ	2.54	0.41
1:D:380:ASP:OD1	1:D:380:ASP:C	2.59	0.41
1:E:543:LEU:HD23	1:E:543:LEU:HA	1.84	0.41
1:F:248:TYR:HB2	1:F:284:TRP:CZ3	2.55	0.41
1:F:371:ASN:HB3	1:F:373:ASP:H	1.85	0.41
1:G:302:ASP:C	1:G:302:ASP:OD1	2.58	0.41
1:H:800:THR:CG2	1:H:802:ALA:H	2.08	0.41
1:B:248:TYR:O	1:B:250:GLN:N	2.54	0.41
1:B:425:ARG:HG2	1:B:425:ARG:H	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:ASN:HD22	1:B:470:ASN:N	2.17	0.41
1:C:312:TYR:O	1:C:316:GLN:HG2	2.21	0.41
1:E:430:TYR:CG	1:E:977:LYS:HD3	2.56	0.41
1:F:604:ASN:OD1	1:F:606:ASN:N	2.46	0.41
1:F:698:ARG:HD3	1:F:698:ARG:HA	1.90	0.41
1:G:293:ARG:CB	1:G:297:MET:CE	2.98	0.41
1:A:1073:LEU:HD23	1:A:1080:LEU:HD21	1.97	0.41
1:A:478:ALA:HB1	1:A:481:ASN:HD22	1.86	0.41
1:A:965:PRO:HD2	1:A:998:SER:HA	2.02	0.41
1:B:758:ALA:HB3	1:B:759:HIS:ND1	2.35	0.41
1:D:350:GLU:C	1:D:352:ASN:H	2.24	0.41
1:F:869:LYS:CD	1:F:871:GLU:OE1	2.69	0.41
1:G:1080:LEU:HB3	1:G:1081:PRO:HD2	2.03	0.41
1:H:837:ALA:HA	1:H:838:PRO:HD3	1.89	0.41
1:B:1025:ARG:HH11	1:B:1025:ARG:HD2	1.70	0.41
1:C:251:VAL:HG21	1:C:259:PHE:HZ	1.81	0.41
1:D:999:SER:C	1:D:1001:LYS:N	2.74	0.41
1:E:458:ASN:O	1:E:459:PHE:C	2.59	0.41
1:F:759:HIS:O	1:F:791:THR:HG21	2.21	0.41
1:F:799:PHE:HE1	1:F:819:TRP:CZ3	2.39	0.41
1:G:1069:THR:HG22	1:G:1070:TYR:O	2.20	0.41
1:G:346:LYS:HE2	1:G:355:TRP:CE3	2.56	0.41
1:H:278:LEU:CA	1:H:283:THR:O	2.68	0.41
1:H:439:ASP:C	1:H:439:ASP:OD1	2.57	0.41
1:H:877:VAL:HG13	1:H:881:ASN:ND2	2.36	0.41
1:H:854:ARG:HD3	1:H:892:ASP:OD2	2.21	0.41
1:H:430:TYR:CD1	1:H:977:LYS:HG2	2.56	0.41
1:A:277:ILE:HD12	1:A:293:ARG:NH2	2.35	0.40
1:A:299:TRP:NE1	1:A:1081:PRO:HB3	2.36	0.40
1:A:365:LYS:HA	1:A:365:LYS:HD3	1.98	0.40
1:A:544:LEU:HD11	1:A:549:LYS:HE2	2.03	0.40
1:B:1064:ASP:C	1:B:1064:ASP:OD1	2.58	0.40
1:B:371:ASN:OD1	1:B:372:SER:N	2.54	0.40
1:C:1061:VAL:HG12	1:C:1070:TYR:CD1	2.57	0.40
1:E:1064:ASP:OD1	1:E:1067:THR:HG23	2.21	0.40
1:F:495:LYS:HE3	1:F:495:LYS:HB2	1.91	0.40
1:F:698:ARG:O	1:F:708:ILE:HA	2.22	0.40
1:F:709:THR:CG2	1:F:736:ILE:CD1	2.86	0.40
1:G:300:TRP:CD1	1:G:306:GLN:HA	2.56	0.40
1:G:789:ARG:HH11	1:G:789:ARG:HD2	1.76	0.40
1:H:877:VAL:HG13	1:H:881:ASN:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PHE:CD2	1:A:259:PHE:N	2.88	0.40
1:B:466:ASP:OD2	1:B:943:LYS:HE2	2.17	0.40
1:B:769:LEU:HD23	1:B:769:LEU:HA	1.81	0.40
1:C:256:ALA:HB1	1:C:261:HIS:CE1	2.56	0.40
1:C:460:GLY:HA3	1:C:470:ASN:ND2	2.36	0.40
1:D:245:PHE:C	1:D:247:GLN:N	2.72	0.40
1:D:474:ILE:HA	1:D:954:ALA:O	2.20	0.40
1:E:1016:GLN:HA	1:E:1023:PHE:CE2	2.56	0.40
1:E:347:ILE:HA	1:E:352:ASN:O	2.21	0.40
1:E:442:ASN:O	1:E:446:GLN:HG3	2.21	0.40
1:F:771:THR:O	1:F:809:ASN:ND2	2.54	0.40
1:G:259:PHE:N	1:G:259:PHE:CD2	2.89	0.40
1:B:1016:GLN:NE2	1:G:748:SER:HA	2.24	0.40
1:H:299:TRP:C	1:H:300:TRP:CE3	2.94	0.40
1:B:974:ARG:HE	1:B:1053:ILE:HG21	1.87	0.40
1:B:930:ASN:C	1:B:932:TYR:N	2.72	0.40
1:E:260:GLU:OE2	1:E:292:PHE:HD1	2.05	0.40
1:F:261:HIS:CD2	1:F:264:HIS:CA	3.03	0.40
1:G:874:THR:HB	1:G:932:TYR:HB3	2.02	0.40
1:G:943:LYS:HG2	1:G:943:LYS:HZ2	1.69	0.40
1:H:281:GLY:O	1:H:282:LYS:CB	2.69	0.40
1:H:663:PHE:CZ	1:H:670:MET:HG2	2.56	0.40
1:A:288:THR:C	1:A:290:LYS:N	2.75	0.40
1:A:669:TYR:CZ	1:A:874:THR:HG23	2.56	0.40
1:B:525:LEU:HA	1:B:525:LEU:HD12	1.84	0.40
1:C:408:ARG:HD2	1:C:413:GLN:O	2.21	0.40
1:D:271:TRP:CD1	1:D:294:PRO:CA	3.02	0.40
1:E:252:TYR:CB	1:E:258:ASN:HD21	2.09	0.40
1:E:938:LEU:HD12	1:E:938:LEU:O	2.22	0.40
1:E:957:VAL:O	1:E:957:VAL:HG12	2.21	0.40
1:F:486:LEU:HA	1:F:486:LEU:HD23	1.89	0.40
1:G:800:THR:HG22	1:G:801:ALA:N	2.36	0.40
1:H:475:ARG:CA	1:H:953:MET:CE	3.00	0.40
1:B:503:ASN:OD1	1:B:505:LYS:HB3	2.21	0.40
1:B:657:VAL:CG1	1:B:658:TYR:N	2.84	0.40
1:B:689:LYS:HD2	1:B:690:TYR:HE1	1.87	0.40
1:B:794:ARG:H	1:B:794:ARG:HG2	1.66	0.40
1:B:797:LEU:HB3	1:B:799:PHE:CE2	2.56	0.40
1:D:1063:LYS:NZ	1:D:1068:ASN:HD21	2.19	0.40
1:D:245:PHE:CD1	1:D:245:PHE:N	2.88	0.40
1:D:391:ASN:OD1	1:D:404:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:670:MET:HE1	1:E:877:VAL:HG12	2.02	0.40
1:F:322:THR:CG2	1:F:323:TYR:N	2.84	0.40
1:F:882:VAL:O	1:F:882:VAL:HG22	2.21	0.40
1:G:1001:LYS:HE2	1:G:1001:LYS:HB2	1.58	0.40
1:G:365:LYS:HD3	1:G:365:LYS:HA	2.00	0.40
1:G:476:VAL:HG22	1:G:956:TRP:HE3	1.87	0.40
1:H:277:ILE:CG1	1:H:291:ASP:HB3	2.45	0.40
1:H:315:ALA:O	1:H:318:GLY:HA2	2.22	0.40
1:H:356:LEU:C	1:H:358:GLN:H	2.25	0.40
1:H:444:VAL:HG11	1:H:1038:VAL:HG22	2.03	0.40
1:H:619:LYS:HA	1:H:619:LYS:HD2	1.31	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	840/844 (100%)	791 (94%)	45 (5%)	4 (0%)	29	64
1	B	745/844 (88%)	693 (93%)	41 (6%)	11 (2%)	10	39
1	C	842/844 (100%)	809 (96%)	29 (3%)	4 (0%)	29	64
1	D	842/844 (100%)	789 (94%)	46 (6%)	7 (1%)	19	54
1	E	842/844 (100%)	791 (94%)	41 (5%)	10 (1%)	13	44
1	F	842/844 (100%)	783 (93%)	53 (6%)	6 (1%)	22	57
1	G	842/844 (100%)	796 (94%)	43 (5%)	3 (0%)	34	69
1	H	804/844 (95%)	743 (92%)	53 (7%)	8 (1%)	15	49
All	All	6599/6752 (98%)	6195 (94%)	351 (5%)	53 (1%)	19	54

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	713	TYR
1	B	761	ASN
1	D	351	LYS
1	G	281	GLY
1	G	351	LYS
1	E	281	GLY
1	E	321	GLN
1	E	351	LYS
1	F	801	ALA
1	F	802	ALA
1	H	282	LYS
1	H	291	ASP
1	H	1066	ALA
1	B	611	SER
1	D	281	GLY
1	G	291	ASP
1	E	291	ASP
1	E	1085	VAL
1	H	263	ASP
1	H	281	GLY
1	H	302	ASP
1	A	357	ARG
1	B	247	GLN
1	B	249	ASN
1	B	384	LYS
1	B	904	ASP
1	C	315	ALA
1	C	1000	GLY
1	D	345	GLU
1	D	1000	GLY
1	E	250	GLN
1	E	345	GLU
1	F	257	ALA
1	H	286	GLN
1	B	870	LYS
1	B	977	LYS
1	B	1066	ALA
1	C	316	GLN
1	D	304	GLU
1	D	349	ALA
1	E	302	ASP
1	F	725	ASP
1	A	250	GLN

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Mol	Chain	Res	Type
1	A	345	GLU
1	D	1066	ALA
1	F	785	ALA
1	H	254	THR
1	B	1045	ALA
1	C	761	ASN
1	F	603	ILE
1	A	603	ILE
1	E	274	PRO
1	E	318	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	713/715 (100%)	671 (94%)	42 (6%)	19	50
1	B	628/715 (88%)	575 (92%)	53 (8%)	11	38
1	C	715/715 (100%)	678 (95%)	37 (5%)	23	55
1	D	715/715 (100%)	660 (92%)	55 (8%)	13	41
1	E	715/715 (100%)	665 (93%)	50 (7%)	15	45
1	F	715/715 (100%)	666 (93%)	49 (7%)	15	45
1	G	715/715 (100%)	675 (94%)	40 (6%)	21	52
1	H	683/715 (96%)	645 (94%)	38 (6%)	21	52
All	All	5599/5720 (98%)	5235 (94%)	364 (6%)	17	47

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
1	A	276	TYR
1	A	279	LYS
1	A	286	GLN
1	A	308	GLN

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Mol	Chain	Res	Type
1	A	321	GLN
1	A	325	THR
1	A	350	GLU
1	A	352	ASN
1	A	359	THR
1	A	368	SER
1	A	374	SER
1	A	397	SER
1	A	465	ASN
1	A	505	LYS
1	A	532	MET
1	A	574	GLU
1	A	604	ASN
1	A	606	ASN
1	A	614	MET
1	A	615	GLU
1	A	702	VAL
1	A	726	ARG
1	A	740	ASN
1	A	744	ARG
1	A	782	GLN
1	A	794	ARG
1	A	800	THR
1	A	805	LYS
1	A	832	VAL
1	A	836	THR
1	A	869	LYS
1	A	870	LYS
1	A	880	LYS
1	A	882	VAL
1	A	985	SER
1	A	990	THR
1	A	1001	LYS
1	A	1025	ARG
1	A	1038	VAL
1	A	1052	ASN
1	A	1082	LYS
1	B	248	TYR
1	B	255	ASP
1	B	259	PHE
1	B	263	ASP
1	B	272	TYR

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Mol	Chain	Res	Type
1	B	273	ARG
1	B	374	SER
1	B	390	SER
1	B	394	LYS
1	B	416	LYS
1	B	422	THR
1	B	465	ASN
1	B	470	ASN
1	B	501	HIS
1	B	503	ASN
1	B	532	MET
1	B	540	ARG
1	B	600	LYS
1	B	604	ASN
1	B	605	PRO
1	B	612	PHE
1	B	618	LYS
1	B	626	LYS
1	B	702	VAL
1	B	710	SER
1	B	712	ARG
1	B	715	LYS
1	B	723	THR
1	B	726	ARG
1	B	740	ASN
1	B	759	HIS
1	B	791	THR
1	B	832	VAL
1	B	854	ARG
1	B	871	GLU
1	B	882	VAL
1	B	912	ILE
1	B	913	GLN
1	B	921	ARG
1	B	947	SER
1	B	951	LYS
1	B	974	ARG
1	B	985	SER
1	B	990	THR
1	B	1003	GLN
1	B	1037	SER
1	B	1038	VAL

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Mol	Chain	Res	Type
1	B	1042	GLN
1	B	1044	SER
1	B	1052	ASN
1	B	1063	LYS
1	B	1082	LYS
1	B	1084	LEU
1	C	247	GLN
1	C	290	LYS
1	C	302	ASP
1	C	308	GLN
1	C	320	HIS
1	C	342	LYS
1	C	346	LYS
1	C	352	ASN
1	C	372	SER
1	C	374	SER
1	C	390	SER
1	C	422	THR
1	C	465	ASN
1	C	532	MET
1	C	574	GLU
1	C	604	ASN
1	C	605	PRO
1	C	632	GLU
1	C	702	VAL
1	C	740	ASN
1	C	793	ASP
1	C	800	THR
1	C	832	VAL
1	C	838	PRO
1	C	870	LYS
1	C	880	LYS
1	C	882	VAL
1	C	921	ARG
1	C	951	LYS
1	C	985	SER
1	C	990	THR
1	C	1038	VAL
1	C	1046	LYS
1	C	1052	ASN
1	C	1064	ASP
1	C	1065	GLN

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Mol	Chain	Res	Type
1	C	1074	VAL
1	D	247	GLN
1	D	251	VAL
1	D	258	ASN
1	D	277	ILE
1	D	279	LYS
1	D	282	LYS
1	D	286	GLN
1	D	288	THR
1	D	290	LYS
1	D	304	GLU
1	D	320	HIS
1	D	322	THR
1	D	341	THR
1	D	350	GLU
1	D	352	ASN
1	D	359	THR
1	D	368	SER
1	D	390	SER
1	D	416	LYS
1	D	422	THR
1	D	465	ASN
1	D	502	LYS
1	D	532	MET
1	D	551	LEU
1	D	574	GLU
1	D	604	ASN
1	D	605	PRO
1	D	619	LYS
1	D	702	VAL
1	D	707	ILE
1	D	726	ARG
1	D	729	ARG
1	D	740	ASN
1	D	744	ARG
1	D	782	GLN
1	D	793	ASP
1	D	800	THR
1	D	854	ARG
1	D	861	SER
1	D	870	LYS
1	D	880	LYS

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Mol	Chain	Res	Type
1	D	882	VAL
1	D	904	ASP
1	D	921	ARG
1	D	985	SER
1	D	986	GLN
1	D	988	LYS
1	D	1001	LYS
1	D	1021	GLU
1	D	1025	ARG
1	D	1038	VAL
1	D	1052	ASN
1	D	1076	ASP
1	D	1084	LEU
1	D	1086	ASN
1	G	253	SER
1	G	282	LYS
1	G	283	THR
1	G	322	THR
1	G	352	ASN
1	G	359	THR
1	G	368	SER
1	G	394	LYS
1	G	422	THR
1	G	465	ASN
1	G	532	MET
1	G	574	GLU
1	G	588	ASP
1	G	600	LYS
1	G	604	ASN
1	G	605	PRO
1	G	606	ASN
1	G	632	GLU
1	G	740	ASN
1	G	746	LYS
1	G	782	GLN
1	G	800	THR
1	G	832	VAL
1	G	835	SER
1	G	870	LYS
1	G	882	VAL
1	G	884	LYS
1	G	912	ILE

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Mol	Chain	Res	Type
1	G	921	ARG
1	G	928	LYS
1	G	948	LYS
1	G	977	LYS
1	G	985	SER
1	G	988	LYS
1	G	990	THR
1	G	1046	LYS
1	G	1052	ASN
1	G	1074	VAL
1	G	1075	SER
1	G	1082	LYS
1	E	244	SER
1	E	251	VAL
1	E	253	SER
1	E	259	PHE
1	E	285	THR
1	E	289	GLU
1	E	290	LYS
1	E	291	ASP
1	E	298	THR
1	E	304	GLU
1	E	305	THR
1	E	308	GLN
1	E	316	GLN
1	E	322	THR
1	E	327	THR
1	E	341	THR
1	E	344	GLU
1	E	351	LYS
1	E	359	THR
1	E	368	SER
1	E	372	SER
1	E	374	SER
1	E	390	SER
1	E	505	LYS
1	E	532	MET
1	E	574	GLU
1	E	619	LYS
1	E	632	GLU
1	E	685	LYS
1	E	702	VAL

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Mol	Chain	Res	Type
1	E	740	ASN
1	E	793	ASP
1	E	800	THR
1	E	805	LYS
1	E	832	VAL
1	E	835	SER
1	E	882	VAL
1	E	928	LYS
1	E	955	ASP
1	E	977	LYS
1	E	986	GLN
1	E	988	LYS
1	E	1001	LYS
1	E	1025	ARG
1	E	1044	SER
1	E	1052	ASN
1	E	1074	VAL
1	E	1075	SER
1	E	1076	ASP
1	E	1077	ASN
1	F	253	SER
1	F	308	GLN
1	F	351	LYS
1	F	352	ASN
1	F	357	ARG
1	F	368	SER
1	F	394	LYS
1	F	422	THR
1	F	425	ARG
1	F	465	ASN
1	F	524	TYR
1	F	532	MET
1	F	540	ARG
1	F	551	LEU
1	F	604	ASN
1	F	605	PRO
1	F	612	PHE
1	F	614	MET
1	F	664	THR
1	F	708	ILE
1	F	723	THR
1	F	726	ARG

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Mol	Chain	Res	Type
1	F	730	THR
1	F	740	ASN
1	F	744	ARG
1	F	745	LEU
1	F	748	SER
1	F	752	VAL
1	F	780	SER
1	F	793	ASP
1	F	794	ARG
1	F	803	ASP
1	F	835	SER
1	F	869	LYS
1	F	870	LYS
1	F	873	TYR
1	F	884	LYS
1	F	904	ASP
1	F	921	ARG
1	F	936	ASP
1	F	940	LYS
1	F	977	LYS
1	F	985	SER
1	F	990	THR
1	F	1001	LYS
1	F	1025	ARG
1	F	1039	LYS
1	F	1052	ASN
1	F	1076	ASP
1	H	244	SER
1	H	278	LEU
1	H	279	LYS
1	H	282	LYS
1	H	283	THR
1	H	288	THR
1	H	291	ASP
1	H	306	GLN
1	H	309	TYR
1	H	316	GLN
1	H	368	SER
1	H	390	SER
1	H	394	LYS
1	H	422	THR
1	H	532	MET

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Mol	Chain	Res	Type
1	H	540	ARG
1	H	619	LYS
1	H	702	VAL
1	H	726	ARG
1	H	727	ILE
1	H	729	ARG
1	H	740	ASN
1	H	744	ARG
1	H	800	THR
1	H	832	VAL
1	H	882	VAL
1	H	904	ASP
1	H	927	SER
1	H	928	LYS
1	H	977	LYS
1	H	985	SER
1	H	988	LYS
1	H	990	THR
1	H	1001	LYS
1	H	1052	ASN
1	H	1074	VAL
1	H	1075	SER
1	H	1078	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (187) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	ASN
1	A	261	HIS
1	A	308	GLN
1	A	311	ASN
1	A	367	GLN
1	A	407	ASN
1	A	440	ASN
1	A	458	ASN
1	A	461	ASN
1	A	470	ASN
1	A	481	ASN
1	A	531	ASN
1	A	604	ASN
1	A	639	ASN
1	A	700	GLN

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Mol	Chain	Res	Type
1	A	740	ASN
1	A	759	HIS
1	A	773	ASN
1	A	782	GLN
1	A	846	HIS
1	A	864	GLN
1	A	1052	ASN
1	A	1068	ASN
1	B	258	ASN
1	B	261	HIS
1	B	264	HIS
1	B	392	ASN
1	B	407	ASN
1	B	440	ASN
1	B	458	ASN
1	B	470	ASN
1	B	481	ASN
1	B	503	ASN
1	B	531	ASN
1	B	639	ASN
1	B	740	ASN
1	B	759	HIS
1	B	761	ASN
1	B	846	HIS
1	B	864	GLN
1	B	960	GLN
1	B	986	GLN
1	B	1016	GLN
1	B	1042	GLN
1	B	1052	ASN
1	C	247	GLN
1	C	250	GLN
1	C	258	ASN
1	C	261	HIS
1	C	308	GLN
1	C	311	ASN
1	C	316	GLN
1	C	367	GLN
1	C	407	ASN
1	C	440	ASN
1	C	461	ASN
1	C	470	ASN

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Mol	Chain	Res	Type
1	C	481	ASN
1	C	531	ASN
1	C	639	ASN
1	C	740	ASN
1	C	759	HIS
1	C	782	GLN
1	C	846	HIS
1	C	864	GLN
1	C	913	GLN
1	C	960	GLN
1	C	1052	ASN
1	C	1068	ASN
1	D	258	ASN
1	D	261	HIS
1	D	308	GLN
1	D	311	ASN
1	D	367	GLN
1	D	407	ASN
1	D	440	ASN
1	D	470	ASN
1	D	481	ASN
1	D	531	ASN
1	D	639	ASN
1	D	740	ASN
1	D	759	HIS
1	D	782	GLN
1	D	846	HIS
1	D	864	GLN
1	D	960	GLN
1	D	1027	GLN
1	D	1052	ASN
1	D	1068	ASN
1	G	258	ASN
1	G	261	HIS
1	G	308	GLN
1	G	311	ASN
1	G	316	GLN
1	G	367	GLN
1	G	407	ASN
1	G	440	ASN
1	G	470	ASN
1	G	481	ASN

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Mol	Chain	Res	Type
1	G	531	ASN
1	G	572	ASN
1	G	639	ASN
1	G	740	ASN
1	G	759	HIS
1	G	782	GLN
1	G	846	HIS
1	G	864	GLN
1	G	881	ASN
1	G	1003	GLN
1	G	1052	ASN
1	G	1068	ASN
1	E	250	GLN
1	E	258	ASN
1	E	261	HIS
1	E	308	GLN
1	E	311	ASN
1	E	367	GLN
1	E	371	ASN
1	E	407	ASN
1	E	440	ASN
1	E	458	ASN
1	E	461	ASN
1	E	470	ASN
1	E	481	ASN
1	E	531	ASN
1	E	558	ASN
1	E	639	ASN
1	E	699	ASN
1	E	740	ASN
1	E	759	HIS
1	E	773	ASN
1	E	782	GLN
1	E	846	HIS
1	E	864	GLN
1	E	1052	ASN
1	E	1065	GLN
1	E	1068	ASN
1	F	258	ASN
1	F	261	HIS
1	F	264	HIS
1	F	308	GLN

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Mol	Chain	Res	Type
1	F	311	ASN
1	F	352	ASN
1	F	367	GLN
1	F	407	ASN
1	F	440	ASN
1	F	481	ASN
1	F	531	ASN
1	F	572	ASN
1	F	639	ASN
1	F	740	ASN
1	F	759	HIS
1	F	773	ASN
1	F	846	HIS
1	F	864	GLN
1	F	881	ASN
1	F	913	GLN
1	F	960	GLN
1	F	1003	GLN
1	F	1027	GLN
1	F	1052	ASN
1	F	1068	ASN
1	H	250	GLN
1	H	258	ASN
1	H	261	HIS
1	H	303	GLN
1	H	308	GLN
1	H	311	ASN
1	H	316	GLN
1	H	367	GLN
1	H	407	ASN
1	H	440	ASN
1	H	470	ASN
1	H	481	ASN
1	H	531	ASN
1	H	572	ASN
1	H	639	ASN
1	H	740	ASN
1	H	759	HIS
1	H	773	ASN
1	H	782	GLN
1	H	846	HIS
1	H	864	GLN

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Mol	Chain	Res	Type
1	H	881	ASN
1	H	1016	GLN
1	H	1052	ASN
1	H	1068	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

2 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	GLC	I	1	2	12,12,12	2.56	5 (41%)	17,17,17	4.55	8 (47%)
2	GLC	I	2	2	11,11,12	0.82	0	15,15,17	2.73	7 (46%)

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	GLC	I	1	2	-	2/2/22/22	0/1/1/1
2	GLC	I	2	2	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	GLC	O5-C1	5.13	1.55	1.42
2	I	1	GLC	O5-C5	4.33	1.54	1.44
2	I	1	GLC	C4-C5	3.28	1.59	1.53
2	I	1	GLC	O1-C1	3.08	1.49	1.39
2	I	1	GLC	C1-C2	3.03	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1	GLC	C3-C4-C5	-12.25	88.38	110.24
2	I	1	GLC	O4-C4-C3	-10.07	87.07	110.35
2	I	2	GLC	O5-C1-C2	-6.59	100.60	110.77
2	I	1	GLC	O5-C5-C4	5.82	120.26	109.69
2	I	1	GLC	O2-C2-C3	-4.52	99.91	110.35
2	I	2	GLC	C2-C3-C4	-4.38	103.31	110.89
2	I	2	GLC	O5-C5-C6	-3.74	101.34	107.20
2	I	2	GLC	C1-O5-C5	-3.48	107.48	112.19
2	I	1	GLC	O1-C1-C2	-3.46	99.28	109.03
2	I	1	GLC	O3-C3-C2	-3.37	102.55	110.35
2	I	2	GLC	O6-C6-C5	-2.84	101.55	111.29
2	I	1	GLC	O6-C6-C5	-2.65	102.18	111.29
2	I	1	GLC	O5-C5-C6	-2.50	100.22	106.44
2	I	2	GLC	O2-C2-C1	2.47	114.20	109.15
2	I	2	GLC	O5-C5-C4	-2.22	105.44	110.83

There are no chirality outliers.

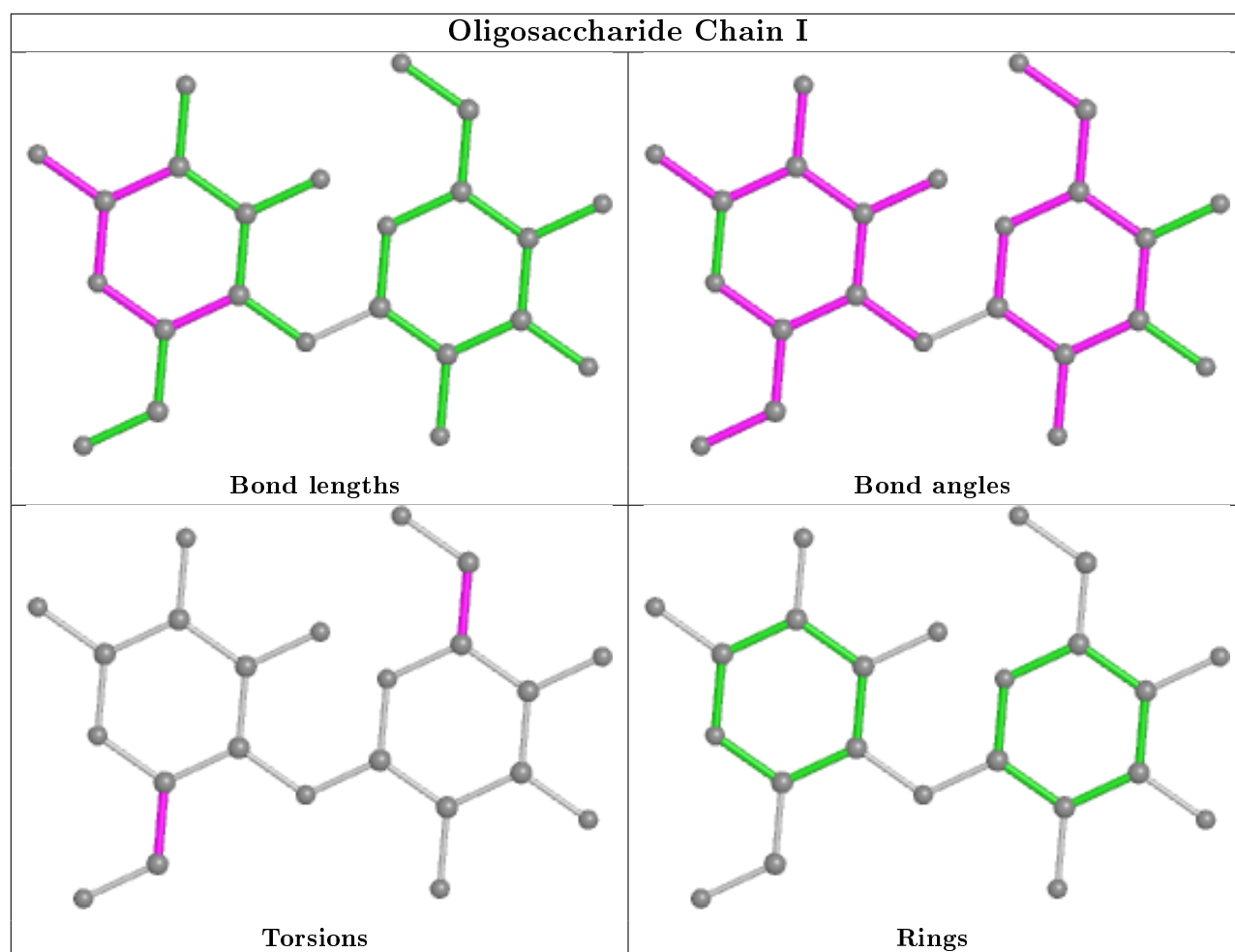
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1	GLC	C4-C5-C6-O6
2	I	1	GLC	O5-C5-C6-O6
2	I	2	GLC	O5-C5-C6-O6
2	I	2	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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



5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MES	G	5001	-	12,12,12	2.58	3 (25%)	14,16,16	7.58	9 (64%)
4	MES	A	5001	-	12,12,12	3.81	7 (58%)	14,16,16	8.87	8 (57%)
4	MES	C	5001	-	12,12,12	3.08	4 (33%)	14,16,16	6.37	6 (42%)
4	MES	F	5001	-	12,12,12	3.17	4 (33%)	14,16,16	7.16	10 (71%)
4	MES	B	5001	-	12,12,12	2.19	4 (33%)	14,16,16	7.86	11 (78%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	H	5001	-	12,12,12	2.62	5 (41%)	14,16,16	6.79	10 (71%)
4	MES	D	5001	-	12,12,12	2.72	5 (41%)	14,16,16	6.59	11 (78%)
4	MES	E	5001	-	12,12,12	2.80	5 (41%)	14,16,16	6.94	10 (71%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	G	5001	-	-	5/6/14/14	0/1/1/1
4	MES	A	5001	-	-	2/6/14/14	0/1/1/1
4	MES	C	5001	-	-	4/6/14/14	0/1/1/1
4	MES	F	5001	-	-	5/6/14/14	0/1/1/1
4	MES	B	5001	-	-	3/6/14/14	0/1/1/1
4	MES	H	5001	-	-	4/6/14/14	0/1/1/1
4	MES	D	5001	-	-	2/6/14/14	0/1/1/1
4	MES	E	5001	-	-	1/6/14/14	0/1/1/1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5001	MES	O2S-S	7.80	1.68	1.45
4	A	5001	MES	O1S-S	7.67	1.67	1.45
4	F	5001	MES	O2S-S	7.27	1.66	1.45
4	C	5001	MES	O1S-S	6.54	1.64	1.45
4	H	5001	MES	O1S-S	5.77	1.62	1.45
4	F	5001	MES	O1S-S	5.77	1.62	1.45
4	C	5001	MES	O2S-S	5.58	1.61	1.45
4	E	5001	MES	O1S-S	5.56	1.61	1.45
4	D	5001	MES	O1S-S	5.45	1.61	1.45
4	E	5001	MES	O2S-S	5.10	1.60	1.45
4	G	5001	MES	O2S-S	5.05	1.59	1.45
4	G	5001	MES	O1S-S	5.01	1.59	1.45
4	A	5001	MES	O3S-S	5.01	1.65	1.47
4	C	5001	MES	O3S-S	5.00	1.65	1.47
4	B	5001	MES	O2S-S	4.80	1.59	1.45
4	H	5001	MES	O2S-S	4.75	1.59	1.45
4	D	5001	MES	O2S-S	4.68	1.58	1.45
4	G	5001	MES	O3S-S	4.42	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5001	MES	O3S-S	4.26	1.62	1.47
4	F	5001	MES	O3S-S	3.91	1.61	1.47
4	B	5001	MES	O1S-S	3.84	1.56	1.45
4	D	5001	MES	O3S-S	3.38	1.59	1.47
4	H	5001	MES	O3S-S	3.20	1.59	1.47
4	B	5001	MES	O3S-S	3.07	1.58	1.47
4	D	5001	MES	C8-S	2.86	1.81	1.77
4	A	5001	MES	C8-S	2.78	1.81	1.77
4	E	5001	MES	C8-S	2.67	1.81	1.77
4	F	5001	MES	C7-C8	2.56	1.59	1.52
4	B	5001	MES	C7-C8	2.53	1.59	1.52
4	D	5001	MES	C5-C6	2.44	1.59	1.50
4	A	5001	MES	C7-C8	2.34	1.58	1.52
4	H	5001	MES	C7-N4	-2.28	1.42	1.47
4	A	5001	MES	C5-N4	2.21	1.53	1.46
4	C	5001	MES	C5-N4	2.20	1.53	1.46
4	H	5001	MES	C5-C6	2.12	1.58	1.50
4	E	5001	MES	C5-C6	2.02	1.58	1.50
4	A	5001	MES	C5-C6	2.02	1.58	1.50

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5001	MES	O1S-S-C8	-23.86	78.18	106.92
4	B	5001	MES	O2S-S-C8	-21.61	80.89	106.92
4	G	5001	MES	O1S-S-C8	-20.68	82.01	106.92
4	A	5001	MES	O2S-S-C8	-20.00	82.84	106.92
4	E	5001	MES	O1S-S-C8	-18.94	84.11	106.92
4	D	5001	MES	O1S-S-C8	-16.14	87.48	106.92
4	F	5001	MES	O2S-S-C8	-15.40	88.37	106.92
4	F	5001	MES	O1S-S-C8	-15.11	88.72	106.92
4	H	5001	MES	O1S-S-C8	-15.00	88.86	106.92
4	B	5001	MES	O1S-S-C8	-14.90	88.97	106.92
4	C	5001	MES	O2S-S-C8	-13.44	90.73	106.92
4	H	5001	MES	O2S-S-C8	-12.85	91.44	106.92
4	E	5001	MES	O2S-S-C8	-12.51	91.85	106.92
4	C	5001	MES	O1S-S-C8	-12.43	91.95	106.92
4	H	5001	MES	O3S-S-C8	-12.40	85.71	105.77
4	D	5001	MES	O3S-S-C8	-11.66	86.92	105.77
4	G	5001	MES	O2S-S-C8	-11.51	93.06	106.92
4	F	5001	MES	O3S-S-C8	-11.25	87.57	105.77
4	G	5001	MES	O3S-S-C8	-10.60	88.62	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	5001	MES	O3S-S-C8	-10.29	89.12	105.77
4	D	5001	MES	O2S-S-C8	-9.16	95.89	106.92
4	C	5001	MES	C5-N4-C3	8.73	128.48	108.83
4	D	5001	MES	C5-N4-C3	8.10	127.07	108.83
4	E	5001	MES	C5-N4-C3	7.73	126.22	108.83
4	B	5001	MES	O3S-S-C8	-6.92	94.58	105.77
4	F	5001	MES	C5-N4-C3	6.89	124.34	108.83
4	E	5001	MES	O3S-S-C8	-6.69	94.94	105.77
4	A	5001	MES	O3S-S-O1S	6.61	127.43	111.27
4	G	5001	MES	C5-N4-C3	6.02	122.37	108.83
4	H	5001	MES	C5-N4-C3	5.88	122.06	108.83
4	A	5001	MES	C5-N4-C3	5.58	121.38	108.83
4	B	5001	MES	C5-N4-C3	5.23	120.59	108.83
4	A	5001	MES	C2-C3-N4	-5.11	102.35	110.10
4	G	5001	MES	C6-C5-N4	-5.07	102.41	110.10
4	F	5001	MES	O3S-S-O2S	4.99	123.46	111.27
4	G	5001	MES	C7-N4-C5	4.83	123.58	111.23
4	B	5001	MES	C2-C3-N4	-4.76	102.89	110.10
4	C	5001	MES	O3S-S-O2S	4.71	122.78	111.27
4	B	5001	MES	O3S-S-O1S	4.47	122.21	111.27
4	G	5001	MES	O3S-S-O1S	4.36	121.93	111.27
4	H	5001	MES	C2-C3-N4	-4.34	103.52	110.10
4	B	5001	MES	C6-C5-N4	-3.83	104.30	110.10
4	F	5001	MES	C7-N4-C5	3.77	120.88	111.23
4	A	5001	MES	C7-N4-C5	3.75	120.83	111.23
4	H	5001	MES	O3S-S-O1S	3.69	120.28	111.27
4	B	5001	MES	C7-N4-C5	3.62	120.50	111.23
4	F	5001	MES	O2S-S-O1S	3.56	126.26	113.95
4	D	5001	MES	O3S-S-O2S	3.48	119.77	111.27
4	D	5001	MES	C2-C3-N4	-3.45	104.88	110.10
4	B	5001	MES	O3S-S-O2S	3.44	119.69	111.27
4	E	5001	MES	C7-N4-C3	3.36	119.82	111.23
4	G	5001	MES	O3S-S-O2S	3.16	119.00	111.27
4	H	5001	MES	C7-N4-C5	3.13	119.23	111.23
4	E	5001	MES	C2-C3-N4	-3.10	105.40	110.10
4	D	5001	MES	O3S-S-O1S	3.10	118.84	111.27
4	E	5001	MES	O3S-S-O2S	3.06	118.74	111.27
4	C	5001	MES	O3S-S-O1S	3.03	118.68	111.27
4	B	5001	MES	C7-N4-C3	3.00	118.91	111.23
4	H	5001	MES	C7-N4-C3	2.91	118.68	111.23
4	D	5001	MES	C6-C5-N4	2.89	114.49	110.10
4	E	5001	MES	O3S-S-O1S	2.88	118.31	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5001	MES	C2-C3-N4	-2.87	105.75	110.10
4	G	5001	MES	C2-C3-N4	-2.82	105.82	110.10
4	F	5001	MES	C6-O1-C2	2.82	119.32	109.89
4	D	5001	MES	C7-N4-C3	2.62	117.94	111.23
4	D	5001	MES	C6-O1-C2	2.62	118.63	109.89
4	H	5001	MES	O3S-S-O2S	2.61	117.64	111.27
4	E	5001	MES	O2S-S-O1S	2.60	122.94	113.95
4	A	5001	MES	C7-N4-C3	2.55	117.76	111.23
4	F	5001	MES	C6-C5-N4	-2.49	106.33	110.10
4	E	5001	MES	C6-C5-N4	2.35	113.66	110.10
4	H	5001	MES	O2S-S-O1S	2.30	121.92	113.95
4	A	5001	MES	O2S-S-O1S	2.21	121.61	113.95
4	D	5001	MES	O2S-S-O1S	2.15	121.39	113.95
4	B	5001	MES	O1-C6-C5	-2.09	107.20	111.80

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5001	MES	C8-C7-N4-C5
4	C	5001	MES	C8-C7-N4-C5
4	G	5001	MES	N4-C7-C8-S
4	G	5001	MES	C7-C8-S-O2S
4	D	5001	MES	C8-C7-N4-C5
4	F	5001	MES	C8-C7-N4-C5
4	F	5001	MES	C7-C8-S-O1S
4	F	5001	MES	C7-C8-S-O3S
4	B	5001	MES	C8-C7-N4-C5
4	B	5001	MES	N4-C7-C8-S
4	H	5001	MES	C8-C7-N4-C5
4	E	5001	MES	C8-C7-N4-C5
4	C	5001	MES	C7-C8-S-O3S
4	G	5001	MES	C7-C8-S-O3S
4	H	5001	MES	C7-C8-S-O3S
4	G	5001	MES	C8-C7-N4-C3
4	D	5001	MES	C8-C7-N4-C3
4	F	5001	MES	C8-C7-N4-C3
4	C	5001	MES	C7-C8-S-O1S
4	C	5001	MES	C7-C8-S-O2S
4	G	5001	MES	C7-C8-S-O1S
4	F	5001	MES	C7-C8-S-O2S
4	H	5001	MES	C7-C8-S-O1S

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Mol	Chain	Res	Type	Atoms
4	H	5001	MES	C7-C8-S-O2S
4	B	5001	MES	C7-C8-S-O3S
4	A	5001	MES	N4-C7-C8-S

There are no ring outliers.

8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	5001	MES	2	0
4	A	5001	MES	4	0
4	C	5001	MES	1	0
4	F	5001	MES	1	0
4	B	5001	MES	1	0
4	H	5001	MES	1	0
4	D	5001	MES	1	0
4	E	5001	MES	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	842/844 (99%)	-0.22	16 (1%) 66 46	23, 36, 90, 112	0
1	B	749/844 (88%)	-0.03	32 (4%) 35 17	30, 51, 98, 148	0
1	C	844/844 (100%)	-0.34	3 (0%) 92 84	25, 35, 61, 71	0
1	D	844/844 (100%)	-0.28	14 (1%) 70 49	25, 37, 89, 110	0
1	E	844/844 (100%)	-0.19	22 (2%) 56 33	22, 36, 111, 136	0
1	F	844/844 (100%)	-0.16	4 (0%) 91 81	39, 55, 78, 91	0
1	G	844/844 (100%)	-0.36	4 (0%) 91 81	24, 36, 72, 85	0
1	H	808/844 (95%)	-0.19	23 (2%) 53 30	25, 43, 101, 144	0
All	All	6619/6752 (98%)	-0.22	118 (1%) 68 47	22, 40, 88, 148	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1087	PRO	5.8
1	E	1081	PRO	5.4
1	H	1087	PRO	5.0
1	H	277	ILE	4.8
1	A	1087	PRO	4.7
1	D	1087	PRO	4.6
1	E	285	THR	4.5
1	G	1087	PRO	4.3
1	A	286	GLN	4.1
1	H	1086	ASN	4.1
1	H	303	GLN	4.0
1	D	286	GLN	3.9
1	F	1087	PRO	3.8
1	A	352	ASN	3.8
1	D	247	GLN	3.7
1	C	1087	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	1087	PRO	3.6
1	B	795	GLY	3.6
1	H	286	GLN	3.6
1	B	274	PRO	3.6
1	D	249	ASN	3.6
1	B	1085	VAL	3.6
1	E	273	ARG	3.4
1	H	276	TYR	3.3
1	B	1086	ASN	3.3
1	E	290	LYS	3.3
1	A	1085	VAL	3.3
1	E	283	THR	3.2
1	B	246	ALA	3.2
1	H	1082	LYS	3.1
1	C	1077	ASN	3.1
1	B	819	TRP	3.1
1	A	292	PHE	3.1
1	H	249	ASN	3.1
1	B	249	ASN	3.0
1	H	1076	ASP	3.0
1	B	247	GLN	3.0
1	B	1077	ASN	3.0
1	E	1086	ASN	3.0
1	B	1072	SER	2.9
1	E	303	GLN	2.9
1	B	273	ARG	2.9
1	B	259	PHE	2.9
1	B	1084	LEU	2.8
1	B	272	TYR	2.8
1	D	1086	ASN	2.7
1	H	247	GLN	2.7
1	E	286	GLN	2.7
1	H	318	GLY	2.7
1	E	253	SER	2.7
1	A	1076	ASP	2.7
1	E	249	ASN	2.7
1	B	726	ARG	2.7
1	F	289	GLU	2.6
1	A	274	PRO	2.6
1	H	281	GLY	2.6
1	H	285	THR	2.6
1	H	273	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1081	PRO	2.6
1	B	248	TYR	2.5
1	F	761	ASN	2.5
1	H	1084	LEU	2.5
1	H	317	LEU	2.5
1	D	351	LYS	2.4
1	H	244	SER	2.4
1	B	250	GLN	2.4
1	B	1063	LYS	2.4
1	E	299	TRP	2.4
1	E	275	LYS	2.4
1	B	1065	GLN	2.4
1	D	306	GLN	2.4
1	D	1079	PHE	2.4
1	D	277	ILE	2.4
1	A	1081	PRO	2.3
1	H	1085	VAL	2.3
1	B	1083	SER	2.3
1	E	322	THR	2.3
1	B	718	LEU	2.3
1	E	1084	LEU	2.3
1	F	823	GLY	2.3
1	B	271	TRP	2.3
1	H	287	SER	2.3
1	B	1068	ASN	2.3
1	D	292	PHE	2.2
1	B	256	ALA	2.2
1	E	330	LEU	2.2
1	A	1084	LEU	2.2
1	E	254	THR	2.2
1	A	313	MET	2.2
1	D	275	LYS	2.2
1	G	289	GLU	2.2
1	A	1077	ASN	2.2
1	D	289	GLU	2.2
1	A	317	LEU	2.2
1	G	286	GLN	2.2
1	E	276	TYR	2.2
1	H	245	PHE	2.2
1	E	1085	VAL	2.1
1	H	1081	PRO	2.1
1	B	253	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1078	THR	2.1
1	B	1079	PHE	2.1
1	C	1076	ASP	2.1
1	A	285	THR	2.1
1	H	298	THR	2.1
1	E	321	GLN	2.1
1	A	353	THR	2.1
1	A	1086	ASN	2.1
1	B	822	VAL	2.1
1	E	252	TYR	2.1
1	D	317	LEU	2.1
1	B	632	GLU	2.0
1	D	1067	THR	2.0
1	A	351	LYS	2.0
1	E	1078	THR	2.0
1	B	258	ASN	2.0
1	G	1086	ASN	2.0
1	H	271	TRP	2.0

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

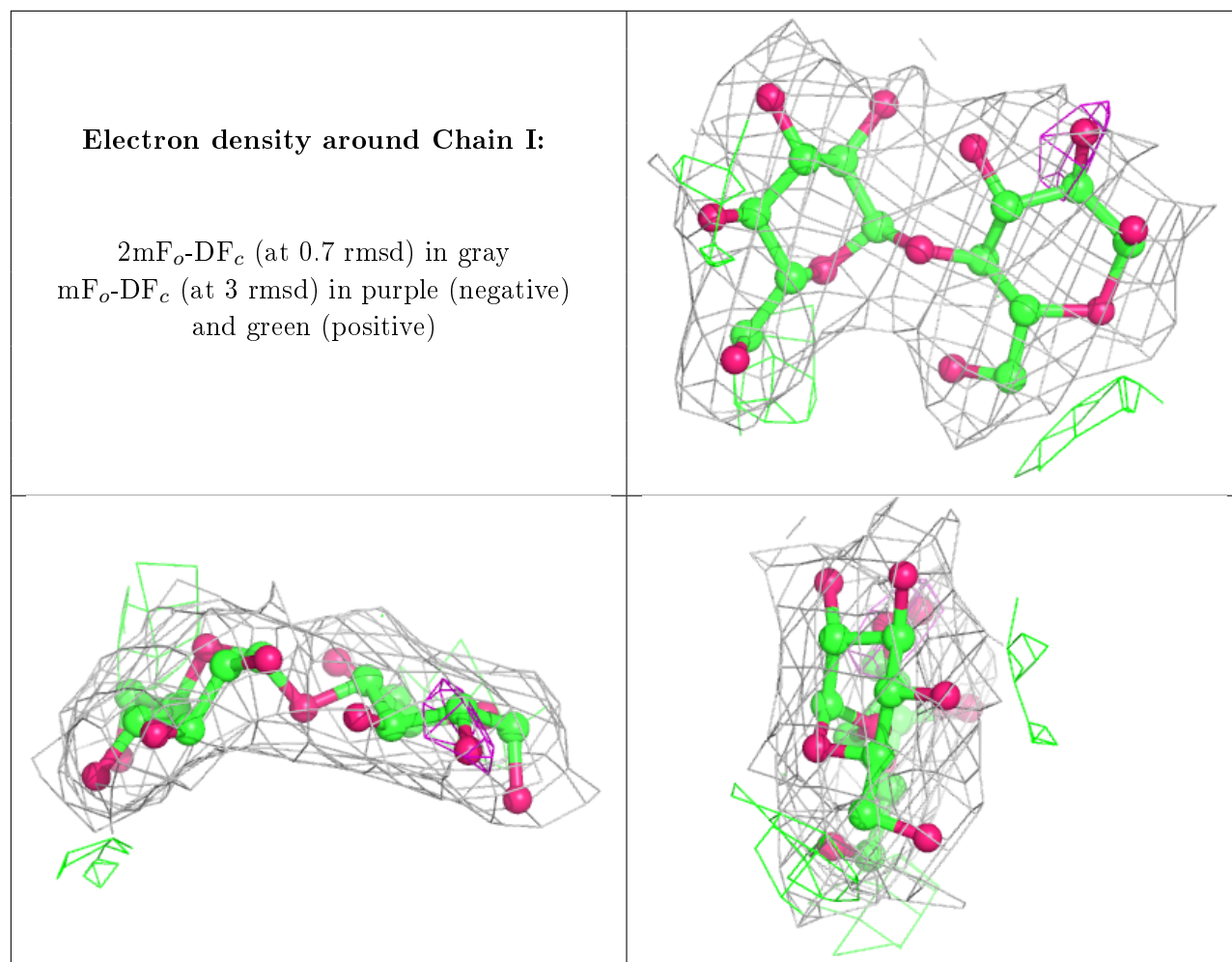
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLC	I	2	11/12	0.94	0.20	30,32,34,35	0
2	GLC	I	1	12/12	0.95	0.14	31,36,39,40	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.



6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
4	MES	A	5001	12/12	0.85	0.26	31,33,33,34	0
4	MES	D	5001	12/12	0.86	0.27	32,34,36,36	0
4	MES	E	5001	12/12	0.88	0.24	32,35,37,37	0
3	CA	C	4001	1/1	0.89	0.17	29,29,29,29	0
4	MES	C	5001	12/12	0.90	0.20	30,31,32,33	0
4	MES	F	5001	12/12	0.90	0.22	38,38,39,39	0
3	CA	E	4001	1/1	0.91	0.17	32,32,32,32	0
4	MES	G	5001	12/12	0.91	0.19	29,31,32,33	0
4	MES	H	5001	12/12	0.91	0.21	30,32,34,35	0
4	MES	B	5001	12/12	0.92	0.23	39,41,43,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	F	4001	1/1	0.94	0.17	40,40,40,40	0
3	CA	B	4001	1/1	0.96	0.19	32,32,32,32	0
3	CA	G	4001	1/1	0.96	0.17	28,28,28,28	0
3	CA	D	4001	1/1	0.96	0.15	30,30,30,30	0
3	CA	A	4001	1/1	0.96	0.15	29,29,29,29	0
3	CA	H	4001	1/1	0.97	0.16	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.