



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:49 PM UTC

PDB ID : 3AIB / pdb_00003aib
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 types of validation reports are described at

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

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

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

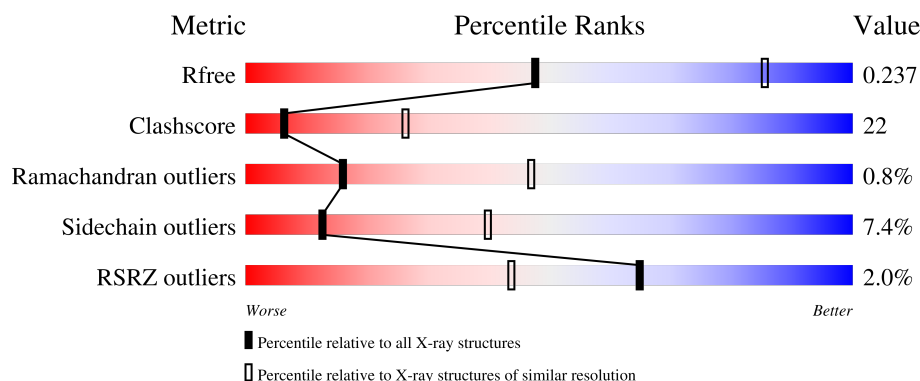
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	844	0.2% 67% 28% 5%
1	B	844	2% 48% 33% 7% 11%
1	C	844	0.2% 70% 26% .
1	D	844	2% 65% 29% 5%
1	E	844	4% 65% 30% 5%

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Mol	Chain	Length	Quality of chain
1	F	844	
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	A	5001	-	X	-	-
4	MES	B	5001	-	X	-	-
4	MES	D	5001	-	X	-	-
4	MES	F	5001	-	X	-	-
4	MES	G	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 (CCD ID: CA) (formula: Ca).

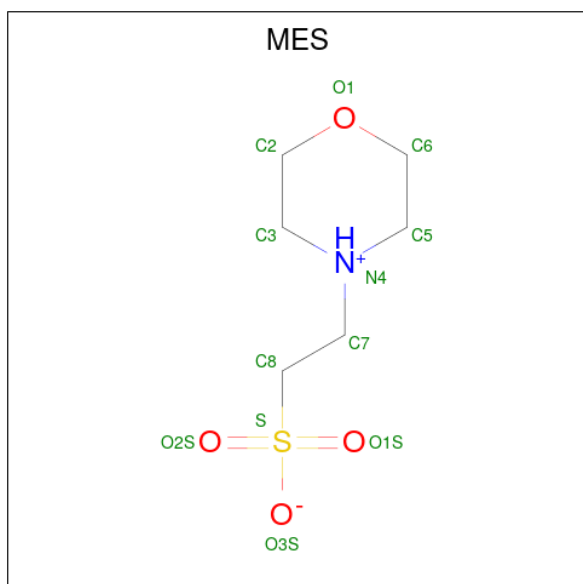
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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		

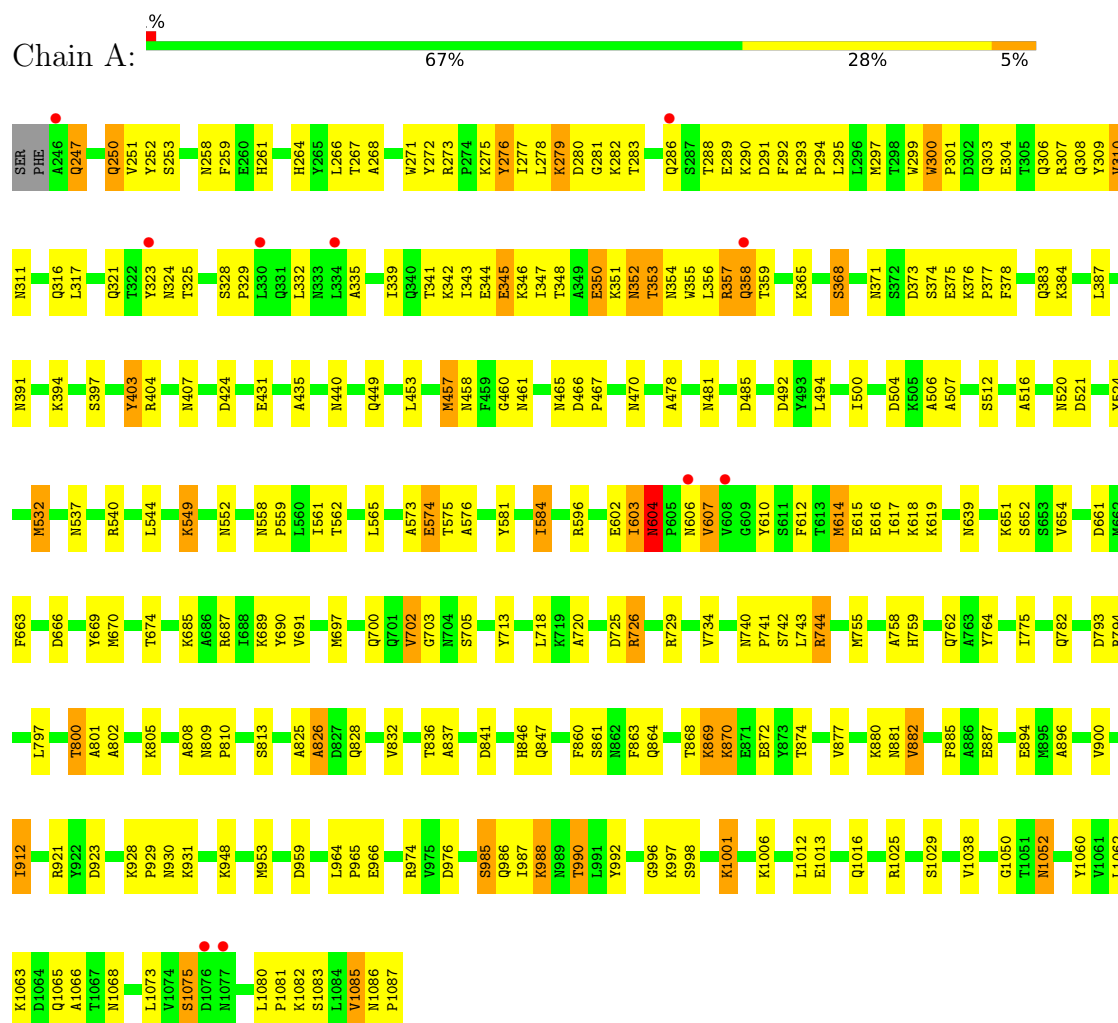
- Molecule 5 is water.

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		

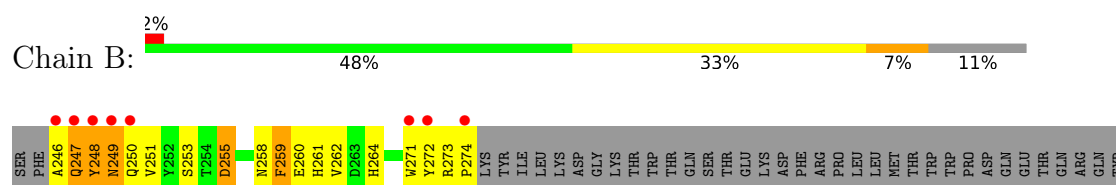
3 Residue-property plots

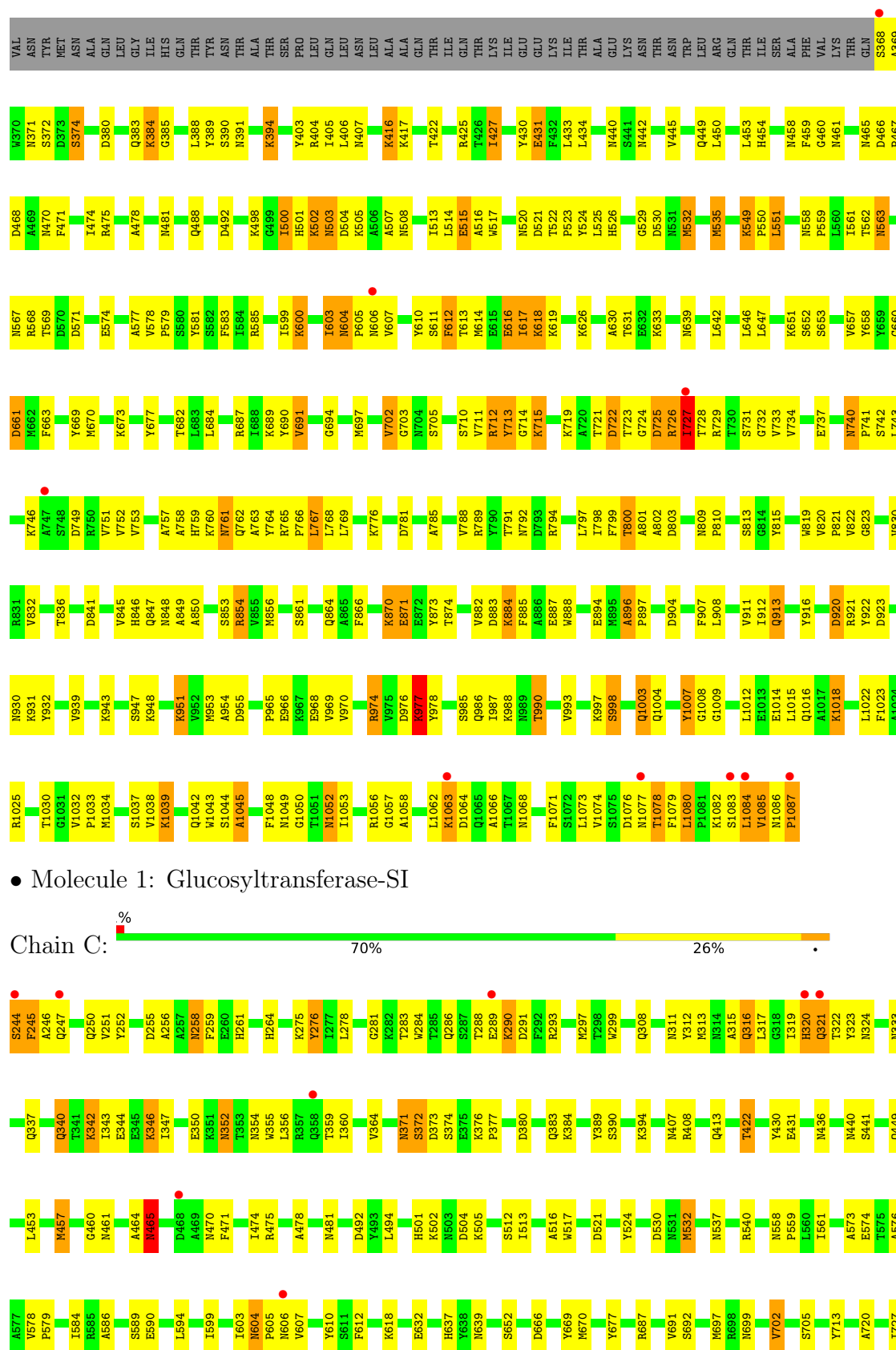
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



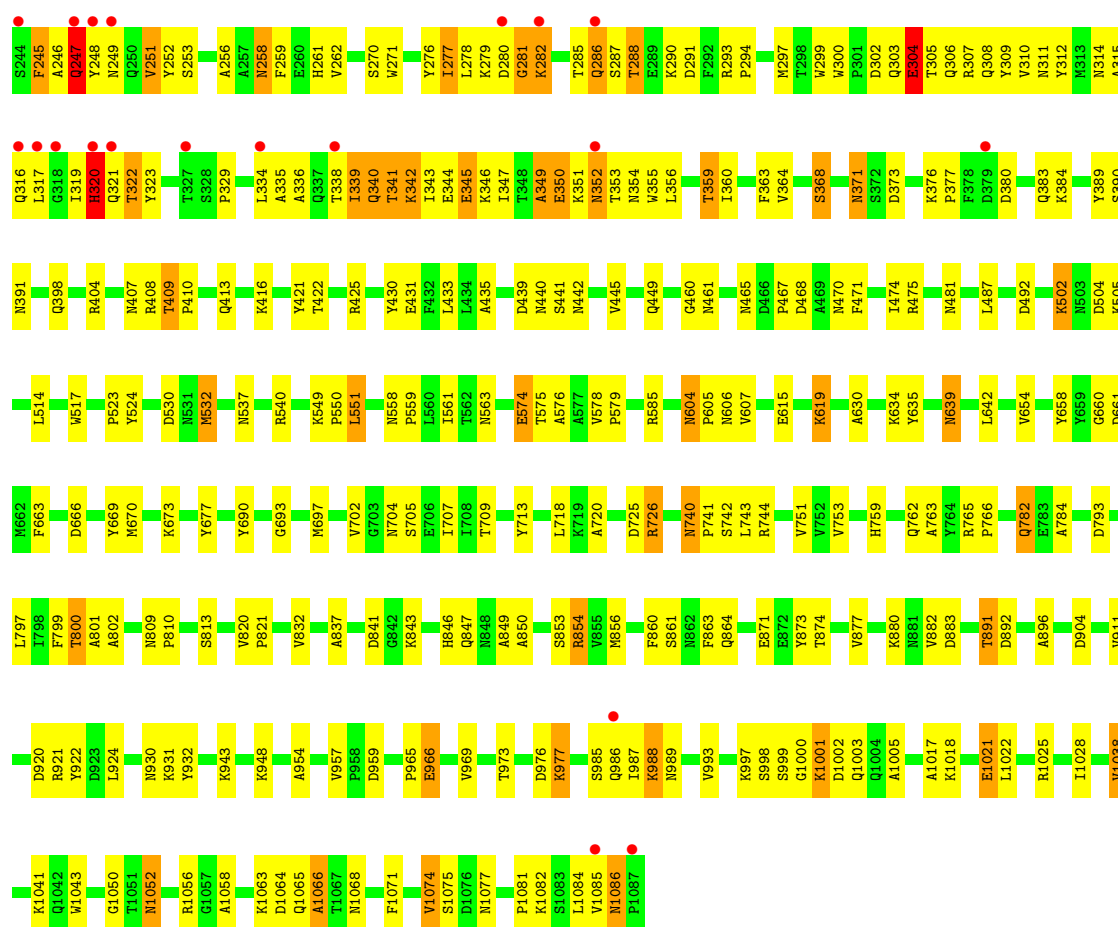
• Molecule 1: Glucosyltransferase-SI





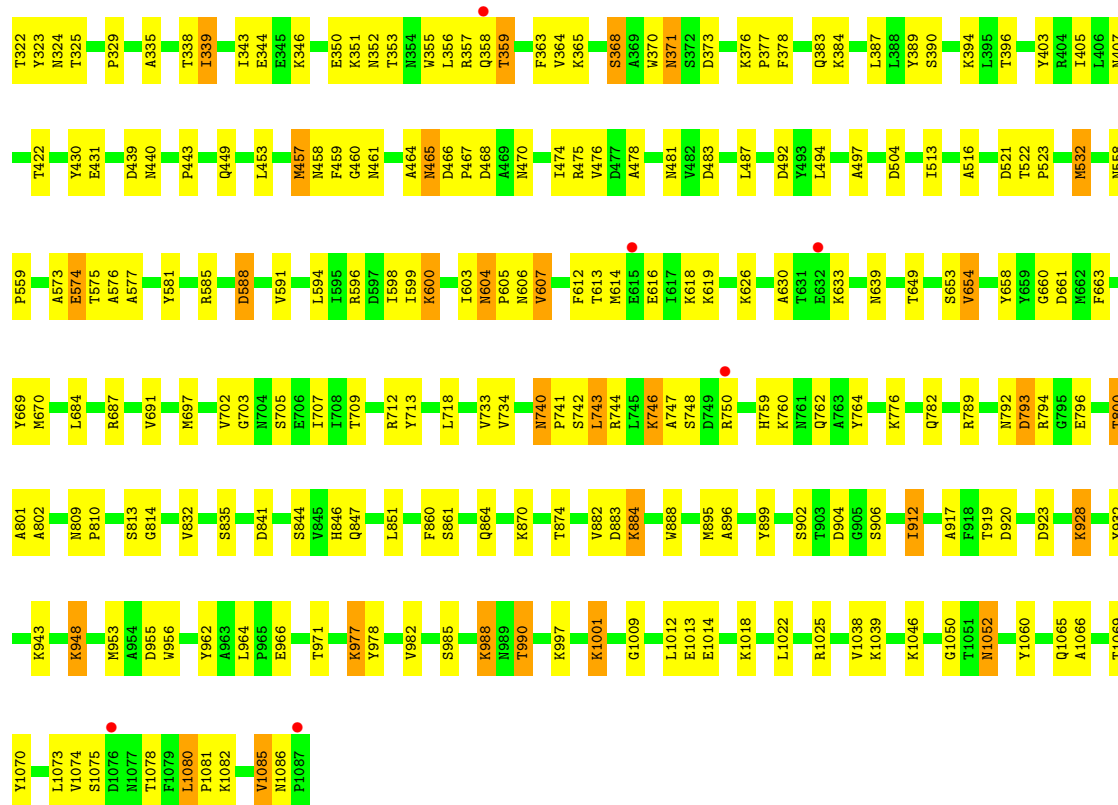


• Molecule 1: Glucosyltransferase-SI

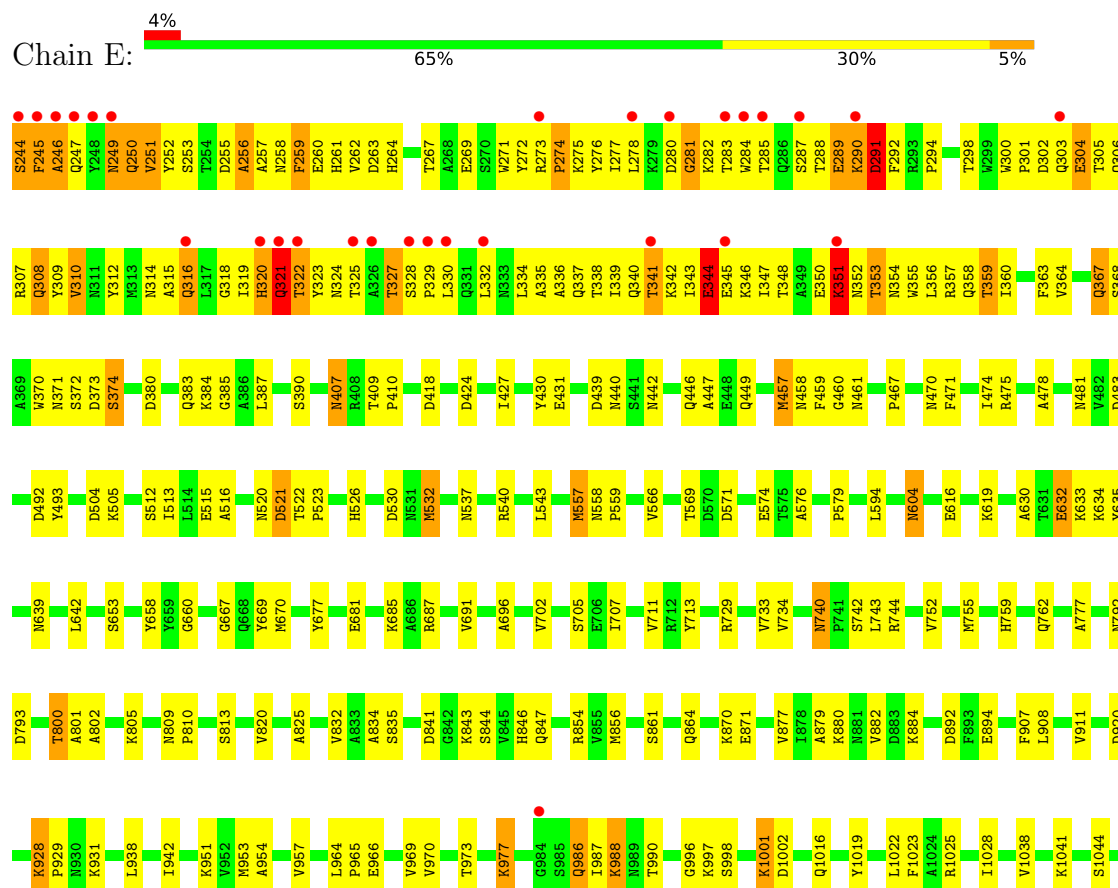


• Molecule 1: Glucosyltransferase-SI



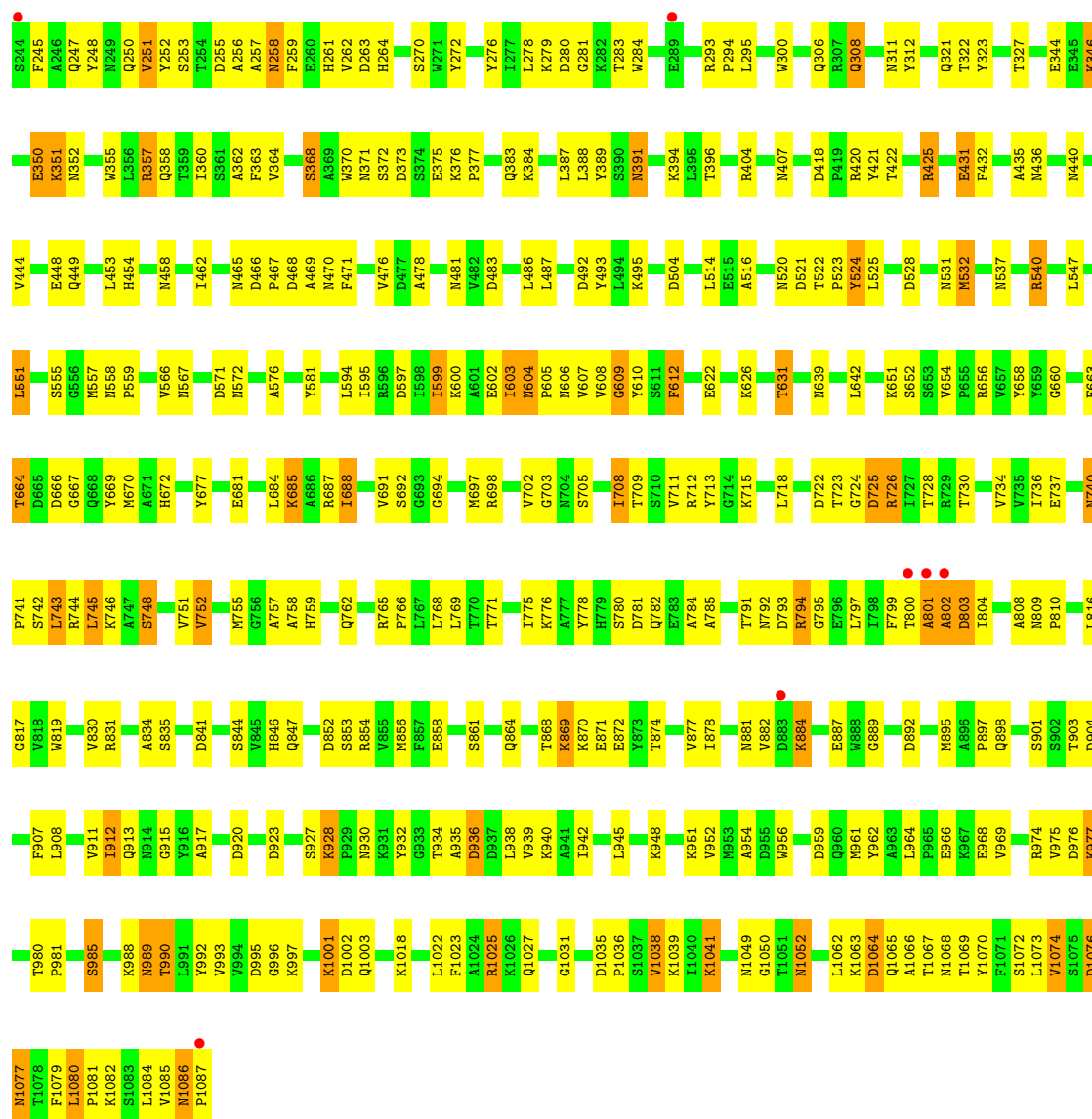


- Molecule 1: Glucosyltransferase-SI

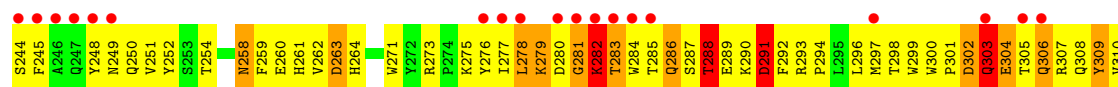


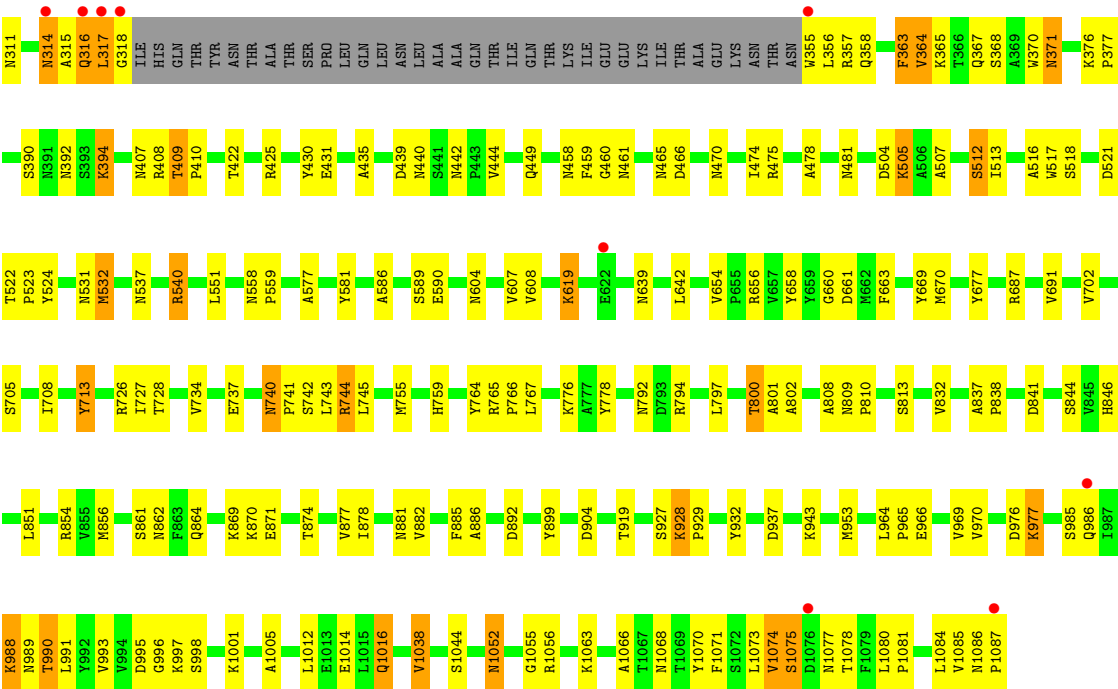


• Molecule 1: Glucosyltransferase-SI

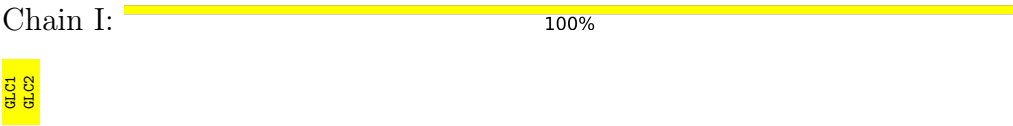


• Molecule 1: Glucosyltransferase-SI





● 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) 97.7 (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 , 0.237	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 , 30.9	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MES, GLC

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	1.30	17/6784 (0.3%)	1.27	19/9213 (0.2%)
1	B	1.18	7/5990 (0.1%)	1.30	40/8132 (0.5%)
1	C	1.35	18/6802 (0.3%)	1.25	26/9237 (0.3%)
1	D	1.30	11/6802 (0.2%)	1.27	38/9237 (0.4%)
1	E	1.30	14/6802 (0.2%)	1.28	36/9237 (0.4%)
1	F	1.07	5/6802 (0.1%)	1.19	27/9237 (0.3%)
1	G	1.33	12/6802 (0.2%)	1.28	28/9237 (0.3%)
1	H	1.19	7/6516 (0.1%)	1.23	27/8845 (0.3%)
All	All	1.26	91/53300 (0.2%)	1.26	241/72375 (0.3%)

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	314	ASN	CG-ND2	-10.39	1.11	1.33
1	D	340	GLN	CA-CB	10.32	1.70	1.53
1	A	507	ALA	CA-CB	-8.64	1.39	1.53
1	C	586	ALA	CA-CB	-7.37	1.42	1.53
1	B	403	TYR	N-CA	-7.34	1.41	1.46
1	A	403	TYR	N-CA	-7.29	1.41	1.46
1	A	606	ASN	N-CA	7.20	1.54	1.46
1	E	320	HIS	C-O	6.90	1.32	1.24
1	H	371	ASN	CA-C	-6.83	1.44	1.52
1	C	371	ASN	CA-C	-6.76	1.43	1.52
1	E	820	VAL	CA-CB	-6.53	1.48	1.55
1	B	1033	PRO	CA-C	-6.51	1.45	1.52
1	D	720	ALA	CA-CB	-6.49	1.42	1.53
1	C	1059	GLY	C-O	-6.46	1.19	1.24
1	B	515	GLU	CA-C	6.43	1.60	1.53
1	D	249	ASN	CG-ND2	6.29	1.46	1.33
1	G	358	GLN	CD-OE1	6.28	1.35	1.23
1	E	1028	ILE	CA-CB	-6.23	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1075	SER	N-CA	6.21	1.53	1.46
1	H	577	ALA	CA-CB	-6.21	1.43	1.53
1	C	720	ALA	CA-CB	-6.13	1.42	1.53
1	B	616	GLU	N-CA	-6.12	1.39	1.46
1	G	573	ALA	CA-CB	-6.06	1.44	1.53
1	C	573	ALA	CA-CB	-5.98	1.44	1.53
1	H	586	ALA	CA-CB	-5.95	1.43	1.53
1	A	720	ALA	CA-CB	-5.90	1.43	1.53
1	A	808	ALA	C-O	-5.86	1.17	1.24
1	A	614	MET	CA-C	-5.84	1.45	1.52
1	C	837	ALA	CA-CB	-5.83	1.45	1.53
1	G	750	ARG	CZ-NH1	5.80	1.40	1.32
1	A	775	ILE	N-CA	-5.79	1.39	1.46
1	E	970	VAL	CA-CB	-5.74	1.45	1.54
1	D	371	ASN	CA-C	-5.70	1.45	1.52
1	D	340	GLN	CB-CG	-5.68	1.35	1.52
1	F	251	VAL	CA-CB	-5.66	1.48	1.54
1	C	244	SER	CB-OG	5.64	1.53	1.42
1	A	726	ARG	CG-CD	5.64	1.69	1.52
1	G	654	VAL	N-CA	-5.63	1.42	1.46
1	C	965	PRO	C-O	-5.62	1.17	1.24
1	D	1038	VAL	C-O	-5.61	1.18	1.24
1	A	1075	SER	N-CA	5.60	1.53	1.46
1	E	447	ALA	CA-CB	-5.60	1.44	1.53
1	G	577	ALA	CA-CB	-5.59	1.44	1.53
1	C	319	ILE	CA-CB	-5.59	1.47	1.54
1	F	688	ILE	CA-CB	5.58	1.60	1.54
1	G	607	VAL	CA-C	5.57	1.60	1.52
1	A	562	THR	CA-CB	-5.57	1.45	1.53
1	B	563	ASN	CA-C	-5.55	1.45	1.52
1	B	1087	PRO	CB-CG	5.55	1.77	1.49
1	E	777	ALA	CA-CB	-5.53	1.44	1.53
1	G	814	GLY	C-O	-5.51	1.21	1.24
1	F	1086	ASN	CA-C	5.50	1.58	1.52
1	C	1053	ILE	CA-CB	-5.50	1.48	1.54
1	D	563	ASN	CA-C	-5.49	1.46	1.52
1	E	321	GLN	CA-C	5.47	1.60	1.52
1	E	566	VAL	CA-CB	5.47	1.61	1.54
1	C	699	ASN	C-O	-5.41	1.17	1.24
1	C	917	ALA	CA-CB	-5.39	1.45	1.53
1	G	1080	LEU	N-CA	5.38	1.49	1.46
1	B	1039	LYS	CB-CG	-5.38	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	879	ALA	CA-CB	-5.38	1.44	1.53
1	A	506	ALA	CA-CB	-5.36	1.44	1.53
1	C	849	ALA	CA-CB	-5.34	1.45	1.53
1	D	390	SER	CA-C	-5.34	1.45	1.52
1	E	1075	SER	N-CA	5.33	1.52	1.46
1	E	834	ALA	CA-CB	-5.33	1.44	1.53
1	A	358	GLN	CD-OE1	5.32	1.33	1.23
1	A	837	ALA	CA-CB	-5.29	1.45	1.53
1	A	808	ALA	CA-CB	-5.29	1.45	1.53
1	G	844	SER	CA-C	-5.27	1.46	1.53
1	A	573	ALA	CA-CB	-5.24	1.45	1.53
1	G	497	ALA	CA-CB	-5.22	1.44	1.53
1	D	693	GLY	C-O	-5.21	1.18	1.24
1	H	303	GLN	CA-C	5.20	1.59	1.52
1	G	955	ASP	N-CA	-5.18	1.40	1.46
1	D	763	ALA	CA-CB	-5.17	1.46	1.53
1	D	849	ALA	CA-CB	-5.17	1.44	1.53
1	C	794	ARG	CZ-NH1	5.16	1.40	1.32
1	C	863	PHE	N-CA	-5.15	1.40	1.46
1	C	692	SER	CA-C	-5.10	1.46	1.52
1	A	726	ARG	CD-NE	5.08	1.53	1.46
1	G	396	THR	CA-CB	5.08	1.57	1.53
1	C	1028	ILE	CA-CB	-5.08	1.48	1.54
1	F	743	LEU	CA-C	5.07	1.59	1.52
1	E	825	ALA	CA-CB	-5.05	1.45	1.53
1	F	911	VAL	C-O	-5.05	1.18	1.24
1	E	632	GLU	CG-CD	5.03	1.64	1.52
1	H	808	ALA	CA-CB	-5.02	1.45	1.53
1	E	752	VAL	C-O	-5.01	1.18	1.24
1	A	604	ASN	C-O	5.01	1.29	1.24
1	H	507	ALA	CA-CB	-5.01	1.45	1.53

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	245	PHE	N-CA-C	-13.27	97.08	113.01
1	H	289	GLU	N-CA-C	-13.27	97.13	113.18
1	H	245	PHE	N-CA-C	12.50	126.08	111.71
1	E	344	GLU	N-CA-C	11.91	124.25	111.03
1	E	320	HIS	N-CA-C	11.49	126.06	111.24
1	H	245	PHE	CB-CA-C	-11.35	89.64	110.63
1	E	245	PHE	N-CA-C	-9.67	101.50	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	740	ASN	CA-C-N	9.57	129.22	119.56
1	B	740	ASN	C-N-CA	9.57	129.22	119.56
1	D	959	ASP	N-CA-C	9.29	122.39	111.71
1	B	653	SER	CA-C-N	-9.15	116.00	122.59
1	B	653	SER	C-N-CA	-9.15	116.00	122.59
1	B	661	ASP	N-CA-C	-8.96	102.48	113.50
1	E	249	ASN	CA-CB-CG	8.83	121.43	112.60
1	A	328	SER	CA-C-N	-8.82	108.81	119.84
1	A	328	SER	C-N-CA	-8.82	108.81	119.84
1	D	320	HIS	N-CA-C	8.70	121.91	111.82
1	H	363	PHE	CA-CB-CG	8.67	122.47	113.80
1	C	319	ILE	N-CA-C	-8.64	97.62	109.55
1	G	604	ASN	CA-C-N	8.33	130.25	119.84
1	G	604	ASN	C-N-CA	8.33	130.25	119.84
1	B	574	GLU	N-CA-C	-8.20	102.42	111.36
1	F	959	ASP	N-CA-C	8.16	119.95	111.14
1	C	245	PHE	N-CA-C	-7.82	103.89	113.19
1	A	300	TRP	CA-C-N	7.81	127.53	119.56
1	A	300	TRP	C-N-CA	7.81	127.53	119.56
1	F	936	ASP	N-CA-C	7.72	120.59	111.71
1	B	549	LYS	CA-C-N	7.71	127.70	119.76
1	B	549	LYS	C-N-CA	7.71	127.70	119.76
1	E	653	SER	CA-C-N	-7.70	117.05	122.59
1	E	653	SER	C-N-CA	-7.70	117.05	122.59
1	B	722	ASP	N-CA-C	7.66	121.05	110.24
1	D	339	ILE	CB-CA-C	-7.66	101.80	112.14
1	D	911	VAL	N-CA-C	-7.60	104.45	111.67
1	E	246	ALA	N-CA-C	-7.52	103.02	111.07
1	D	247	GLN	N-CA-C	7.52	119.56	111.36
1	E	344	GLU	CB-CA-C	-7.49	99.35	110.95
1	G	1085	VAL	CB-CA-C	-7.30	104.30	111.30
1	C	911	VAL	N-CA-C	-7.19	104.77	111.45
1	B	1076	ASP	N-CA-C	-7.18	104.78	113.97
1	F	1002	ASP	N-CA-C	7.18	119.83	110.43
1	G	653	SER	CA-C-N	-7.17	117.42	122.59
1	G	653	SER	C-N-CA	-7.17	117.42	122.59
1	B	727	ILE	N-CA-C	7.06	117.78	110.36
1	B	725	ASP	N-CA-C	-7.03	98.95	108.86
1	E	1028	ILE	N-CA-C	7.01	117.72	110.36
1	D	1017	ALA	N-CA-C	-6.92	103.43	110.97
1	H	317	LEU	N-CA-C	-6.91	102.86	112.25
1	B	488	GLN	N-CA-C	-6.90	103.84	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	328	SER	CA-C-N	-6.80	111.34	119.84
1	E	328	SER	C-N-CA	-6.80	111.34	119.84
1	B	603	ILE	CA-C-N	-6.73	114.71	122.52
1	B	603	ILE	C-N-CA	-6.73	114.71	122.52
1	B	1062	LEU	N-CA-C	6.68	119.98	109.96
1	D	1018	LYS	N-CA-C	6.67	118.64	111.36
1	B	896	ALA	CA-C-N	-6.54	113.23	119.90
1	B	896	ALA	C-N-CA	-6.54	113.23	119.90
1	C	517	TRP	N-CA-C	6.47	119.33	111.82
1	A	1085	VAL	CB-CA-C	-6.38	105.37	111.05
1	F	1002	ASP	N-CA-CB	-6.37	101.15	110.26
1	C	291	ASP	N-CA-C	6.37	119.53	110.68
1	E	256	ALA	N-CA-C	-6.36	104.39	111.71
1	H	1075	SER	N-CA-C	6.35	119.01	111.71
1	H	1005	ALA	N-CA-C	-6.30	104.33	111.07
1	E	594	LEU	N-CA-C	-6.23	104.57	111.36
1	A	885	PHE	N-CA-C	-6.21	104.59	111.36
1	G	291	ASP	N-CA-C	6.19	123.98	110.80
1	E	418	ASP	CA-C-N	6.18	125.87	119.56
1	E	418	ASP	C-N-CA	6.18	125.87	119.56
1	A	674	THR	N-CA-C	-6.16	101.66	110.59
1	D	619	LYS	N-CA-C	-6.15	104.65	111.36
1	D	837	ALA	CA-C-N	-6.12	113.64	119.76
1	D	837	ALA	C-N-CA	-6.12	113.64	119.76
1	G	626	LYS	N-CA-C	-6.11	104.53	111.07
1	C	321	GLN	N-CA-C	-6.06	100.53	109.81
1	F	396	THR	CB-CA-C	-6.06	102.11	111.74
1	D	753	VAL	N-CA-C	6.04	116.56	107.80
1	H	661	ASP	N-CA-C	-6.00	105.96	113.28
1	G	964	LEU	CA-C-N	5.99	125.38	118.85
1	G	964	LEU	C-N-CA	5.99	125.38	118.85
1	G	371	ASN	CB-CA-C	-5.99	98.53	111.11
1	B	517	TRP	N-CA-C	5.97	117.87	111.36
1	B	1080	LEU	N-CA-C	5.95	115.15	108.25
1	D	517	TRP	N-CA-C	5.93	117.82	111.36
1	H	505	LYS	N-CA-C	-5.93	104.90	111.36
1	B	427	ILE	N-CA-C	-5.92	106.73	112.29
1	F	928	LYS	CA-C-N	-5.88	114.20	120.03
1	F	928	LYS	C-N-CA	-5.88	114.20	120.03
1	C	441	SER	N-CA-C	-5.87	106.16	113.38
1	H	885	PHE	N-CA-C	-5.86	104.84	112.23
1	C	371	ASN	CB-CA-C	-5.86	98.81	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1075	SER	N-CA-C	5.84	120.95	111.37
1	B	920	ASP	N-CA-C	5.83	119.42	107.69
1	B	1007	TYR	N-CA-C	5.82	120.66	113.50
1	B	968	GLU	CA-C-N	-5.81	115.61	122.93
1	B	968	GLU	C-N-CA	-5.81	115.61	122.93
1	A	826	ALA	N-CA-C	-5.79	105.05	111.71
1	B	562	THR	N-CA-C	5.77	120.59	113.50
1	C	666	ASP	CA-C-N	-5.76	112.00	121.92
1	C	666	ASP	C-N-CA	-5.76	112.00	121.92
1	H	989	ASN	CB-CA-C	-5.75	103.73	111.89
1	H	767	LEU	N-CA-C	-5.75	105.04	112.68
1	C	422	THR	N-CA-CB	-5.71	102.99	110.88
1	A	549	LYS	CA-C-N	5.71	125.72	119.89
1	A	549	LYS	C-N-CA	5.71	125.72	119.89
1	B	1085	VAL	N-CA-C	5.71	116.47	111.56
1	H	364	VAL	N-CA-C	-5.70	103.31	111.17
1	A	959	ASP	N-CA-C	5.68	117.55	111.36
1	E	353	THR	N-CA-C	-5.67	104.57	113.02
1	D	549	LYS	CA-C-N	5.66	125.67	119.90
1	D	549	LYS	C-N-CA	5.66	125.67	119.90
1	F	1080	LEU	CA-C-N	5.65	126.90	119.84
1	F	1080	LEU	C-N-CA	5.65	126.90	119.84
1	E	407	ASN	N-CA-C	5.64	119.46	112.24
1	G	603	ILE	CA-C-N	-5.63	115.60	122.64
1	G	603	ILE	C-N-CA	-5.63	115.60	122.64
1	C	465	ASN	CB-CA-C	-5.63	103.73	111.73
1	E	320	HIS	CB-CA-C	-5.63	101.57	110.86
1	A	552	ASN	N-CA-C	5.62	119.39	112.54
1	E	942	ILE	N-CA-C	-5.62	105.05	110.72
1	B	431	GLU	N-CA-C	5.61	117.19	111.14
1	C	885	PHE	N-CA-C	-5.61	105.25	111.36
1	A	1075	SER	N-CA-C	5.59	117.46	111.36
1	D	320	HIS	N-CA-CB	-5.59	101.61	110.28
1	D	441	SER	N-CA-C	-5.59	106.50	113.38
1	B	911	VAL	N-CA-C	-5.58	105.66	111.58
1	D	1028	ILE	N-CA-C	5.57	115.77	110.42
1	F	1001	LYS	CA-C-N	5.57	130.28	120.87
1	F	1001	LYS	C-N-CA	5.57	130.28	120.87
1	H	517	TRP	N-CA-C	5.55	119.22	112.23
1	F	622	GLU	N-CA-C	-5.55	104.87	111.03
1	H	249	ASN	OD1-CG-ND2	-5.54	117.06	122.60
1	D	270	SER	N-CA-C	5.52	118.24	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	713	TYR	N-CA-C	5.51	117.28	111.28
1	C	276	TYR	N-CA-C	5.50	117.78	109.41
1	G	284	TRP	N-CA-C	-5.50	101.71	109.96
1	A	368	SER	N-CA-C	5.49	117.69	111.11
1	D	639	ASN	N-CA-C	5.48	118.99	111.54
1	D	630	ALA	N-CA-C	5.47	118.17	109.96
1	D	1005	ALA	N-CA-C	-5.47	106.11	112.89
1	H	512	SER	N-CA-C	5.47	118.61	110.14
1	A	1006	LYS	N-CA-C	5.47	117.32	111.36
1	F	283	THR	N-CA-C	5.46	119.11	107.70
1	D	475	ARG	N-CA-C	-5.43	100.55	109.40
1	C	794	ARG	N-CA-C	-5.43	106.33	113.17
1	F	1077	ASN	N-CA-C	5.43	119.06	111.30
1	F	391	ASN	N-CA-C	5.42	118.11	111.82
1	C	702	VAL	CB-CA-C	-5.42	102.02	110.69
1	E	1075	SER	CA-C-N	5.41	127.53	120.28
1	E	1075	SER	C-N-CA	5.41	127.53	120.28
1	E	367	GLN	N-CA-C	5.41	117.33	108.52
1	E	604	ASN	CA-C-N	5.40	125.73	119.47
1	E	604	ASN	C-N-CA	5.40	125.73	119.47
1	D	891	THR	N-CA-C	-5.40	107.06	113.97
1	E	1019	TYR	CA-C-N	5.39	125.21	119.28
1	E	1019	TYR	C-N-CA	5.39	125.21	119.28
1	D	784	ALA	N-CA-C	-5.38	105.42	112.41
1	E	987	ILE	CB-CA-C	-5.38	106.55	112.68
1	C	289	GLU	N-CA-C	-5.37	105.83	112.38
1	A	713	TYR	N-CA-C	5.36	119.08	112.54
1	F	1041	LYS	N-CA-C	-5.34	106.90	113.41
1	H	409	THR	CA-C-N	-5.34	113.69	119.24
1	H	409	THR	C-N-CA	-5.34	113.69	119.24
1	E	616	GLU	N-CA-C	-5.34	105.46	111.28
1	D	690	TYR	CA-C-N	-5.33	115.95	122.93
1	D	690	TYR	C-N-CA	-5.33	115.95	122.93
1	G	978	TYR	N-CA-C	-5.33	106.63	113.02
1	G	353	THR	N-CA-C	-5.33	105.06	112.30
1	F	889	GLY	N-CA-C	-5.32	107.94	115.43
1	B	753	VAL	CB-CA-C	-5.31	104.33	110.91
1	G	319	ILE	N-CA-CB	5.31	117.53	110.26
1	F	609	GLY	CA-C-N	-5.30	114.30	123.25
1	F	609	GLY	C-N-CA	-5.30	114.30	123.25
1	C	340	GLN	N-CA-C	-5.29	105.51	111.28
1	G	793	ASP	CB-CA-C	-5.29	101.68	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	398	GLN	N-CA-C	-5.29	106.66	113.01
1	D	409	THR	CA-C-N	-5.29	113.29	119.32
1	D	409	THR	C-N-CA	-5.29	113.29	119.32
1	C	283	THR	N-CA-C	5.27	117.66	108.76
1	G	899	TYR	CA-CB-CG	-5.25	104.45	113.90
1	H	518	SER	N-CA-C	5.25	117.85	110.23
1	D	249	ASN	N-CA-C	5.25	118.84	112.23
1	F	431	GLU	N-CA-C	5.25	117.08	111.36
1	F	631	THR	N-CA-C	-5.23	105.66	111.36
1	E	667	GLY	N-CA-C	5.22	119.26	112.68
1	F	1062	LEU	N-CA-C	5.22	117.78	109.96
1	B	753	VAL	N-CA-C	5.21	116.09	108.58
1	F	1018	LYS	N-CA-C	5.21	118.10	111.69
1	D	989	ASN	CB-CA-C	-5.21	104.89	111.86
1	G	619	LYS	N-CA-C	-5.20	105.69	111.36
1	B	569	THR	N-CA-C	-5.19	104.54	111.24
1	E	521	ASP	N-CA-C	5.18	116.93	111.28
1	B	403	TYR	CA-CB-CG	-5.18	104.58	113.90
1	C	372	SER	N-CA-C	-5.18	106.92	113.18
1	G	368	SER	N-CA-C	5.17	117.31	111.11
1	F	989	ASN	CB-CA-C	-5.17	104.93	111.86
1	C	343	ILE	CB-CA-C	-5.17	105.25	112.02
1	B	1039	LYS	N-CA-C	5.16	117.82	109.40
1	E	792	ASN	CA-C-N	-5.15	114.41	122.65
1	E	792	ASN	C-N-CA	-5.15	114.41	122.65
1	H	886	ALA	N-CA-C	-5.15	105.75	111.36
1	B	1048	PHE	N-CA-C	5.15	117.95	109.72
1	D	1075	SER	N-CA-C	5.14	116.57	111.07
1	H	435	ALA	N-CA-C	5.13	115.60	108.00
1	D	425	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	D	966	GLU	N-CA-C	5.13	117.85	109.59
1	H	737	GLU	N-CA-C	5.13	117.60	109.50
1	E	1041	LYS	N-CA-C	-5.13	107.16	113.41
1	B	977	LYS	CB-CA-C	-5.12	100.23	110.42
1	E	557	MET	N-CA-C	5.11	119.52	113.28
1	A	353	THR	N-CA-C	-5.10	106.18	114.09
1	D	977	LYS	CA-CB-CG	5.10	124.30	114.10
1	F	425	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	G	743	LEU	N-CA-C	5.10	117.94	110.30
1	A	661	ASP	N-CA-C	-5.09	107.12	113.38
1	E	931	LYS	N-CA-C	-5.09	106.33	112.54
1	B	767	LEU	N-CA-C	-5.09	104.71	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	245	PHE	N-CA-C	-5.09	107.14	113.19
1	F	462	ILE	CB-CA-C	-5.08	105.21	112.22
1	E	911	VAL	N-CA-C	-5.08	106.73	111.45
1	C	594	LEU	N-CA-C	-5.06	105.84	111.36
1	H	288	THR	CB-CA-C	5.06	122.10	112.43
1	G	982	VAL	N-CA-C	5.06	116.92	109.63
1	D	1041	LYS	N-CA-C	-5.05	107.25	113.41
1	B	1018	LYS	N-CA-C	5.05	118.59	112.23
1	B	468	ASP	N-CA-C	-5.04	107.10	113.20
1	H	899	TYR	CA-CB-CG	-5.04	104.83	113.90
1	D	338	THR	N-CA-C	-5.03	105.87	111.36
1	A	617	ILE	N-CA-C	5.03	115.64	110.36
1	H	1055	GLY	N-CA-C	-5.03	107.88	115.32
1	B	691	VAL	N-CA-C	5.03	114.84	107.15
1	F	901	SER	N-CA-C	5.02	117.72	110.28
1	C	652	SER	CB-CA-C	-5.02	103.61	111.39
1	C	501	HIS	N-CA-C	-5.02	107.15	113.28
1	G	902	SER	CA-C-N	-5.02	114.61	122.49
1	G	902	SER	C-N-CA	-5.02	114.61	122.49
1	H	608	VAL	CB-CA-C	-5.02	104.10	110.98
1	G	249	ASN	N-CA-C	5.01	118.65	112.54
1	C	637	HIS	N-CA-C	5.01	117.69	110.28
1	G	1012	LEU	CA-C-N	-5.01	112.16	120.68
1	G	1012	LEU	C-N-CA	-5.01	112.16	120.68

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6643	0	6475	256	0
1	B	5868	0	5704	356	0
1	C	6660	0	6489	195	0
1	D	6660	0	6489	278	0
1	E	6660	0	6489	323	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	6660	0	6489	368	0
1	G	6660	0	6489	225	0
1	H	6378	0	6201	284	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
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	2285	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 22.

All (2285) 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:CB	1:B:1087:PRO:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:669:TYR:CE2	1:B:670:MET:HE3	1.65	1.30
1:F:669:TYR:CE2	1:F:670:MET:HE2	1.72	1.24
1:H:669:TYR:CE2	1:H:670:MET:HE2	1.73	1.21
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: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:D:669:TYR:CE2	1:D:670:MET:HE2	1.80	1.15
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: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
1:H:248:TYR:HB3	1:H:276:TYR:HB2	1.27	1.13
1:E:475:ARG:CB	1:E:953:MET:HE2	1.78	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: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:C:475:ARG:HB2	1:C:953:MET:HE2	1.12	1.11
1:D:277:ILE:HD13	1:D:291:ASP:HB3	1.30	1.11
1:H:278:LEU:HD21	1:H:281:GLY:HA2	1.29	1.11
1:E:513:ILE:HG12	1:E:953:MET:HE1	1.21	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:HH11	1:B:712:ARG:HG3	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:CE	1.80	1.10
1:F:709:THR:HG22	1:F:736:ILE:HD13	1.34	1.09
1:H:513:ILE:CG1	1:H:953:MET:HE1	1.82	1.09
1:B:712:ARG:HH11	1:B:712:ARG:CG	1.64	1.09
1:D:336:ALA:HA	1:D:339:ILE:HD12	1.29	1.09
1:G:800:THR:HG22	1:G:802:ALA:N	1.67	1.09
1:F:726:ARG:HH11	1:F:726:ARG:HG2	1.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:726:ARG:HG2	1:D:726:ARG:HH11	1.13	1.07
1:H:800:THR:HG22	1:H:802:ALA:H	1.18	1.07
1:B:262:VAL:HG12	1:B:969:VAL:HG23	1.30	1.06
1:B:854:ARG:HG2	1:B:854:ARG:HH11	1.20	1.06
1:E:513:ILE:CG1	1:E:953:MET:HE1	1.84	1.06
1:D:303:GLN:NE2	1:D:329:PRO:HG3	1.69	1.06
1:E:1085:VAL:HG23	1:E:1086:ASN:N	1.56	1.05
1:H:669:TYR:HE2	1:H:670:MET:HE2	0.96	1.05
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:B:513:ILE:HD13	1:B:856:MET:HE1	1.39	1.04
1:F:261:HIS:HD2	1:F:264:HIS:H	1.06	1.04
1:F:726:ARG:HG2	1:F:726:ARG:NH1	1.64	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
1:G:513:ILE:HG12	1:G:953:MET:HE1	1.35	1.03
1:E:271:TRP:CE2	1:E:357:ARG:HD3	1.92	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: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:HA	1:H:316:GLN:NE2	1.68	1.02
1:G:475:ARG:CB	1:G:953:MET:HE2	1.88	1.02
1:H:316:GLN:HA	1:H:316:GLN:HE21	1.19	1.02
1:B:610:TYR:HA	1:B:612:PHE:CE2	1.95	1.01
1:D:303:GLN:HE22	1:D:329:PRO:HG3	1.22	1.01
1:G:316:GLN:NE2	1:G:316:GLN:HA	1.71	1.01
1:B:861:SER:H	1:B:864:GLN:HE21	1.07	1.00
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:669:TYR:HE2	1:B:670:MET:HE3	1.22	1.00
1:A:275:LYS:C	1:A:276:TYR:HD2	1.69	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:974:ARG:HG3	1:B:974:ARG:HH11	1.21	0.99
1:E:330:LEU:HD12	1:E:330:LEU:O	1.62	0.99
1:F:669:TYR:HE2	1:F:670:MET:HE2	1.10	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:H	1:B:1052:ASN:HD22	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:H:669:TYR:CE2	1:H:670:MET:CE	2.45	0.98
1:F:669:TYR:CE2	1:F:670:MET:CE	2.46	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:E:670:MET:HE3	1:E:877:VAL:HG12	1.46	0.97
1:B:974:ARG:HG3	1:B:974:ARG:NH1	1.78	0.97
1:D:726:ARG:HH11	1:D:726:ARG:CG	1.78	0.97
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:E:669:TYR:CE2	1:E:670:MET:HE2	1.98	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
1:H:475:ARG:HB2	1:H:953:MET:HE2	1.47	0.96
4:A:5001:MES:C5	4:A:5001:MES:O2S	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:B:800:THR:HG22	1:B:802:ALA:H	0.81	0.95
1:E:475:ARG:HB2	1:E:953:MET:HE2	0.96	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: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:G:335:ALA:O	1:G:339:ILE:HD12	1.65	0.95
1:E:273:ARG:HH11	1:E:289:GLU:HA	1.32	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:800:THR:HG22	1:E:802:ALA:H	1.28	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:A:273:ARG:HH21	1:A:288:THR:C	1.75	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:OE1	1:B:871:GLU:N	2.00	0.94
1:G:861:SER:H	1:G:864:GLN:HE21	1.13	0.94
1:G:475:ARG:HB2	1:G:953:MET:HE2	0.94	0.94
1:E:320:HIS:O	1:E:321:GLN:O	1.86	0.94
1:D:303:GLN:CD	1:D:329:PRO:HG3	1.92	0.93
1:C:639:ASN:HD21	1:C:813:SER:H	1.15	0.93
1:B:394:LYS:H	1:B:394:LYS:CD	1.80	0.93
1:B:1074:VAL:HG12	1:B:1077:ASN:HB3	1.48	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:OE1	1:B:1003:GLN:CA	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
1:F:745:LEU:H	1:F:745:LEU:HD12	1.33	0.93
1:B:513:ILE:HG21	1:B:856:MET:HE1	1.50	0.92
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:H:513:ILE:HG12	1:H:953:MET:HE1	0.95	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:HA	1:G:316:GLN:HE21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:513:ILE:CG1	1:G:953:MET:HE1	2.01	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: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:E:513:ILE:CD1	1:E:953:MET:HE1	2.03	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: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:HD3	1:B:951:LYS:N	1.86	0.88
1:D:726:ARG:HG2	1:D:726:ARG:NH1	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
1:E:669:TYR:HE2	1:E:670:MET:HE2	1.34	0.87
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:475:ARG:CB	1:G:953:MET:CE	2.52	0.85
1:C:475:ARG:HB2	1:C:953:MET:HE3	1.54	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:HD22	1:F:1052:ASN:H	1.23	0.84
1:H:1052:ASN:HD22	1:H:1052:ASN:H	1.19	0.84
1:B:440:ASN:HD21	1:B:449:GLN:HE21	1.23	0.84
1:B:513:ILE:HD13	1:B:856:MET:CE	2.08	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:HH11	1:F:726:ARG:CB	1.90	0.84
1:B:631:THR:HG23	1:B:809:ASN:CA	2.08	0.84
1:C:513:ILE:HG12	1:C:953:MET:HE1	1.59	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:H:513:ILE:HD13	1:H:856:MET:HE1	1.58	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:ASP:HB3	1:D:1022:LEU:HD22	1.61	0.83
1:B:513:ILE:HG12	1:B:953:MET:HE1	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:HH11	1:F:357:ARG:CG	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:D:293:ARG:HB3	1:D:297:MET:HE2	1.61	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:1065:GLN:HG3	1:D:1066:ALA:N	1.90	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:A:740:ASN:HD22	1:A:740:ASN:C	1.88	0.81
1:D:303:GLN:HE22	1:D:329:PRO:CG	1.93	0.81
1:D:669:TYR:HE2	1:D:670:MET:CE	1.89	0.81
1:G:614:MET:HG3	1:G:618:LYS:HE3	1.61	0.81
1:E:513:ILE:HD13	1:E:856:MET:HE1	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
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:G:1052:ASN:H	1:G:1052:ASN:HD22	1.28	0.81
1:E:740:ASN:ND2	1:E:742:SER:H	1.79	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:G:251:VAL:HG21	1:G:259:PHE:HZ	1.47	0.80
1:E:861:SER:N	1:E:864:GLN:HE21	1.77	0.80
1:H:466:ASP:OD2	1:H:943:LYS:CE	2.28	0.80
1:H:1085:VAL:CG2	1:H:1086:ASN:H	1.93	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:H:475:ARG:CB	1:H:953:MET:HE2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD3	1:H:394:LYS:H	1.40	0.80
1:H:740:ASN:C	1:H:740:ASN:HD22	1.90	0.80
1:B:1074:VAL:CG1	1:B:1077:ASN:CB	2.59	0.80
1:G:740:ASN:C	1:G:740:ASN:HD22	1.90	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:H	1:F:708:ILE:HD13	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:H:317:LEU:O	1:H:318:GLY:C	2.25	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: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
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:D:300:TRP:CG	1:D:306:GLN:HB2	2.18	0.78
1:D:1065:GLN:HG3	1:D:1066:ALA:H	1.46	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:G:346:LYS:HD3	1:G:355:TRP:CZ2	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:492:ASP:HB3	1:G:1022:LEU:CD2	2.15	0.76
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:B:871:GLU:H	1:B:871:GLU:CD	1.93	0.76
1:G:740:ASN:HD22	1:G:742:SER:H	1.33	0.76
1:D:740:ASN:HD22	1:D:740:ASN:C	1.91	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
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:C:475:ARG:CA	1:C:953:MET:HE3	2.15	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:HD22	1:E:1052:ASN:H	1.31	0.76
1:H:861:SER:N	1:H:864:GLN:HE21	1.84	0.76
1:B:513:ILE:HG12	1:B:953:MET:CE	2.16	0.75
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:F:516:ALA:HB1	1:F:521:ASP:OD2	1.86	0.75
1:E:271:TRP:CG	1:E:357:ARG:NH1	2.55	0.75
1:H:475:ARG:CA	1:H:953:MET:HE2	2.16	0.75
1:C:460:GLY:N	1:C:470:ASN:ND2	2.35	0.75
1:C:1063:LYS:HE2	1:C:1068:ASN:ND2	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:669:TYR:CD2	1:B:670:MET:HE3	2.22	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:407:ASN:ND2	1:F:431:GLU:H	1.86	0.74
1:F:1070:TYR:CD2	5:F:242:HOH:O	2.41	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:355:TRP:HE3	1:D:359:THR:HG21	1.52	0.74
1:D:999:SER:O	1:D:1001:LYS:N	2.21	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:A:275:LYS:C	1:A:276:TYR:CD2	2.60	0.73
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:E:670:MET:HE3	1:E:877:VAL:CG1	2.17	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
1:E:244:SER:N	1:E:246:ALA:H	1.85	0.73
1:E:740:ASN:HD22	1:E:740:ASN:C	1.95	0.73
1:F:1052:ASN:H	1:F:1052:ASN:ND2	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:H:734:VAL:HB	1:H:755:MET:HE1	1.71	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:N	1:B:259:PHE:CD2	2.56	0.73
1:B:416:LYS:HE2	1:F:551:LEU:HD12	1.71	0.73
1:B:726:ARG:HG2	1:B:727:ILE:H	1.54	0.73
1:F:745:LEU:CD1	1:F:801:ALA:HA	2.17	0.73
1:D:740:ASN:HD22	1:D:742:SER:H	1.33	0.73
1:D:1052:ASN:H	1:D:1052:ASN:ND2	1.82	0.73
1:C:513:ILE:CG1	1:C:953:MET:HE1	2.19	0.73
1:G:478:ALA:HB1	1:G:481:ASN:HD22	1.54	0.73
1:E:1001:LYS:O	1:E:1001:LYS:CG	2.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1068:ASN:CG	1:E:1068:ASN:O	2.32	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:H:355:TRP:CG	1:H:356:LEU:H	2.06	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:C:670:MET:HE1	1:C:885:PHE:HZ	1.55	0.72
1:E:965:PRO:HD2	1:E:997:LYS:O	1.88	0.72
1:E:1001:LYS:O	1:E:1001:LYS:HG2	1.89	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:E:320:HIS:O	1:E:321:GLN:C	2.33	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:504:ASP:OD1	1:D:846:HIS:HD2	1.73	0.71
1:D:841:ASP:OD1	1:D:846:HIS:HE1	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:276:TYR:CD2	1:A:276:TYR:N	2.58	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: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
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:B:513:ILE:CG1	1:B:953:MET:HE1	2.22	0.69
1:D:759:HIS:HD2	1:D:762:GLN:OE1	1.75	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:H	1:H:1052:ASN:ND2	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:G:247:GLN:O	1:G:250:GLN:HG2	1.92	0.68
1:F:1067:THR:CG2	1:F:1069:THR:OG1	2.41	0.68
1:B:272:TYR:CD1	1:B:272:TYR:C	2.71	0.68
1:D:1052:ASN:HD22	1:D:1052:ASN:N	1.89	0.68
1:F:800:THR:O	1:F:801:ALA:C	2.34	0.68
1:H:304:GLU:OE1	1:H:304:GLU:CA	2.37	0.68
1:B:1063:LYS:HZ3	1:B:1068:ASN:CA	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:513:ILE:HG23	1:B:953:MET:HE1	1.74	0.67
1:E:271:TRP:CH2	1:E:357:ARG:HG2	2.29	0.67
1:E:272:TYR:CD1	1:E:272:TYR:C	2.73	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:H:285:THR:O	1:H:286:GLN:C	2.37	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: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
1:D:310:VAL:HG22	1:D:339:ILE:HD11	1.76	0.67
1:A:440:ASN:HD21	1:A:449:GLN:NE2	1.85	0.67
1:A:1063:LYS:HE2	1:A:1068:ASN:ND2	2.10	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:604:ASN:C	1:B:604:ASN:OD1	2.38	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:G:293:ARG:HB3	1:G:297:MET:HE2	1.76	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:B:651:LYS:O	1:B:652:SER:HB2	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:669:TYR:CD2	1:D:670:MET:CE	2.79	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:535:MET:HE2	1:B:583:PHE:CE2	2.31	0.65
1:B:682:THR:HG22	1:B:767:LEU:HD11	1.77	0.65
1:D:245:PHE:O	1:D:246:ALA:C	2.37	0.65
1:F:256:ALA:C	1:F:258:ASN:H	2.02	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:H:363:PHE:C	1:H:365:LYS:N	2.49	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:C:740:ASN:C	1:C:740:ASN:HD22	2.02	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
1:H:1071:PHE:CD1	1:H:1081:PRO:HD3	2.31	0.65
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:D:344:GLU:O	1:D:345:GLU:C	2.40	0.65
1:D:293:ARG:CB	1:D:297:MET:HE2	2.26	0.65
1:E:1064:ASP:HB2	1:E:1071:PHE:CE1	2.31	0.65
1:C:475:ARG:CB	1:C:953:MET:HE3	2.16	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:G:383:GLN:O	1:G:384:LYS:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:469:ALA:CB	1:F:939:VAL:HG13	2.27	0.64
1:F:801:ALA:O	1:F:803:ASP:N	2.30	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:G:1085:VAL:CG2	1:G:1086:ASN:N	2.60	0.64
1:E:759:HIS:HD2	1:E:762:GLN:OE1	1.79	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: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:293:ARG:HG3	1:D:297:MET:HE1	1.80	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:HE21	1:A:782:GLN:HA	1.63	0.64
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:D:280:ASP:C	1:D:282:LYS:N	2.55	0.64
1:A:304:GLU:OE1	1:A:304:GLU:HA	1.97	0.64
1:G:475:ARG:CA	1:G:953:MET:HE3	2.28	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: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:H:271:TRP:CD1	1:H:294:PRO:HA	2.33	0.63
1:H:303:GLN:O	1:H:304:GLU:C	2.40	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:801:ALA:O	1:F:802:ALA:C	2.41	0.63
1:H:356:LEU:O	1:H:357:ARG:C	2.41	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:E:330:LEU:HD12	1:E:330:LEU:C	2.21	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:G:244:SER:C	1:G:246:ALA:H	2.05	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:H:278:LEU:HD11	1:H:281:GLY:C	2.21	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:356:LEU:C	1:A:358:GLN:H	2.06	0.62
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:G:988:LYS:H	1:G:990:THR:HG23	1.64	0.62
1:F:664:THR:OG1	1:F:672:HIS:HB2	1.99	0.62
1:H:1012:LEU:O	1:H:1016:GLN:HG3	1.99	0.62
1:A:639:ASN:ND2	1:A:813:SER:H	1.96	0.62
1:F:642:LEU:N	1:F:642:LEU:HD12	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:A:740:ASN:C	1:A:740:ASN:ND2	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:VAL:HG12	1:B:969:VAL:CG2	2.19	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: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:513:ILE:HD11	1:E:953:MET:HE1	1.81	0.62
1:F:321:GLN:HG3	1:F:322:THR:N	2.15	0.62
1:F:847:GLN:NE2	1:F:852:ASP:OD1	2.30	0.62
1:E:367:GLN:O	1:E:370:TRP:N	2.26	0.62
1:F:1076:ASP:OD2	1:F:1076:ASP:C	2.42	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:H	1:E:1052:ASN:ND2	1.97	0.62
1:G:461:ASN:H	1:G:470:ASN:HD21	1.45	0.62
1:E:272:TYR:CD1	1:E:273:ARG:C	2.77	0.62
1:F:734:VAL:HB	1:F:755:MET:HE1	1.81	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:E:272:TYR:HD1	1:E:273:ARG:C	2.07	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:513:ILE:CG2	1:B:856:MET:HE1	2.28	0.61
1:B:715:LYS:CG	1:B:830:VAL:HB	2.28	0.61
1:C:492:ASP:CG	1:C:1025:ARG:NH1	2.58	0.61
1:E:288:THR:H	1:E:291:ASP:CG	2.08	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
1:E:271:TRP:CZ2	1:E:357:ARG:CG	2.84	0.61
1:E:273:ARG:HH11	1:E:289:GLU:CA	2.10	0.61
1:G:278:LEU:O	1:G:344:GLU:HG3	1.99	0.61
1:G:513:ILE:CD1	1:G:953:MET:HE1	2.30	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:B:259:PHE:N	1:B:259:PHE:HD2	1.97	0.61
1:D:293:ARG:CG	1:D:297:MET:HE1	2.31	0.61
1:E:346:LYS:O	1:E:350:GLU:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:670:MET:HE3	1:H:877:VAL:HG12	1.82	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:B:450:LEU:HD22	1:B:1034:MET:HE1	1.83	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:H:280:ASP:O	1:H:281:GLY:C	2.44	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:C:492:ASP:CG	1:C:1025:ARG:HH11	2.07	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:726:ARG:HG2	1:B:727:ILE:N	2.16	0.60
1:B:1052:ASN:N	1:B:1052:ASN:ND2	2.45	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: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:669:TYR:HE2	1:C:670:MET:CE	2.14	0.60
1:C:1071:PHE:CD1	1:C:1081:PRO:HD3	2.36	0.60
1:D:368:SER:O	1:D:371:ASN:HB2	2.01	0.60
1:G:355:TRP:CG	1:G:356:LEU:H	2.18	0.60
1:F:740:ASN:HD22	1:F:740:ASN:C	2.09	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:356:LEU:C	1:A:358:GLN:N	2.58	0.60
1:A:424:ASP:HB3	1:A:520:ASN:ND2	2.17	0.60
1:C:1076:ASP:OD2	1:C:1077:ASN:HB2	2.02	0.60
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:G:460:GLY:N	1:G:470:ASN:HD22	1.98	0.60
1:E:474:ILE:O	1:E:953:MET:HE3	2.01	0.60
1:F:801:ALA:O	1:F:804:ILE:N	2.34	0.60
1:H:669:TYR:CD2	1:H:670:MET:HE3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASN:OD1	1:A:354:ASN:HB2	2.02	0.60
1:A:602:GLU:C	1:A:603:ILE:HG13	2.26	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:HD22	1:C:1052:ASN:N	1.94	0.60
1:G:669:TYR:CD1	1:G:874:THR:HG23	2.36	0.60
1:F:708:ILE:HD11	1:F:737:GLU:HB2	1.81	0.60
1:H:475:ARG:HB2	1:H:953:MET:CE	2.26	0.60
1:D:471:PHE:CG	1:D:954:ALA:HB2	2.37	0.60
1:G:904:ASP:OD2	1:G:906:SER:HB3	2.02	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:A:278:LEU:HD12	1:A:283:THR:N	2.16	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:C:1063:LYS:HE2	1:C:1068:ASN:CG	2.26	0.60
1:E:281:GLY:CA	1:E:341:THR:CG2	2.80	0.60
1:A:316:GLN:OE1	1:A:316:GLN:HA	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:557:MET:HE2	1:F:708:ILE:HD12	1.83	0.59
1:F:1085:VAL:HG23	1:F:1086:ASN:N	2.16	0.59
1:H:792:ASN:C	1:H:792:ASN:OD1	2.45	0.59
1:G:440:ASN:ND2	1:G:449:GLN:HE21	1.93	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:F:514:LEU:HD21	1:F:532:MET:HG3	1.84	0.59
1:H:307:ARG:O	1:H:310:VAL:HB	2.02	0.59
1:B:551:LEU:HD12	1:B:551:LEU:O	2.03	0.59
1:B:1063:LYS:HZ1	1:B:1068:ASN:HB3	1.63	0.59
1:D:277:ILE:HD11	1:D:291:ASP:HB3	1.77	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:669:TYR:CD2	1:D:670:MET:HE3	2.37	0.59
1:G:244:SER:C	1:G:246:ALA:N	2.59	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: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:G:1052:ASN:H	1:G:1052:ASN:ND2	1.98	0.59
1:B:713:TYR:O	1:B:732:GLY:CA	2.48	0.59
1:F:407:ASN:HD22	1:F:431:GLU:N	2.00	0.59
1:F:1063:LYS:HE3	1:F:1068:ASN:ND2	2.17	0.59
1:G:904:ASP:OD2	1:G:906:SER:CB	2.50	0.59
1:F:917:ALA:HA	1:F:962:TYR:CD1	2.37	0.59
1:H:288:THR:C	1:H:290:LYS:H	2.09	0.59
1:H:355:TRP:CD2	1:H:356:LEU:N	2.71	0.59
1:H:513:ILE:CD1	1:H:953:MET:HE1	2.32	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:G:705:SER:HB3	1:G:743:LEU:HD13	1.84	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:H:474:ILE:O	1:H:953:MET:HE3	2.01	0.59
1:C:999:SER:C	1:C:1001:LYS:H	2.10	0.59
1:E:407:ASN:ND2	1:E:431:GLU:H	2.01	0.59
1:H:260:GLU:HG3	1:H:271:TRP:O	2.03	0.59
1:H:278:LEU:HA	1:H:283:THR:O	2.03	0.58
1:H:461:ASN:H	1:H:470:ASN:HD21	1.51	0.58
1:F:740:ASN:HD22	1:F:741:PRO:N	2.00	0.58
1:G:304:GLU:OE1	1:G:304:GLU:HA	2.02	0.58
1:E:306:GLN:O	1:E:309:TYR:HB3	2.02	0.58
1:H:363:PHE:C	1:H:365:LYS:H	2.10	0.58
1:A:300:TRP:CG	1:A:306:GLN:HG3	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:363:PHE:O	1:H:364:VAL:C	2.42	0.58
1:H:740:ASN:C	1:H:740:ASN:ND2	2.61	0.58
1:C:380:ASP:OD1	1:C:977:LYS:HE3	2.03	0.58
1:G:574:GLU:HG3	1:G:575:THR:N	2.14	0.58
1:F:376:LYS:HB3	1:F:377:PRO:HA	1.85	0.58
1:H:874:THR:HG22	1:H:878:ILE:HD12	1.86	0.58
1:A:288:THR:C	1:A:290:LYS:H	2.12	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: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:G:407:ASN:ND2	1:G:431:GLU:H	2.00	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: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:B:258:ASN:C	1:B:259:PHE:CD2	2.82	0.58
1:A:272:TYR:CE2	1:A:295:LEU:HD23	2.39	0.58
1:A:1085:VAL:HG23	1:A:1086:ASN:N	2.19	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:604:ASN:C	1:D:604:ASN:OD1	2.47	0.57
1:D:841:ASP:HB2	5:D:101:HOH:O	2.03	0.57
1:G:1065:GLN:HG3	1:G:1066:ALA:H	1.69	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:A:574:GLU:HG3	1:A:575:THR:N	2.18	0.57
1:G:792:ASN:HD21	1:G:796:GLU:HB2	1.70	0.57
1:E:271:TRP:CD1	1:E:357:ARG:NH1	2.72	0.57
1:A:310:VAL:HG21	1:A:335:ALA:HB3	1.86	0.57
1:B:930:ASN:O	1:B:931:LYS:C	2.46	0.57
1:D:854:ARG:HD3	1:D:892:ASP:OD2	2.04	0.57
1:F:261:HIS:CD2	1:F:264:HIS:N	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:669:TYR:HE2	1:C:670:MET:HE3	1.70	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:H:765:ARG:HB2	1:H:766:PRO:HD2	1.87	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:280:ASP:C	1:D:282:LYS:H	2.13	0.57
1:D:639:ASN:HD21	1:D:813:SER:N	1.90	0.57
1:F:458:ASN:HA	1:F:470:ASN:OD1	2.05	0.57
1:B:1003:GLN:OE1	1:B:1003:GLN:N	2.37	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:OE1	1:A:449:GLN:HA	2.05	0.57
1:B:1063:LYS:HZ3	1:B:1068:ASN:CB	2.18	0.57
1:C:513:ILE:CD1	1:C:953:MET:HE1	2.34	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:C:669:TYR:CE2	1:C:670:MET:CE	2.87	0.57
1:G:390:SER:HB2	1:G:971:THR:HB	1.86	0.57
1:G:474:ILE:C	1:G:953:MET:HE3	2.29	0.57
1:A:616:GLU:O	1:A:619:LYS:HB3	2.04	0.57
1:B:974:ARG:HH11	1:B:974:ARG:CG	2.04	0.57
1:B:1086:ASN:N	1:B:1087:PRO:HD3	2.18	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:B:1063:LYS:HZ3	1:B:1068:ASN:HA	1.70	0.56
1:C:457:MET:HE1	1:C:494:LEU:HD21	1.87	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:471:PHE:CG	1:E:954:ALA:HB2	2.40	0.56
1:E:475:ARG:CA	1:E:953:MET:HE2	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLN:O	1:A:250:GLN:HG2	2.05	0.56
1:B:248:TYR:C	1:B:250:GLN:H	2.12	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:G:280:ASP:O	1:G:282:LYS:N	2.39	0.56
1:E:322:THR:CG2	1:E:323:TYR:N	2.69	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:H:669:TYR:CD2	1:H:670:MET:CE	2.88	0.56
1:C:250:GLN:NE2	1:C:275:LYS:NZ	2.53	0.56
1:C:1000:GLY:HA3	5:C:171:HOH:O	2.04	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:356:LEU:C	1:H:358:GLN:N	2.62	0.56
1:A:316:GLN:OE1	1:A:316:GLN:CA	2.52	0.56
1:E:669:TYR:CE2	1:E:670:MET:CE	2.83	0.56
1:F:745:LEU:HD13	1:F:801:ALA:CB	2.34	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: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:HD12	1:D:551:LEU:O	2.05	0.56
1:F:261:HIS:CD2	1:F:264:HIS:HA	2.41	0.56
1:A:253:SER:HB3	1:A:258:ASN:OD1	2.06	0.56
1:A:868:THR:O	1:A:868:THR:HG22	2.05	0.56
1:D:334:LEU:O	1:D:335:ALA:C	2.47	0.56
1:F:576:ALA:HB3	1:F:847:GLN:HB3	1.88	0.56
1:H:302:ASP:O	1:H:303:GLN:C	2.48	0.56
1:H:504:ASP:OD1	1:H:846:HIS:HD2	1.89	0.56
1:C:320:HIS:ND1	1:C:320:HIS:N	2.52	0.56
1:H:300:TRP:HB3	1:H:305:THR:HG23	1.88	0.56
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:B:740:ASN:HD22	1:B:740:ASN:C	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:999:SER:O	1:D:999:SER:OG	2.24	0.55
1:D:1071:PHE:CD1	1:D:1081:PRO:HD3	2.42	0.55
1:F:454:HIS:ND1	1:F:493:TYR:OH	2.31	0.55
1:F:606:ASN:O	1:F:607:VAL:C	2.49	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:A:734:VAL:HB	1:A:755:MET:HE1	1.86	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:A:273:ARG:NH2	1:A:288:THR:C	2.57	0.55
1:B:1063:LYS:NZ	1:B:1068:ASN:OD1	2.40	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:715:LYS:HD2	1:B:830:VAL:CA	2.35	0.55
1:B:1085:VAL:HG23	1:B:1086:ASN:N	2.21	0.55
1:G:363:PHE:O	1:G:364:VAL:C	2.48	0.55
1:E:307:ARG:HD2	1:E:324:ASN:O	2.07	0.55
1:F:726:ARG:CG	1:F:726:ARG:NH1	2.31	0.55
1:H:271:TRP:CZ2	1:H:294:PRO:HG3	2.41	0.55
1:H:794:ARG:HG2	1:H:794:ARG:HH11	1.72	0.55
1:C:278:LEU:O	1:C:344:GLU:HG3	2.07	0.55
1:F:752:VAL:O	1:F:752:VAL:HG12	2.07	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:A:485:ASP:OD2	1:A:1029:SER:OG	2.22	0.55
1:B:631:THR:HG23	1:B:809:ASN:C	2.31	0.55
1:F:765:ARG:HD3	1:F:784:ALA:HB3	1.87	0.55
1:A:453:LEU:HD11	1:A:457:MET:HE1	1.89	0.55
1:B:260:GLU:HG3	1:B:271:TRP:O	2.07	0.55
1:B:492:ASP:HB3	1:B:1022:LEU:CD2	2.37	0.55
1:D:666:ASP:HA	1:D:863:PHE:O	2.06	0.55
1:G:310:VAL:HG11	1:G:335:ALA:HB1	1.89	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:311:ASN:ND2	1:G:323:TYR:H	2.03	0.55
1:E:350:GLU:C	1:E:352:ASN:H	2.13	0.55
1:F:794:ARG:HH11	1:F:794:ARG:CG	2.20	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:B:1085:VAL:C	1:B:1087:PRO:HD3	2.32	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:E:291:ASP:N	1:E:291:ASP:OD1	2.38	0.54
1:F:245:PHE:O	1:F:247:GLN:N	2.40	0.54
1:F:1067:THR:HG22	1:F:1067:THR:O	2.06	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:436:ASN:HB2	1:C:961:MET:O	2.08	0.54
1:C:800:THR:HG22	1:C:802:ALA:N	2.17	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:G:293:ARG:HB3	1:G:297:MET:CE	2.37	0.54
1:E:256:ALA:HB1	1:E:261:HIS:CE1	2.42	0.54
1:E:280:ASP:C	1:E:282:LYS:N	2.65	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:324:ASN:OD1	1:G:324:ASN:C	2.51	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: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:G:475:ARG:N	1:G:953:MET:HE3	2.23	0.53
1:G:713:TYR:O	1:G:759:HIS:HE1	1.91	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:HG2	1:E:515:GLU:O	2.07	0.53
1:F:698:ARG:HB2	1:F:709:THR:OG1	2.08	0.53
1:B:478:ALA:HB1	1:B:481:ASN:HD22	1.73	0.53
1:C:670:MET:HE1	1:C:885:PHE:CZ	2.38	0.53
1:F:531:ASN:ND2	1:F:844:SER:OG	2.42	0.53
1:F:651:LYS:O	1:F:652:SER:HB2	2.07	0.53
1:A:304:GLU:OE1	1:A:304:GLU:CA	2.53	0.53
1:B:407:ASN:ND2	1:B:431:GLU:N	2.55	0.53
1:B:1012:LEU:O	1:B:1016:GLN:HB2	2.09	0.53
1:D:248:TYR:HB3	1:D:276:TYR:HB2	1.90	0.53
1:E:380:ASP:C	1:E:380:ASP:OD1	2.51	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:H:288:THR:C	1:H:290:LYS:N	2.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:268:ALA:HB2	1:G:370:TRP:CE2	2.44	0.53
1:E:630:ALA:O	1:E:633:LYS:NZ	2.41	0.53
1:F:259:PHE:CD2	1:F:259:PHE:N	2.76	0.53
1:F:311:ASN:ND2	1:F:323:TYR:H	1.97	0.53
1:A:342:LYS:HA	1:A:345:GLU:OE1	2.08	0.53
1:A:1085:VAL:HG23	1:A:1086:ASN:H	1.74	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:871:GLU:H	1:H:871:GLU:CD	2.16	0.53
1:H:1087:PRO:OXT	1:H:1087:PRO:CD	2.56	0.53
1:C:261:HIS:CD2	1:C:264:HIS:HA	2.44	0.53
1:G:376:LYS:HA	1:G:377:PRO:C	2.33	0.53
1:G:581:TYR:HA	1:G:654:VAL:O	2.08	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:F:930:ASN:OD1	1:F:930:ASN:C	2.51	0.53
1:H:278:LEU:CD1	1:H:283:THR:N	2.71	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: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:E:347:ILE:HG13	1:E:355:TRP:HE1	1.73	0.53
1:F:483:ASP:C	1:F:483:ASP:OD1	2.50	0.53
1:F:639:ASN:HD22	1:F:642:LEU:HD13	1.73	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:A:868:THR:HB	1:A:872:GLU:OE1	2.08	0.53
1:D:987:ILE:O	1:D:987:ILE:HG22	2.08	0.53
1:G:280:ASP:C	1:G:282:LYS:N	2.66	0.53
1:G:457:MET:HE1	1:G:494:LEU:HD21	1.90	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
1:B:762:GLN:HG3	1:B:763:ALA:H	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:669:TYR:CE2	1:C:670:MET:HE3	2.44	0.52
1:E:558:ASN:N	1:E:559:PRO:CD	2.73	0.52
1:D:1052:ASN:ND2	1:D:1052:ASN:N	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:H:309:TYR:C	1:H:309:TYR:CD2	2.88	0.52
1:B:614:MET:HE3	1:B:618:LYS:HD2	1.92	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:N	1:E:259:PHE:CD2	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: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:585:ARG:CD	1:B:661:ASP:OD1	2.57	0.52
1:B:920:ASP:CG	1:B:923:ASP:HB2	2.34	0.52
1:D:293:ARG:CB	1:D:297:MET:HE1	2.39	0.52
1:D:973:THR:HG23	1:D:988:LYS:HA	1.92	0.52
1:F:631:THR:HG21	1:F:808:ALA:O	2.10	0.52
1:F:694:GLY:HA3	1:F:718:LEU:O	2.08	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:246:ALA:O	1:B:247:GLN:C	2.51	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:G:319:ILE:HD13	1:G:338:THR:HG22	1.90	0.52
1:F:765:ARG:HB2	1:F:784:ALA:HB1	1.92	0.52
1:F:874:THR:O	1:F:878:ILE:HG13	2.10	0.52
1:C:561:ILE:HG12	1:C:697:MET:HB3	1.90	0.52
1:D:504:ASP:OD1	1:D:846:HIS:CD2	2.59	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:957:VAL:O	1:D:957:VAL:HG12	2.09	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:E:319:ILE:HD11	1:E:342:LYS:HD2	1.90	0.52
1:F:794:ARG:NH1	1:F:794:ARG:CG	2.73	0.52
1:E:385:GLY:C	1:E:1053:ILE:HG23	2.35	0.51
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: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: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: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:F:256:ALA:HA	1:F:1073:LEU:HD13	1.92	0.51
1:F:1035:ASP:C	1:F:1035:ASP:OD1	2.53	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:663:PHE:O	1:F:664:THR:C	2.54	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:321:GLN:HG2	1:C:322:THR:H	1.76	0.51
1:C:492:ASP:HB3	1:C:1022:LEU:CD2	2.41	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:A:988:LYS:C	1:A:990:THR:HG22	2.35	0.51
1:B:407:ASN:ND2	1:B:431:GLU:HB2	2.26	0.51
1:C:604:ASN:C	1:C:604:ASN:OD1	2.53	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:E:325:THR:C	1:E:327:THR:H	2.18	0.51
1:E:707:ILE:C	1:E:707:ILE:HD12	2.35	0.51
1:F:256:ALA:C	1:F:258:ASN:N	2.65	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:303:GLN:O	1:E:304:GLU:C	2.52	0.51
1:E:440:ASN:ND2	1:E:449:GLN:HE21	1.88	0.51
1:E:677:TYR:C	1:E:677:TYR:CD2	2.88	0.51
1:F:322:THR:HG22	1:F:323:TYR:N	2.24	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: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:C:1000:GLY:CA	5:C:171:HOH:O	2.59	0.51
1:E:271:TRP:CH2	1:E:357:ARG:CG	2.94	0.51
1:B:639:ASN:ND2	1:B:813:SER:H	1.99	0.51
1:B:729:ARG:HD2	1:B:758:ALA:O	2.11	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:D:344:GLU:C	1:D:346:LYS:N	2.68	0.50
1:G:558:ASN:N	1:G:559:PRO:CD	2.73	0.50
1:E:337:GLN:O	1:E:340:GLN:CB	2.59	0.50
1:F:524:TYR:C	1:F:524:TYR:CD2	2.89	0.50
1:A:356:LEU:O	1:A:357:ARG:C	2.52	0.50
1:B:781:ASP:OD2	1:B:822:VAL:HG13	2.11	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:440:ASN:HD21	1:F:449:GLN:NE2	2.03	0.50
1:F:1074:VAL:HG13	1:F:1077:ASN:HB3	1.93	0.50
1:D:873:TYR:O	1:D:874:THR:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:TYR:HB3	1:G:276:TYR:HB2	1.94	0.50
1:G:483:ASP:C	1:G:483:ASP:OD1	2.53	0.50
1:H:308:GLN:NE2	1:H:367:GLN:OE1	2.44	0.50
1:B:1030:THR:HB	1:B:1032:VAL:HG22	1.94	0.50
1:E:320:HIS:C	1:E:321:GLN:O	2.54	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:B:535:MET:HE2	1:B:583:PHE:HE2	1.74	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:D:871:GLU:H	1:D:871:GLU:CD	2.18	0.50
1:D:930:ASN:O	1:D:931:LYS:C	2.54	0.50
1:G:1052:ASN:ND2	1:G:1052:ASN:N	2.58	0.50
1:E:530:ASP:O	1:E:844:SER:HB2	2.11	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:F:1052:ASN:ND2	1:F:1052:ASN:N	2.54	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:B:513:ILE:CG2	1:B:953:MET:HE1	2.42	0.50
1:D:965:PRO:HD2	1:D:997:LYS:O	2.12	0.50
1:H:298:THR:C	1:H:300:TRP:CZ3	2.90	0.50
1:H:928:LYS:HE2	1:H:929:PRO:O	2.12	0.50
1:G:344:GLU:OE1	1:G:344:GLU:HA	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: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:G:245:PHE:O	1:G:246:ALA:C	2.55	0.50
1:E:713:TYR:O	1:E:759:HIS:HE1	1.94	0.50
1:E:734:VAL:HB	1:E:755:MET:HE1	1.93	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:O	1:C:999:SER:OG	2.29	0.49
1:G:271:TRP:HZ2	1:G:357:ARG:HA	1.77	0.49
1:G:1080:LEU:HB3	1:G:1081:PRO:CD	2.42	0.49
1:F:765:ARG:HG2	1:F:781:ASP:OD1	2.12	0.49
1:H:278:LEU:CG	1:H:281:GLY:HA2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:740:ASN:ND2	1:D:740:ASN:C	2.61	0.49
1:D:800:THR:CG2	1:D:801:ALA:N	2.74	0.49
1:E:407:ASN:ND2	1:E:431:GLU:N	2.60	0.49
1:H:407:ASN:ND2	1:H:431:GLU:N	2.60	0.49
1:H:993:VAL:O	1:H:1056:ARG:NH1	2.45	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:280:ASP:O	1:D:281:GLY:C	2.54	0.49
1:D:965:PRO:HD2	1:D:998:SER:HA	1.94	0.49
1:G:293:ARG:CB	1:G:297:MET:HE2	2.42	0.49
1:G:457:MET:HE3	1:G:494:LEU:HD23	1.94	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:E:271:TRP:CZ2	1:E:357:ARG:HG2	2.47	0.49
1:F:537:ASN:OD1	1:F:540:ARG:NH1	2.44	0.49
1:F:1067:THR:HG21	1:F:1069:THR:OG1	2.12	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:312:TYR:C	1:C:312:TYR:CD2	2.90	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:G:860:PHE:CG	1:G:896:ALA:HB2	2.47	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: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: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:B:988:LYS:N	1:B:990:THR:HG23	2.27	0.49
1:G:599:ILE:O	1:G:600:LYS:C	2.56	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:604:ASN:C	1:F:606:ASN:H	2.21	0.49
1:F:927:SER:OG	1:F:928:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:GLY:O	1:B:712:ARG:HD2	2.12	0.49
1:F:725:ASP:C	1:F:725:ASP:OD1	2.54	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:B:746:LYS:HB2	1:B:749:ASP:CG	2.38	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:H:581:TYR:HA	1:H:654:VAL:O	2.13	0.49
1:A:252:TYR:CE2	1:A:273:ARG:NH1	2.78	0.49
1:A:868:THR:O	1:A:868:THR:CG2	2.61	0.49
1:D:286:GLN:O	1:D:287:SER:C	2.52	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:F:458:ASN:C	1:F:470:ASN:OD1	2.55	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:278:LEU:O	1:D:344:GLU:HG3	2.12	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:F:698:ARG:HB2	1:F:709:THR:HG1	1.78	0.49
1:F:816:LEU:HD12	1:F:817:GLY:H	1.78	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:B:253:SER:C	1:B:255:ASP:H	2.20	0.49
1:C:513:ILE:HD11	1:C:953:MET:HE1	1.95	0.49
1:C:1052:ASN:H	1:C:1052:ASN:ND2	1.95	0.49
1:G:387:LEU:O	1:G:1050:GLY:HA3	2.13	0.49
1:E:280:ASP:C	1:E:282:LYS:H	2.21	0.49
1:F:279:LYS:O	1:F:280:ASP:HB3	2.12	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: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:E:474:ILE:C	1:E:953:MET:HE3	2.38	0.48
1:F:711:VAL:CG2	1:F:734:VAL:HG23	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:244:SER:C	1:C:246:ALA:H	2.21	0.48
1:C:987:ILE:HG12	1:C:1058:ALA:HB2	1.94	0.48
1:D:1081:PRO:O	1:D:1082:LYS:C	2.55	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:C:669:TYR:CE2	1:C:670:MET:HE2	2.47	0.48
1:D:262:VAL:HG12	1:D:969:VAL:HG23	1.94	0.48
1:D:514:LEU:HD21	1:D:532:MET:HG3	1.94	0.48
1:D:524:TYR:CD2	1:D:524:TYR:C	2.91	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:A:309:TYR:C	1:A:309:TYR:CD2	2.91	0.48
1:A:397:SER:HB3	5:A:1093:HOH:O	2.14	0.48
1:B:669:TYR:CE2	1:B:670:MET:HE2	2.44	0.48
1:B:760:LYS:O	1:B:761:ASN:C	2.57	0.48
1:D:987:ILE:HG12	1:D:1058:ALA:HB2	1.94	0.48
1:F:514:LEU:HD11	1:F:525:LEU:HD13	1.95	0.48
1:F:726:ARG:HD3	1:F:726:ARG:H	1.79	0.48
1:H:280:ASP:O	1:H:281:GLY:O	2.30	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:G:301:PRO:O	1:G:302:ASP:HB3	2.14	0.48
1:E:634:LYS:HD3	1:E:635:TYR:CE2	2.49	0.48
1:E:1068:ASN:O	1:E:1068:ASN:OD1	2.30	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:H:841:ASP:OD1	1:H:846:HIS:HE1	1.97	0.48
1:B:380:ASP:C	1:B:380:ASP:OD1	2.56	0.48
1:B:1063:LYS:NZ	1:B:1068:ASN:CA	2.76	0.48
1:G:453:LEU:CD1	1:G:474:ILE:HG21	2.44	0.48
1:E:460:GLY:H	1:E:470:ASN:ND2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:639:ASN:HB3	1:E:642:LEU:HB2	1.95	0.48
1:F:669:TYR:CD2	1:F:670:MET:HE3	2.49	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: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: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:F:766:PRO:HA	1:F:819:TRP:CD1	2.49	0.48
1:H:513:ILE:HG21	1:H:856:MET:HE1	1.96	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:H:364:VAL:HG13	1:H:370:TRP:CE3	2.49	0.48
1:H:677:TYR:CD2	1:H:677:TYR:C	2.92	0.48
1:C:356:LEU:HA	1:C:359:THR:HG22	1.96	0.48
1:D:585:ARG:HD3	1:D:661:ASP:OD1	2.13	0.48
1:G:356:LEU:O	1:G:357:ARG:C	2.56	0.48
1:E:604:ASN:C	1:E:604:ASN:OD1	2.56	0.48
1:F:466:ASP:C	1:F:468:ASP:H	2.21	0.48
1:F:917:ALA:HB1	1:F:962:TYR:CD1	2.49	0.48
1:A:1065:GLN:HG3	1:A:1066:ALA:N	2.28	0.47
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:305:THR:C	1:H:307:ARG:N	2.71	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:502:LYS:C	1:B:503:ASN:HD22	2.22	0.47
1:B:558:ASN:N	1:B:559:PRO:CD	2.77	0.47
1:C:457:MET:HE1	1:C:494:LEU:CD2	2.43	0.47
1:C:599:ILE:HA	1:C:603:ILE:HB	1.96	0.47
1:D:502:LYS:HD2	1:D:502:LYS:HA	1.49	0.47
1:E:263:ASP:O	1:E:264:HIS:HB2	2.13	0.47
1:E:337:GLN:O	1:E:338:THR:C	2.56	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:H	1:F:708:ILE:CD1	2.21	0.47
1:H:261:HIS:HD2	1:H:264:HIS:N	2.09	0.47
1:H:288:THR:H	1:H:291:ASP:CG	2.21	0.47
1:H:604:ASN:C	1:H:604:ASN:OD1	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LYS:O	1:A:276:TYR:CD2	2.66	0.47
1:A:407:ASN:ND2	1:A:431:GLU:H	2.12	0.47
1:A:524:TYR:C	1:A:524:TYR:CD2	2.92	0.47
1:B:530:ASP:O	1:B:845:VAL:HG23	2.14	0.47
1:B:577:ALA:C	1:B:578:VAL:HG23	2.39	0.47
1:G:356:LEU:HA	1:G:359:THR:CG2	2.44	0.47
1:G:457:MET:HE1	1:G:494:LEU:CD2	2.44	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: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:244:SER:C	1:E:246:ALA:H	2.20	0.47
1:E:319:ILE:CD1	1:E:342:LYS:HE2	2.43	0.47
1:F:976:ASP:C	1:F:976:ASP:OD1	2.57	0.47
1:B:896:ALA:HB1	1:B:932:TYR:CE2	2.50	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:262:VAL:O	1:H:263:ASP:C	2.55	0.47
1:H:310:VAL:O	1:H:311:ASN:C	2.56	0.47
1:B:822:VAL:HG12	1:B:823:GLY:N	2.30	0.47
1:B:1064:ASP:HB2	1:B:1071:PHE:CZ	2.48	0.47
1:D:276:TYR:HA	1:D:285:THR:O	2.14	0.47
1:G:883:ASP:OD1	1:G:948:LYS:HE3	2.15	0.47
1:E:273:ARG:NH1	1:E:289:GLU:HA	2.15	0.47
1:H:639:ASN:HD22	1:H:642:LEU:HD13	1.79	0.47
1:B:603:ILE:HG22	1:B:604:ASN:N	2.30	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:727:ILE:HG23	1:C:727:ILE:HD12	1.60	0.47
1:C:729:ARG:HD2	1:C:758:ALA:O	2.14	0.47
1:D:355:TRP:CG	1:D:356:LEU:H	2.32	0.47
1:D:669:TYR:HE2	1:D:670:MET:HE1	1.78	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:917:ALA:CB	1:F:962:TYR:CE1	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:964:LEU:CD1	1:F:996:GLY:HA2	2.41	0.47
1:F:1063:LYS:HE3	1:F:1068:ASN:CG	2.39	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:475:ARG:CB	1:E:953:MET:CE	2.62	0.47
1:E:733:VAL:HG22	1:E:734:VAL:N	2.29	0.47
1:E:854:ARG:NH1	1:E:892:ASP:OD2	2.44	0.47
1:F:669:TYR:CD2	1:F:670:MET:CE	2.95	0.47
1:F:702:VAL:O	1:F:703:GLY:C	2.57	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:576:ALA:HB3	1:C:847:GLN:HB3	1.97	0.47
1:C:584:ILE:O	1:C:584:ILE:HG13	2.13	0.47
1:G:718:LEU:HD23	1:G:718:LEU:HA	1.65	0.47
1:E:277:ILE:HD12	1:E:291:ASP:CG	2.39	0.47
1:F:751:VAL:O	1:F:751:VAL:HG12	2.13	0.47
1:F:1027:GLN:O	1:F:1031:GLY:N	2.46	0.47
1:B:471:PHE:CG	1:B:954:ALA:HB2	2.49	0.47
1:B:578:VAL:HG13	1:B:579:PRO:HD2	1.98	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:G:733:VAL:HG22	1:G:734:VAL:N	2.30	0.47
1:E:670:MET:CE	1:E:877:VAL:HG12	2.32	0.47
1:F:263:ASP:OD2	1:F:968:GLU:HA	2.15	0.47
1:C:321:GLN:HG2	1:C:322:THR:N	2.30	0.46
1:G:687:ARG:HA	1:G:691:VAL:HG23	1.97	0.46
1:E:290:LYS:HE2	1:E:290:LYS:HB2	1.54	0.46
1:H:285:THR:O	1:H:286:GLN:O	2.32	0.46
1:H:356:LEU:HD12	1:H:356:LEU:HA	1.76	0.46
1:H:442:ASN:OD1	1:H:442:ASN:C	2.57	0.46
1:H:871:GLU:OE1	1:H:871:GLU:N	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:D:409:THR:O	1:D:410:PRO:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:687:ARG:HA	1:E:691:VAL:HG23	1.98	0.46
1:F:312:TYR:C	1:F:312:TYR:CD2	2.93	0.46
1:F:476:VAL:HG22	1:F:956:TRP:HE3	1.80	0.46
1:F:571:ASP:C	1:F:571:ASP:OD1	2.58	0.46
1:F:642:LEU:N	1:F:642:LEU:CD1	2.77	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:475:ARG:N	1:C:953:MET:HE3	2.30	0.46
1:C:974:ARG:HG2	1:C:987:ILE:HB	1.96	0.46
1:E:973:THR:HG23	1:E:988:LYS:HA	1.97	0.46
1:H:607:VAL:O	1:H:607:VAL:HG13	2.15	0.46
1:B:529:GLY:O	1:B:530:ASP:C	2.57	0.46
1:B:702:VAL:O	1:B:703:GLY:C	2.58	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:E:461:ASN:OD1	1:E:467:PRO:HA	2.15	0.46
1:F:581:TYR:HA	1:F:654:VAL:O	2.16	0.46
1:F:712:ARG:HH11	1:F:712:ARG:HG3	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:F:934:THR:O	1:F:935:ALA:C	2.59	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:574:GLU:HG3	1:D:575:THR:N	2.26	0.46
1:D:578:VAL:HG13	1:D:579:PRO:HD2	1.98	0.46
1:E:571:ASP:C	1:E:571:ASP:OD1	2.58	0.46
1:F:724:GLY:HA3	1:F:728:THR:CB	2.46	0.46
1:A:565:LEU:HA	1:A:565:LEU:HD23	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:O	1:D:339:ILE:HG22	2.14	0.46
1:D:726:ARG:CG	1:D:726:ARG:NH1	2.52	0.46
1:D:854:ARG:HH11	1:D:892:ASP:CG	2.23	0.46
1:G:800:THR:HG23	1:G:801:ALA:N	2.31	0.46
1:F:487:LEU:HD22	1:F:532:MET:HE3	1.98	0.46
1:F:664:THR:HB	1:F:667:GLY:H	1.81	0.46
1:F:692:SER:OG	1:F:715:LYS:HA	2.15	0.46
1:H:356:LEU:O	1:H:358:GLN:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:797:LEU:HD23	1:H:797:LEU:HA	1.62	0.46
1:B:460:GLY:C	1:B:466:ASP:O	2.59	0.46
1:B:461:ASN:OD1	1:B:467:PRO:HB3	2.16	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: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: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:705:SER:HB3	1:E:743:LEU:HD13	1.97	0.46
1:H:516:ALA:HB1	1:H:521:ASP:OD2	2.15	0.46
1:A:324:ASN:C	1:A:324:ASN:OD1	2.58	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:B:1003:GLN:O	1:B:1004:GLN:C	2.57	0.46
1:C:558:ASN:N	1:C:559:PRO:CD	2.79	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: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:551:LEU:CD2	1:F:741:PRO:HG2	2.45	0.46
1:H:355:TRP:O	1:H:356:LEU:C	2.59	0.46
1:B:272:TYR:CD1	1:B:273:ARG:N	2.84	0.46
1:C:524:TYR:C	1:C:524:TYR:CD2	2.94	0.46
1:C:677:TYR:C	1:C:677:TYR:CD2	2.94	0.46
1:C:797:LEU:HD23	1:C:797:LEU:HA	1.86	0.46
1:C:1027:GLN:HA	1:C:1027:GLN:OE1	2.16	0.46
1:G:928:LYS:HE3	1:G:928:LYS:HB2	1.70	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:B:430:TYR:HB3	1:B:978:TYR:CE1	2.51	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:ASP:C	1:D:380:ASP:OD1	2.59	0.46
1:G:302:ASP:C	1:G:302:ASP:OD1	2.58	0.46
1:G:977:LYS:HB2	1:G:977:LYS:HE2	1.59	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: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:H51	4:C:5001:MES:H82	1.43	0.45
1:G:794:ARG:HG2	1:G:794:ARG:HH11	1.81	0.45
1:E:301:PRO:O	1:E:1065:GLN:CG	2.64	0.45
1:F:372:SER:O	1:F:373:ASP:C	2.58	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:515:GLU:O	1:B:515:GLU:HG2	2.16	0.45
1:B:800:THR:HG22	1:B:801:ALA:N	2.08	0.45
1:B:1073:LEU:CD1	1:B:1080:LEU:HD21	2.42	0.45
1:C:297:MET:SD	1:C:340:GLN:HG3	2.55	0.45
1:D:350:GLU:C	1:D:352:ASN:H	2.24	0.45
1:E:346:LYS:HG2	1:E:355:TRP:CZ2	2.51	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:H:993:VAL:CG1	1:H:1056:ARG:NH1	2.71	0.45
1:A:407:ASN:ND2	1:A:431:GLU:N	2.64	0.45
1:C:1034:MET:HB2	1:C:1034:MET:HE3	1.81	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:999:SER:C	1:D:1001:LYS:N	2.74	0.45
1:G:319:ILE:CD1	1:G:338:THR:HG22	2.45	0.45
1:E:458:ASN:O	1:E:459:PHE:C	2.59	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:H:439:ASP:OD1	1:H:439:ASP:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ASN:HB3	1:B:445:VAL:HB	1.99	0.45
1:B:1064:ASP:C	1:B:1064:ASP:OD1	2.58	0.45
1:C:957:VAL:O	1:C:957:VAL:HG12	2.16	0.45
1:D:317:LEU:HD13	1:D:342:LYS:HB3	1.96	0.45
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: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:300:TRP:CE3	1:H:300:TRP:N	2.85	0.45
1:H:408:ARG:HA	1:H:408:ARG:HD3	1.74	0.45
1:A:759:HIS:HD2	1:A:762:GLN:OE1	2.00	0.45
1:B:513:ILE:CD1	1:B:953:MET:HE1	2.46	0.45
1:B:687:ARG:HA	1:B:691:VAL:HG23	1.97	0.45
1:B:930:ASN:C	1:B:932:TYR:N	2.72	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: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:D:245:PHE:C	1:D:247:GLN:N	2.72	0.45
1:G:776:LYS:HD2	5:G:80:HOH:O	2.16	0.45
1:G:1052:ASN:HD22	1:G:1052:ASN:N	2.03	0.45
1:E:280:ASP:OD1	1:E:348:THR:HG21	2.16	0.45
1:E:301:PRO:O	1:E:1065:GLN:HG3	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:H:299:TRP:C	1:H:300:TRP:CE3	2.94	0.45
1:A:279:LYS:HB3	1:A:279:LYS:HE2	1.78	0.45
1:C:407:ASN:HD21	1:C:431:GLU:H	1.64	0.45
1:E:457:MET:HE2	1:E:493:TYR:HE2	1.81	0.45
1:C:475:ARG:HA	1:C:953:MET:HE3	1.98	0.45
1:E:308:GLN:HE21	1:E:308:GLN:HB3	1.54	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:F:1041:LYS:HA	1:F:1041:LYS:HD2	1.69	0.45
1:F:1070:TYR:HD2	5:F:242:HOH:O	1.89	0.45
1:H:315:ALA:O	1:H:318:GLY:CA	2.65	0.45
1:H:356:LEU:C	1:H:358:GLN:H	2.25	0.45
1:H:928:LYS:HE3	1:H:928:LYS:HB2	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:C	1:A:290:LYS:N	2.75	0.45
1:A:976:ASP:C	1:A:976:ASP:OD1	2.60	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:309:TYR:CD2	1:D:309:TYR:C	2.94	0.45
1:D:642:LEU:HD12	1:D:642:LEU:N	2.32	0.45
1:D:924:LEU:N	1:D:924:LEU:CD1	2.80	0.45
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:E:281:GLY:H	1:E:344:GLU:HB2	1.81	0.45
1:H:475:ARG:N	1:H:953:MET:HE2	2.31	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:B:871:GLU:N	1:B:871:GLU:CD	2.68	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: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:N	1:H:394:LYS:CD	2.55	0.45
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.67	0.45
1:A:376:LYS:HE2	1:A:378:PHE:CZ	2.52	0.45
1:D:670:MET:HE3	1:D:877:VAL:HG12	1.99	0.45
1:G:310:VAL:CG1	1:G:335:ALA:HB1	2.47	0.45
1:G:474:ILE:O	1:G:953:MET:HE3	2.17	0.45
1:G:792:ASN:ND2	1:G:796:GLU:HB2	2.32	0.45
1:E:271:TRP:CG	1:E:357:ARG:HH12	2.35	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: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:B:1074:VAL:HG13	1:B:1077:ASN:H	1.82	0.44
1:E:460:GLY:N	1:E:470:ASN:ND2	2.65	0.44
1:F:467:PRO:HA	1:F:470:ASN:ND2	2.32	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:F:1025:ARG:HG2	1:F:1027:GLN:NE2	2.32	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:A:355:TRP:CG	1:A:356:LEU:H	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:GLN:O	1:A:384:LYS:HB2	2.18	0.44
1:A:458:ASN:C	1:A:470:ASN:ND2	2.75	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:B:856:MET:HE3	1:B:953:MET:SD	2.56	0.44
1:G:267:THR:C	1:G:269:GLU:N	2.72	0.44
1:G:492:ASP:CB	1:G:1022:LEU:HD22	2.33	0.44
1:E:255:ASP:C	1:E:257:ALA:N	2.73	0.44
1:E:275:LYS:C	1:E:276:TYR:CD2	2.96	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
1:H:745:LEU:HD12	1:H:745:LEU:N	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
1:C:999:SER:C	1:C:1001:LYS:N	2.73	0.44
1:D:578:VAL:CG1	1:D:579:PRO:HD2	2.48	0.44
4:D:5001:MES:H52	4:D:5001:MES:H82	1.18	0.44
1:G:244:SER:N	1:G:246:ALA:H	2.16	0.44
1:E:347:ILE:HG12	1:E:352:ASN:O	2.17	0.44
1:E:669:TYR:HE2	1:E:670:MET:CE	2.18	0.44
1:F:514:LEU:CD2	1:F:532:MET:HG3	2.47	0.44
1:H:293:ARG:HB3	1:H:297:MET:HE2	1.99	0.44
1:H:303:GLN:O	1:H:307:ARG:N	2.50	0.44
1:C:471:PHE:CG	1:C:954:ALA:HB2	2.52	0.44
1:D:530:ASP:HB2	1:D:843:LYS:HB3	1.98	0.44
1:D:809:ASN:HB2	1:D:810:PRO:HD2	1.99	0.44
1:G:389:TYR:CE1	1:G:1050:GLY:HA2	2.52	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: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: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: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:A:1001:LYS:HB2	1:A:1001:LYS:HE2	1.69	0.44
1:C:288:THR:C	1:C:290:LYS:N	2.73	0.44
1:G:740:ASN:HD22	1:G:741:PRO:CD	2.30	0.44
1:E:303:GLN:OE1	1:E:332:LEU:HD13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:LEU:O	1:E:360:ILE:HG12	2.18	0.44
1:F:752:VAL:O	1:F:752:VAL:CG1	2.65	0.44
1:F:797:LEU:HD23	1:F:797:LEU:HA	1.74	0.44
1:B:599:ILE:HA	1:B:603:ILE:HB	1.99	0.44
1:G:613:THR:OG1	1:G:616:GLU:HG3	2.17	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:A:300:TRP:CD2	1:A:300:TRP:N	2.85	0.44
1:B:714:GLY:O	1:B:715:LYS:C	2.58	0.44
1:B:721:THR:O	1:B:757:ALA:HB2	2.18	0.44
1:B:976:ASP:O	1:B:977:LYS:C	2.60	0.44
1:B:1077:ASN:O	1:B:1078:THR:C	2.61	0.44
1:C:333:ASN:O	1:C:337:GLN:HG3	2.17	0.44
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:F:801:ALA:C	1:F:803:ASP:N	2.76	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:350:GLU:O	1:A:351:LYS:C	2.60	0.44
1:A:869:LYS:O	1:A:870:LYS:C	2.60	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:CA	1:D:782:GLN:NE2	2.81	0.44
1:D:988:LYS:O	1:D:988:LYS:HG3	2.16	0.44
1:G:280:ASP:O	1:G:281:GLY:C	2.60	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:E:271:TRP:CH2	1:E:357:ARG:NE	2.86	0.44
1:H:759:HIS:CD2	1:H:764:TYR:OH	2.71	0.44
1:B:567:ASN:OD1	1:B:567:ASN:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:797:LEU:HD23	1:D:797:LEU:HA	1.84	0.44
1:D:948:LYS:HD3	1:D:948:LYS:HA	1.75	0.44
1:G:759:HIS:CD2	1:G:764:TYR:OH	2.71	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: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: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: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:D:551:LEU:HD12	1:D:551:LEU:C	2.43	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:F:988:LYS:C	1:F:990:THR:HG22	2.43	0.43
1:H:260:GLU:OE2	1:H:357:ARG:NH2	2.37	0.43
1:H:298:THR:C	1:H:300:TRP:CH2	2.95	0.43
1:H:460:GLY:N	1:H:470:ASN:ND2	2.66	0.43
1:A:375:GLU:OE2	1:A:992:TYR:OH	2.24	0.43
1:B:249:ASN:O	1:B:1084:LEU:HD22	2.18	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:E:439:ASP:OD1	1:E:439:ASP:C	2.61	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:H	1:F:745:LEU:CD1	2.18	0.43
1:B:433:LEU:HG	1:B:434:LEU:HG	2.00	0.43
1:B:630:ALA:O	1:B:633:LYS:NZ	2.48	0.43
1:B:908:LEU:C	1:B:908:LEU:HD12	2.43	0.43
1:C:324:ASN:C	1:C:324:ASN:OD1	2.61	0.43
1:C:350:GLU:C	1:C:352:ASN:H	2.26	0.43
1:G:449:GLN:OE1	1:G:449:GLN:HA	2.18	0.43
1:E:287:SER:HB3	1:E:291:ASP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:608:VAL:O	1:F:609:GLY:C	2.61	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:H:301:PRO:O	1:H:302:ASP:HB3	2.18	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:669:TYR:CE1	1:F:874:THR:HG23	2.53	0.43
1:F:712:ARG:NH1	1:F:712:ARG:HG3	2.32	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:C:606:ASN:O	1:C:607:VAL:C	2.61	0.43
1:D:1071:PHE:CE1	1:D:1081:PRO:HD3	2.52	0.43
1:G:280:ASP:C	1:G:282:LYS:H	2.25	0.43
1:E:1085:VAL:O	1:E:1087:PRO:HD3	2.18	0.43
1:F:469:ALA:C	1:F:942:ILE:HG21	2.43	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:883:ASP:OD1	1:C:948:LYS:HE3	2.18	0.43
1:C:917:ALA:HB1	1:C:962:TYR:CG	2.54	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:439:ASP:OD1	1:D:439:ASP:C	2.60	0.43
1:D:820:VAL:HB	1:D:821:PRO:HD2	2.01	0.43
1:G:371:ASN:HB3	1:G:373:ASP:N	2.25	0.43
1:E:1067:THR:OG1	1:E:1069:THR:HB	2.18	0.43
1:F:677:TYR:CD2	1:F:677:TYR:C	2.96	0.43
1:F:681:GLU:OE2	1:F:884:LYS:NZ	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:ALA:O	1:B:897:PRO:C	2.56	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:G:594:LEU:O	1:G:598:ILE:HG13	2.19	0.43
1:E:272:TYR:HE1	1:E:274:PRO:CA	2.32	0.43
1:F:364:VAL:HG13	1:F:370:TRP:CE3	2.53	0.43
1:B:272:TYR:CE1	1:B:274:PRO:CD	3.01	0.43
1:B:513:ILE:HG12	1:B:953:MET:HE2	1.98	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:C:740:ASN:C	1:C:740:ASN:ND2	2.69	0.43
1:D:487:LEU:HD22	1:D:532:MET:HE3	1.99	0.43
1:E:261:HIS:CD2	1:E:264:HIS:N	2.79	0.43
1:E:288:THR:C	1:E:290:LYS:N	2.76	0.43
1:F:375:GLU:OE2	1:F:992:TYR:OH	2.27	0.43
1:F:854:ARG:NH1	1:F:892:ASP:OD2	2.48	0.43
1:H:444:VAL:CG1	1:H:1038:VAL:HG22	2.48	0.43
1:H:1073:LEU:HD21	1:H:1080:LEU:HD21	2.00	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:389:TYR:CE1	1:B:970:VAL:HG21	2.54	0.43
1:B:391:ASN:OD1	1:B:404:ARG:HD2	2.18	0.43
1:B:604:ASN:O	1:B:604:ASN:CG	2.61	0.43
1:G:585:ARG:HD3	1:G:661:ASP:OD1	2.19	0.43
1:E:1067:THR:O	1:E:1068:ASN:C	2.62	0.43
1:F:861:SER:N	1:F:864:GLN:NE2	2.52	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:C:244:SER:C	1:C:246:ALA:N	2.76	0.43
1:C:464:ALA:O	1:C:465:ASN:HB2	2.19	0.43
1:C:1002:ASP:OD1	1:C:1002:ASP:N	2.33	0.43
1:D:320:HIS:ND1	1:D:320:HIS:N	2.63	0.43
1:D:350:GLU:O	1:D:352:ASN:N	2.52	0.43
1:E:409:THR:O	1:E:410:PRO:C	2.60	0.43
1:E:457:MET:HE2	1:E:493:TYR:CE2	2.53	0.43
1:E:483:ASP:OD1	1:E:483:ASP:C	2.62	0.43
1:H:300:TRP:CD2	1:H:306:GLN:HG2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:551:LEU:O	1:H:551:LEU:HD12	2.19	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:718:LEU:HD23	1:A:718:LEU:HA	1.79	0.42
1:A:759:HIS:CD2	1:A:764:TYR:OH	2.72	0.42
1:B:416:LYS:CE	1:F:551:LEU:HD11	2.37	0.42
1:B:458:ASN:O	1:B:459:PHE:C	2.62	0.42
1:B:689:LYS:CD	1:B:690:TYR:CE1	3.02	0.42
1:B:1007:TYR:O	1:B:1008:GLY:C	2.62	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:E:322:THR:HG23	1:E:323:TYR:N	2.35	0.42
1:E:1086:ASN:HA	1:E:1087:PRO:HD3	1.71	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:907:PHE:O	1:F:908:LEU:C	2.61	0.42
1:F:1067:THR:CG2	1:F:1067:THR:O	2.67	0.42
1:H:278:LEU:HD13	1:H:283:THR:N	2.35	0.42
1:H:744:ARG:HD3	1:H:744:ARG:HA	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:G:256:ALA:C	1:G:258:ASN:H	2.26	0.42
1:G:430:TYR:CZ	1:G:977:LYS:HD2	2.54	0.42
1:G:740:ASN:ND2	1:G:740:ASN:C	2.63	0.42
1:G:1065:GLN:HG3	1:G:1066:ALA:N	2.34	0.42
1:F:599:ILE:HG22	1:F:600:LYS:N	2.35	0.42
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:D:725:ASP:C	1:D:725:ASP:OD1	2.59	0.42
1:G:281:GLY:H	1:G:344:GLU:CB	2.30	0.42
1:G:895:MET:HB3	1:G:895:MET:HE2	1.84	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:323:TYR:CD1	1:F:327:THR:HG21	2.55	0.42
1:F:358:GLN:O	1:F:358:GLN:HG2	2.18	0.42
1:F:874:THR:HB	1:F:932:TYR:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:912:ILE:HA	1:F:912:ILE:HD12	1.80	0.42
1:F:935:ALA:O	1:F:938:LEU:HB3	2.18	0.42
1:F:1073:LEU:HD21	1:F:1080:LEU:HD21	2.01	0.42
1:H:919:THR:O	1:H:919:THR:HG22	2.19	0.42
1:H:976:ASP:OD1	1:H:976:ASP:C	2.62	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:A:725:ASP:C	1:A:725:ASP:OD1	2.63	0.42
1:A:930:ASN:O	1:A:931:LYS:C	2.57	0.42
1:B:389:TYR:CZ	1:B:1050:GLY:HA2	2.55	0.42
1:B:646:LEU:O	1:B:647:LEU:C	2.60	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:G:466:ASP:C	1:G:468:ASP:H	2.26	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:F:567:ASN:C	1:F:567:ASN:OD1	2.63	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:H:669:TYR:HD2	1:H:670:MET:HE3	1.82	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:B:760:LYS:C	1:B:762:GLN:N	2.77	0.42
1:B:873:TYR:O	1:B:874:THR:C	2.60	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: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: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: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:417:LYS:CE	1:F:555:SER:HB3	2.49	0.42
1:B:1023:PHE:HB3	1:G:747:ALA:HB3	2.01	0.42
1:C:705:SER:HB3	1:C:743:LEU:HD13	2.02	0.42
1:C:938:LEU:O	1:C:939:VAL:C	2.63	0.42
1:D:278:LEU:HG	1:D:281:GLY:CA	2.31	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:440:ASN:HD21	1:E:449:GLN:NE2	1.89	0.42
1:E:907:PHE:O	1:E:908:LEU:C	2.63	0.42
1:E:1077:ASN:OD1	1:E:1077:ASN:C	2.61	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:610:TYR:HA	1:C:612:PHE:CE2	2.54	0.42
1:C:1052:ASN:N	1:C:1052:ASN:ND2	2.58	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:D:606:ASN:O	1:D:607:VAL:C	2.63	0.42
1:D:993:VAL:O	1:D:1056:ARG:NH1	2.53	0.42
1:G:316:GLN:N	1:G:316:GLN:CD	2.76	0.42
1:G:794:ARG:HG2	1:G:794:ARG:NH1	2.34	0.42
1:F:603:ILE:HG22	1:F:604:ASN:N	2.34	0.42
1:F:604:ASN:C	1:F:606:ASN:N	2.78	0.42
1:F:711:VAL:HG22	1:F:734:VAL:CG2	2.48	0.42
1:F:951:LYS:HD3	1:F:951:LYS:HA	1.79	0.42
1:H:800:THR:HG23	1:H:801:ALA:N	2.34	0.42
1:A:278:LEU:HG	1:A:281:GLY:C	2.45	0.42
1:D:1022:LEU:N	1:D:1022:LEU:HD23	2.35	0.42
1:G:311:ASN:O	1:G:312:TYR:C	2.62	0.42
1:G:630:ALA:O	1:G:633:LYS:NZ	2.51	0.42
1:F:300:TRP:CD2	1:F:306:GLN:HG3	2.54	0.42
1:A:300:TRP:HB3	1:A:301:PRO:HD2	2.02	0.42
1:A:825:ALA:O	1:A:826:ALA:C	2.63	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:D:277:ILE:HD13	1:D:291:ASP:CG	2.44	0.42
1:G:403:TYR:CE2	1:G:443:PRO:HD2	2.55	0.42
1:E:951:LYS:HD3	1:E:951:LYS:HA	1.81	0.42
1:F:684:LEU:HD23	1:F:684:LEU:HA	1.88	0.42
1:F:746:LYS:C	1:F:748:SER:N	2.76	0.42
1:F:856:MET:HE3	1:F:856:MET:HB2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:394:LYS:H	1:H:394:LYS:CD	2.21	0.42
1:H:794:ARG:HG2	1:H:794:ARG:NH1	2.34	0.42
1:B:670:MET:HE1	1:B:885:PHE:HZ	1.84	0.42
1:B:725:ASP:O	1:B:726:ARG:C	2.63	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: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:E:557:MET:C	1:E:559:PRO:HD2	2.44	0.42
1:E:681:GLU:OE2	1:E:884:LYS:NZ	2.53	0.42
1:F:344:GLU:OE1	1:F:344:GLU:HA	2.19	0.42
1:F:432:PHE:HB2	1:F:977:LYS:HA	2.00	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:409:THR:O	1:H:410:PRO:C	2.62	0.42
1:A:561:ILE:HG12	1:A:697:MET:HE2	2.02	0.41
1:B:561:ILE:HG12	1:B:697:MET:HB3	2.01	0.41
1:B:617:ILE:O	1:B:617:ILE:CG2	2.66	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:D:1021:GLU:O	1:D:1022:LEU:C	2.62	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:E:271:TRP:CD1	1:E:294:PRO:HA	2.55	0.41
1:E:576:ALA:HB3	1:E:847:GLN:HB3	2.01	0.41
1:E:729:ARG:NH2	1:E:762:GLN:HB2	2.35	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:895:MET:HE2	1:F:895:MET:HB3	1.86	0.41
1:F:988:LYS:O	1:F:990:THR:HG22	2.19	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:B:759:HIS:ND1	1:B:759:HIS:N	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:670:MET:HE3	1:D:877:VAL:CG1	2.50	0.41
1:G:513:ILE:HD11	1:G:953:MET:HE1	2.02	0.41
1:G:1014:GLU:HG3	1:G:1018:LYS:HE3	2.01	0.41
1:E:344:GLU:OE1	1:E:344:GLU:HA	2.19	0.41
1:F:602:GLU:C	1:F:603:ILE:HG13	2.45	0.41
1:F:664:THR:HG22	1:F:666:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:930:ASN:OD1	1:F:932:TYR:N	2.46	0.41
4:F:5001:MES:H82	4:F:5001:MES:H52	1.15	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
1:A:344:GLU:O	1:A:345:GLU:C	2.63	0.41
4:A:5001:MES:H51	4:A:5001:MES:H81	1.34	0.41
1:B:248:TYR:C	1:B:250:GLN:N	2.77	0.41
1:B:660:GLY:HA2	1:B:663:PHE:O	2.19	0.41
1:B:848:ASN:O	1:B:849:ALA:C	2.59	0.41
1:C:313:MET:HE3	1:C:313:MET:HB3	1.86	0.41
1:D:314:ASN:O	1:D:319:ILE:N	2.53	0.41
1:D:976:ASP:O	1:D:977:LYS:C	2.62	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: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:424:ASP:HB3	1:E:520:ASN:CG	2.45	0.41
1:E:809:ASN:CB	1:E:810:PRO:CD	2.98	0.41
1:F:458:ASN:CA	1:F:470:ASN:OD1	2.68	0.41
1:F:799:PHE:N	1:F:799:PHE:CD2	2.88	0.41
1:F:895:MET:HE2	1:F:898:GLN:NE2	2.36	0.41
1:H:285:THR:C	1:H:286:GLN:O	2.63	0.41
1:H:299:TRP:C	1:H:300:TRP:CD2	2.98	0.41
1:H:1074:VAL:CG2	1:H:1077:ASN:HB2	2.49	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:C:293:ARG:HG3	1:C:297:MET:HE1	2.01	0.41
1:D:389:TYR:CZ	1:D:1050:GLY:HA2	2.55	0.41
1:D:1063:LYS:CE	1:D:1068:ASN:ND2	2.83	0.41
1:G:278:LEU:HG	1:G:281:GLY:C	2.46	0.41
1:G:370:TRP:CD1	1:G:1060:TYR:HA	2.55	0.41
1:E:267:THR:C	1:E:269:GLU:N	2.78	0.41
1:E:894:GLU:HA	1:E:953:MET:HB3	2.01	0.41
1:F:504:ASP:HB3	1:F:834:ALA:HB1	2.02	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: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:H:278:LEU:HD12	1:H:278:LEU:C	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:425:ARG:HH11	1:H:425:ARG:HD3	1.72	0.41
1:H:458:ASN:O	1:H:459:PHE:C	2.64	0.41
1:A:689:LYS:HD3	1:A:828:GLN:HB3	2.02	0.41
1:B:1063:LYS:NZ	1:B:1068:ASN:CG	2.79	0.41
1:C:988:LYS:N	1:C:990:THR:HG23	2.35	0.41
1:D:449:GLN:OE1	1:D:449:GLN:HA	2.19	0.41
1:D:854:ARG:HB3	1:D:891:THR:OG1	2.20	0.41
1:D:997:LYS:HA	1:D:1043:TRP:O	2.21	0.41
1:G:439:ASP:OD1	1:G:439:ASP:C	2.62	0.41
1:G:884:LYS:HA	1:G:884:LYS:HD3	1.74	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:F:362:ALA:O	1:F:363:PHE:C	2.64	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: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:D:363:PHE:O	1:D:364:VAL:C	2.63	0.41
1:G:458:ASN:O	1:G:459:PHE:C	2.63	0.41
1:G:884:LYS:HD2	1:G:888:TRP:CZ2	2.56	0.41
1:H:305:THR:CG2	1:H:306:GLN:H	2.34	0.41
1:H:1084:LEU:HA	1:H:1084:LEU:HD23	1.56	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:792:ASN:OD1	1:B:792:ASN:C	2.63	0.41
1:B:987:ILE:CG1	1:B:1058:ALA:HB2	2.51	0.41
1:D:883:ASP:OD1	1:D:948:LYS:HE3	2.21	0.41
1:G:1073:LEU:HD21	1:G:1080:LEU:HD21	2.03	0.41
1:F:945:LEU:HD13	1:F:952:VAL:HG22	2.02	0.41
1:F:1081:PRO:O	1:F:1082:LYS:C	2.63	0.41
1:H:589:SER:O	1:H:590:GLU:HB2	2.21	0.41
1:A:921:ARG:HH11	1:A:921:ARG:HD3	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:383:GLN:O	1:D:384:LYS:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:800:THR:CG2	1:H:802:ALA:H	2.08	0.41
1:A:457:MET:HE2	1:A:457:MET:HB2	1.94	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:A:1073:LEU:HD23	1:A:1080:LEU:HD21	1.97	0.41
1:B:248:TYR:O	1:B:250:GLN:N	2.54	0.41
1:B:425:ARG:H	1:B:425:ARG:HG2	1.66	0.41
1:B:470:ASN:N	1:B:470:ASN:HD22	2.17	0.41
1:B:758:ALA:HB3	1:B:759:HIS:ND1	2.35	0.41
1:C:312:TYR:O	1:C:316:GLN:HG2	2.21	0.41
1:C:589:SER:O	1:C:590:GLU:HB2	2.19	0.41
1:D:288:THR:H	1:D:291:ASP:CG	2.28	0.41
1:G:1080:LEU:HB3	1:G:1081:PRO:HD2	2.03	0.41
1:E:350:GLU:C	1:E:352:ASN:N	2.78	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:HA	1:F:698:ARG:HD3	1.90	0.41
1:F:869:LYS:CD	1:F:871:GLU:OE1	2.69	0.41
1:H:837:ALA:HA	1:H:838:PRO:HD3	1.89	0.41
1:H:861:SER:O	1:H:862:ASN:C	2.61	0.41
1:B:524:TYR:CD2	1:B:524:TYR:C	2.99	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:654:VAL:HG11	1:D:856:MET:HE3	2.03	0.41
1:G:346:LYS:HE2	1:G:355:TRP:CE3	2.56	0.41
1:G:487:LEU:O	1:G:532:MET:HE1	2.21	0.41
1:G:1069:THR:HG22	1:G:1070:TYR:O	2.20	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:H:278:LEU:CA	1:H:283:THR:O	2.68	0.41
1:H:430:TYR:CD1	1:H:977:LYS:HG2	2.56	0.41
1:H:524:TYR:CD2	1:H:524:TYR:C	2.98	0.41
1:H:854:ARG:HD3	1:H:892:ASP:OD2	2.21	0.41
1:H:877:VAL:HG13	1:H:881:ASN:ND2	2.36	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:HD3	1:A:365:LYS:HA	1.98	0.40
1:A:544:LEU:HD11	1:A:549:LYS:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ASN:OD1	1:B:372:SER:N	2.54	0.40
1:B:976:ASP:C	1:B:976:ASP:OD1	2.62	0.40
1:C:1061:VAL:HG12	1:C:1070:TYR:CD1	2.57	0.40
1:D:550:PRO:O	1:D:551:LEU:C	2.63	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:E:1064:ASP:OD1	1:E:1067:THR:HG23	2.21	0.40
1:F:495:LYS:HB2	1:F:495:LYS:HE3	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:H:305:THR:O	1:H:306:GLN:C	2.63	0.40
1:H:877:VAL:HG13	1:H:881:ASN:HD21	1.86	0.40
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:B:1016:GLN:NE2	1:G:748:SER:HA	2.24	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:474:ILE:HA	1:D:954:ALA:O	2.20	0.40
1:G:259:PHE:CD2	1:G:259:PHE:N	2.89	0.40
1:G:702:VAL:O	1:G:703:GLY:C	2.64	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:E:1016:GLN:HA	1:E:1023:PHE:CE2	2.56	0.40
1:F:771:THR:O	1:F:809:ASN:ND2	2.54	0.40
1:B:974:ARG:HE	1:B:1053:ILE:HG21	1.87	0.40
1:C:350:GLU:C	1:C:352:ASN:N	2.79	0.40
1:G:293:ARG:CB	1:G:297:MET:CE	2.98	0.40
1:G:874:THR:HB	1:G:932:TYR:HB3	2.02	0.40
1:G:943:LYS:HZ2	1:G:943:LYS:HG2	1.69	0.40
1:E:260:GLU:OE2	1:E:292:PHE:HD1	2.05	0.40
1:E:355:TRP:CG	1:E:356:LEU:H	2.40	0.40
1:F:261:HIS:CD2	1:F:264:HIS:CA	3.03	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:299:TRP:C	1:A:300:TRP:CD2	2.99	0.40
1:A:669:TYR:CZ	1:A:874:THR:HG23	2.56	0.40
1:B:525:LEU:HD12	1:B:525:LEU:HA	1.84	0.40
1:C:245:PHE:O	1:C:246:ALA:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:THR:O	1:D:306:GLN:C	2.65	0.40
1:G:800:THR:HG22	1:G:801:ALA:N	2.36	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:HD23	1:F:486:LEU:HA	1.89	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:245:PHE:N	1:D:245:PHE:CD1	2.88	0.40
1:D:391:ASN:OD1	1:D:404:ARG:HD2	2.22	0.40
1:D:1063:LYS:NZ	1:D:1068:ASN:HD21	2.19	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:G:1001:LYS:HB2	1:G:1001:LYS:HE2	1.58	0.40
1:F:322:THR:CG2	1:F:323:TYR:N	2.84	0.40
1:F:882:VAL:HG22	1:F:882:VAL:O	2.21	0.40
1:F:1076:ASP:CG	1:F:1077:ASN:HB2	2.46	0.40
1:H:277:ILE:CG1	1:H:291:ASP:HB3	2.45	0.40
1:H:279:LYS:O	1:H:280:ASP:C	2.64	0.40
1:H:315:ALA:O	1:H:318:GLY:HA2	2.22	0.40
1:H:444:VAL:HG11	1:H:1038:VAL:HG22	2.03	0.40
1:H:619:LYS:HD2	1:H:619:LYS:HA	1.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	840/844 (100%)	791 (94%)	45 (5%)	4 (0%)	24 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	745/844 (88%)	693 (93%)	41 (6%)	11 (2%)	8	32
1	C	842/844 (100%)	809 (96%)	29 (3%)	4 (0%)	24	57
1	D	842/844 (100%)	789 (94%)	46 (6%)	7 (1%)	16	47
1	E	842/844 (100%)	791 (94%)	41 (5%)	10 (1%)	10	37
1	F	842/844 (100%)	783 (93%)	53 (6%)	6 (1%)	18	49
1	G	842/844 (100%)	796 (94%)	43 (5%)	3 (0%)	30	61
1	H	804/844 (95%)	743 (92%)	53 (7%)	8 (1%)	12	41
All	All	6599/6752 (98%)	6195 (94%)	351 (5%)	53 (1%)	16	47

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	668 (94%)	45 (6%)	16	45
1	B	628/715 (88%)	566 (90%)	62 (10%)	7	29
1	C	715/715 (100%)	673 (94%)	42 (6%)	18	48
1	D	715/715 (100%)	660 (92%)	55 (8%)	12	38
1	E	715/715 (100%)	658 (92%)	57 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	715/715 (100%)	659 (92%)	56 (8%)	11	38
1	G	715/715 (100%)	664 (93%)	51 (7%)	13	41
1	H	683/715 (96%)	634 (93%)	49 (7%)	13	40
All	All	5599/5720 (98%)	5182 (93%)	417 (7%)	13	40

All (417) 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
1	A	310	VAL
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	394	LYS
1	A	457	MET
1	A	465	ASN
1	A	532	MET
1	A	574	GLU
1	A	584	ILE
1	A	604	ASN
1	A	607	VAL
1	A	614	MET
1	A	615	GLU
1	A	618	LYS
1	A	702	VAL
1	A	726	ARG
1	A	744	ARG
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

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Mol	Chain	Res	Type
1	A	880	LYS
1	A	882	VAL
1	A	912	ILE
1	A	985	SER
1	A	988	LYS
1	A	990	THR
1	A	1001	LYS
1	A	1013	GLU
1	A	1038	VAL
1	A	1052	ASN
1	A	1075	SER
1	A	1082	LYS
1	B	248	TYR
1	B	255	ASP
1	B	259	PHE
1	B	374	SER
1	B	390	SER
1	B	394	LYS
1	B	405	ILE
1	B	416	LYS
1	B	422	THR
1	B	465	ASN
1	B	498	LYS
1	B	500	ILE
1	B	501	HIS
1	B	502	LYS
1	B	503	ASN
1	B	532	MET
1	B	535	MET
1	B	551	LEU
1	B	600	LYS
1	B	604	ASN
1	B	605	PRO
1	B	612	PHE
1	B	617	ILE
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	719	LYS

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Mol	Chain	Res	Type
1	B	723	THR
1	B	726	ARG
1	B	727	ILE
1	B	776	LYS
1	B	791	THR
1	B	800	THR
1	B	832	VAL
1	B	836	THR
1	B	854	ARG
1	B	871	GLU
1	B	882	VAL
1	B	884	LYS
1	B	912	ILE
1	B	913	GLN
1	B	921	ARG
1	B	939	VAL
1	B	947	SER
1	B	951	LYS
1	B	974	ARG
1	B	985	SER
1	B	990	THR
1	B	998	SER
1	B	1003	GLN
1	B	1037	SER
1	B	1038	VAL
1	B	1042	GLN
1	B	1044	SER
1	B	1052	ASN
1	B	1063	LYS
1	B	1078	THR
1	B	1082	LYS
1	B	1084	LEU
1	C	247	GLN
1	C	258	ASN
1	C	290	LYS
1	C	308	GLN
1	C	320	HIS
1	C	342	LYS
1	C	346	LYS
1	C	347	ILE
1	C	352	ASN
1	C	372	SER

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Mol	Chain	Res	Type
1	C	374	SER
1	C	390	SER
1	C	394	LYS
1	C	422	THR
1	C	457	MET
1	C	465	ASN
1	C	505	LYS
1	C	532	MET
1	C	574	GLU
1	C	604	ASN
1	C	605	PRO
1	C	618	LYS
1	C	632	GLU
1	C	702	VAL
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	884	LYS
1	C	912	ILE
1	C	928	LYS
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	1065	GLN
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

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Mol	Chain	Res	Type
1	D	320	HIS
1	D	322	THR
1	D	341	THR
1	D	342	LYS
1	D	350	GLU
1	D	352	ASN
1	D	359	THR
1	D	368	SER
1	D	416	LYS
1	D	422	THR
1	D	465	ASN
1	D	502	LYS
1	D	505	LYS
1	D	532	MET
1	D	551	LEU
1	D	574	GLU
1	D	604	ASN
1	D	605	PRO
1	D	615	GLU
1	D	619	LYS
1	D	702	VAL
1	D	707	ILE
1	D	726	ARG
1	D	740	ASN
1	D	744	ARG
1	D	782	GLN
1	D	793	ASP
1	D	800	THR
1	D	832	VAL
1	D	854	ARG
1	D	880	LYS
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

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Mol	Chain	Res	Type
1	D	1074	VAL
1	D	1084	LEU
1	D	1086	ASN
1	G	253	SER
1	G	258	ASN
1	G	275	LYS
1	G	282	LYS
1	G	283	THR
1	G	322	THR
1	G	339	ILE
1	G	350	GLU
1	G	352	ASN
1	G	359	THR
1	G	368	SER
1	G	394	LYS
1	G	405	ILE
1	G	422	THR
1	G	457	MET
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	707	ILE
1	G	740	ASN
1	G	744	ARG
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
1	G	928	LYS
1	G	948	LYS
1	G	977	LYS
1	G	985	SER

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Mol	Chain	Res	Type
1	G	988	LYS
1	G	990	THR
1	G	1001	LYS
1	G	1013	GLU
1	G	1025	ARG
1	G	1038	VAL
1	G	1046	LYS
1	G	1052	ASN
1	G	1074	VAL
1	G	1075	SER
1	G	1078	THR
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	310	VAL
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	457	MET
1	E	505	LYS
1	E	532	MET
1	E	574	GLU
1	E	619	LYS
1	E	632	GLU

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Mol	Chain	Res	Type
1	E	685	LYS
1	E	702	VAL
1	E	711	VAL
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	870	LYS
1	E	880	LYS
1	E	882	VAL
1	E	928	LYS
1	E	977	LYS
1	E	986	GLN
1	E	988	LYS
1	E	1001	LYS
1	E	1025	ARG
1	E	1038	VAL
1	E	1044	SER
1	E	1052	ASN
1	E	1069	THR
1	E	1074	VAL
1	E	1075	SER
1	E	1076	ASP
1	E	1077	ASN
1	E	1078	THR
1	F	253	SER
1	F	258	ASN
1	F	308	GLN
1	F	346	LYS
1	F	350	GLU
1	F	351	LYS
1	F	357	ARG
1	F	368	SER
1	F	394	LYS
1	F	422	THR
1	F	425	ARG
1	F	453	LEU
1	F	465	ASN
1	F	524	TYR
1	F	532	MET

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Mol	Chain	Res	Type
1	F	540	ARG
1	F	551	LEU
1	F	599	ILE
1	F	604	ASN
1	F	605	PRO
1	F	612	PHE
1	F	626	LYS
1	F	664	THR
1	F	685	LYS
1	F	708	ILE
1	F	723	THR
1	F	726	ARG
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	793	ASP
1	F	794	ARG
1	F	803	ASP
1	F	835	SER
1	F	869	LYS
1	F	870	LYS
1	F	884	LYS
1	F	904	ASP
1	F	912	ILE
1	F	936	ASP
1	F	940	LYS
1	F	977	LYS
1	F	980	THR
1	F	985	SER
1	F	990	THR
1	F	1001	LYS
1	F	1025	ARG
1	F	1038	VAL
1	F	1039	LYS
1	F	1052	ASN
1	F	1064	ASP
1	F	1074	VAL
1	F	1076	ASP
1	H	244	SER

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Mol	Chain	Res	Type
1	H	258	ASN
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	303	GLN
1	H	304	GLU
1	H	306	GLN
1	H	309	TYR
1	H	316	GLN
1	H	368	SER
1	H	390	SER
1	H	392	ASN
1	H	394	LYS
1	H	422	THR
1	H	465	ASN
1	H	505	LYS
1	H	532	MET
1	H	540	ARG
1	H	619	LYS
1	H	702	VAL
1	H	708	ILE
1	H	726	ARG
1	H	727	ILE
1	H	728	THR
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	986	GLN
1	H	988	LYS
1	H	990	THR
1	H	1001	LYS
1	H	1014	GLU

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Mol	Chain	Res	Type
1	H	1016	GLN
1	H	1038	VAL
1	H	1052	ASN
1	H	1074	VAL
1	H	1075	SER
1	H	1078	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (221) 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	412	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	558	ASN
1	A	572	ASN
1	A	604	ASN
1	A	639	ASN
1	A	699	ASN
1	A	700	GLN
1	A	740	ASN
1	A	759	HIS
1	A	773	ASN
1	A	782	GLN
1	A	811	GLN
1	A	828	GLN
1	A	846	HIS
1	A	864	GLN
1	A	960	GLN
1	A	989	ASN
1	A	1052	ASN
1	A	1068	ASN
1	B	261	HIS

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Mol	Chain	Res	Type
1	B	264	HIS
1	B	392	ASN
1	B	407	ASN
1	B	412	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	558	ASN
1	B	639	ASN
1	B	699	ASN
1	B	740	ASN
1	B	759	HIS
1	B	761	ASN
1	B	782	GLN
1	B	846	HIS
1	B	864	GLN
1	B	960	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	331	GLN
1	C	367	GLN
1	C	407	ASN
1	C	440	ASN
1	C	461	ASN
1	C	470	ASN
1	C	481	ASN
1	C	531	ASN
1	C	558	ASN
1	C	639	ASN
1	C	676	ASN
1	C	740	ASN

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Mol	Chain	Res	Type
1	C	759	HIS
1	C	761	ASN
1	C	773	ASN
1	C	782	GLN
1	C	811	GLN
1	C	846	HIS
1	C	864	GLN
1	C	913	GLN
1	C	1052	ASN
1	D	258	ASN
1	D	261	HIS
1	D	308	GLN
1	D	311	ASN
1	D	316	GLN
1	D	407	ASN
1	D	412	ASN
1	D	440	ASN
1	D	470	ASN
1	D	481	ASN
1	D	558	ASN
1	D	639	ASN
1	D	699	ASN
1	D	700	GLN
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	1016	GLN
1	D	1027	GLN
1	D	1052	ASN
1	D	1068	ASN
1	G	250	GLN
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	412	ASN

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Mol	Chain	Res	Type
1	G	440	ASN
1	G	470	ASN
1	G	481	ASN
1	G	558	ASN
1	G	572	ASN
1	G	604	ASN
1	G	639	ASN
1	G	699	ASN
1	G	740	ASN
1	G	759	HIS
1	G	761	ASN
1	G	782	GLN
1	G	846	HIS
1	G	864	GLN
1	G	875	ASN
1	G	898	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	352	ASN
1	E	367	GLN
1	E	407	ASN
1	E	412	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	700	GLN
1	E	740	ASN
1	E	759	HIS
1	E	773	ASN
1	E	782	GLN
1	E	811	GLN

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Mol	Chain	Res	Type
1	E	846	HIS
1	E	864	GLN
1	E	986	GLN
1	E	1016	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
1	F	311	ASN
1	F	352	ASN
1	F	367	GLN
1	F	407	ASN
1	F	440	ASN
1	F	458	ASN
1	F	481	ASN
1	F	531	ASN
1	F	558	ASN
1	F	639	ASN
1	F	676	ASN
1	F	699	ASN
1	F	740	ASN
1	F	759	HIS
1	F	761	ASN
1	F	773	ASN
1	F	782	GLN
1	F	846	HIS
1	F	864	GLN
1	F	881	ASN
1	F	913	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

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Mol	Chain	Res	Type
1	H	316	GLN
1	H	367	GLN
1	H	407	ASN
1	H	412	ASN
1	H	440	ASN
1	H	470	ASN
1	H	481	ASN
1	H	531	ASN
1	H	558	ASN
1	H	572	ASN
1	H	639	ASN
1	H	699	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
1	H	881	ASN
1	H	1016	GLN
1	H	1052	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

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	2.58	5 (41%)	17,17,17	4.48	8 (47%)
2	GLC	I	2	2	11,11,12	0.80	0	15,15,17	2.32	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	5.24	1.55	1.42
2	I	1	GLC	O5-C5	4.28	1.54	1.44
2	I	1	GLC	C4-C5	3.25	1.59	1.53
2	I	1	GLC	O1-C1	3.14	1.49	1.39
2	I	1	GLC	C1-C2	3.12	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	-12.05	88.38	110.23
2	I	1	GLC	O4-C4-C3	-9.89	87.07	110.38
2	I	1	GLC	O5-C5-C4	5.86	120.26	109.70
2	I	1	GLC	O2-C2-C3	-4.44	99.91	110.38
2	I	2	GLC	C2-C3-C4	-4.29	103.31	110.86
2	I	2	GLC	O5-C1-C2	-4.27	100.60	110.79
2	I	2	GLC	C1-O5-C5	-3.51	107.48	112.19
2	I	1	GLC	O1-C1-C2	-3.34	99.28	108.98
2	I	1	GLC	O3-C3-C2	-3.32	102.55	110.38
2	I	2	GLC	O5-C5-C6	-3.25	101.34	107.66
2	I	2	GLC	O6-C6-C5	-2.87	101.55	111.33
2	I	1	GLC	O6-C6-C5	-2.69	102.18	111.33
2	I	1	GLC	O5-C5-C6	-2.51	100.22	106.44
2	I	2	GLC	O5-C5-C4	-2.22	105.44	110.83
2	I	2	GLC	O2-C2-C1	2.17	114.20	109.22

There are no chirality outliers.

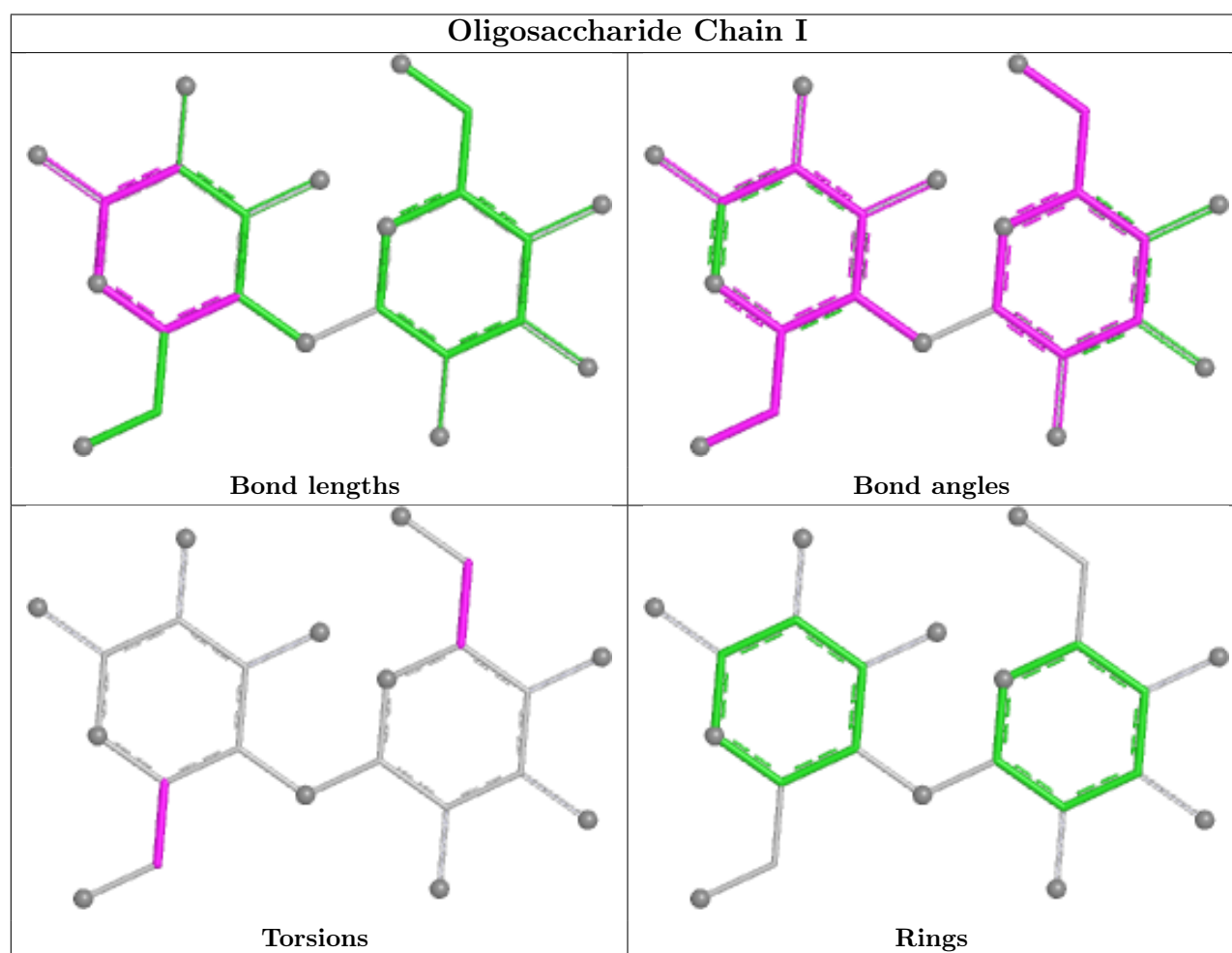
All (4) torsion outliers are listed below:

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	2.63	3 (25%)	15,16,16	6.18	10 (66%)
4	MES	F	5001	-	12,12,12	3.28	4 (33%)	15,16,16	5.97	11 (73%)
4	MES	B	5001	-	12,12,12	2.26	4 (33%)	15,16,16	6.34	12 (80%)
4	MES	A	5001	-	12,12,12	3.92	7 (58%)	15,16,16	7.05	9 (60%)
4	MES	E	5001	-	12,12,12	2.87	5 (41%)	15,16,16	5.81	11 (73%)
4	MES	D	5001	-	12,12,12	2.79	6 (50%)	15,16,16	5.53	12 (80%)
4	MES	C	5001	-	12,12,12	3.16	4 (33%)	15,16,16	5.43	7 (46%)
4	MES	H	5001	-	12,12,12	2.70	5 (41%)	15,16,16	5.63	11 (73%)

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	F	5001	-	-	5/6/14/14	0/1/1/1
4	MES	B	5001	-	-	3/6/14/14	0/1/1/1
4	MES	A	5001	-	-	2/6/14/14	0/1/1/1
4	MES	E	5001	-	-	1/6/14/14	0/1/1/1
4	MES	D	5001	-	-	2/6/14/14	0/1/1/1
4	MES	C	5001	-	-	4/6/14/14	0/1/1/1
4	MES	H	5001	-	-	4/6/14/14	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5001	MES	O2S-S	8.13	1.68	1.45
4	A	5001	MES	O1S-S	8.00	1.67	1.45
4	F	5001	MES	O2S-S	7.58	1.66	1.45
4	C	5001	MES	O1S-S	6.81	1.64	1.45
4	H	5001	MES	O1S-S	6.01	1.62	1.45
4	F	5001	MES	O1S-S	6.01	1.62	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	5001	MES	O2S-S	5.81	1.61	1.45
4	E	5001	MES	O1S-S	5.78	1.61	1.45
4	D	5001	MES	O1S-S	5.67	1.61	1.45
4	E	5001	MES	O2S-S	5.30	1.60	1.45
4	G	5001	MES	O2S-S	5.26	1.59	1.45
4	G	5001	MES	O1S-S	5.21	1.59	1.45
4	B	5001	MES	O2S-S	4.99	1.59	1.45
4	H	5001	MES	O2S-S	4.94	1.59	1.45
4	D	5001	MES	O2S-S	4.86	1.58	1.45
4	A	5001	MES	O3S-S	4.81	1.65	1.47
4	C	5001	MES	O3S-S	4.81	1.65	1.47
4	G	5001	MES	O3S-S	4.26	1.63	1.47
4	E	5001	MES	O3S-S	4.11	1.62	1.47
4	B	5001	MES	O1S-S	3.99	1.56	1.45
4	F	5001	MES	O3S-S	3.79	1.61	1.47
4	D	5001	MES	O3S-S	3.29	1.59	1.47
4	H	5001	MES	O3S-S	3.13	1.59	1.47
4	B	5001	MES	O3S-S	3.01	1.58	1.47
4	D	5001	MES	C8-S	2.84	1.81	1.77
4	A	5001	MES	C8-S	2.76	1.81	1.77
4	F	5001	MES	C7-C8	2.71	1.59	1.52
4	B	5001	MES	C7-C8	2.68	1.59	1.52
4	E	5001	MES	C8-S	2.65	1.81	1.77
4	D	5001	MES	C5-C6	2.52	1.59	1.50
4	A	5001	MES	C7-C8	2.48	1.58	1.52
4	H	5001	MES	C7-N4	-2.30	1.42	1.47
4	A	5001	MES	C5-N4	2.27	1.53	1.46
4	C	5001	MES	C5-N4	2.26	1.53	1.46
4	H	5001	MES	C5-C6	2.18	1.58	1.50
4	E	5001	MES	C5-C6	2.08	1.58	1.50
4	A	5001	MES	C5-C6	2.08	1.58	1.50
4	D	5001	MES	C7-C8	2.04	1.57	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5001	MES	O1S-S-C8	-18.89	78.18	106.73
4	B	5001	MES	O2S-S-C8	-17.10	80.89	106.73
4	G	5001	MES	O1S-S-C8	-16.36	82.01	106.73
4	A	5001	MES	O2S-S-C8	-15.81	82.84	106.73
4	E	5001	MES	O1S-S-C8	-14.97	84.11	106.73
4	D	5001	MES	O1S-S-C8	-12.73	87.48	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	5001	MES	O2S-S-C8	-12.15	88.37	106.73
4	F	5001	MES	O1S-S-C8	-11.92	88.72	106.73
4	H	5001	MES	O1S-S-C8	-11.83	88.86	106.73
4	B	5001	MES	O1S-S-C8	-11.75	88.97	106.73
4	C	5001	MES	O2S-S-C8	-10.59	90.73	106.73
4	H	5001	MES	O3S-S-C8	-10.38	85.71	106.00
4	H	5001	MES	O2S-S-C8	-10.12	91.44	106.73
4	E	5001	MES	O2S-S-C8	-9.85	91.85	106.73
4	C	5001	MES	O1S-S-C8	-9.78	91.95	106.73
4	D	5001	MES	O3S-S-C8	-9.76	86.92	106.00
4	F	5001	MES	O3S-S-C8	-9.42	87.57	106.00
4	C	5001	MES	C5-N4-C3	9.12	128.48	108.84
4	G	5001	MES	O2S-S-C8	-9.05	93.06	106.73
4	G	5001	MES	O3S-S-C8	-8.88	88.62	106.00
4	C	5001	MES	O3S-S-C8	-8.63	89.12	106.00
4	D	5001	MES	C5-N4-C3	8.46	127.07	108.84
4	E	5001	MES	C5-N4-C3	8.07	126.22	108.84
4	F	5001	MES	C5-N4-C3	7.20	124.34	108.84
4	D	5001	MES	O2S-S-C8	-7.17	95.89	106.73
4	A	5001	MES	O3S-S-O1S	6.41	127.43	111.40
4	G	5001	MES	C5-N4-C3	6.28	122.37	108.84
4	H	5001	MES	C5-N4-C3	6.14	122.06	108.84
4	B	5001	MES	O3S-S-C8	-5.84	94.58	106.00
4	A	5001	MES	C5-N4-C3	5.82	121.38	108.84
4	E	5001	MES	C8-C7-N4	-5.78	90.49	112.36
4	E	5001	MES	O3S-S-C8	-5.66	94.94	106.00
4	B	5001	MES	C5-N4-C3	5.45	120.59	108.84
4	C	5001	MES	C8-C7-N4	-5.44	91.79	112.36
4	F	5001	MES	C8-C7-N4	-5.25	92.50	112.36
4	A	5001	MES	C2-C3-N4	-5.11	102.35	110.12
4	G	5001	MES	C6-C5-N4	-5.07	102.41	110.12
4	F	5001	MES	O3S-S-O2S	4.82	123.46	111.40
4	B	5001	MES	C2-C3-N4	-4.76	102.89	110.12
4	H	5001	MES	C8-C7-N4	-4.65	94.78	112.36
4	G	5001	MES	C7-N4-C5	4.63	123.58	111.24
4	C	5001	MES	O3S-S-O2S	4.55	122.78	111.40
4	H	5001	MES	C2-C3-N4	-4.34	103.52	110.12
4	B	5001	MES	O3S-S-O1S	4.32	122.21	111.40
4	G	5001	MES	O3S-S-O1S	4.21	121.93	111.40
4	D	5001	MES	C8-C7-N4	-4.04	97.06	112.36
4	B	5001	MES	C6-C5-N4	-3.83	104.30	110.12
4	F	5001	MES	O2S-S-O1S	3.83	126.26	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	5001	MES	C8-C7-N4	-3.66	98.53	112.36
4	B	5001	MES	C8-C7-N4	-3.65	98.56	112.36
4	F	5001	MES	C7-N4-C5	3.62	120.88	111.24
4	A	5001	MES	C7-N4-C5	3.60	120.83	111.24
4	H	5001	MES	O3S-S-O1S	3.55	120.28	111.40
4	B	5001	MES	C7-N4-C5	3.47	120.50	111.24
4	D	5001	MES	C2-C3-N4	-3.45	104.88	110.12
4	D	5001	MES	O3S-S-O2S	3.35	119.77	111.40
4	B	5001	MES	O3S-S-O2S	3.31	119.69	111.40
4	E	5001	MES	C7-N4-C3	3.22	119.82	111.24
4	E	5001	MES	C2-C3-N4	-3.11	105.40	110.12
4	G	5001	MES	O3S-S-O2S	3.04	119.00	111.40
4	H	5001	MES	C7-N4-C5	3.00	119.23	111.24
4	D	5001	MES	O3S-S-O1S	2.97	118.84	111.40
4	E	5001	MES	O3S-S-O2S	2.94	118.74	111.40
4	F	5001	MES	C6-O1-C2	2.92	119.32	109.88
4	C	5001	MES	O3S-S-O1S	2.91	118.68	111.40
4	B	5001	MES	C7-N4-C3	2.88	118.91	111.24
4	F	5001	MES	C2-C3-N4	-2.88	105.75	110.12
4	D	5001	MES	C6-C5-N4	2.87	114.49	110.12
4	A	5001	MES	C8-C7-N4	-2.85	101.58	112.36
4	G	5001	MES	C2-C3-N4	-2.83	105.82	110.12
4	E	5001	MES	O2S-S-O1S	2.80	122.94	113.82
4	H	5001	MES	C7-N4-C3	2.79	118.68	111.24
4	E	5001	MES	O3S-S-O1S	2.76	118.31	111.40
4	D	5001	MES	C6-O1-C2	2.71	118.63	109.88
4	D	5001	MES	C7-N4-C3	2.51	117.94	111.24
4	H	5001	MES	O3S-S-O2S	2.50	117.64	111.40
4	F	5001	MES	C6-C5-N4	-2.50	106.33	110.12
4	H	5001	MES	O2S-S-O1S	2.49	121.92	113.82
4	A	5001	MES	C7-N4-C3	2.45	117.76	111.24
4	A	5001	MES	O2S-S-O1S	2.39	121.61	113.82
4	E	5001	MES	C6-C5-N4	2.33	113.66	110.12
4	D	5001	MES	O2S-S-O1S	2.33	121.39	113.82
4	B	5001	MES	O1-C6-C5	-2.12	107.20	111.77

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	B	5001	MES	C8-C7-N4-C5

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

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	F	5001	MES	1	0
4	B	5001	MES	1	0
4	A	5001	MES	4	0
4	E	5001	MES	1	0
4	D	5001	MES	1	0
4	C	5001	MES	1	0
4	H	5001	MES	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.33	10 (1%) 76 58	23, 36, 90, 112	0
1	B	749/844 (88%)	-0.04	17 (2%) 61 39	30, 51, 98, 148	0
1	C	844/844 (100%)	-0.46	11 (1%) 75 56	25, 35, 61, 71	0
1	D	844/844 (100%)	-0.28	20 (2%) 59 38	25, 36, 89, 110	0
1	E	844/844 (100%)	-0.23	30 (3%) 46 26	22, 36, 111, 136	0
1	F	844/844 (100%)	-0.11	7 (0%) 82 65	39, 55, 78, 91	0
1	G	844/844 (100%)	-0.39	7 (0%) 82 65	24, 36, 72, 85	0
1	H	808/844 (95%)	-0.27	28 (3%) 47 27	25, 43, 101, 144	0
All	All	6619/6752 (98%)	-0.27	130 (1%) 65 44	22, 40, 88, 148	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	303	GLN	5.5
1	H	318	GLY	5.4
1	B	246	ALA	5.0
1	H	249	ASN	4.8
1	H	282	LYS	4.8
1	E	273	ARG	4.7
1	E	303	GLN	4.6
1	B	249	ASN	4.5
1	H	245	PHE	4.4
1	H	297	MET	4.2
1	H	277	ILE	4.2
1	D	249	ASN	4.2
1	B	248	TYR	4.1
1	H	247	GLN	3.9
1	D	244	SER	3.9
1	H	280	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	H	317	LEU	3.8
1	E	249	ASN	3.7
1	A	606	ASN	3.7
1	E	278	LEU	3.6
1	B	274	PRO	3.4
1	E	1081	PRO	3.4
1	D	320	HIS	3.4
1	B	1087	PRO	3.4
1	H	1087	PRO	3.3
1	A	1076	ASP	3.3
1	E	325	THR	3.3
1	C	1077	ASN	3.2
1	H	284	TRP	3.2
1	C	244	SER	3.2
1	C	1076	ASP	3.1
1	H	283	THR	3.1
1	E	248	TYR	3.1
1	B	272	TYR	3.1
1	A	246	ALA	3.1
1	E	320	HIS	3.1
1	E	330	LEU	3.0
1	F	801	ALA	3.0
1	E	351	LYS	3.0
1	G	358	GLN	3.0
1	E	321	GLN	3.0
1	A	1077	ASN	3.0
1	H	1076	ASP	2.9
1	E	322	THR	2.9
1	D	286	GLN	2.9
1	G	244	SER	2.9
1	E	285	THR	2.9
1	E	284	TRP	2.8
1	H	355	TRP	2.8
1	A	358	GLN	2.8
1	H	246	ALA	2.8
1	A	330	LEU	2.8
1	H	244	SER	2.8
1	G	615	GLU	2.8
1	B	1077	ASN	2.8
1	F	244	SER	2.8
1	D	327	THR	2.8
1	H	281	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	278	LEU	2.8
1	H	276	TYR	2.7
1	C	321	GLN	2.7
1	D	280	ASP	2.7
1	E	326	ALA	2.7
1	B	1084	LEU	2.7
1	B	247	GLN	2.7
1	D	247	GLN	2.7
1	D	321	GLN	2.7
1	C	468	ASP	2.7
1	E	247	GLN	2.6
1	C	1087	PRO	2.6
1	G	1087	PRO	2.6
1	E	329	PRO	2.6
1	E	290	LYS	2.6
1	B	250	GLN	2.5
1	D	334	LEU	2.5
1	E	244	SER	2.5
1	E	280	ASP	2.5
1	F	800	THR	2.5
1	H	314	ASN	2.5
1	D	316	GLN	2.5
1	B	727	ILE	2.4
1	C	289	GLU	2.4
1	H	306	GLN	2.4
1	G	1076	ASP	2.4
1	D	282	LYS	2.4
1	H	305	THR	2.4
1	E	984	GLY	2.4
1	E	316	GLN	2.4
1	B	1083	SER	2.4
1	A	286	GLN	2.4
1	C	358	GLN	2.4
1	D	317	LEU	2.4
1	E	283	THR	2.3
1	D	318	GLY	2.3
1	G	750	ARG	2.3
1	D	379	ASP	2.3
1	E	345	GLU	2.2
1	B	747	ALA	2.2
1	C	247	GLN	2.2
1	D	986	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	289	GLU	2.2
1	E	287	SER	2.2
1	C	320	HIS	2.2
1	E	341	THR	2.2
1	H	248	TYR	2.2
1	E	332	LEU	2.2
1	D	1085	VAL	2.2
1	B	368	SER	2.2
1	F	1087	PRO	2.2
1	E	245	PHE	2.2
1	F	883	ASP	2.2
1	B	606	ASN	2.1
1	H	285	THR	2.1
1	F	802	ALA	2.1
1	E	246	ALA	2.1
1	H	986	GLN	2.1
1	E	328	SER	2.1
1	A	608	VAL	2.1
1	G	632	GLU	2.1
1	D	248	TYR	2.1
1	H	316	GLN	2.1
1	D	1087	PRO	2.1
1	D	352	ASN	2.0
1	B	271	TRP	2.0
1	B	1063	LYS	2.0
1	A	334	LEU	2.0
1	C	606	ASN	2.0
1	A	323	TYR	2.0
1	D	338	THR	2.0
1	H	622	GLU	2.0

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

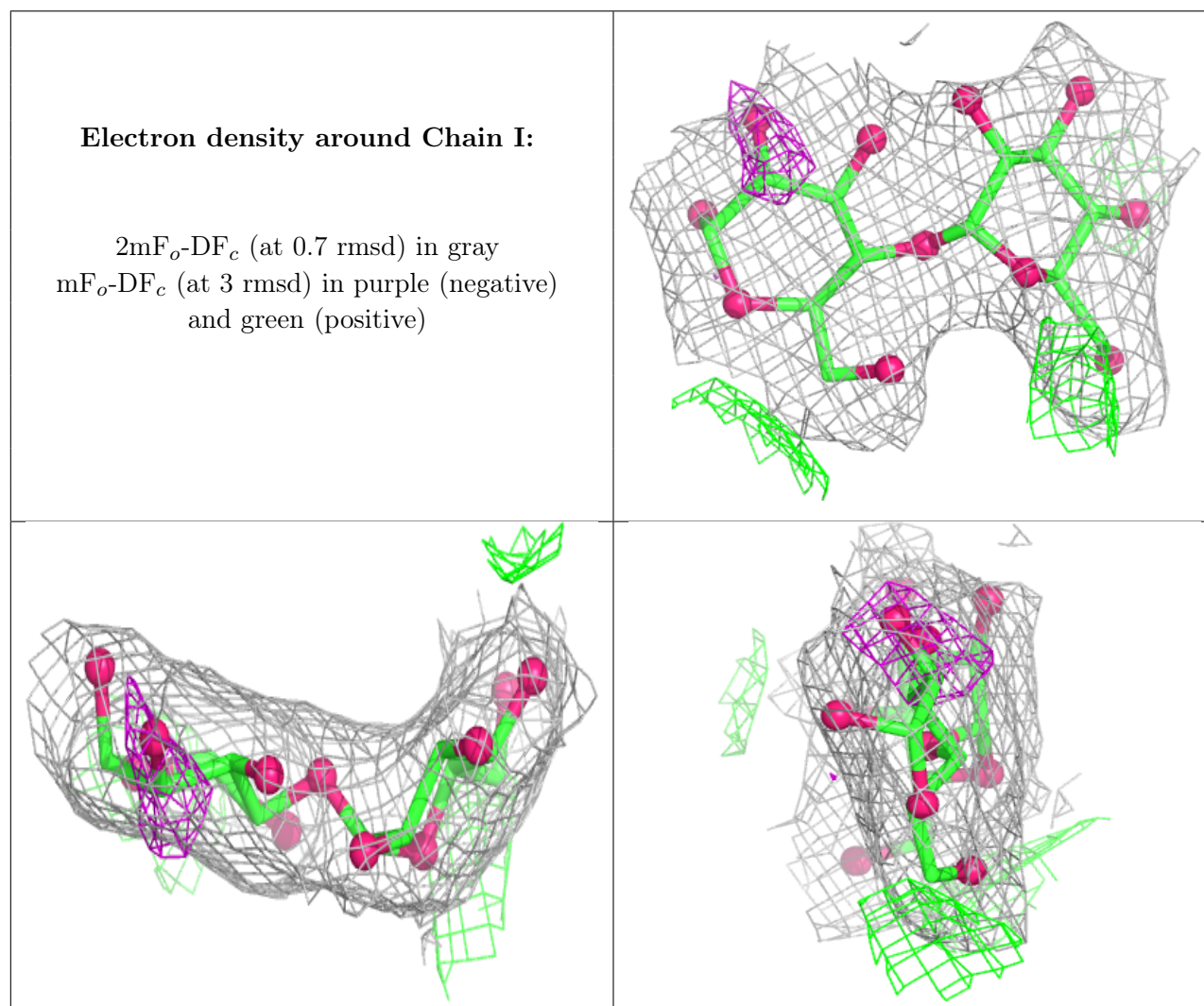
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GLC	I	2	11/12	0.91	0.11	30,32,34,35	0
2	GLC	I	1	12/12	0.92	0.09	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MES	A	5001	12/12	0.77	0.23	31,33,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MES	D	5001	12/12	0.81	0.23	32,34,36,36	0
4	MES	E	5001	12/12	0.81	0.23	32,35,37,37	0
4	MES	C	5001	12/12	0.82	0.23	30,31,32,33	0
4	MES	G	5001	12/12	0.85	0.21	29,31,32,33	0
4	MES	H	5001	12/12	0.86	0.20	30,32,34,35	0
4	MES	F	5001	12/12	0.87	0.20	38,38,39,39	0
4	MES	B	5001	12/12	0.89	0.20	39,41,43,44	0
3	CA	B	4001	1/1	0.94	0.05	32,32,32,32	0
3	CA	C	4001	1/1	0.95	0.05	29,29,29,29	0
3	CA	H	4001	1/1	0.96	0.05	32,32,32,32	0
3	CA	G	4001	1/1	0.96	0.05	28,28,28,28	0
3	CA	E	4001	1/1	0.96	0.07	32,32,32,32	0
3	CA	A	4001	1/1	0.97	0.06	29,29,29,29	0
3	CA	D	4001	1/1	0.97	0.04	30,30,30,30	0
3	CA	F	4001	1/1	0.97	0.06	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.