



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 04:42 PM UTC

PDB ID : 3S28 / pdb_00003s28
Title : The crystal structure of sucrose synthase-1 in complex with a breakdown product of the UDP-glucose
Authors : Zheng, Y.; Garavito, R.M.
Deposited on : 2011-05-16
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

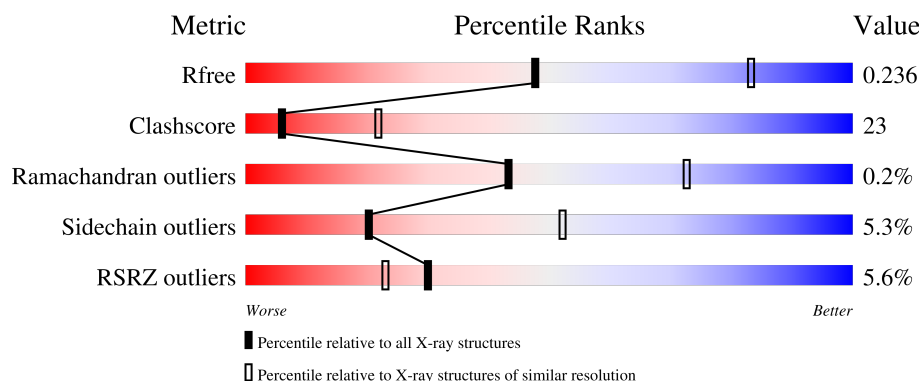
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	816	5% 62% 31% • •
1	B	816	9% 61% 32% • •
1	C	816	4% 57% 35% • •
1	D	816	4% 64% 29% • •
1	E	816	5% 65% 27% • •

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Mol	Chain	Length	Quality of chain
1	F	816	
1	G	816	
1	H	816	

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	NHF	D	904[B]	-	-	X	-
5	SO4	A	912	-	-	X	-
5	SO4	B	913	-	-	X	-
5	SO4	D	913	-	-	X	-
5	SO4	F	912	-	-	X	-
5	SO4	F	913	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 51388 atoms, of which 264 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 Sucrose synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	0	0
			6289	4039	1069	1159	22			
1	B	780	Total	C	N	O	S	0	0	0
			6158	3949	1050	1137	22			
1	C	781	Total	C	N	O	S	0	0	0
			6290	4045	1066	1157	22			
1	D	781	Total	C	N	O	S	0	0	0
			6280	4035	1062	1161	22			
1	E	781	Total	C	N	O	S	0	0	0
			6271	4028	1062	1159	22			
1	F	781	Total	C	N	O	S	0	0	0
			6292	4042	1070	1158	22			
1	G	781	Total	C	N	O	S	0	0	0
			6299	4045	1070	1162	22			
1	H	780	Total	C	N	O	S	0	0	0
			6243	4007	1063	1151	22			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	809	VAL	-	expression tag	UNP P49040
A	810	GLU	-	expression tag	UNP P49040
A	811	HIS	-	expression tag	UNP P49040
A	812	HIS	-	expression tag	UNP P49040
A	813	HIS	-	expression tag	UNP P49040
A	814	HIS	-	expression tag	UNP P49040
A	815	HIS	-	expression tag	UNP P49040
A	816	HIS	-	expression tag	UNP P49040
B	809	VAL	-	expression tag	UNP P49040
B	810	GLU	-	expression tag	UNP P49040
B	811	HIS	-	expression tag	UNP P49040
B	812	HIS	-	expression tag	UNP P49040
B	813	HIS	-	expression tag	UNP P49040

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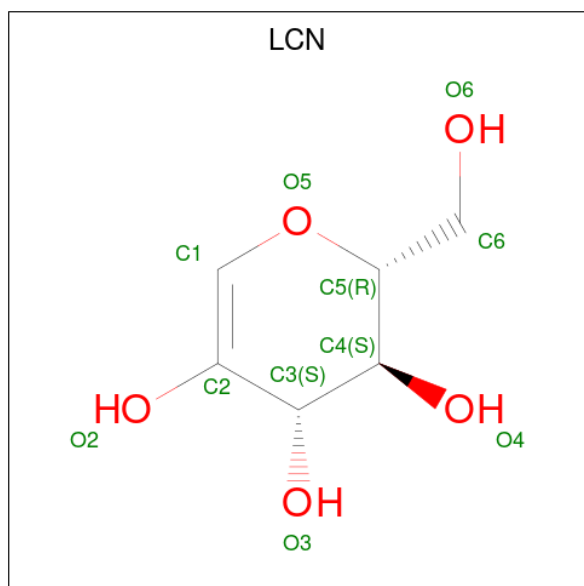
Chain	Residue	Modelled	Actual	Comment	Reference
B	814	HIS	-	expression tag	UNP P49040
B	815	HIS	-	expression tag	UNP P49040
B	816	HIS	-	expression tag	UNP P49040
C	809	VAL	-	expression tag	UNP P49040
C	810	GLU	-	expression tag	UNP P49040
C	811	HIS	-	expression tag	UNP P49040
C	812	HIS	-	expression tag	UNP P49040
C	813	HIS	-	expression tag	UNP P49040
C	814	HIS	-	expression tag	UNP P49040
C	815	HIS	-	expression tag	UNP P49040
C	816	HIS	-	expression tag	UNP P49040
D	809	VAL	-	expression tag	UNP P49040
D	810	GLU	-	expression tag	UNP P49040
D	811	HIS	-	expression tag	UNP P49040
D	812	HIS	-	expression tag	UNP P49040
D	813	HIS	-	expression tag	UNP P49040
D	814	HIS	-	expression tag	UNP P49040
D	815	HIS	-	expression tag	UNP P49040
D	816	HIS	-	expression tag	UNP P49040
E	809	VAL	-	expression tag	UNP P49040
E	810	GLU	-	expression tag	UNP P49040
E	811	HIS	-	expression tag	UNP P49040
E	812	HIS	-	expression tag	UNP P49040
E	813	HIS	-	expression tag	UNP P49040
E	814	HIS	-	expression tag	UNP P49040
E	815	HIS	-	expression tag	UNP P49040
E	816	HIS	-	expression tag	UNP P49040
F	809	VAL	-	expression tag	UNP P49040
F	810	GLU	-	expression tag	UNP P49040
F	811	HIS	-	expression tag	UNP P49040
F	812	HIS	-	expression tag	UNP P49040
F	813	HIS	-	expression tag	UNP P49040
F	814	HIS	-	expression tag	UNP P49040
F	815	HIS	-	expression tag	UNP P49040
F	816	HIS	-	expression tag	UNP P49040
G	809	VAL	-	expression tag	UNP P49040
G	810	GLU	-	expression tag	UNP P49040
G	811	HIS	-	expression tag	UNP P49040
G	812	HIS	-	expression tag	UNP P49040
G	813	HIS	-	expression tag	UNP P49040
G	814	HIS	-	expression tag	UNP P49040
G	815	HIS	-	expression tag	UNP P49040

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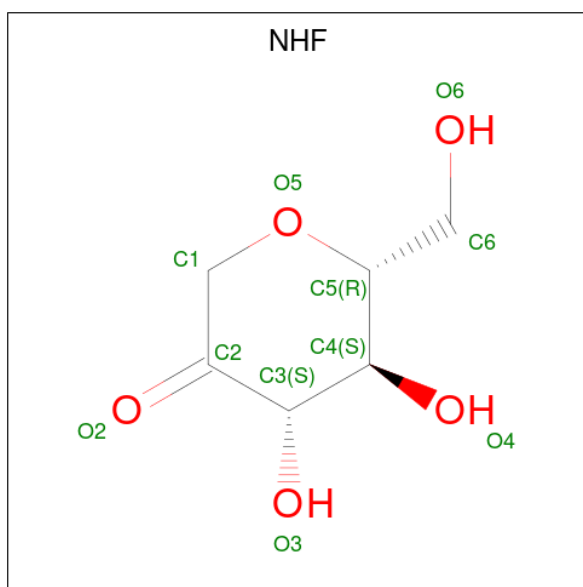
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	H	N	O	P	
			36	9	11	2	12	2	
								0	0

- Molecule 3 is 1,5-anhydro-D-arabino-hex-1-enitol (CCD ID: LCN) (formula: $C_6H_{10}O_5$).



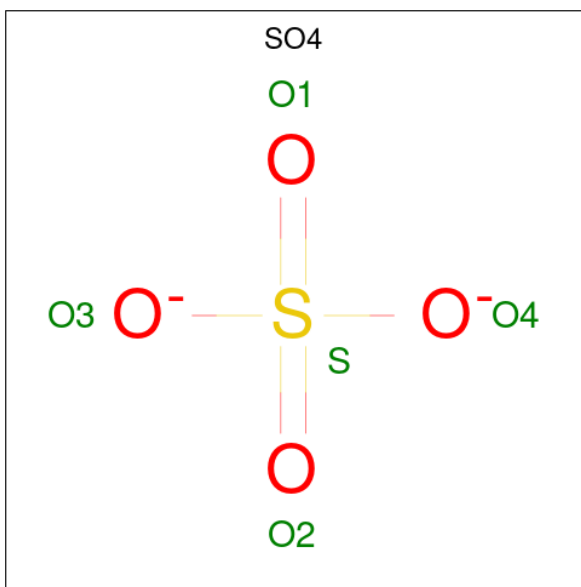
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O		
			21	6	10	5	0	1
3	B	1	Total	C	H	O		
			21	6	10	5	0	1
3	C	1	Total	C	H	O		
			21	6	10	5	0	1
3	D	1	Total	C	H	O		
			21	6	10	5	0	1
3	E	1	Total	C	H	O		
			21	6	10	5	0	1
3	F	1	Total	C	H	O		
			21	6	10	5	0	1
3	G	1	Total	C	H	O		
			21	6	10	5	0	1
3	H	1	Total	C	H	O		
			21	6	10	5	0	1

- Molecule 4 is 1,5-anhydro-D-fructose (CCD ID: NHF) (formula: $C_6H_{10}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	1
			21	6	10	5		
4	B	1	Total	C	H	O	0	1
			21	6	10	5		
4	C	1	Total	C	H	O	0	1
			21	6	10	5		
4	D	1	Total	C	H	O	0	1
			21	6	10	5		
4	E	1	Total	C	H	O	0	1
			21	6	10	5		
4	F	1	Total	C	H	O	0	1
			21	6	10	5		
4	G	1	Total	C	H	O	0	1
			21	6	10	5		
4	H	1	Total	C	H	O	0	1
			21	6	10	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



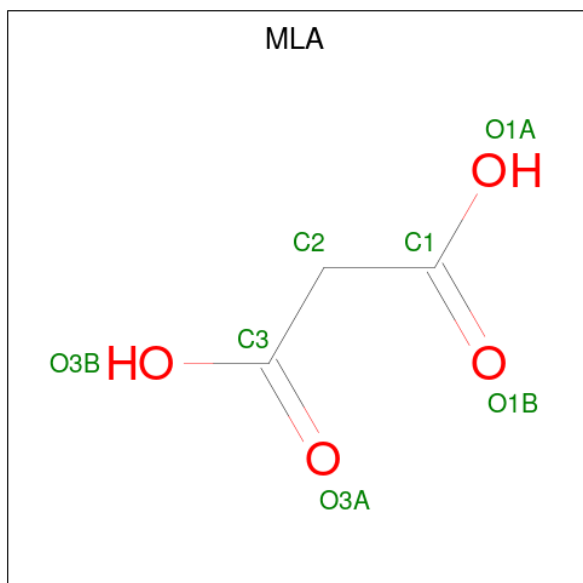
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		
5	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	F	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	G	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		
5	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is MALONIC ACID (CCD ID: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			9	3	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	H	O	0	0
			9	3	2	4		
6	C	1	Total	C	H	O	0	0
			9	3	2	4		
6	D	1	Total	C	H	O	0	0
			9	3	2	4		
6	E	1	Total	C	H	O	0	0
			9	3	2	4		
6	F	1	Total	C	H	O	0	0
			9	3	2	4		
6	G	1	Total	C	H	O	0	0
			9	3	2	4		
6	H	1	Total	C	H	O	0	0
			9	3	2	4		

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	K	0	0
			1	1		
7	B	1	Total	K	0	0
			1	1		
7	C	1	Total	K	0	0
			1	1		
7	D	1	Total	K	0	0
			1	1		
7	E	1	Total	K	0	0
			1	1		
7	F	1	Total	K	0	0
			1	1		
7	G	1	Total	K	0	0
			1	1		
7	H	1	Total	K	0	0
			1	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	69	Total	O	0	0
			69	69		
8	B	55	Total	O	0	0
			55	55		

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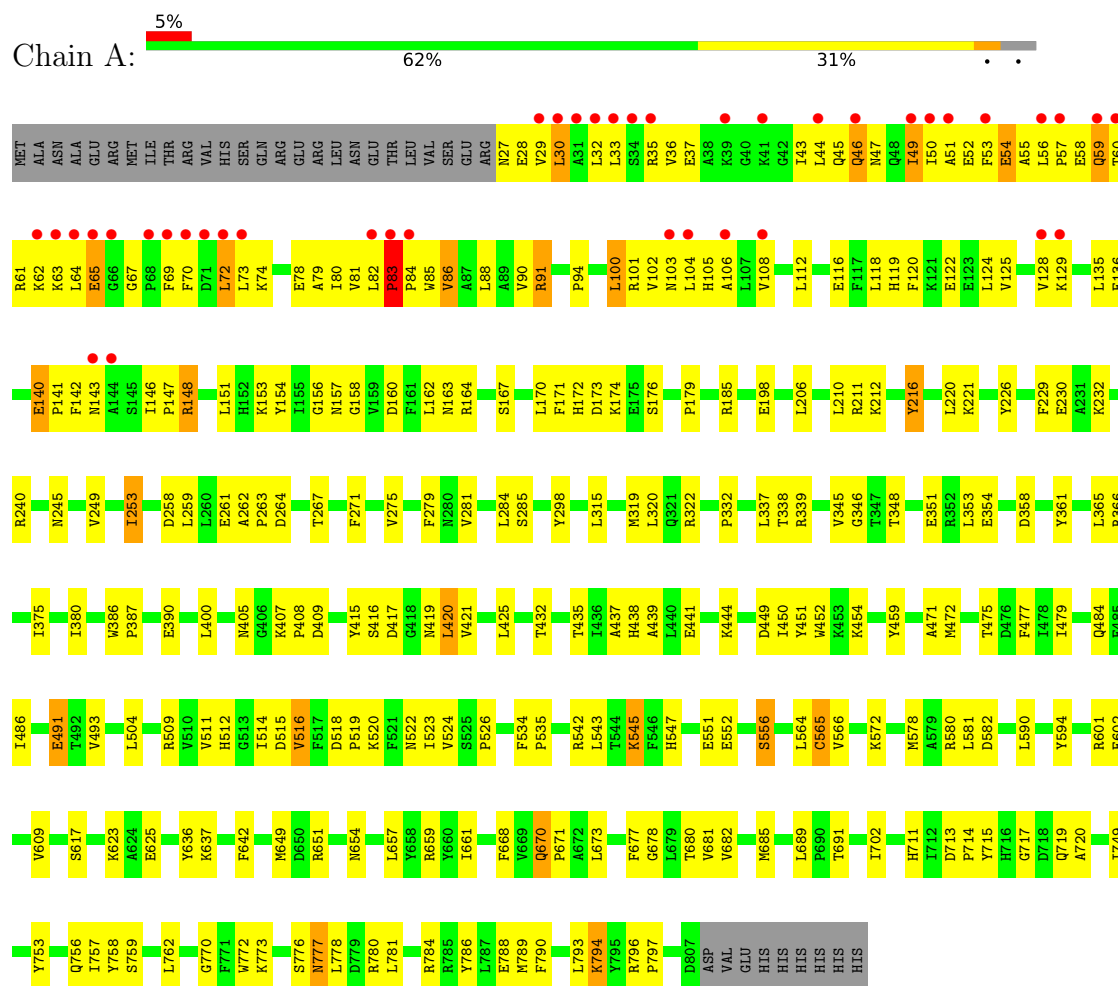
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	24	Total 24	O 24	0	0
8	D	54	Total 54	O 54	0	0
8	E	50	Total 50	O 50	0	0
8	F	79	Total 79	O 79	0	0
8	G	62	Total 62	O 62	0	0
8	H	49	Total 49	O 49	0	0

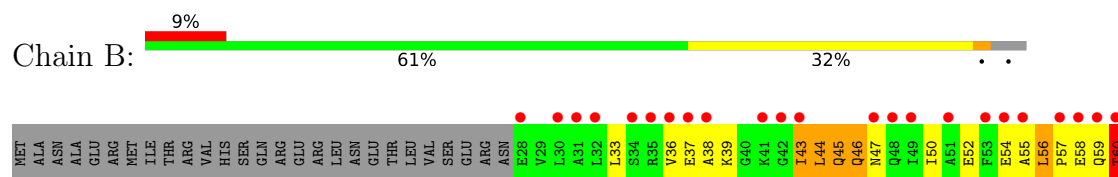
3 Residue-property plots

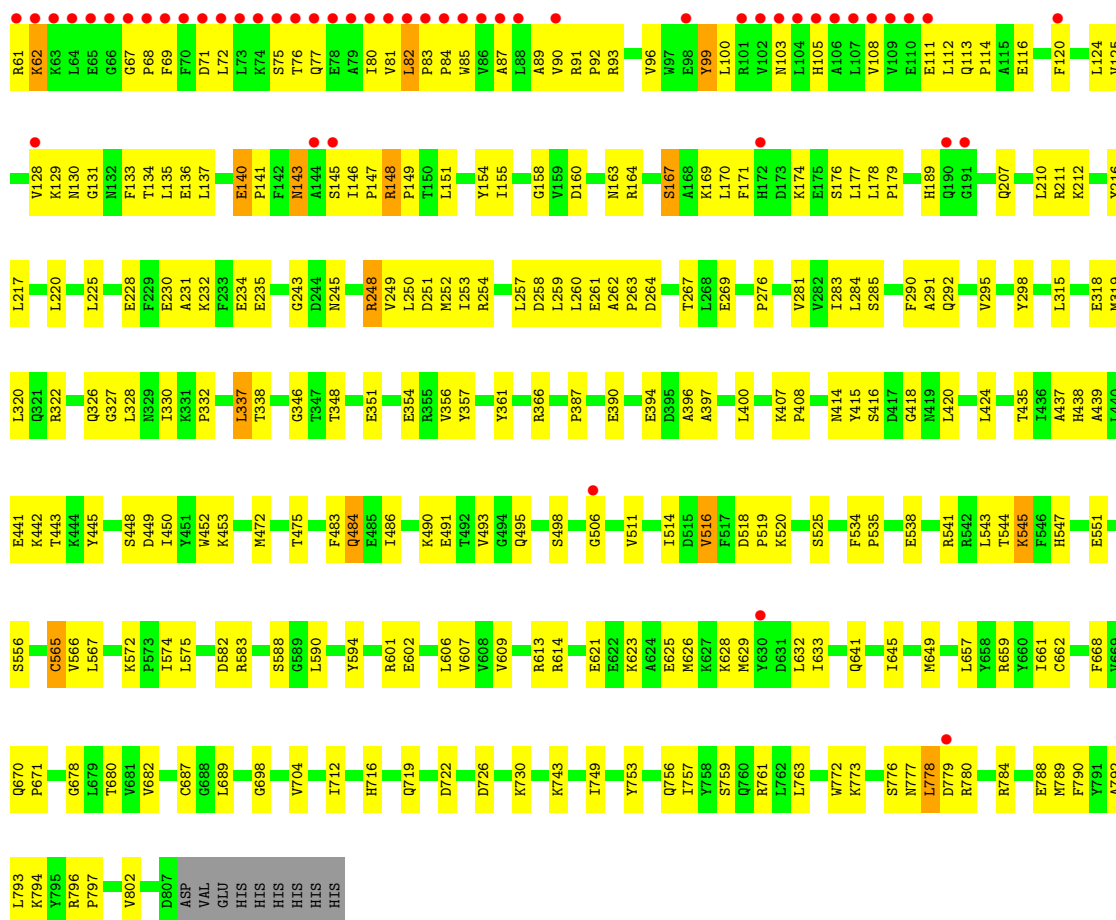
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Sucrose synthase 1

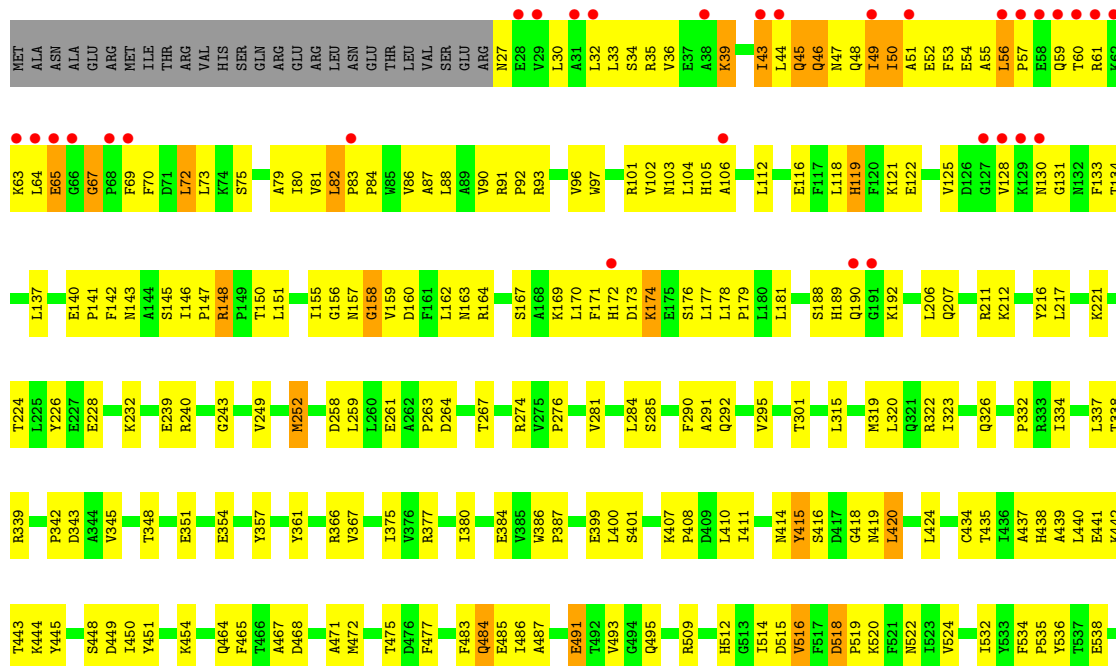


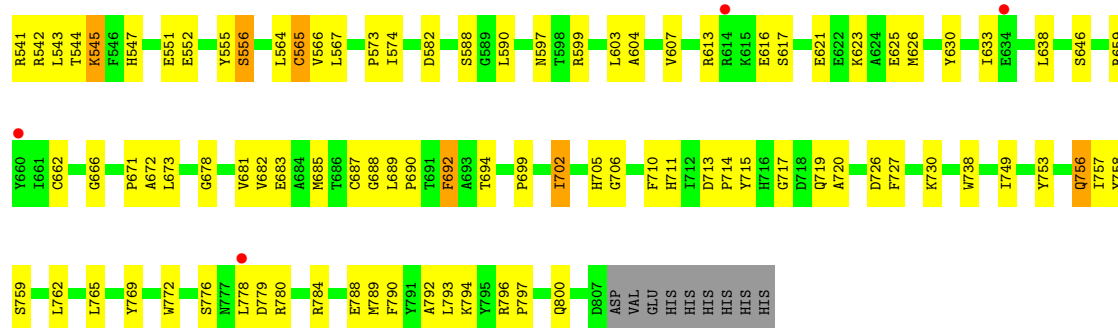
• Molecule 1: Sucrose synthase 1





• Molecule 1: Sucrose synthase 1

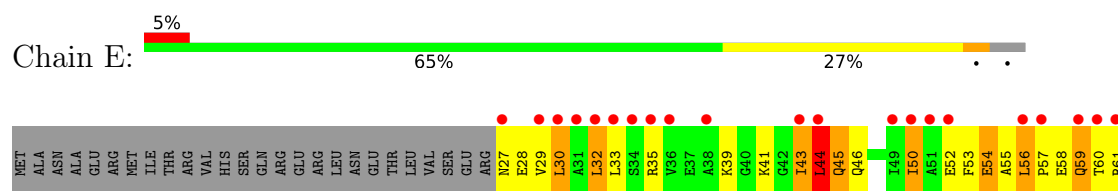


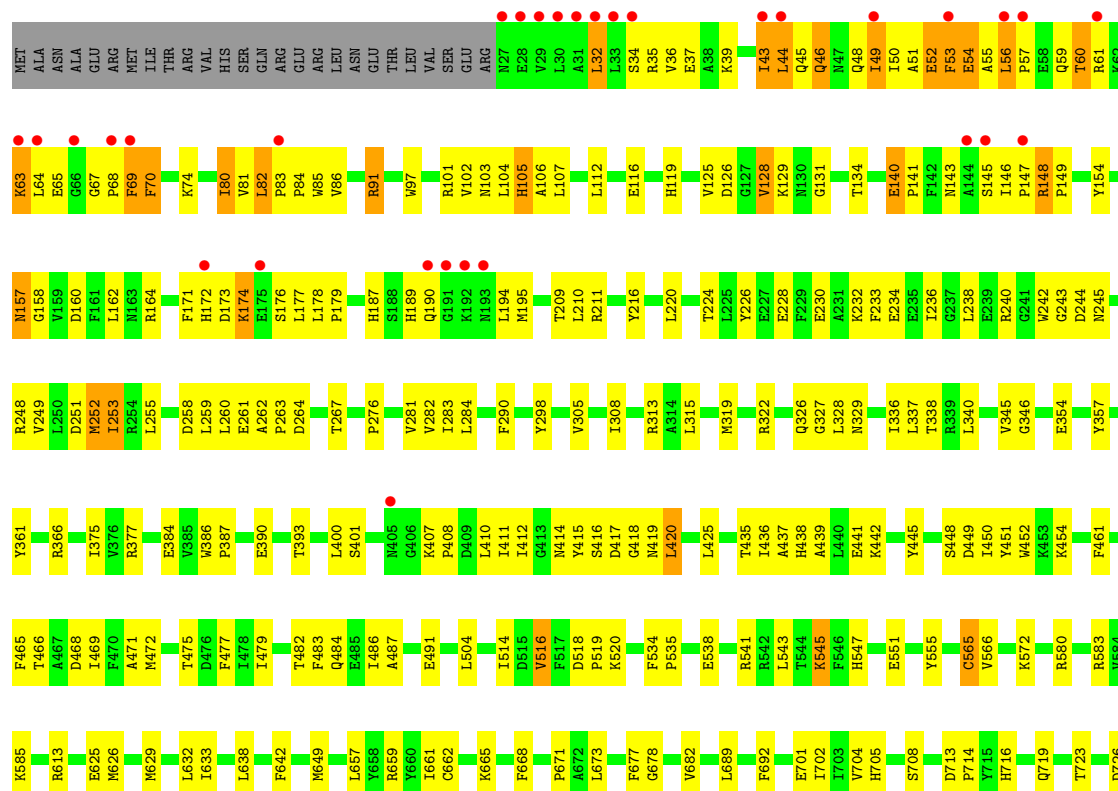


● Molecule 1: Sucrose synthase 1



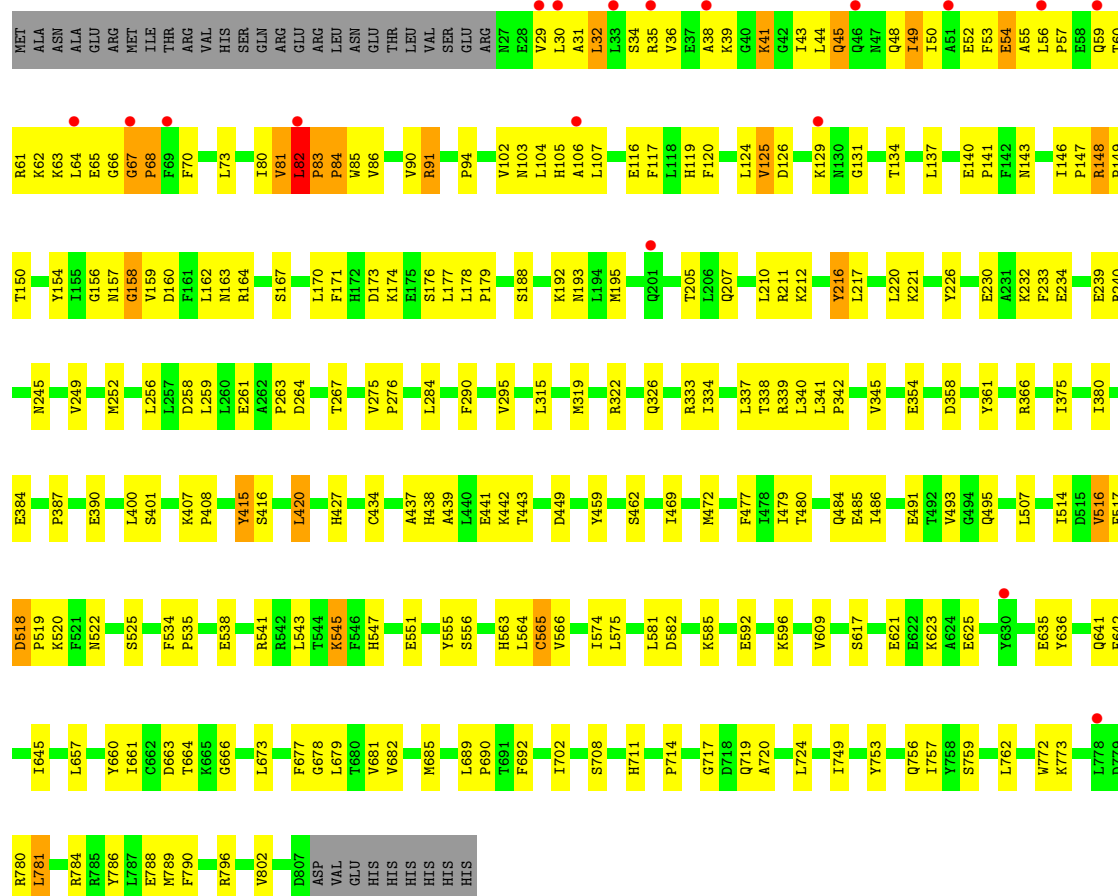
● Molecule 1: Sucrose synthase 1



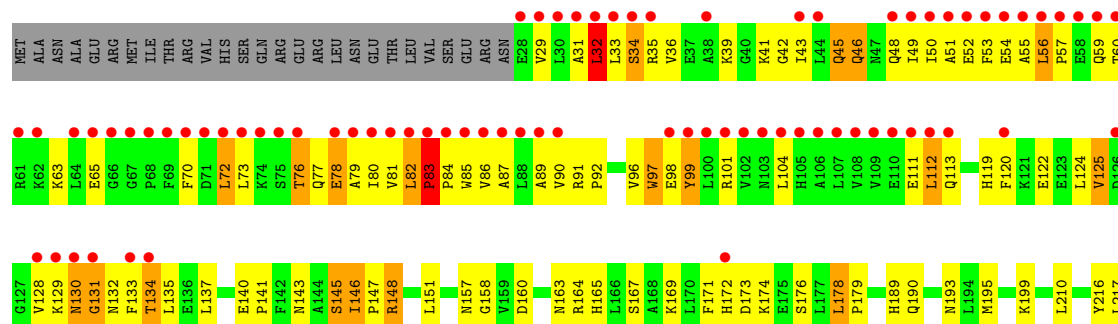




• Molecule 1: Sucrose synthase 1



• Molecule 1: Sucrose synthase 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	276.75Å 261.88Å 160.19Å 90.00° 108.70° 90.00°	Depositor
Resolution (Å)	24.98 – 2.80 24.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.98-2.80) 99.6 (24.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.7_650	Depositor
R, R_{free}	0.188 , 0.236 0.188 , 0.236	Depositor DCC
R_{free} test set	13263 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	51388	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.65 % 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 2.1188e-03. 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: SO4, LCN, NHF, MLA, UDP, K

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/6436	0.86	9/8714 (0.1%)
1	B	0.45	0/6304	0.92	13/8549 (0.2%)
1	C	0.41	0/6437	0.86	16/8718 (0.2%)
1	D	0.45	0/6427	0.89	18/8707 (0.2%)
1	E	0.44	0/6417	0.94	18/8693 (0.2%)
1	F	0.48	0/6439	0.91	16/8719 (0.2%)
1	G	0.46	0/6446	0.92	22/8728 (0.3%)
1	H	0.45	0/6390	0.90	17/8655 (0.2%)
All	All	0.45	0/51296	0.90	129/69483 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	3
All	All	0	8

There are no bond length outliers.

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	83	PRO	CA-C-N	14.72	134.24	119.82
1	E	83	PRO	C-N-CA	14.72	134.24	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	82	LEU	CA-C-N	11.82	132.56	120.38
1	E	82	LEU	C-N-CA	11.82	132.56	120.38
1	G	82	LEU	CA-C-N	11.46	132.19	120.38
1	G	82	LEU	C-N-CA	11.46	132.19	120.38
1	F	565	CYS	CB-CA-C	-9.29	104.74	115.79
1	A	565	CYS	CB-CA-C	-9.25	104.78	115.79
1	H	82	LEU	CA-C-N	8.96	129.61	120.38
1	H	82	LEU	C-N-CA	8.96	129.61	120.38
1	D	565	CYS	CB-CA-C	-8.40	105.80	115.79
1	F	53	PHE	N-CA-C	-8.31	102.16	111.14
1	H	565	CYS	CB-CA-C	-8.05	106.21	115.79
1	B	83	PRO	N-CA-C	8.03	120.50	110.70
1	D	295	VAL	N-CA-C	7.60	121.71	113.43
1	E	565	CYS	CB-CA-C	-7.56	106.80	115.79
1	G	565	CYS	CB-CA-C	-7.55	106.80	115.79
1	B	565	CYS	CB-CA-C	-7.51	106.86	115.79
1	C	361	TYR	N-CA-C	7.34	122.42	113.17
1	E	83	PRO	N-CA-C	7.30	119.60	110.70
1	H	361	TYR	N-CA-C	7.30	122.36	113.17
1	D	361	TYR	N-CA-C	7.29	122.36	113.17
1	D	91	ARG	CA-C-N	7.28	126.54	118.97
1	D	91	ARG	C-N-CA	7.28	126.54	118.97
1	H	76	THR	N-CA-C	7.10	118.81	111.14
1	F	44	LEU	CB-CA-C	-7.05	106.47	116.34
1	H	518	ASP	CA-C-N	7.02	126.70	119.82
1	H	518	ASP	C-N-CA	7.02	126.70	119.82
1	C	82	LEU	CA-C-N	-6.80	113.37	120.38
1	C	82	LEU	C-N-CA	-6.80	113.37	120.38
1	B	81	VAL	N-CA-C	6.80	117.44	107.37
1	F	91	ARG	CA-C-N	6.80	126.05	118.97
1	F	91	ARG	C-N-CA	6.80	126.05	118.97
1	D	518	ASP	CA-C-N	6.59	126.28	119.82
1	D	518	ASP	C-N-CA	6.59	126.28	119.82
1	E	44	LEU	CB-CA-C	-6.56	107.16	116.34
1	G	555	TYR	N-CA-C	6.56	121.43	113.17
1	C	518	ASP	CA-C-N	6.55	126.24	119.56
1	C	518	ASP	C-N-CA	6.55	126.24	119.56
1	E	361	TYR	N-CA-C	6.51	121.38	113.17
1	D	82	LEU	CA-C-N	-6.46	113.72	120.38
1	D	82	LEU	C-N-CA	-6.46	113.72	120.38
1	H	32	LEU	N-CA-C	-6.42	105.07	113.17
1	A	91	ARG	CA-C-N	6.40	125.63	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ARG	C-N-CA	6.40	125.63	118.97
1	G	157	ASN	N-CA-C	6.38	120.77	112.92
1	G	91	ARG	CA-C-N	6.35	125.58	118.97
1	G	91	ARG	C-N-CA	6.35	125.58	118.97
1	C	565	CYS	CB-CA-C	-6.29	108.30	115.79
1	F	361	TYR	N-CA-C	6.29	121.10	113.17
1	F	555	TYR	N-CA-C	6.10	120.85	113.17
1	B	60	THR	N-CA-C	6.09	117.02	108.00
1	G	84	PRO	N-CA-C	-6.06	106.16	113.98
1	G	518	ASP	CA-C-N	6.00	125.70	119.82
1	G	518	ASP	C-N-CA	6.00	125.70	119.82
1	B	62	LYS	N-CA-C	-5.95	106.02	113.28
1	C	158	GLY	N-CA-C	5.95	120.08	112.83
1	G	459	TYR	N-CA-C	5.91	120.49	113.28
1	A	157	ASN	N-CA-C	5.91	120.19	112.92
1	H	459	TYR	N-CA-C	5.88	120.18	112.89
1	G	361	TYR	N-CA-C	5.84	120.53	113.17
1	A	361	TYR	N-CA-C	5.84	120.53	113.17
1	C	67	GLY	CA-C-N	5.81	125.01	118.97
1	C	67	GLY	C-N-CA	5.81	125.01	118.97
1	E	91	ARG	CA-C-N	5.79	124.99	118.97
1	E	91	ARG	C-N-CA	5.79	124.99	118.97
1	G	68	PRO	CA-C-N	-5.79	113.91	122.41
1	G	68	PRO	C-N-CA	-5.79	113.91	122.41
1	B	361	TYR	N-CA-C	5.77	120.44	113.17
1	C	532	ILE	N-CA-C	5.75	117.27	111.00
1	F	346	GLY	N-CA-C	-5.71	107.50	114.92
1	B	346	GLY	N-CA-C	-5.68	107.82	115.21
1	E	65	GLU	N-CA-C	5.64	120.28	113.17
1	D	555	TYR	N-CA-C	5.63	120.26	113.17
1	D	459	TYR	N-CA-C	5.62	120.14	113.28
1	F	671	PRO	CA-C-O	-5.62	117.05	121.38
1	D	678	GLY	N-CA-C	5.61	126.48	113.18
1	E	555	TYR	N-CA-C	5.60	120.23	113.17
1	B	678	GLY	N-CA-C	5.59	126.43	113.18
1	E	384	GLU	N-CA-C	5.59	120.21	113.17
1	G	384	GLU	N-CA-C	5.57	120.19	113.17
1	B	55	ALA	N-CA-C	-5.53	106.23	112.87
1	D	157	ASN	N-CA-C	5.49	119.68	112.92
1	H	157	ASN	N-CA-C	5.47	119.65	112.92
1	A	459	TYR	N-CA-C	5.46	120.00	113.23
1	G	158	GLY	N-CA-C	5.45	120.52	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	83	PRO	N-CA-C	5.45	117.35	110.70
1	H	78	GLU	N-CA-C	5.43	116.71	108.07
1	G	67	GLY	CA-C-N	5.42	126.62	119.84
1	G	67	GLY	C-N-CA	5.42	126.62	119.84
1	D	671	PRO	CA-C-O	-5.42	117.21	121.38
1	A	346	GLY	N-CA-C	-5.40	108.19	115.21
1	G	295	VAL	N-CA-C	5.38	121.30	113.39
1	H	97	TRP	N-CA-C	5.38	117.18	108.41
1	H	158	GLY	N-CA-C	5.38	120.42	113.27
1	C	285	SER	CA-C-N	5.37	124.70	118.85
1	C	285	SER	C-N-CA	5.37	124.70	118.85
1	F	377	ARG	N-CA-C	5.36	118.29	111.69
1	G	83	PRO	N-CA-C	5.36	117.24	110.70
1	A	678	GLY	N-CA-C	5.36	125.88	113.18
1	B	72	LEU	N-CA-C	-5.34	106.61	113.23
1	E	456	ASP	N-CA-C	5.33	116.89	111.14
1	C	384	GLU	N-CA-C	5.30	119.85	113.17
1	B	44	LEU	CB-CA-C	-5.27	110.06	117.23
1	F	44	LEU	N-CA-C	5.25	115.78	108.00
1	C	678	GLY	N-CA-C	5.22	125.55	113.18
1	C	555	TYR	N-CA-C	5.21	119.73	113.17
1	B	38	ALA	N-CA-C	-5.19	106.80	113.02
1	B	69	PHE	N-CA-C	-5.18	106.80	113.02
1	H	713	ASP	CA-C-N	5.17	124.84	119.56
1	H	713	ASP	C-N-CA	5.17	124.84	119.56
1	E	459	TYR	N-CA-C	5.17	119.64	113.23
1	F	678	GLY	N-CA-C	5.13	125.33	113.18
1	G	415	TYR	CB-CA-C	-5.12	109.69	115.79
1	F	384	GLU	N-CA-C	5.12	119.62	113.17
1	E	67	GLY	CA-C-N	5.11	124.28	118.97
1	E	67	GLY	C-N-CA	5.11	124.28	118.97
1	H	678	GLY	N-CA-C	5.10	125.26	113.18
1	E	157	ASN	N-CA-C	5.09	119.18	112.92
1	F	329	ASN	N-CA-C	5.09	119.58	113.17
1	H	456	ASP	N-CA-C	5.09	116.91	111.36
1	D	285	SER	CA-C-N	5.07	124.38	118.85
1	D	285	SER	C-N-CA	5.07	124.38	118.85
1	F	34	SER	N-CA-C	-5.05	105.85	111.36
1	D	384	GLU	N-CA-C	5.04	119.52	113.17
1	G	678	GLY	N-CA-C	5.04	125.11	113.18
1	F	157	ASN	N-CA-C	5.02	119.09	112.92
1	C	415	TYR	CB-CA-C	-5.02	109.82	115.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	VAL	N-CA-C	5.01	115.80	108.58

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	PRO	Peptide
1	B	71	ASP	Peptide
1	E	81	VAL	Peptide
1	F	82	LEU	Peptide
1	G	81	VAL	Peptide
1	H	130	ASN	Peptide
1	H	131	GLY	Peptide
1	H	83	PRO	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6289	0	6220	296	0
1	B	6158	0	5959	306	0
1	C	6290	0	6242	330	0
1	D	6280	0	6206	285	0
1	E	6271	0	6194	276	0
1	F	6292	0	6234	302	0
1	G	6299	0	6240	274	0
1	H	6243	0	6130	327	0
2	A	25	11	11	3	0
2	B	25	11	11	1	0
2	C	25	11	11	1	0
2	D	25	11	11	4	0
2	E	25	11	11	1	0
2	F	25	11	11	1	0
2	G	25	11	11	4	0
2	H	25	11	11	4	0
3	A	11	10	10	1	0
3	B	11	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	11	10	10	0	0
3	D	11	10	10	1	0
3	E	11	10	10	0	0
3	F	11	10	10	1	0
3	G	11	10	10	1	0
3	H	11	10	10	0	0
4	A	11	10	10	2	0
4	B	11	10	10	2	0
4	C	11	10	10	1	0
4	D	11	10	10	6	0
4	E	11	10	10	2	0
4	F	11	10	10	0	0
4	G	11	10	10	1	0
4	H	11	10	10	4	0
5	A	15	0	0	3	0
5	B	15	0	0	5	0
5	C	15	0	0	1	0
5	D	15	0	0	2	0
5	E	15	0	0	1	0
5	F	15	0	0	5	0
5	G	15	0	0	2	0
5	H	15	0	0	1	0
6	A	7	2	2	0	0
6	B	7	2	2	0	0
6	C	7	2	2	0	0
6	D	7	2	2	0	0
6	E	7	2	2	1	0
6	F	7	2	2	1	0
6	G	7	2	2	0	0
6	H	7	2	2	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	A	69	0	0	0	0
8	B	55	0	0	2	0
8	C	24	0	0	0	0
8	D	54	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	E	50	0	0	1	0
8	F	79	0	0	2	0
8	G	62	0	0	1	0
8	H	49	0	0	1	0
All	All	51124	264	49689	2283	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 23.

All (2283) 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:46:GLN:HG2	1:B:50:ILE:CB	1.66	1.25
1:G:66:GLY:C	1:G:68:PRO:HD3	1.60	1.24
1:E:789:MET:HB3	1:H:789:MET:CE	1.68	1.22
1:F:789:MET:CE	1:G:789:MET:HB3	1.71	1.21
1:H:82:LEU:HB2	1:H:83:PRO:HD2	1.20	1.19
1:C:83:PRO:HG2	1:C:84:PRO:HD3	1.20	1.15
1:E:81:VAL:CG1	1:E:86:VAL:HB	1.77	1.15
1:D:48:GLN:HA	1:D:51:ALA:HB2	1.19	1.14
1:A:789:MET:HE2	1:D:789:MET:CE	1.77	1.13
1:F:39:LYS:HG2	1:F:104:LEU:HD13	1.27	1.13
1:B:37:GLU:CB	1:B:59:GLN:HA	1.79	1.12
1:B:281:VAL:HG21	1:B:319:MET:HE1	1.18	1.12
1:B:146:ILE:HG22	1:B:147:PRO:HD2	1.28	1.11
1:C:545:LYS:H	1:C:545:LYS:HD3	1.10	1.11
1:B:789:MET:CE	1:C:789:MET:HB3	1.81	1.10
1:B:315:LEU:HG	1:B:319:MET:HE3	1.32	1.10
1:H:545:LYS:H	1:H:545:LYS:HD3	1.12	1.10
1:B:45:GLN:HB3	1:B:80:ILE:HA	1.12	1.09
1:B:89:ALA:HB1	1:B:99:TYR:HD1	1.11	1.09
1:H:80:ILE:HD11	1:H:87:ALA:HB3	1.27	1.09
1:B:789:MET:CE	1:C:789:MET:HE2	1.83	1.09
1:B:82:LEU:O	1:B:84:PRO:HD2	1.53	1.07
1:F:789:MET:CE	1:G:789:MET:HE2	1.83	1.07
1:G:543:LEU:HB3	1:G:545:LYS:HE3	1.37	1.07
1:E:46:GLN:HB3	1:E:50:ILE:HB	1.26	1.06
1:E:789:MET:HE2	1:H:789:MET:HE2	1.10	1.06
1:G:83:PRO:HB2	1:G:85:TRP:H	1.18	1.06
1:B:89:ALA:HB1	1:B:99:TYR:CD1	1.90	1.05
1:C:143:ASN:HB3	1:C:148:ARG:NH2	1.72	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:ILE:HG23	1:H:147:PRO:HD2	1.35	1.05
1:A:789:MET:HE2	1:D:789:MET:HE2	1.08	1.04
1:G:45:GLN:HE21	1:G:45:GLN:HA	1.21	1.03
1:B:87:ALA:HB2	1:B:120:PHE:CE2	1.94	1.03
1:E:82:LEU:N	1:E:83:PRO:HD3	1.70	1.03
1:H:31:ALA:HA	1:H:33:LEU:HD23	1.37	1.03
1:A:315:LEU:HG	1:A:319:MET:HE3	1.39	1.03
1:D:48:GLN:HA	1:D:51:ALA:CB	1.88	1.02
1:F:789:MET:HE2	1:G:789:MET:HE2	1.06	1.02
1:B:112:LEU:HD22	1:B:116:GLU:HB2	1.41	1.01
1:F:146:ILE:HG22	1:F:147:PRO:HD2	1.42	1.01
1:G:315:LEU:HG	1:G:319:MET:HE2	1.41	1.01
1:D:41:LYS:HE2	1:D:54:GLU:HG3	1.44	1.00
1:H:82:LEU:HD21	1:H:86:VAL:HA	1.43	1.00
1:H:315:LEU:HG	1:H:319:MET:HE2	1.42	1.00
1:B:146:ILE:CG2	1:B:147:PRO:HD2	1.91	1.00
1:E:53:PHE:O	1:E:57:PRO:HG2	1.61	1.00
1:F:789:MET:HB3	1:G:789:MET:CE	1.91	1.00
1:G:119:HIS:CE1	1:G:129:LYS:HD3	1.94	1.00
1:C:148:ARG:HH11	1:C:148:ARG:CG	1.75	0.99
1:B:789:MET:HE2	1:C:789:MET:HE2	1.00	0.99
1:D:173:ASP:HB3	1:D:176:SER:HB3	1.46	0.98
1:C:83:PRO:CG	1:C:84:PRO:HD3	1.93	0.98
1:E:143:ASN:HB3	1:E:148:ARG:NH2	1.79	0.98
1:D:103:ASN:CB	1:D:106:ALA:HB3	1.93	0.98
1:D:216:TYR:HE1	1:D:220:LEU:HD11	1.27	0.97
1:H:72:LEU:HD13	1:H:90:VAL:HG11	1.44	0.97
1:G:56:LEU:HB3	1:G:57:PRO:HD3	1.46	0.97
1:B:789:MET:HB3	1:C:789:MET:CE	1.95	0.97
1:H:146:ILE:HG23	1:H:147:PRO:CD	1.93	0.97
1:H:82:LEU:CD2	1:H:86:VAL:HA	1.95	0.96
1:F:281:VAL:HG21	1:F:319:MET:HE1	1.46	0.96
1:C:545:LYS:HD3	1:C:545:LYS:N	1.78	0.96
1:E:85:TRP:HB3	1:E:103:ASN:HA	1.48	0.96
1:B:89:ALA:CB	1:B:99:TYR:HD1	1.78	0.96
1:D:83:PRO:O	1:D:104:LEU:HD12	1.65	0.96
1:B:789:MET:HE2	1:C:789:MET:CE	1.94	0.96
1:H:80:ILE:CD1	1:H:87:ALA:HB3	1.95	0.96
1:H:216:TYR:CE2	1:H:232:LYS:HG2	2.00	0.95
1:H:545:LYS:HD3	1:H:545:LYS:N	1.80	0.95
1:B:148:ARG:CG	1:B:148:ARG:HH11	1.78	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:83:PRO:HB2	1:H:84:PRO:HD2	1.49	0.95
1:D:217:LEU:HD11	1:D:233:PHE:HZ	1.30	0.95
1:A:146:ILE:HG23	1:A:147:PRO:HD2	1.48	0.94
1:C:137:LEU:HD11	1:C:790:PHE:CE1	2.02	0.94
1:E:85:TRP:CB	1:E:103:ASN:HA	1.97	0.94
1:F:789:MET:HE2	1:G:789:MET:CE	1.96	0.94
1:B:60:THR:HG23	1:B:61:ARG:H	1.29	0.94
1:B:100:LEU:CB	1:B:111:GLU:HA	1.97	0.94
1:H:39:LYS:CG	1:H:104:LEU:HD13	1.97	0.94
1:B:545:LYS:HD3	1:B:545:LYS:H	1.29	0.94
1:B:146:ILE:HG22	1:B:147:PRO:CD	1.97	0.94
1:H:46:GLN:HB2	1:H:79:ALA:HB3	1.50	0.94
1:B:789:MET:HE1	1:C:789:MET:HB3	1.47	0.93
1:F:173:ASP:HB3	1:F:176:SER:HB3	1.49	0.93
1:A:103:ASN:CB	1:A:106:ALA:HB3	1.96	0.93
1:A:789:MET:CE	1:D:789:MET:HE2	1.97	0.93
1:H:315:LEU:HG	1:H:319:MET:CE	1.98	0.93
1:H:39:LYS:HG2	1:H:104:LEU:HD13	1.48	0.93
1:C:148:ARG:HH11	1:C:148:ARG:HG2	1.33	0.93
1:E:35:ARG:HD2	1:E:104:LEU:HA	1.51	0.93
1:H:39:LYS:HG2	1:H:104:LEU:HD22	1.50	0.93
1:H:545:LYS:H	1:H:545:LYS:CD	1.76	0.92
1:H:146:ILE:HG22	1:H:147:PRO:O	1.69	0.92
1:E:789:MET:HE2	1:H:789:MET:CE	2.00	0.92
1:D:146:ILE:HD11	1:D:772:TRP:CZ2	2.05	0.92
1:H:112:LEU:HD12	1:H:112:LEU:N	1.84	0.92
1:B:281:VAL:CG2	1:B:319:MET:HE1	1.99	0.92
1:G:319:MET:HE1	1:G:334:ILE:HD11	1.51	0.92
1:B:45:GLN:HB3	1:B:80:ILE:CA	1.99	0.92
1:C:547:HIS:O	1:C:551:GLU:HG2	1.70	0.92
1:F:315:LEU:HG	1:F:319:MET:HE3	1.50	0.92
1:F:327:GLY:O	1:F:328:LEU:HD23	1.67	0.92
1:H:148:ARG:HH11	1:H:148:ARG:HG3	1.35	0.91
1:A:83:PRO:HB2	1:A:84:PRO:HD2	1.49	0.91
1:H:668:PHE:HB2	1:H:689:LEU:HD23	1.50	0.91
1:F:52:GLU:O	1:F:57:PRO:HD2	1.70	0.91
1:A:59:GLN:HG3	1:A:60:THR:H	1.36	0.91
1:E:81:VAL:HG12	1:E:86:VAL:HB	1.49	0.91
1:G:32:LEU:O	1:G:36:VAL:HG23	1.71	0.91
1:E:315:LEU:HG	1:E:319:MET:HE2	1.50	0.90
1:E:789:MET:CE	1:H:789:MET:HE2	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:MET:HB3	1:D:789:MET:CE	2.02	0.90
1:C:543:LEU:HB3	1:C:545:LYS:CE	2.00	0.90
1:G:66:GLY:C	1:G:68:PRO:CD	2.43	0.90
1:B:60:THR:HG23	1:B:61:ARG:N	1.83	0.89
1:E:83:PRO:HB2	1:E:85:TRP:HD1	1.35	0.89
1:D:315:LEU:HG	1:D:319:MET:HE3	1.51	0.89
1:D:56:LEU:HB3	1:D:57:PRO:HD3	1.55	0.89
1:G:49:ILE:H	1:G:49:ILE:HD12	1.34	0.89
1:B:163:ASN:HD21	1:B:269:GLU:HG3	1.37	0.89
1:G:83:PRO:HD2	1:G:85:TRP:O	1.72	0.88
1:G:82:LEU:HD12	1:G:83:PRO:CG	2.03	0.88
1:H:130:ASN:HD21	1:H:506:GLY:H	1.18	0.88
1:C:32:LEU:O	1:C:36:VAL:HG23	1.73	0.88
1:D:103:ASN:HD21	1:F:106:ALA:CB	1.86	0.88
1:H:33:LEU:HA	1:H:36:VAL:HG23	1.55	0.88
1:B:43:ILE:HD13	1:B:44:LEU:H	1.37	0.88
1:A:35:ARG:NH2	1:A:86:VAL:HG12	1.89	0.87
1:D:173:ASP:HB3	1:D:176:SER:CB	2.04	0.87
1:A:789:MET:CE	1:D:789:MET:HB3	2.05	0.87
1:D:52:GLU:O	1:D:57:PRO:HD2	1.75	0.87
1:A:543:LEU:HB3	1:A:545:LYS:HE3	1.57	0.87
1:H:83:PRO:HB2	1:H:84:PRO:CD	2.05	0.87
1:H:99:TYR:O	1:H:111:GLU:HG2	1.74	0.86
1:H:131:GLY:O	1:H:134:THR:HG23	1.74	0.86
1:H:39:LYS:HG2	1:H:104:LEU:CD1	2.05	0.86
1:H:82:LEU:HB2	1:H:83:PRO:CD	2.05	0.86
1:B:76:THR:CB	1:B:90:VAL:HG22	2.06	0.86
1:H:39:LYS:CE	1:H:104:LEU:HD13	2.05	0.86
1:H:46:GLN:CB	1:H:79:ALA:HB3	2.05	0.86
1:H:291:ALA:HB3	1:H:295:VAL:HG11	1.58	0.86
1:D:784:ARG:O	1:D:788:GLU:HG3	1.75	0.86
1:F:789:MET:HB3	1:G:789:MET:HE1	1.58	0.86
1:H:80:ILE:HD11	1:H:87:ALA:CB	2.05	0.85
1:B:82:LEU:HD22	1:B:84:PRO:CD	2.07	0.85
1:B:46:GLN:CG	1:B:50:ILE:CB	2.54	0.85
1:B:113:GLN:HG3	1:B:114:PRO:HD2	1.57	0.84
1:G:82:LEU:N	1:G:83:PRO:HD3	1.92	0.84
1:H:39:LYS:HG2	1:H:104:LEU:CD2	2.07	0.84
1:B:148:ARG:HH11	1:B:148:ARG:HG2	1.40	0.84
1:E:315:LEU:HG	1:E:319:MET:CE	2.06	0.84
1:B:545:LYS:HD3	1:B:545:LYS:N	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:GLN:HB3	1:H:51:ALA:HB2	1.60	0.84
1:B:43:ILE:HD13	1:B:44:LEU:N	1.91	0.84
1:C:146:ILE:HG23	1:C:147:PRO:HD2	1.57	0.84
1:A:43:ILE:O	1:A:44:LEU:HG	1.77	0.83
1:D:41:LYS:CE	1:D:54:GLU:HG3	2.08	0.83
1:E:789:MET:HB3	1:H:789:MET:HE2	1.59	0.83
1:E:151:LEU:HD23	1:F:211:ARG:HH22	1.42	0.83
1:B:210:LEU:HD22	1:B:253:ILE:HG23	1.59	0.83
1:C:543:LEU:HB3	1:C:545:LYS:HE3	1.59	0.83
1:F:789:MET:HE1	1:G:789:MET:HB3	1.58	0.83
1:C:146:ILE:HG22	1:C:147:PRO:O	1.78	0.83
1:E:230:GLU:O	1:E:234:GLU:HG3	1.78	0.82
1:E:72:LEU:O	1:E:72:LEU:HD13	1.79	0.82
1:D:327:GLY:O	1:D:328:LEU:HD23	1.79	0.82
1:C:545:LYS:H	1:C:545:LYS:CD	1.92	0.82
1:B:82:LEU:HD11	1:B:120:PHE:CE2	2.15	0.82
1:F:67:GLY:N	1:F:68:PRO:HD2	1.94	0.82
1:H:39:LYS:HE2	1:H:104:LEU:HD13	1.61	0.81
1:H:543:LEU:HA	1:H:545:LYS:HE3	1.62	0.81
1:A:54:GLU:HG3	1:A:55:ALA:N	1.93	0.81
1:B:628:LYS:O	1:B:632:LEU:HG	1.79	0.81
1:H:111:GLU:C	1:H:112:LEU:HD12	2.04	0.81
1:H:34:SER:OG	1:H:55:ALA:HB1	1.79	0.81
1:C:796:ARG:HB2	1:C:797:PRO:HD3	1.62	0.81
1:D:33:LEU:O	1:D:37:GLU:HG3	1.81	0.81
1:G:545:LYS:HD3	1:G:545:LYS:H	1.45	0.81
1:H:82:LEU:CB	1:H:83:PRO:HD2	2.02	0.81
1:B:124:LEU:HD23	1:B:124:LEU:O	1.80	0.81
1:G:366:ARG:HD3	8:G:824:HOH:O	1.80	0.81
1:H:35:ARG:O	1:H:39:LYS:HB2	1.80	0.81
1:C:65:GLU:HA	1:C:65:GLU:OE2	1.81	0.81
1:E:41:LYS:HE2	1:E:54:GLU:OE1	1.80	0.81
1:D:60:THR:O	1:D:63:LYS:HD3	1.80	0.81
1:G:216:TYR:HE1	1:G:220:LEU:HD11	1.45	0.81
1:B:281:VAL:HG21	1:B:319:MET:CE	2.08	0.80
1:F:173:ASP:HB3	1:F:176:SER:CB	2.11	0.80
1:A:545:LYS:H	1:A:545:LYS:HD3	1.45	0.80
1:B:100:LEU:HA	1:B:112:LEU:HB2	1.63	0.80
1:D:48:GLN:CA	1:D:51:ALA:HB2	2.08	0.80
1:A:682:VAL:HG13	1:A:749:ILE:HD12	1.63	0.80
1:D:103:ASN:HB2	1:D:106:ALA:HB3	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:789:MET:CE	1:H:789:MET:HB3	2.11	0.80
1:A:281:VAL:HG21	1:A:319:MET:HE1	1.64	0.80
1:B:366:ARG:HD3	8:B:835:HOH:O	1.81	0.80
1:E:789:MET:HB3	1:H:789:MET:HE1	1.62	0.80
1:C:43:ILE:O	1:C:44:LEU:HG	1.82	0.80
1:F:46:GLN:HB2	1:F:50:ILE:HB	1.64	0.80
1:A:81:VAL:HA	1:A:86:VAL:HG23	1.63	0.80
1:B:668:PHE:HB2	1:B:689:LEU:HD23	1.63	0.80
1:F:789:MET:HE3	1:G:789:MET:HB3	1.63	0.80
1:G:67:GLY:N	1:G:68:PRO:CD	2.45	0.80
1:H:39:LYS:CG	1:H:104:LEU:HD22	2.12	0.80
1:E:216:TYR:CE1	1:E:220:LEU:HD11	2.18	0.79
1:D:125:VAL:HG11	1:D:505:PRO:HG2	1.64	0.79
1:A:83:PRO:HB2	1:A:84:PRO:CD	2.12	0.79
1:F:315:LEU:O	1:F:319:MET:HG3	1.82	0.79
1:B:112:LEU:HD22	1:B:116:GLU:CB	2.12	0.79
1:A:146:ILE:HG22	1:A:147:PRO:O	1.83	0.79
1:C:400:LEU:HD12	1:C:401:SER:N	1.96	0.79
1:C:574:ILE:HG23	1:C:607:VAL:HG23	1.65	0.79
1:H:668:PHE:HB2	1:H:689:LEU:CD2	2.11	0.79
1:D:146:ILE:HG22	1:D:147:PRO:O	1.82	0.79
1:D:216:TYR:CE2	1:D:232:LYS:HG2	2.17	0.79
1:E:81:VAL:CG1	1:E:86:VAL:CB	2.61	0.78
1:G:31:ALA:CB	1:G:35:ARG:HH21	1.97	0.78
1:G:784:ARG:O	1:G:788:GLU:HG3	1.83	0.78
1:H:87:ALA:HB2	1:H:120:PHE:CE2	2.17	0.78
1:D:103:ASN:HB3	1:D:106:ALA:HB3	1.65	0.78
1:H:56:LEU:HD21	1:H:65:GLU:HG3	1.63	0.78
1:C:756:GLN:HG2	1:C:757:ILE:N	1.98	0.78
1:E:83:PRO:CB	1:E:84:PRO:HD2	2.12	0.78
1:E:83:PRO:HB2	1:E:85:TRP:CD1	2.19	0.78
1:A:82:LEU:HD12	1:A:120:PHE:CD1	2.19	0.78
1:D:216:TYR:CE1	1:D:220:LEU:HD11	2.14	0.78
1:F:400:LEU:HD12	1:F:401:SER:N	1.99	0.78
1:H:124:LEU:O	1:H:124:LEU:HD23	1.84	0.78
1:D:43:ILE:O	1:D:44:LEU:HD22	1.84	0.77
1:A:32:LEU:O	1:A:36:VAL:HG23	1.85	0.77
1:A:46:GLN:HB2	1:A:79:ALA:O	1.85	0.77
1:A:146:ILE:CG2	1:A:147:PRO:HD2	2.13	0.77
1:E:82:LEU:H	1:E:83:PRO:HD3	1.49	0.77
1:H:338:THR:HG23	1:H:366:ARG:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ARG:HG2	1:C:148:ARG:NH1	1.97	0.77
1:H:80:ILE:CG1	1:H:87:ALA:HB3	2.15	0.77
1:B:276:PRO:HG3	1:B:326:GLN:HG3	1.67	0.77
1:C:55:ALA:O	1:C:59:GLN:HB2	1.85	0.77
1:F:789:MET:CE	1:G:789:MET:CB	2.60	0.77
1:H:145:SER:HB3	1:H:779:ASP:OD2	1.85	0.77
1:C:86:VAL:CG1	1:C:102:VAL:HG22	2.15	0.77
1:B:543:LEU:HA	1:B:545:LYS:HE3	1.65	0.77
1:D:103:ASN:ND2	1:F:106:ALA:HB1	2.00	0.77
1:G:39:LYS:HB2	1:G:104:LEU:HD13	1.67	0.77
1:A:85:TRP:CE3	1:A:101:ARG:HG2	2.20	0.77
1:C:543:LEU:HB3	1:C:545:LYS:HE2	1.67	0.77
1:A:35:ARG:HH22	1:A:86:VAL:HG12	1.50	0.76
1:E:60:THR:HG23	1:E:62:LYS:H	1.48	0.76
1:E:81:VAL:HG13	1:E:86:VAL:CG2	2.16	0.76
1:E:148:ARG:HH11	1:E:148:ARG:HG3	1.49	0.76
1:E:319:MET:HE3	1:E:334:ILE:HD11	1.66	0.76
1:D:103:ASN:HD21	1:F:106:ALA:HB1	1.48	0.76
1:D:281:VAL:HG21	1:D:319:MET:HE1	1.67	0.76
1:F:45:GLN:HB3	1:F:80:ILE:HA	1.67	0.76
1:B:76:THR:CA	1:B:90:VAL:HG13	2.16	0.76
1:E:82:LEU:H	1:E:82:LEU:HD23	1.49	0.76
1:G:216:TYR:CE1	1:G:220:LEU:HD11	2.19	0.76
1:B:315:LEU:HG	1:B:319:MET:CE	2.13	0.76
1:C:87:ALA:O	1:C:88:LEU:HD23	1.86	0.76
1:F:37:GLU:HG2	1:F:54:GLU:OE2	1.86	0.76
1:A:315:LEU:HG	1:A:319:MET:CE	2.15	0.76
1:G:82:LEU:HD12	1:G:83:PRO:CD	2.15	0.76
1:G:719:GLN:HG3	5:G:913:SO4:O3	1.84	0.76
1:G:82:LEU:HD12	1:G:83:PRO:HD3	1.66	0.76
1:B:82:LEU:O	1:B:82:LEU:HD13	1.86	0.76
1:F:105:HIS:O	1:F:106:ALA:HB3	1.84	0.76
1:A:35:ARG:HH21	1:A:102:VAL:CB	1.99	0.75
1:B:76:THR:HA	1:B:90:VAL:HG13	1.68	0.75
1:D:217:LEU:HD11	1:D:233:PHE:CZ	2.18	0.75
1:F:719:GLN:HG3	5:F:913:SO4:O2	1.86	0.75
1:B:248:ARG:HB3	1:B:248:ARG:HH11	1.48	0.75
1:F:65:GLU:C	1:F:68:PRO:HD2	2.12	0.75
1:F:146:ILE:CG2	1:F:147:PRO:HD2	2.14	0.75
1:G:319:MET:CE	1:G:334:ILE:HD11	2.17	0.75
1:C:32:LEU:O	1:C:32:LEU:HD13	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:LEU:HG	1:D:319:MET:CE	2.15	0.75
1:C:34:SER:HA	1:C:59:GLN:HE22	1.50	0.75
1:H:31:ALA:HA	1:H:33:LEU:CD2	2.14	0.75
1:C:451:TYR:HB3	1:C:454:LYS:HE2	1.68	0.75
1:A:45:GLN:HA	1:A:45:GLN:HE21	1.51	0.75
1:B:89:ALA:HB2	1:B:99:TYR:HB3	1.68	0.75
1:F:69:PHE:C	1:F:69:PHE:CD1	2.63	0.75
1:A:72:LEU:HD22	1:A:90:VAL:HG11	1.67	0.75
1:G:60:THR:O	1:G:63:LYS:HD3	1.86	0.75
1:F:83:PRO:O	1:F:104:LEU:HD12	1.86	0.75
1:G:54:GLU:HG3	1:G:55:ALA:N	2.00	0.75
1:H:173:ASP:HB3	1:H:176:SER:HB3	1.69	0.75
1:F:315:LEU:HG	1:F:319:MET:CE	2.17	0.75
1:A:60:THR:HG23	1:A:62:LYS:CB	2.16	0.74
1:E:35:ARG:CD	1:E:104:LEU:HA	2.16	0.74
1:E:83:PRO:HG2	1:E:85:TRP:O	1.86	0.74
1:A:339:ARG:HH12	1:A:380:ILE:HG13	1.50	0.74
1:C:53:PHE:HA	1:C:57:PRO:CG	2.15	0.74
1:G:49:ILE:H	1:G:49:ILE:CD1	2.00	0.74
1:H:719:GLN:HG3	5:H:913:SO4:O2	1.87	0.74
1:F:59:GLN:HG2	1:F:60:THR:N	2.00	0.74
1:G:31:ALA:HB1	1:G:35:ARG:HH21	1.52	0.74
1:C:564:LEU:HD13	1:C:613:ARG:HH22	1.52	0.74
1:E:327:GLY:C	1:E:328:LEU:HD23	2.11	0.74
1:F:327:GLY:C	1:F:328:LEU:HD23	2.11	0.74
1:H:80:ILE:HG12	1:H:87:ALA:O	1.87	0.74
1:G:83:PRO:HB2	1:G:85:TRP:N	2.00	0.74
1:F:224:THR:HG23	1:F:228:GLU:HG3	1.70	0.74
1:B:189:HIS:ND1	1:B:330:ILE:HD13	2.02	0.74
1:G:43:ILE:HA	1:G:81:VAL:O	1.88	0.74
1:E:45:GLN:HB3	1:E:80:ILE:HA	1.69	0.73
1:D:27:ASN:HB2	1:D:30:LEU:HD23	1.68	0.73
1:H:72:LEU:CD1	1:H:90:VAL:HG11	2.19	0.73
1:C:104:LEU:HD22	1:C:104:LEU:H	1.53	0.73
1:F:789:MET:CB	1:G:789:MET:CE	2.66	0.73
1:E:81:VAL:HG13	1:E:86:VAL:HB	1.70	0.73
1:E:486:ILE:HG22	1:E:516:VAL:HG22	1.70	0.73
1:B:87:ALA:HB2	1:B:120:PHE:HE2	1.53	0.73
1:C:53:PHE:O	1:C:57:PRO:HG2	1.88	0.73
1:F:51:ALA:O	1:F:52:GLU:HB3	1.86	0.73
1:F:216:TYR:CE2	1:F:232:LYS:HG2	2.23	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:GLN:O	1:H:78:GLU:HA	1.88	0.73
1:E:72:LEU:HD22	1:E:90:VAL:HG11	1.69	0.73
1:E:789:MET:HE1	1:H:789:MET:HB3	1.69	0.73
1:B:82:LEU:C	1:B:84:PRO:HD2	2.13	0.73
1:E:146:ILE:CG2	1:E:147:PRO:HD2	2.19	0.73
1:E:151:LEU:HD23	1:F:211:ARG:NH2	2.04	0.73
1:E:281:VAL:HG21	1:E:319:MET:HE1	1.71	0.73
1:B:92:PRO:HG2	1:B:96:VAL:CG2	2.18	0.72
1:F:673:LEU:HD23	1:F:714:PRO:HB2	1.69	0.72
1:A:789:MET:CE	1:D:789:MET:CE	2.62	0.72
1:B:789:MET:HB3	1:C:789:MET:HE1	1.71	0.72
1:G:66:GLY:O	1:G:68:PRO:HD3	1.89	0.72
1:A:789:MET:HG2	1:D:789:MET:HE3	1.70	0.72
1:G:82:LEU:H	1:G:83:PRO:HD3	1.54	0.72
1:A:210:LEU:HD22	1:A:253:ILE:HG23	1.70	0.72
1:F:216:TYR:CD2	1:F:232:LYS:HG2	2.23	0.72
1:D:82:LEU:HD13	1:D:84:PRO:HD2	1.71	0.71
1:E:43:ILE:HG13	1:E:82:LEU:HA	1.72	0.71
1:H:39:LYS:HG2	1:H:104:LEU:CG	2.19	0.71
1:E:82:LEU:N	1:E:83:PRO:CD	2.51	0.71
1:G:119:HIS:HE1	1:G:129:LYS:HD3	1.54	0.71
1:G:82:LEU:HD12	1:G:83:PRO:HG3	1.71	0.71
1:C:420:LEU:HD23	1:C:467:ALA:CB	2.20	0.71
1:C:50:ILE:O	1:C:54:GLU:HB3	1.90	0.71
1:D:756:GLN:HG3	1:D:757:ILE:HD13	1.73	0.71
1:F:103:ASN:OD1	1:F:106:ALA:HB3	1.90	0.71
1:B:298:TYR:CE1	1:B:649:MET:HE1	2.25	0.71
1:C:441:GLU:OE1	1:C:441:GLU:HA	1.90	0.71
1:F:146:ILE:HG22	1:F:147:PRO:CD	2.19	0.71
1:H:76:THR:HA	1:H:89:ALA:O	1.90	0.71
1:H:148:ARG:HH11	1:H:148:ARG:CG	2.03	0.71
1:B:56:LEU:CB	1:B:57:PRO:CD	2.68	0.71
1:E:125:VAL:HG11	1:E:505:PRO:HG2	1.71	0.71
1:G:682:VAL:HG13	1:G:749:ILE:HD12	1.73	0.71
1:A:789:MET:HB3	1:D:789:MET:HE1	1.70	0.70
1:H:91:ARG:HD2	1:H:97:TRP:CZ2	2.25	0.70
1:H:112:LEU:N	1:H:112:LEU:CD1	2.54	0.70
1:G:212:LYS:HE2	1:G:232:LYS:NZ	2.06	0.70
1:G:230:GLU:O	1:G:234:GLU:HG3	1.91	0.70
1:B:545:LYS:H	1:B:545:LYS:CD	1.87	0.70
1:C:534:PHE:HB2	1:C:535:PRO:CD	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:756:GLN:HG3	1:D:757:ILE:CD1	2.21	0.70
1:E:85:TRP:HB2	1:E:103:ASN:HA	1.72	0.70
1:F:125:VAL:HG21	1:F:450:ILE:HG12	1.72	0.70
1:F:59:GLN:C	1:F:60:THR:HG22	2.17	0.70
1:B:245:ASN:O	1:B:249:VAL:HG23	1.90	0.70
1:G:67:GLY:N	1:G:68:PRO:HD3	2.06	0.70
1:G:518:ASP:OD1	1:G:520:LYS:HG2	1.91	0.70
1:A:756:GLN:HG2	1:A:757:ILE:N	2.05	0.70
1:F:547:HIS:O	1:F:551:GLU:HG2	1.92	0.70
1:F:65:GLU:HA	1:F:68:PRO:CG	2.21	0.70
1:F:245:ASN:O	1:F:249:VAL:HG23	1.92	0.70
1:D:146:ILE:HG23	1:D:147:PRO:HD2	1.73	0.70
1:E:789:MET:HB3	1:H:789:MET:HE3	1.70	0.70
1:C:137:LEU:HD11	1:C:790:PHE:CZ	2.27	0.69
1:C:146:ILE:CG2	1:C:147:PRO:HD2	2.21	0.69
1:A:249:VAL:O	1:A:253:ILE:HG13	1.92	0.69
1:H:111:GLU:HA	1:H:112:LEU:HD12	1.73	0.69
1:A:124:LEU:O	1:A:124:LEU:HD23	1.90	0.69
1:C:281:VAL:HG21	1:C:319:MET:HE1	1.74	0.69
1:C:315:LEU:O	1:C:319:MET:HG3	1.93	0.69
1:D:103:ASN:HD21	1:F:106:ALA:HB2	1.56	0.69
1:G:49:ILE:HD12	1:G:49:ILE:N	2.06	0.69
1:H:174:LYS:HD2	1:H:174:LYS:N	2.08	0.69
1:B:82:LEU:HD22	1:B:84:PRO:HD2	1.74	0.69
1:B:582:ASP:HB2	1:B:621:GLU:OE1	1.92	0.69
1:E:69:PHE:O	1:E:73:LEU:HB2	1.93	0.69
1:H:39:LYS:CB	1:H:104:LEU:HD22	2.22	0.69
1:E:35:ARG:CG	1:E:104:LEU:HA	2.22	0.69
1:H:486:ILE:HG22	1:H:516:VAL:HG22	1.74	0.69
1:G:81:VAL:HG22	1:G:86:VAL:HG23	1.75	0.69
1:H:217:LEU:HD11	1:H:233:PHE:HZ	1.58	0.69
1:E:255:LEU:HD22	1:E:267:THR:HG23	1.75	0.69
1:G:63:LYS:O	1:G:65:GLU:HG2	1.91	0.69
1:H:189:HIS:CD2	1:H:190:GLN:HG3	2.28	0.69
1:H:111:GLU:CA	1:H:112:LEU:HD12	2.23	0.69
1:G:48:GLN:NE2	1:G:52:GLU:HB3	2.08	0.69
1:C:131:GLY:HA3	1:C:134:THR:HG23	1.74	0.68
1:H:82:LEU:HD11	1:H:120:PHE:CZ	2.28	0.68
1:H:146:ILE:CG2	1:H:147:PRO:N	2.56	0.68
1:A:547:HIS:O	1:A:551:GLU:HG3	1.93	0.68
1:B:207:GLN:HG3	1:B:211:ARG:NH2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:ASN:HB3	1:E:148:ARG:HH22	1.57	0.68
1:G:407:LYS:HB2	1:G:408:PRO:CD	2.23	0.68
1:G:635:GLU:HG2	1:G:636:TYR:CD2	2.28	0.68
1:A:789:MET:CG	1:D:789:MET:HE3	2.24	0.68
1:E:44:LEU:HA	1:E:124:LEU:HD11	1.75	0.68
1:C:86:VAL:HG12	1:C:102:VAL:HG22	1.73	0.68
1:C:290:PHE:O	1:C:366:ARG:NH1	2.26	0.68
1:E:217:LEU:HD11	1:E:233:PHE:HZ	1.58	0.68
1:F:48:GLN:O	1:F:51:ALA:O	2.11	0.68
1:H:130:ASN:HB3	1:H:134:THR:HG21	1.73	0.68
1:D:43:ILE:HG22	1:D:82:LEU:HA	1.75	0.68
1:G:82:LEU:CD1	1:G:83:PRO:HG3	2.24	0.68
1:A:33:LEU:O	1:A:36:VAL:HB	1.94	0.68
1:B:84:PRO:O	1:B:85:TRP:HD1	1.77	0.68
1:F:543:LEU:HB3	1:F:545:LYS:HE3	1.74	0.68
1:C:34:SER:CA	1:C:59:GLN:HE22	2.06	0.68
1:C:535:PRO:HD2	1:C:538:GLU:OE2	1.94	0.68
1:D:39:LYS:HB2	1:D:104:LEU:HD13	1.74	0.68
1:A:73:LEU:HD23	1:A:73:LEU:O	1.93	0.68
1:B:43:ILE:CD1	1:B:44:LEU:H	2.05	0.68
1:E:30:LEU:HD11	1:E:62:LYS:O	1.94	0.68
1:E:65:GLU:HG3	1:E:70:PHE:HB2	1.75	0.68
1:A:30:LEU:HD12	1:A:62:LYS:O	1.92	0.68
1:A:45:GLN:HE22	1:A:80:ILE:CD1	2.06	0.68
1:C:681:VAL:O	1:C:685:MET:HG3	1.94	0.68
1:E:146:ILE:HG22	1:E:147:PRO:HD2	1.75	0.68
1:F:43:ILE:HG23	1:F:44:LEU:N	2.09	0.68
1:F:55:ALA:O	1:F:59:GLN:HB2	1.93	0.68
1:A:170:LEU:HD23	1:A:176:SER:OG	1.93	0.68
1:F:209:THR:HG23	1:F:236:ILE:HB	1.75	0.68
1:F:486:ILE:HG22	1:F:516:VAL:HG22	1.74	0.68
1:G:582:ASP:HB2	1:G:621:GLU:OE1	1.94	0.68
1:A:216:TYR:HD1	1:A:216:TYR:C	2.02	0.67
1:A:298:TYR:HE1	1:A:649:MET:HE1	1.57	0.67
1:B:82:LEU:CD1	1:B:82:LEU:H	2.06	0.67
1:D:145:SER:HB3	1:D:779:ASP:OD2	1.94	0.67
1:F:276:PRO:HG3	1:F:326:GLN:HG3	1.74	0.67
1:H:137:LEU:HD11	1:H:790:PHE:CE1	2.29	0.67
1:A:486:ILE:HG22	1:A:516:VAL:HG22	1.75	0.67
1:C:552:GLU:O	1:C:556:SER:HB3	1.94	0.67
1:H:276:PRO:HG3	1:H:326:GLN:HG3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ILE:HG22	1:A:50:ILE:N	2.10	0.67
1:A:72:LEU:O	1:A:72:LEU:HD13	1.94	0.67
1:D:103:ASN:ND2	1:F:106:ALA:CB	2.58	0.67
1:E:789:MET:HG3	1:H:135:LEU:HD11	1.77	0.67
1:F:407:LYS:HB2	1:F:408:PRO:CD	2.25	0.67
1:A:298:TYR:CE1	1:A:649:MET:HE1	2.29	0.67
1:B:89:ALA:CB	1:B:99:TYR:CD1	2.63	0.67
1:D:298:TYR:CE1	1:D:649:MET:HE1	2.29	0.67
1:H:130:ASN:ND2	1:H:506:GLY:H	1.92	0.67
1:B:93:ARG:O	1:B:96:VAL:HG22	1.95	0.67
1:B:327:GLY:O	1:B:328:LEU:HD23	1.95	0.67
1:E:148:ARG:HG3	1:E:148:ARG:NH1	2.09	0.67
1:F:400:LEU:HD12	1:F:400:LEU:C	2.20	0.67
1:B:148:ARG:HH11	1:B:148:ARG:HG3	1.57	0.67
1:D:81:VAL:HG22	1:D:86:VAL:HG23	1.77	0.67
1:D:633:ILE:HA	1:D:638:LEU:HD12	1.75	0.67
1:H:319:MET:HE3	1:H:334:ILE:HD11	1.76	0.67
1:B:789:MET:HB3	1:C:789:MET:HE2	1.76	0.66
1:C:83:PRO:HG2	1:C:84:PRO:CD	2.13	0.66
1:A:56:LEU:HB3	1:A:57:PRO:HD3	1.77	0.66
1:A:82:LEU:HB3	1:A:83:PRO:HD2	1.77	0.66
1:H:87:ALA:CB	1:H:120:PHE:CE2	2.77	0.66
1:D:82:LEU:HD12	1:D:82:LEU:C	2.20	0.66
1:E:116:GLU:O	1:E:119:HIS:HB2	1.96	0.66
1:D:116:GLU:O	1:D:119:HIS:HB2	1.96	0.66
1:E:83:PRO:CB	1:E:84:PRO:CD	2.72	0.66
1:A:420:LEU:HD13	1:A:420:LEU:C	2.20	0.66
1:C:105:HIS:O	1:C:106:ALA:HB3	1.95	0.66
1:E:46:GLN:HB3	1:E:50:ILE:CB	2.16	0.66
1:G:480:THR:HB	1:G:485:GLU:OE1	1.96	0.66
1:C:131:GLY:CA	1:C:134:THR:HG23	2.25	0.66
1:F:83:PRO:HG2	1:F:84:PRO:HD3	1.78	0.66
1:F:756:GLN:HG2	1:F:757:ILE:H	1.61	0.66
1:H:33:LEU:HD21	1:H:59:GLN:NE2	2.11	0.66
1:A:124:LEU:HD23	1:A:124:LEU:C	2.20	0.66
1:C:173:ASP:OD2	1:C:176:SER:HB2	1.96	0.66
1:D:216:TYR:CD2	1:D:232:LYS:HG2	2.31	0.66
1:E:762:LEU:O	1:E:762:LEU:HD12	1.95	0.66
1:H:590:LEU:HB2	1:H:671:PRO:HG3	1.77	0.66
1:F:116:GLU:O	1:F:119:HIS:HB2	1.96	0.66
1:F:281:VAL:CG2	1:F:319:MET:HE1	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:45:GLN:NE2	1:H:80:ILE:HG22	2.11	0.66
1:A:245:ASN:O	1:A:249:VAL:HG23	1.95	0.66
1:B:52:GLU:O	1:B:56:LEU:CB	2.44	0.65
1:C:315:LEU:HG	1:C:319:MET:HE3	1.77	0.65
1:E:226:TYR:CE2	1:E:240:ARG:HG2	2.31	0.65
1:E:131:GLY:HA3	1:E:134:THR:HG23	1.77	0.65
1:D:146:ILE:CD1	1:D:772:TRP:CZ2	2.79	0.65
1:G:319:MET:HE1	1:G:334:ILE:CD1	2.23	0.65
1:A:216:TYR:HD1	1:A:216:TYR:O	1.78	0.65
1:E:135:LEU:HD11	1:H:789:MET:HG3	1.78	0.65
1:F:145:SER:HB3	1:F:779:ASP:OD2	1.96	0.65
1:C:148:ARG:HH11	1:C:148:ARG:HG3	1.59	0.65
1:C:319:MET:O	1:C:323:ILE:HG13	1.96	0.65
1:D:400:LEU:HD12	1:D:401:SER:N	2.12	0.65
1:D:561:LYS:HD3	1:D:613:ARG:O	1.96	0.65
1:C:315:LEU:HG	1:C:319:MET:CE	2.27	0.65
1:D:319:MET:O	1:D:323:ILE:HG13	1.96	0.65
1:G:103:ASN:HB3	1:G:106:ALA:O	1.97	0.65
1:A:65:GLU:HA	1:A:65:GLU:OE2	1.96	0.65
1:B:435:THR:HG23	1:B:475:THR:HB	1.79	0.65
1:B:89:ALA:CB	1:B:99:TYR:HB3	2.26	0.65
1:B:547:HIS:O	1:B:551:GLU:HG2	1.97	0.65
1:C:56:LEU:HB3	1:C:57:PRO:HD3	1.79	0.65
1:C:86:VAL:HG12	1:C:102:VAL:CG2	2.27	0.65
1:F:140:GLU:N	1:F:141:PRO:HD2	2.11	0.65
1:A:29:VAL:O	1:A:33:LEU:HG	1.96	0.65
1:A:143:ASN:HB3	1:A:148:ARG:NH2	2.12	0.65
1:B:92:PRO:HG2	1:B:96:VAL:HG21	1.78	0.65
1:C:673:LEU:HD23	1:C:714:PRO:HB2	1.79	0.65
1:D:438:HIS:ND1	4:D:904[B]:NHF:H6	2.11	0.65
1:F:52:GLU:HA	1:F:55:ALA:HB3	1.79	0.65
1:H:146:ILE:HG23	1:H:147:PRO:N	2.12	0.65
1:C:82:LEU:HB3	1:C:83:PRO:HD2	1.79	0.65
1:D:103:ASN:HD22	1:D:108:VAL:HG12	1.62	0.65
1:H:131:GLY:C	1:H:134:THR:HG23	2.22	0.65
1:A:789:MET:HE1	1:D:789:MET:HB3	1.78	0.64
1:F:249:VAL:O	1:F:253:ILE:HG13	1.96	0.64
1:G:195:MET:HE1	1:G:252:MET:HE1	1.77	0.64
1:H:82:LEU:HD23	1:H:86:VAL:HA	1.79	0.64
1:A:54:GLU:HG3	1:A:55:ALA:H	1.61	0.64
1:A:407:LYS:HB2	1:A:408:PRO:CD	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:LEU:O	1:C:81:VAL:HG12	1.96	0.64
1:A:405:ASN:ND2	1:F:61:ARG:HD3	2.12	0.64
1:D:148:ARG:HH11	1:D:148:ARG:HG3	1.61	0.64
1:E:173:ASP:HB3	1:E:176:SER:HB3	1.80	0.64
1:F:387:PRO:HD3	1:F:802:VAL:HB	1.78	0.64
1:E:441:GLU:HA	1:E:441:GLU:OE1	1.97	0.64
1:G:217:LEU:HD11	1:G:233:PHE:HZ	1.62	0.64
1:G:565:CYS:HB2	1:G:642:PHE:O	1.97	0.64
1:B:264:ASP:OD1	1:B:267:THR:HB	1.97	0.64
1:C:295:VAL:HB	1:C:301:THR:HG21	1.80	0.64
1:D:176:SER:O	1:D:179:PRO:HD2	1.97	0.64
1:H:249:VAL:O	1:H:253:ILE:HG13	1.98	0.64
1:A:46:GLN:HB3	1:A:79:ALA:HB3	1.78	0.64
1:B:670:GLN:HG3	1:B:670:GLN:O	1.97	0.64
1:E:105:HIS:O	1:E:106:ALA:HB3	1.97	0.64
1:F:49:ILE:O	1:F:53:PHE:CB	2.45	0.64
1:A:262:ALA:HB3	1:B:154:TYR:OH	1.98	0.64
1:D:103:ASN:HD22	1:D:108:VAL:CG1	2.10	0.64
1:D:518:ASP:OD1	1:D:520:LYS:HG2	1.96	0.64
1:E:255:LEU:CD2	1:E:267:THR:HG23	2.27	0.64
1:D:39:LYS:HZ1	1:D:104:LEU:HB3	1.62	0.64
1:A:216:TYR:HE1	1:A:220:LEU:HD11	1.63	0.64
1:D:102:VAL:HG23	1:D:108:VAL:O	1.98	0.64
1:E:170:LEU:HD22	1:E:177:LEU:HD23	1.79	0.64
1:H:131:GLY:CA	1:H:134:THR:HG23	2.28	0.64
1:B:100:LEU:HA	1:B:112:LEU:H	1.63	0.64
1:F:83:PRO:HG2	1:F:84:PRO:CD	2.28	0.64
1:A:681:VAL:O	1:A:685:MET:HG3	1.98	0.63
1:H:33:LEU:HA	1:H:36:VAL:CG2	2.27	0.63
1:A:512:HIS:CE1	1:A:515:ASP:HB2	2.32	0.63
1:G:45:GLN:HA	1:G:45:GLN:NE2	2.03	0.63
1:H:790:PHE:O	1:H:794:LYS:HB3	1.98	0.63
1:A:419:ASN:OD1	1:A:435:THR:HB	1.98	0.63
1:B:36:VAL:O	1:B:39:LYS:CB	2.45	0.63
1:B:726:ASP:O	1:B:730:LYS:HG3	1.98	0.63
1:E:319:MET:CE	1:E:334:ILE:HD11	2.28	0.63
1:F:35:ARG:CD	1:F:104:LEU:HD23	2.28	0.63
1:G:216:TYR:C	1:G:216:TYR:HD1	2.05	0.63
1:A:262:ALA:HB1	1:B:164:ARG:HD2	1.80	0.63
1:B:76:THR:HA	1:B:90:VAL:HA	1.80	0.63
1:D:438:HIS:ND1	4:D:904[B]:NHF:C6	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:GLU:OE1	1:D:541:ARG:HD3	1.98	0.63
1:G:400:LEU:C	1:G:400:LEU:HD12	2.23	0.63
1:H:48:GLN:O	1:H:52:GLU:HB3	1.98	0.63
1:A:216:TYR:CE1	1:A:220:LEU:HD11	2.33	0.63
1:B:143:ASN:HB3	1:B:780:ARG:NH1	2.13	0.63
1:B:789:MET:CE	1:C:789:MET:CE	2.68	0.63
1:C:87:ALA:C	1:C:88:LEU:HD23	2.22	0.63
1:D:298:TYR:HE1	1:D:649:MET:HE1	1.64	0.63
1:F:35:ARG:HB2	1:F:35:ARG:CZ	2.28	0.63
1:F:282:VAL:HG13	1:F:337:LEU:HD23	1.80	0.63
1:A:60:THR:HG23	1:A:62:LYS:H	1.64	0.63
1:C:53:PHE:HA	1:C:57:PRO:HG3	1.79	0.63
1:D:216:TYR:HD1	1:D:216:TYR:C	2.07	0.63
1:G:84:PRO:O	1:G:104:LEU:HG	1.99	0.63
1:C:93:ARG:HH21	1:C:96:VAL:HG21	1.62	0.63
1:G:35:ARG:HH12	1:G:107:LEU:CB	2.10	0.63
1:G:339:ARG:HH12	1:G:380:ILE:HG13	1.62	0.63
1:H:319:MET:CE	1:H:334:ILE:HD11	2.28	0.63
1:H:670:GLN:HG3	1:H:670:GLN:O	1.98	0.63
1:C:80:ILE:CD1	1:C:121:LYS:CG	2.77	0.63
1:C:259:LEU:O	1:C:263:PRO:HG3	1.97	0.63
1:C:442:LYS:HD2	1:C:449:ASP:HB3	1.80	0.63
1:D:125:VAL:HG13	1:D:126:ASP:N	2.14	0.63
1:F:39:LYS:HG2	1:F:104:LEU:CD1	2.17	0.63
1:G:83:PRO:CB	1:G:84:PRO:HD2	2.29	0.63
1:C:445:TYR:O	1:C:448:SER:HB3	1.99	0.63
1:C:765:LEU:HD22	1:C:769:TYR:HE2	1.64	0.63
1:D:160:ASP:O	1:D:164:ARG:HG3	1.99	0.63
1:E:46:GLN:CB	1:E:50:ILE:HB	2.17	0.63
1:E:327:GLY:O	1:E:328:LEU:HD23	1.99	0.63
1:G:338:THR:HG23	1:G:366:ARG:HG2	1.81	0.63
1:G:486:ILE:HG22	1:G:516:VAL:HG22	1.81	0.63
1:G:689:LEU:HD12	1:G:690:PRO:HD2	1.80	0.63
1:A:216:TYR:C	1:A:216:TYR:CD1	2.75	0.62
1:B:609:VAL:HG22	1:B:645:ILE:HB	1.81	0.62
1:F:86:VAL:HG12	1:F:102:VAL:O	1.99	0.62
1:F:143:ASN:HB3	1:F:148:ARG:NH2	2.14	0.62
1:A:789:MET:CE	1:D:789:MET:CB	2.76	0.62
1:C:143:ASN:HA	1:C:780:ARG:HH12	1.64	0.62
1:C:613:ARG:HG3	1:C:626:MET:HE2	1.81	0.62
1:D:411:ILE:HG13	1:D:431:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:LYS:HE2	1:H:104:LEU:CD1	2.29	0.62
1:H:55:ALA:O	1:H:59:GLN:HB2	1.98	0.62
1:G:48:GLN:HE22	1:G:52:GLU:HB3	1.63	0.62
1:A:84:PRO:O	1:A:104:LEU:N	2.28	0.62
1:A:160:ASP:O	1:A:164:ARG:HG3	2.00	0.62
1:G:216:TYR:C	1:G:216:TYR:CD1	2.77	0.62
1:C:72:LEU:C	1:C:72:LEU:HD13	2.25	0.62
1:E:82:LEU:N	1:E:82:LEU:HD23	2.13	0.62
1:F:613:ARG:HG3	1:F:626:MET:HE2	1.80	0.62
1:H:42:GLY:O	1:H:81:VAL:HB	2.00	0.62
1:H:131:GLY:HA3	1:H:134:THR:HG23	1.82	0.62
1:B:60:THR:CG2	1:B:61:ARG:N	2.56	0.62
1:B:680:THR:HG23	2:B:901:UDP:O1A	1.98	0.62
1:F:65:GLU:O	1:F:68:PRO:HD2	1.99	0.62
1:F:67:GLY:N	1:F:68:PRO:CD	2.61	0.62
1:A:54:GLU:CG	1:A:55:ALA:N	2.63	0.62
1:C:143:ASN:HB3	1:C:148:ARG:HH21	1.62	0.62
1:H:77:GLN:O	1:H:78:GLU:HB3	1.99	0.62
1:E:534:PHE:HB2	1:E:535:PRO:CD	2.29	0.62
1:A:103:ASN:CB	1:A:106:ALA:CB	2.76	0.62
1:B:160:ASP:O	1:B:164:ARG:HG3	2.00	0.62
1:B:538:GLU:OE1	1:B:541:ARG:HD3	2.00	0.62
1:D:83:PRO:HB2	1:D:84:PRO:HD3	1.81	0.62
1:H:407:LYS:HB2	1:H:408:PRO:CD	2.30	0.62
1:A:125:VAL:HG21	1:A:450:ILE:HG12	1.82	0.61
1:E:81:VAL:HG13	1:E:86:VAL:CB	2.27	0.61
1:F:59:GLN:O	1:F:60:THR:HG22	2.00	0.61
1:F:534:PHE:HB2	1:F:535:PRO:CD	2.30	0.61
1:F:782:GLU:HG3	1:G:141:PRO:HB2	1.82	0.61
1:G:54:GLU:HG3	1:G:55:ALA:H	1.62	0.61
1:G:83:PRO:HG2	1:G:85:TRP:HB2	1.82	0.61
1:G:119:HIS:CE1	1:G:129:LYS:CD	2.78	0.61
1:G:479:ILE:CD1	1:G:762:LEU:HD13	2.30	0.61
1:A:27:ASN:HB3	1:A:30:LEU:HB2	1.81	0.61
1:A:72:LEU:HD13	1:A:72:LEU:C	2.25	0.61
1:E:181:LEU:HD13	1:E:206:LEU:HD22	1.81	0.61
1:G:54:GLU:CG	1:G:55:ALA:N	2.63	0.61
1:A:45:GLN:HA	1:A:45:GLN:NE2	2.15	0.61
1:D:148:ARG:HG3	1:D:148:ARG:NH1	2.13	0.61
1:F:85:TRP:CZ3	1:F:101:ARG:HD2	2.35	0.61
1:G:146:ILE:HG23	1:G:147:PRO:HD2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:LEU:HD23	1:C:467:ALA:HB1	1.81	0.61
1:C:588:SER:HB3	1:C:625:GLU:OE2	2.00	0.61
1:D:80:ILE:HD13	1:D:117:PHE:CZ	2.35	0.61
1:D:170:LEU:HD23	1:D:176:SER:OG	2.01	0.61
1:F:756:GLN:HG2	1:F:757:ILE:N	2.15	0.61
1:H:119:HIS:CE1	1:H:129:LYS:CB	2.84	0.61
1:A:789:MET:CB	1:D:789:MET:CE	2.77	0.61
1:C:518:ASP:OD1	1:C:520:LYS:HG2	2.01	0.61
1:F:789:MET:CE	1:G:789:MET:CE	2.69	0.61
1:H:770:GLY:O	1:H:773:LYS:HB2	2.01	0.61
1:A:116:GLU:O	1:A:119:HIS:HB2	2.01	0.61
1:A:770:GLY:O	1:A:773:LYS:HB2	1.99	0.61
1:D:171:PHE:HD1	1:D:263:PRO:HD2	1.65	0.61
1:H:82:LEU:HG	1:H:85:TRP:O	2.00	0.61
1:G:34:SER:N	1:G:59:GLN:HE22	1.98	0.61
1:H:140:GLU:N	1:H:141:PRO:HD2	2.16	0.61
1:B:424:LEU:HD22	1:C:133:PHE:CE1	2.35	0.61
1:C:80:ILE:CD1	1:C:121:LYS:HG3	2.31	0.61
1:D:216:TYR:C	1:D:216:TYR:CD1	2.79	0.61
1:E:315:LEU:O	1:E:319:MET:HG3	1.99	0.61
1:F:46:GLN:HB3	1:F:50:ILE:CD1	2.31	0.61
1:G:441:GLU:OE1	1:G:441:GLU:HA	2.00	0.61
1:A:88:LEU:HB2	1:A:100:LEU:CD2	2.31	0.61
1:C:400:LEU:HD12	1:C:400:LEU:C	2.25	0.61
1:D:50:ILE:O	1:D:53:PHE:N	2.33	0.61
1:F:46:GLN:HB3	1:F:50:ILE:HD12	1.82	0.61
1:G:163:ASN:O	1:G:167:SER:HB2	2.01	0.61
1:D:39:LYS:HB2	1:D:39:LYS:HZ2	1.66	0.60
1:E:35:ARG:HG2	1:E:104:LEU:HA	1.82	0.60
1:G:82:LEU:N	1:G:83:PRO:CD	2.62	0.60
1:H:76:THR:CA	1:H:89:ALA:O	2.48	0.60
1:A:158:GLY:HA3	1:A:519:PRO:O	2.01	0.60
1:A:491:GLU:CD	1:A:491:GLU:H	2.09	0.60
1:D:181:LEU:HD13	1:D:206:LEU:HD22	1.82	0.60
1:B:128:VAL:HG22	1:B:129:LYS:H	1.64	0.60
1:B:668:PHE:HB2	1:B:689:LEU:CD2	2.30	0.60
1:E:27:ASN:OD1	1:E:30:LEU:HB3	2.00	0.60
1:F:298:TYR:CE1	1:F:649:MET:HE1	2.36	0.60
1:A:545:LYS:H	1:A:545:LYS:CD	2.15	0.60
1:B:58:GLU:O	1:B:59:GLN:CB	2.49	0.60
1:B:148:ARG:HG2	1:B:148:ARG:NH1	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:400:LEU:C	1:H:400:LEU:HD12	2.25	0.60
1:B:92:PRO:HG2	1:B:96:VAL:HG23	1.83	0.60
1:D:290:PHE:O	1:D:366:ARG:NH1	2.32	0.60
1:H:53:PHE:O	1:H:57:PRO:HG2	2.01	0.60
1:B:354:GLU:OE1	1:B:366:ARG:NH2	2.31	0.60
1:D:486:ILE:HG22	1:D:516:VAL:HG22	1.83	0.60
1:B:682:VAL:HG13	1:B:749:ILE:HD12	1.83	0.60
1:D:52:GLU:HG2	1:D:57:PRO:CD	2.31	0.60
1:D:125:VAL:HG13	1:D:126:ASP:H	1.67	0.60
1:D:796:ARG:HB2	1:D:797:PRO:HD3	1.83	0.60
1:F:59:GLN:C	1:F:60:THR:CG2	2.74	0.60
1:F:116:GLU:HA	1:F:119:HIS:HD2	1.65	0.60
1:G:702:ILE:HA	1:G:753:TYR:OH	2.02	0.60
1:H:131:GLY:HA3	1:H:134:THR:CG2	2.31	0.60
1:B:315:LEU:O	1:B:319:MET:HG3	2.01	0.60
1:E:81:VAL:HG13	1:E:86:VAL:HG23	1.83	0.60
1:E:162:LEU:HD11	1:E:772:TRP:CE3	2.37	0.60
1:F:53:PHE:O	1:F:57:PRO:HB2	2.02	0.60
1:F:105:HIS:O	1:F:106:ALA:CB	2.50	0.60
1:G:81:VAL:HG22	1:G:86:VAL:CG2	2.32	0.60
1:G:407:LYS:HB2	1:G:408:PRO:HD2	1.84	0.60
1:H:131:GLY:O	1:H:133:PHE:C	2.45	0.60
1:A:56:LEU:HD23	1:A:70:PHE:HE1	1.66	0.60
1:B:441:GLU:HA	1:B:441:GLU:OE1	2.02	0.60
1:D:146:ILE:HD11	1:D:772:TRP:CH2	2.36	0.60
1:F:131:GLY:O	1:F:134:THR:HG23	2.02	0.60
1:G:146:ILE:HG22	1:G:147:PRO:O	2.02	0.60
1:A:762:LEU:HD12	1:A:762:LEU:O	2.02	0.59
1:C:534:PHE:HB2	1:C:535:PRO:HD2	1.84	0.59
1:A:30:LEU:HD22	1:A:30:LEU:H	1.67	0.59
1:B:170:LEU:HD22	1:B:177:LEU:HD23	1.84	0.59
1:C:60:THR:O	1:C:63:LYS:HD3	2.03	0.59
1:C:101:ARG:HB3	1:C:112:LEU:HD22	1.83	0.59
1:C:407:LYS:HB2	1:C:408:PRO:CD	2.32	0.59
1:D:233:PHE:O	1:D:236:ILE:HG12	2.02	0.59
1:E:43:ILE:HG23	1:E:44:LEU:N	2.16	0.59
1:E:249:VAL:O	1:E:253:ILE:HG13	2.02	0.59
1:F:789:MET:HE2	1:G:789:MET:HB3	1.77	0.59
1:A:789:MET:HE2	1:D:789:MET:HB3	1.81	0.59
2:D:901:UDP:O2B	4:D:904[B]:NHF:H1	2.02	0.59
1:G:158:GLY:HA3	1:G:519:PRO:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:SER:HB3	1:C:779:ASP:OD2	2.02	0.59
1:D:43:ILE:HA	1:D:81:VAL:O	2.03	0.59
1:G:53:PHE:HA	1:G:57:PRO:HG2	1.84	0.59
1:D:30:LEU:N	1:D:30:LEU:HD22	2.17	0.59
1:F:125:VAL:CG2	1:F:450:ILE:HG12	2.31	0.59
1:F:451:TYR:HB3	1:F:454:LYS:HE2	1.85	0.59
1:G:82:LEU:CB	1:G:83:PRO:HD3	2.32	0.59
1:C:702:ILE:HA	1:C:753:TYR:OH	2.01	0.59
1:E:131:GLY:CA	1:E:134:THR:HG23	2.32	0.59
1:F:284:LEU:HD13	1:F:337:LEU:HB2	1.84	0.59
1:F:479:ILE:HD11	1:F:762:LEU:HD13	1.84	0.59
1:G:83:PRO:HB3	1:G:84:PRO:HD2	1.84	0.59
1:H:534:PHE:HB2	1:H:535:PRO:CD	2.33	0.59
1:B:158:GLY:HA3	1:B:519:PRO:O	2.03	0.59
1:E:290:PHE:O	1:E:366:ARG:NH1	2.30	0.59
1:F:226:TYR:CE2	1:F:240:ARG:HG2	2.38	0.59
1:H:148:ARG:CG	1:H:148:ARG:NH1	2.65	0.59
1:H:224:THR:HG23	1:H:228:GLU:HG3	1.84	0.59
1:A:534:PHE:HB2	1:A:535:PRO:CD	2.33	0.59
1:D:407:LYS:HB2	1:D:408:PRO:CD	2.33	0.59
1:F:67:GLY:H	1:F:68:PRO:HD2	1.66	0.59
1:G:354:GLU:OE1	1:G:366:ARG:NH2	2.31	0.59
1:H:113:GLN:N	1:H:113:GLN:OE1	2.36	0.59
1:H:169:LYS:HG2	1:H:176:SER:OG	2.03	0.59
1:A:84:PRO:O	1:A:104:LEU:CB	2.51	0.59
1:B:435:THR:HG23	1:B:475:THR:CB	2.31	0.59
1:E:216:TYR:O	1:E:216:TYR:HD1	1.85	0.59
1:E:668:PHE:HB2	1:E:689:LEU:HD23	1.85	0.59
1:B:534:PHE:HB2	1:B:535:PRO:CD	2.33	0.59
1:D:390:GLU:OE1	1:D:796:ARG:HD2	2.03	0.59
1:F:216:TYR:HD1	1:F:216:TYR:O	1.85	0.59
1:F:437:ALA:C	1:F:439:ALA:H	2.10	0.59
1:H:224:THR:CG2	1:H:228:GLU:HG3	2.33	0.59
1:F:65:GLU:HA	1:F:68:PRO:HG3	1.85	0.58
1:C:574:ILE:HG23	1:C:607:VAL:CG2	2.31	0.58
1:D:171:PHE:CD1	1:D:263:PRO:HD2	2.38	0.58
1:E:30:LEU:O	1:E:33:LEU:HB2	2.03	0.58
1:G:45:GLN:HE21	1:G:45:GLN:CA	2.01	0.58
1:H:616:GLU:OE1	1:H:616:GLU:HA	2.03	0.58
1:B:276:PRO:HG3	1:B:326:GLN:CG	2.33	0.58
1:B:629:MET:O	1:B:633:ILE:HG13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:491:GLU:H	1:C:491:GLU:CD	2.11	0.58
1:E:72:LEU:HD13	1:E:72:LEU:C	2.27	0.58
1:C:224:THR:CG2	1:C:228:GLU:HG3	2.33	0.58
1:E:43:ILE:HG12	1:E:44:LEU:H	1.68	0.58
1:E:794:LYS:HA	1:E:794:LYS:HE2	1.85	0.58
1:F:233:PHE:CD1	1:F:238:LEU:HD12	2.38	0.58
1:B:90:VAL:HG12	1:B:91:ARG:H	1.67	0.58
1:B:169:LYS:HG2	1:B:176:SER:OG	2.03	0.58
1:D:174:LYS:N	1:D:174:LYS:HD2	2.19	0.58
1:F:224:THR:CG2	1:F:228:GLU:HG3	2.33	0.58
1:G:547:HIS:O	1:G:551:GLU:HG3	2.03	0.58
1:H:538:GLU:OE1	1:H:541:ARG:HD3	2.04	0.58
1:B:90:VAL:HG12	1:B:91:ARG:N	2.17	0.58
1:B:216:TYR:CD2	1:B:232:LYS:HG2	2.38	0.58
1:E:55:ALA:O	1:E:59:GLN:HB2	2.04	0.58
1:F:390:GLU:OE1	1:F:796:ARG:HD2	2.03	0.58
1:G:45:GLN:HE22	1:G:80:ILE:HG13	1.69	0.58
1:G:245:ASN:O	1:G:249:VAL:HG23	2.04	0.58
1:H:32:LEU:HD22	1:H:35:ARG:NH1	2.19	0.58
1:A:711:HIS:HE1	5:A:912:SO4:O1	1.87	0.58
1:B:82:LEU:HD11	1:B:120:PHE:CZ	2.38	0.58
1:C:264:ASP:OD1	1:C:267:THR:HB	2.04	0.58
1:F:534:PHE:HB2	1:F:535:PRO:HD2	1.84	0.58
1:G:534:PHE:HB2	1:G:535:PRO:CD	2.33	0.58
1:A:441:GLU:OE1	1:A:444:LYS:HD3	2.03	0.58
1:C:80:ILE:HD13	1:C:121:LYS:HG2	1.86	0.58
1:G:188:SER:HB2	1:G:192:LYS:O	2.03	0.58
1:H:217:LEU:HD11	1:H:233:PHE:CZ	2.39	0.58
1:B:250:LEU:O	1:B:254:ARG:HG3	2.04	0.58
1:D:435:THR:HG23	1:D:475:THR:HB	1.84	0.58
1:E:146:ILE:HG22	1:E:147:PRO:CD	2.33	0.58
1:E:414:ASN:O	1:E:418:GLY:HA3	2.04	0.58
1:B:82:LEU:CD1	1:B:120:PHE:CE2	2.85	0.57
1:A:56:LEU:O	1:A:59:GLN:HB3	2.05	0.57
1:B:178:LEU:HB2	1:B:179:PRO:HD3	1.86	0.57
1:F:668:PHE:HB2	1:F:689:LEU:HD23	1.86	0.57
1:F:789:MET:HE3	1:G:789:MET:CB	2.29	0.57
1:H:322:ARG:O	1:H:326:GLN:HG2	2.05	0.57
1:F:43:ILE:HG23	1:F:44:LEU:HD23	1.86	0.57
1:F:216:TYR:HD1	1:F:216:TYR:C	2.13	0.57
1:B:761:ARG:CZ	1:B:761:ARG:HB3	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:545:LYS:H	1:F:545:LYS:HD3	1.68	0.57
1:A:146:ILE:CG2	1:A:147:PRO:CD	2.83	0.57
1:A:259:LEU:HD21	1:A:267:THR:HG22	1.87	0.57
1:F:85:TRP:CD2	1:F:101:ARG:HD3	2.39	0.57
1:G:80:ILE:HD12	1:G:80:ILE:N	2.19	0.57
1:G:143:ASN:HB3	1:G:148:ARG:NH2	2.18	0.57
1:H:199:LYS:NZ	1:H:234:GLU:O	2.34	0.57
1:A:85:TRP:HE3	1:A:101:ARG:HG2	1.68	0.57
1:E:39:LYS:O	1:E:39:LYS:HD3	2.05	0.57
1:A:176:SER:O	1:A:179:PRO:HD2	2.05	0.57
1:E:101:ARG:CB	1:E:112:LEU:HD21	2.35	0.57
1:G:195:MET:HE1	1:G:252:MET:CE	2.34	0.57
1:D:441:GLU:OE1	1:D:441:GLU:HA	2.05	0.57
1:B:719:GLN:HG3	5:B:913:SO4:O1	2.04	0.57
1:C:52:GLU:O	1:C:57:PRO:HD2	2.05	0.57
1:E:543:LEU:HB3	1:E:545:LYS:HE3	1.86	0.57
1:H:472:MET:HG2	1:H:514:ILE:HD13	1.85	0.56
1:A:173:ASP:HB3	1:A:176:SER:HB3	1.87	0.56
1:B:259:LEU:O	1:B:263:PRO:HG3	2.04	0.56
1:C:207:GLN:HA	1:C:207:GLN:NE2	2.20	0.56
1:F:756:GLN:HG3	1:F:757:ILE:HD13	1.86	0.56
1:G:56:LEU:CB	1:G:57:PRO:HD3	2.27	0.56
1:H:56:LEU:CD2	1:H:65:GLU:HG3	2.34	0.56
1:A:171:PHE:CD1	1:A:263:PRO:HD2	2.39	0.56
1:A:451:TYR:HB3	1:A:454:LYS:HE2	1.88	0.56
1:B:534:PHE:HB2	1:B:535:PRO:HD2	1.86	0.56
1:C:339:ARG:HH12	1:C:380:ILE:HG13	1.70	0.56
1:F:32:LEU:O	1:F:35:ARG:HB3	2.06	0.56
1:F:46:GLN:C	1:F:46:GLN:HE21	2.13	0.56
1:F:101:ARG:HB2	1:F:112:LEU:HD21	1.87	0.56
1:A:206:LEU:HD12	1:A:206:LEU:O	2.05	0.56
1:A:230:GLU:OE1	1:A:240:ARG:NH1	2.39	0.56
1:A:437:ALA:C	1:A:439:ALA:H	2.13	0.56
1:B:534:PHE:O	1:B:687:CYS:HA	2.05	0.56
1:F:56:LEU:HB2	1:F:57:PRO:HD3	1.86	0.56
1:F:210:LEU:HD22	1:F:253:ILE:HG23	1.86	0.56
1:A:390:GLU:OE1	1:A:796:ARG:HD2	2.06	0.56
1:B:276:PRO:HG3	1:B:326:GLN:CB	2.36	0.56
2:D:901:UDP:O1B	3:D:903[A]:LCN:H3	2.06	0.56
1:E:158:GLY:HA3	1:E:519:PRO:O	2.06	0.56
1:F:216:TYR:CE1	1:F:220:LEU:HD11	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:LEU:HD13	1:H:90:VAL:CG1	2.28	0.56
1:A:206:LEU:HD11	1:A:210:LEU:HD11	1.88	0.56
1:B:614:ARG:HD2	8:B:869:HOH:O	2.05	0.56
1:D:173:ASP:HB3	1:D:176:SER:HB2	1.87	0.56
1:G:171:PHE:CD1	1:G:263:PRO:HD2	2.41	0.56
1:H:39:LYS:HG3	1:H:104:LEU:HB3	1.87	0.56
1:A:140:GLU:HB3	1:A:141:PRO:CD	2.35	0.56
1:A:339:ARG:NH1	1:A:380:ILE:HG13	2.20	0.56
1:B:327:GLY:C	1:B:328:LEU:HD23	2.30	0.56
1:C:226:TYR:CE2	1:C:240:ARG:HG2	2.41	0.56
1:C:435:THR:HG23	1:C:475:THR:HB	1.87	0.56
1:D:81:VAL:HG22	1:D:86:VAL:CG2	2.35	0.56
1:E:338:THR:HG23	1:E:366:ARG:HG2	1.88	0.56
1:E:704:VAL:HA	5:E:912:SO4:O3	2.06	0.56
1:F:35:ARG:HG2	1:F:104:LEU:O	2.06	0.56
1:F:59:GLN:HG2	1:F:60:THR:HG23	1.88	0.56
1:G:137:LEU:HD11	1:G:790:PHE:CZ	2.41	0.56
1:H:131:GLY:O	1:H:133:PHE:N	2.38	0.56
1:H:400:LEU:HD12	1:H:401:SER:N	2.21	0.56
1:A:140:GLU:HB3	1:A:141:PRO:HD3	1.88	0.56
1:B:82:LEU:HD22	1:B:84:PRO:CG	2.35	0.56
1:C:69:PHE:HE1	1:C:73:LEU:HD11	1.70	0.56
1:C:699:PRO:HA	1:C:702:ILE:HG13	1.87	0.56
1:D:56:LEU:HG	1:D:70:PHE:CE1	2.41	0.56
1:F:435:THR:HG23	1:F:475:THR:CB	2.35	0.56
1:G:147:PRO:HB2	1:H:172:HIS:CE1	2.41	0.56
1:G:534:PHE:HB2	1:G:535:PRO:HD2	1.88	0.56
1:H:193:ASN:HB3	1:H:239:GLU:HG3	1.88	0.56
1:B:387:PRO:HD3	1:B:802:VAL:HB	1.87	0.56
1:E:82:LEU:HG	1:E:83:PRO:HG3	1.87	0.56
1:E:173:ASP:HB3	1:E:176:SER:CB	2.35	0.56
1:F:55:ALA:O	1:F:59:GLN:CB	2.54	0.56
1:F:69:PHE:HD1	1:F:70:PHE:N	2.03	0.56
1:F:789:MET:HB3	1:G:789:MET:HE2	1.83	0.56
1:G:52:GLU:CD	1:G:53:PHE:N	2.64	0.56
1:G:400:LEU:HD12	1:G:401:SER:N	2.21	0.56
1:B:45:GLN:CB	1:B:80:ILE:HA	2.08	0.56
1:B:216:TYR:CE1	1:B:220:LEU:HD11	2.41	0.56
1:E:83:PRO:HB3	1:E:84:PRO:HD2	1.88	0.56
1:F:354:GLU:OE1	1:F:366:ARG:NH2	2.38	0.56
1:G:390:GLU:OE1	1:G:796:ARG:HD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:ILE:CG2	1:H:147:PRO:CD	2.79	0.56
1:B:131:GLY:N	1:B:134:THR:HG21	2.20	0.55
1:C:156:GLY:O	1:C:522:ASN:HA	2.05	0.55
1:C:189:HIS:CE1	1:C:190:GLN:NE2	2.74	0.55
1:E:206:LEU:HD11	1:E:210:LEU:HD11	1.88	0.55
1:H:348:THR:O	1:H:351:GLU:HG2	2.04	0.55
1:A:281:VAL:HG21	1:A:319:MET:CE	2.33	0.55
1:C:207:GLN:OE1	1:C:211:ARG:NH2	2.40	0.55
1:D:32:LEU:O	1:D:36:VAL:HG23	2.06	0.55
1:F:657:LEU:O	1:F:661:ILE:HG12	2.05	0.55
1:A:56:LEU:HD23	1:A:70:PHE:CE1	2.40	0.55
1:A:477:PHE:HA	1:A:520:LYS:HB2	1.87	0.55
1:C:599:ARG:O	1:C:603:LEU:HD12	2.05	0.55
1:D:174:LYS:HD2	1:D:174:LYS:H	1.70	0.55
1:E:366:ARG:HD3	8:E:854:HOH:O	2.06	0.55
1:F:259:LEU:HD21	1:F:267:THR:HG22	1.87	0.55
1:F:789:MET:HG2	1:G:789:MET:HE3	1.88	0.55
1:H:552:GLU:O	1:H:556:SER:HB3	2.06	0.55
1:C:140:GLU:N	1:C:141:PRO:HD2	2.21	0.55
1:C:468:ASP:O	1:C:472:MET:HB2	2.06	0.55
1:D:82:LEU:CD1	1:D:84:PRO:HD2	2.37	0.55
1:D:140:GLU:N	1:D:141:PRO:HD2	2.21	0.55
1:E:32:LEU:O	1:E:35:ARG:HB3	2.06	0.55
1:G:479:ILE:HD11	1:G:762:LEU:HD13	1.88	0.55
1:A:264:ASP:OD1	1:A:267:THR:HB	2.07	0.55
1:C:48:GLN:HG2	1:C:49:ILE:HD13	1.87	0.55
1:G:315:LEU:HG	1:G:319:MET:CE	2.27	0.55
1:D:146:ILE:CG2	1:D:147:PRO:HD2	2.36	0.55
1:D:670:GLN:HG3	1:D:670:GLN:O	2.06	0.55
1:F:435:THR:HG23	1:F:475:THR:HB	1.87	0.55
1:H:128:VAL:HG12	1:H:129:LYS:N	2.22	0.55
1:A:407:LYS:HB2	1:A:408:PRO:HD2	1.89	0.55
1:C:80:ILE:CD1	1:C:121:LYS:HG2	2.37	0.55
1:C:92:PRO:HD2	1:C:96:VAL:O	2.07	0.55
1:E:111:GLU:C	1:E:112:LEU:HD23	2.31	0.55
1:E:216:TYR:CD1	1:E:216:TYR:C	2.84	0.55
1:E:417:ASP:O	1:E:421:VAL:HG23	2.06	0.55
1:H:171:PHE:HD1	1:H:263:PRO:HD2	1.72	0.55
1:A:315:LEU:O	1:A:319:MET:HG3	2.06	0.55
1:B:796:ARG:HB2	1:B:797:PRO:HD3	1.89	0.55
1:C:281:VAL:HG21	1:C:319:MET:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:LEU:HD22	1:G:177:LEU:HD23	1.89	0.55
1:B:140:GLU:N	1:B:141:PRO:HD2	2.22	0.55
1:B:437:ALA:C	1:B:439:ALA:H	2.15	0.55
1:C:216:TYR:HD1	1:C:216:TYR:C	2.15	0.55
1:E:390:GLU:OE1	1:E:796:ARG:HD2	2.07	0.55
1:F:216:TYR:C	1:F:216:TYR:CD1	2.84	0.55
1:G:55:ALA:O	1:G:59:GLN:HB2	2.06	0.55
1:G:91:ARG:NH2	1:G:94:PRO:HA	2.22	0.55
1:H:143:ASN:C	1:H:145:SER:H	2.14	0.55
1:A:151:LEU:HD12	1:B:261:GLU:HG2	1.88	0.55
1:C:91:ARG:HD2	1:C:97:TRP:CZ2	2.42	0.55
1:G:56:LEU:HB3	1:G:57:PRO:CD	2.28	0.55
1:A:163:ASN:O	1:A:167:SER:HB2	2.07	0.54
1:D:30:LEU:HD22	1:D:30:LEU:H	1.71	0.54
1:F:85:TRP:CZ3	1:F:103:ASN:HB2	2.42	0.54
1:F:233:PHE:CE1	1:F:238:LEU:HD12	2.43	0.54
1:G:681:VAL:O	1:G:685:MET:HG3	2.07	0.54
1:H:56:LEU:HG	1:H:70:PHE:HE1	1.72	0.54
1:A:136:GLU:HG2	1:A:511:VAL:HG23	1.88	0.54
1:A:526:PRO:O	1:A:753:TYR:HB3	2.07	0.54
1:B:216:TYR:CD1	1:B:220:LEU:HD11	2.42	0.54
1:E:163:ASN:O	1:E:167:SER:HB2	2.07	0.54
1:F:518:ASP:OD1	1:F:520:LYS:HG2	2.08	0.54
1:G:84:PRO:HB2	1:G:103:ASN:HD21	1.72	0.54
1:G:545:LYS:H	1:G:545:LYS:CD	2.18	0.54
1:H:250:LEU:O	1:H:254:ARG:HG3	2.07	0.54
1:E:438:HIS:HB3	4:E:904[B]:NHF:O5	2.07	0.54
1:G:53:PHE:O	1:G:57:PRO:HD2	2.07	0.54
1:G:68:PRO:HG2	1:G:70:PHE:HB2	1.89	0.54
1:G:437:ALA:C	1:G:439:ALA:H	2.15	0.54
1:A:101:ARG:HB2	1:A:112:LEU:HD11	1.88	0.54
1:A:164:ARG:HD2	1:B:262:ALA:HB1	1.89	0.54
1:A:354:GLU:OE1	1:A:366:ARG:NH2	2.40	0.54
1:B:789:MET:HE3	1:C:789:MET:HB3	1.84	0.54
1:C:772:TRP:CZ2	1:C:776:SER:HB3	2.42	0.54
1:E:164:ARG:HD2	1:F:262:ALA:HB1	1.89	0.54
1:E:284:LEU:O	1:E:414:ASN:HB2	2.07	0.54
1:F:472:MET:HG2	1:F:514:ILE:HD13	1.89	0.54
1:G:83:PRO:CB	1:G:85:TRP:H	2.05	0.54
1:G:147:PRO:HB2	1:H:172:HIS:ND1	2.21	0.54
1:G:434:CYS:HB2	1:G:477:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:547:HIS:O	1:G:551:GLU:CG	2.55	0.54
1:A:789:MET:CB	1:D:789:MET:HE3	2.37	0.54
1:C:72:LEU:CD2	1:C:90:VAL:HG21	2.36	0.54
1:D:338:THR:HG23	1:D:366:ARG:HG2	1.89	0.54
1:D:437:ALA:C	1:D:439:ALA:H	2.15	0.54
1:C:292:GLN:HE22	1:C:357:TYR:H	1.53	0.54
1:D:354:GLU:OE1	1:D:366:ARG:NH2	2.41	0.54
1:G:82:LEU:CD1	1:G:83:PRO:HD3	2.36	0.54
1:B:390:GLU:OE1	1:B:796:ARG:HD2	2.08	0.54
1:B:704:VAL:HA	5:B:912:SO4:O3	2.08	0.54
1:E:212:LYS:HE2	1:E:232:LYS:HZ1	1.73	0.54
1:A:46:GLN:OE1	1:A:46:GLN:HA	2.07	0.54
1:A:141:PRO:HB2	1:D:782:GLU:HG3	1.89	0.54
1:A:668:PHE:HB2	1:A:689:LEU:HD23	1.90	0.54
1:B:338:THR:HG23	1:B:366:ARG:HG2	1.89	0.54
1:D:281:VAL:HG21	1:D:319:MET:CE	2.37	0.54
1:E:796:ARG:HB2	1:E:797:PRO:HD3	1.90	0.54
1:F:65:GLU:O	1:F:68:PRO:HG2	2.08	0.54
1:F:85:TRP:CE3	1:F:101:ARG:HD2	2.43	0.54
1:F:338:THR:HG23	1:F:366:ARG:HG2	1.90	0.54
1:H:32:LEU:HD22	1:H:35:ARG:HH12	1.73	0.54
1:H:49:ILE:HD11	1:H:696:LYS:NZ	2.23	0.54
1:H:291:ALA:HB3	1:H:295:VAL:CG1	2.34	0.54
1:H:567:LEU:HD22	1:H:605:ASN:HB3	1.89	0.54
1:H:784:ARG:O	1:H:788:GLU:HG3	2.07	0.54
1:B:84:PRO:O	1:B:85:TRP:CD1	2.58	0.54
1:B:486:ILE:HG22	1:B:516:VAL:HG22	1.89	0.54
1:C:54:GLU:HG3	1:C:55:ALA:N	2.23	0.54
1:E:354:GLU:OE1	1:E:366:ARG:NH2	2.40	0.54
1:A:338:THR:HG23	1:A:366:ARG:HG2	1.88	0.54
1:B:33:LEU:CB	1:B:62:LYS:CB	2.86	0.54
1:B:93:ARG:H	1:B:96:VAL:CG2	2.20	0.54
1:E:83:PRO:HB2	1:E:84:PRO:HD2	1.89	0.54
1:E:438:HIS:ND1	4:E:904[B]:NHF:H6	2.23	0.54
1:E:442:LYS:HD2	1:E:449:ASP:HB3	1.90	0.54
1:H:72:LEU:CD1	1:H:90:VAL:HG21	2.38	0.54
1:H:210:LEU:HD22	1:H:253:ILE:HG23	1.90	0.54
1:H:420:LEU:C	1:H:420:LEU:HD13	2.33	0.54
1:H:651:ARG:HA	1:H:654:ASN:HB2	1.90	0.54
1:B:82:LEU:H	1:B:82:LEU:HD12	1.71	0.53
1:B:292:GLN:OE1	1:B:356:VAL:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ASN:CB	1:C:30:LEU:HD12	2.38	0.53
1:C:564:LEU:HD22	1:C:613:ARG:NH2	2.23	0.53
1:F:81:VAL:HG12	1:F:86:VAL:HG23	1.90	0.53
1:F:756:GLN:CG	1:F:757:ILE:N	2.72	0.53
1:G:35:ARG:HD3	1:G:102:VAL:HG11	1.89	0.53
1:G:290:PHE:O	1:G:366:ARG:NH1	2.41	0.53
1:H:76:THR:O	1:H:89:ALA:HB3	2.08	0.53
1:H:419:ASN:OD1	1:H:435:THR:HB	2.08	0.53
1:H:626:MET:O	1:H:630:TYR:HD2	1.91	0.53
1:A:172:HIS:ND1	1:B:147:PRO:HB2	2.23	0.53
1:B:112:LEU:CD2	1:B:116:GLU:CB	2.86	0.53
1:B:145:SER:HB3	1:B:779:ASP:OD2	2.08	0.53
1:C:172:HIS:ND1	1:D:147:PRO:CG	2.71	0.53
1:C:243:GLY:HA2	1:C:326:GLN:HA	1.90	0.53
1:G:156:GLY:O	1:G:522:ASN:HA	2.08	0.53
1:H:39:LYS:CD	1:H:104:LEU:HD13	2.36	0.53
1:A:136:GLU:HG3	1:A:509:ARG:HD2	1.90	0.53
1:B:131:GLY:H	1:B:134:THR:HG21	1.73	0.53
1:B:574:ILE:HG23	1:B:607:VAL:HG23	1.89	0.53
1:C:566:VAL:HG12	1:C:567:LEU:N	2.22	0.53
1:G:124:LEU:HD23	1:G:124:LEU:O	2.09	0.53
1:H:122:GLU:OE1	1:H:130:ASN:HB2	2.08	0.53
1:H:216:TYR:CD2	1:H:232:LYS:HG2	2.42	0.53
1:B:163:ASN:ND2	1:B:269:GLU:HG3	2.15	0.53
1:B:435:THR:CG2	1:B:475:THR:HB	2.39	0.53
1:C:83:PRO:CB	1:C:84:PRO:HD3	2.39	0.53
1:E:81:VAL:HG12	1:E:86:VAL:CB	2.30	0.53
1:E:176:SER:O	1:E:179:PRO:HD2	2.09	0.53
1:G:173:ASP:HB3	1:G:176:SER:HB3	1.89	0.53
1:A:415:TYR:CG	1:A:416:SER:N	2.77	0.53
1:B:131:GLY:O	1:B:134:THR:HG23	2.08	0.53
1:B:757:ILE:O	1:B:761:ARG:HG2	2.09	0.53
1:C:415:TYR:CG	1:C:416:SER:N	2.76	0.53
1:H:39:LYS:O	1:H:39:LYS:HD3	2.09	0.53
1:H:39:LYS:HA	1:H:104:LEU:HD22	1.90	0.53
1:H:435:THR:HG23	1:H:475:THR:HB	1.91	0.53
1:H:794:LYS:O	1:H:794:LYS:HD3	2.09	0.53
1:H:796:ARG:HB2	1:H:797:PRO:HD3	1.90	0.53
1:A:432:THR:OG1	1:A:773:LYS:HE2	2.07	0.53
1:A:594:TYR:CE1	1:A:601:ARG:HG2	2.44	0.53
1:C:338:THR:HG23	1:C:366:ARG:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:LEU:CB	1:C:545:LYS:HE2	2.38	0.53
1:D:534:PHE:HB2	1:D:535:PRO:CD	2.39	0.53
1:E:178:LEU:N	1:E:179:PRO:CD	2.71	0.53
1:F:483:PHE:CE1	1:F:487:ALA:HB3	2.43	0.53
1:G:171:PHE:HD1	1:G:263:PRO:HD2	1.74	0.53
1:H:46:GLN:HG2	1:H:51:ALA:HA	1.90	0.53
1:A:35:ARG:NH2	1:A:102:VAL:O	2.42	0.53
1:A:400:LEU:C	1:A:400:LEU:HD12	2.33	0.53
1:C:354:GLU:OE1	1:C:366:ARG:NH2	2.42	0.53
1:E:54:GLU:O	1:E:58:GLU:CB	2.56	0.53
1:G:178:LEU:HB2	1:G:179:PRO:HD3	1.90	0.53
1:G:276:PRO:HG3	1:G:326:GLN:HG3	1.89	0.53
1:A:670:GLN:C	1:A:670:GLN:OE1	2.52	0.53
1:C:216:TYR:C	1:C:216:TYR:CD1	2.86	0.53
1:C:672:ALA:HB3	1:C:694:THR:HG21	1.90	0.53
1:D:690:PRO:HA	8:D:861:HOH:O	2.09	0.53
1:E:83:PRO:CG	1:E:85:TRP:O	2.55	0.53
1:F:55:ALA:O	1:F:57:PRO:O	2.27	0.53
1:G:32:LEU:HD11	1:G:105:HIS:O	2.09	0.53
1:G:66:GLY:CA	1:G:68:PRO:HD3	2.37	0.53
1:A:789:MET:HE1	1:D:790:PHE:N	2.24	0.53
1:B:148:ARG:CG	1:B:148:ARG:NH1	2.49	0.53
1:C:46:GLN:HB2	1:C:50:ILE:HG13	1.90	0.53
1:E:437:ALA:C	1:E:439:ALA:H	2.16	0.53
1:E:668:PHE:HB2	1:E:689:LEU:CD2	2.39	0.53
1:H:33:LEU:HD21	1:H:59:GLN:HE21	1.74	0.53
1:H:41:LYS:HD3	1:H:54:GLU:OE1	2.08	0.53
1:H:174:LYS:N	1:H:174:LYS:CD	2.72	0.53
1:A:261:GLU:OE2	1:B:149:PRO:HA	2.09	0.53
1:B:322:ARG:CD	1:B:763:LEU:HD13	2.38	0.53
1:E:396:ALA:O	1:E:400:LEU:HG	2.09	0.53
1:A:420:LEU:HD13	1:A:420:LEU:O	2.09	0.52
1:C:130:ASN:HB2	1:C:509:ARG:HH21	1.74	0.52
1:C:573:PRO:O	1:C:604:ALA:HB1	2.09	0.52
1:D:39:LYS:HZ2	1:D:39:LYS:CB	2.21	0.52
1:E:216:TYR:HD1	1:E:216:TYR:C	2.18	0.52
1:F:46:GLN:HB3	1:F:50:ILE:HG21	1.91	0.52
1:F:56:LEU:CB	1:F:57:PRO:HD3	2.39	0.52
1:F:59:GLN:HG2	1:F:60:THR:H	1.70	0.52
1:F:468:ASP:O	1:F:472:MET:HB2	2.08	0.52
1:F:659:ARG:O	1:F:662:CYS:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:472:MET:HG2	1:G:514:ILE:HD13	1.90	0.52
1:H:45:GLN:NE2	1:H:80:ILE:CG2	2.71	0.52
1:H:82:LEU:CG	1:H:85:TRP:O	2.55	0.52
1:H:189:HIS:CD2	1:H:190:GLN:CG	2.92	0.52
1:B:472:MET:HG2	1:B:514:ILE:HD13	1.91	0.52
1:D:281:VAL:CG2	1:D:319:MET:HE1	2.38	0.52
1:F:171:PHE:HD1	1:F:263:PRO:HD2	1.74	0.52
1:F:756:GLN:HG3	1:F:757:ILE:CD1	2.38	0.52
1:H:518:ASP:OD1	1:H:520:LYS:HG2	2.09	0.52
1:A:386:TRP:N	1:A:387:PRO:HD2	2.25	0.52
1:C:72:LEU:HD21	1:C:90:VAL:HG21	1.92	0.52
1:C:189:HIS:HE1	1:C:190:GLN:NE2	2.07	0.52
1:D:56:LEU:HG	1:D:70:PHE:HE1	1.72	0.52
1:D:56:LEU:HD13	1:D:56:LEU:C	2.34	0.52
1:E:56:LEU:HB3	1:E:57:PRO:HD3	1.91	0.52
1:E:206:LEU:CD1	1:E:210:LEU:HD11	2.40	0.52
1:E:420:LEU:C	1:E:420:LEU:HD13	2.33	0.52
1:E:433:GLN:HG2	1:E:475:THR:OG1	2.10	0.52
1:F:52:GLU:C	1:F:54:GLU:O	2.51	0.52
1:G:538:GLU:OE1	1:G:541:ARG:HD3	2.10	0.52
1:B:137:LEU:HD11	1:B:790:PHE:CZ	2.44	0.52
1:B:790:PHE:N	1:C:789:MET:HE1	2.24	0.52
1:C:217:LEU:HD11	1:C:249:VAL:CG1	2.39	0.52
1:C:438:HIS:ND1	4:C:904[B]:NHF:H6	2.24	0.52
1:D:56:LEU:HB3	1:D:57:PRO:CD	2.35	0.52
1:F:65:GLU:CA	1:F:68:PRO:HG2	2.39	0.52
1:H:354:GLU:OE1	1:H:366:ARG:NH2	2.36	0.52
1:A:46:GLN:CB	1:A:79:ALA:HB3	2.39	0.52
1:A:226:TYR:HA	1:A:229:PHE:CZ	2.44	0.52
1:C:45:GLN:HB2	1:C:79:ALA:O	2.10	0.52
2:G:901:UDP:O2B	3:G:903[A]:LCN:C1	2.58	0.52
1:A:69:PHE:CE1	1:A:73:LEU:HD12	2.45	0.52
1:B:790:PHE:O	1:B:794:LYS:HB3	2.09	0.52
1:D:298:TYR:CE1	1:D:649:MET:CE	2.92	0.52
1:D:400:LEU:HD12	1:D:400:LEU:C	2.34	0.52
1:E:45:GLN:HG2	1:E:80:ILE:HD13	1.92	0.52
1:E:146:ILE:HG23	1:E:147:PRO:HD2	1.91	0.52
1:H:366:ARG:HD3	8:H:851:HOH:O	2.09	0.52
1:A:136:GLU:HG2	1:A:511:VAL:CG2	2.40	0.52
1:A:211:ARG:NH2	1:B:151:LEU:HD23	2.24	0.52
1:B:54:GLU:C	1:B:56:LEU:N	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:HIS:ND1	4:B:904[B]:NHF:H6	2.24	0.52
1:B:544:THR:HA	1:B:547:HIS:ND1	2.24	0.52
1:C:53:PHE:HA	1:C:57:PRO:HG2	1.91	0.52
1:C:86:VAL:CG1	1:C:102:VAL:CG2	2.84	0.52
1:D:48:GLN:CA	1:D:51:ALA:CB	2.76	0.52
1:E:45:GLN:CB	1:E:80:ILE:HD13	2.40	0.52
1:G:146:ILE:CG2	1:G:147:PRO:HD2	2.39	0.52
1:C:116:GLU:O	1:C:119:HIS:HB2	2.10	0.52
1:E:140:GLU:N	1:E:141:PRO:HD2	2.25	0.52
1:E:757:ILE:HG22	1:E:761:ARG:CG	2.39	0.52
1:G:147:PRO:CB	1:H:172:HIS:ND1	2.73	0.52
1:H:90:VAL:O	1:H:98:GLU:O	2.27	0.52
1:H:146:ILE:CG2	1:H:147:PRO:HD2	2.25	0.52
1:H:171:PHE:CD1	1:H:263:PRO:HD2	2.44	0.52
1:H:189:HIS:ND1	1:H:279:PHE:CD2	2.77	0.52
1:H:486:ILE:HG22	1:H:516:VAL:CG2	2.40	0.52
1:F:244:ASP:OD2	1:F:248:ARG:HD3	2.10	0.52
1:H:45:GLN:HG2	1:H:447:ASP:OD1	2.10	0.52
1:H:242:TRP:HA	1:H:252:MET:HE2	1.91	0.52
1:B:82:LEU:CD1	1:B:82:LEU:N	2.70	0.52
1:C:160:ASP:O	1:C:164:ARG:HG3	2.10	0.52
1:C:217:LEU:CD1	1:C:249:VAL:HG12	2.40	0.52
1:C:281:VAL:CG2	1:C:319:MET:HE1	2.40	0.52
1:C:407:LYS:HB2	1:C:408:PRO:HD2	1.92	0.52
1:C:415:TYR:HA	1:C:437:ALA:O	2.10	0.52
1:D:44:LEU:HA	1:D:124:LEU:HD11	1.92	0.52
1:H:76:THR:O	1:H:89:ALA:C	2.53	0.52
1:H:87:ALA:HA	1:H:101:ARG:HA	1.90	0.52
1:B:322:ARG:HD3	1:B:763:LEU:HD13	1.91	0.51
1:E:491:GLU:H	1:E:491:GLU:CD	2.19	0.51
1:E:790:PHE:N	1:H:789:MET:HE1	2.25	0.51
1:A:617:SER:HB3	1:A:623:LYS:HG3	1.91	0.51
1:D:284:LEU:HD22	1:D:284:LEU:N	2.26	0.51
1:A:81:VAL:HA	1:A:86:VAL:CG2	2.35	0.51
1:C:104:LEU:HD22	1:C:104:LEU:N	2.22	0.51
1:C:590:LEU:HB2	1:C:671:PRO:HG3	1.93	0.51
1:E:512:HIS:CE1	1:E:515:ASP:HB2	2.45	0.51
1:F:46:GLN:CB	1:F:50:ILE:HB	2.38	0.51
1:F:49:ILE:HG22	1:F:50:ILE:N	2.24	0.51
1:C:224:THR:HG23	1:C:228:GLU:HG3	1.92	0.51
1:F:420:LEU:C	1:F:420:LEU:HD13	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:207:GLN:OE1	1:G:211:ARG:NH2	2.44	0.51
1:A:46:GLN:HG3	1:A:51:ALA:HB2	1.92	0.51
1:C:35:ARG:O	1:C:104:LEU:HD12	2.10	0.51
1:D:407:LYS:HB2	1:D:408:PRO:HD2	1.92	0.51
1:E:52:GLU:CD	1:E:52:GLU:C	2.78	0.51
1:E:261:GLU:OE2	1:F:149:PRO:HA	2.10	0.51
1:G:162:LEU:HD11	1:G:772:TRP:CD2	2.46	0.51
1:H:33:LEU:HD23	1:H:33:LEU:H	1.75	0.51
1:A:789:MET:HE3	1:D:789:MET:HG2	1.91	0.51
1:B:174:LYS:N	1:B:174:LYS:HD2	2.26	0.51
1:B:716:HIS:HB3	5:B:913:SO4:O1	2.10	0.51
1:C:83:PRO:CG	1:C:84:PRO:CD	2.81	0.51
1:E:415:TYR:CG	1:E:416:SER:N	2.79	0.51
1:E:680:THR:HG23	2:E:901:UDP:O1A	2.10	0.51
1:A:171:PHE:HD1	1:A:263:PRO:HD2	1.75	0.51
1:C:633:ILE:HA	1:C:638:LEU:HD12	1.93	0.51
1:D:50:ILE:O	1:D:51:ALA:C	2.52	0.51
1:D:80:ILE:HD13	1:D:117:PHE:CE2	2.46	0.51
1:D:103:ASN:HB2	1:D:108:VAL:HG12	1.92	0.51
1:D:415:TYR:CG	1:D:416:SER:N	2.79	0.51
1:D:534:PHE:HB2	1:D:535:PRO:HD2	1.93	0.51
1:F:143:ASN:HB3	1:F:148:ARG:HH22	1.74	0.51
1:F:178:LEU:HB2	1:F:179:PRO:HD3	1.93	0.51
1:F:692:PHE:HZ	1:F:727:PHE:CG	2.29	0.51
1:G:427:HIS:ND1	1:G:784:ARG:NH2	2.57	0.51
1:A:47:ASN:O	1:A:51:ALA:N	2.33	0.51
1:A:140:GLU:N	1:A:141:PRO:HD2	2.26	0.51
1:A:153:LYS:HG3	1:A:154:TYR:CD2	2.46	0.51
1:C:178:LEU:N	1:C:179:PRO:CD	2.73	0.51
1:E:46:GLN:HA	1:E:50:ILE:HD12	1.91	0.51
1:E:52:GLU:OE1	1:E:57:PRO:HD3	2.11	0.51
1:H:92:PRO:HD2	1:H:96:VAL:O	2.11	0.51
1:A:772:TRP:CZ2	1:A:776:SER:HB3	2.45	0.51
1:C:574:ILE:CG2	1:C:607:VAL:CG2	2.89	0.51
1:D:613:ARG:HG3	1:D:626:MET:HE2	1.92	0.51
1:G:210:LEU:HD11	1:G:256:LEU:HD23	1.91	0.51
1:B:163:ASN:HD21	1:B:269:GLU:CG	2.18	0.51
1:B:443:THR:HG21	1:B:495:GLN:HA	1.93	0.51
1:E:44:LEU:HA	1:E:124:LEU:HD21	1.93	0.51
1:E:594:TYR:CE1	1:E:601:ARG:HG2	2.46	0.51
1:G:116:GLU:O	1:G:119:HIS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:390:GLU:OE1	1:H:796:ARG:HD2	2.11	0.51
1:B:47:ASN:O	1:B:50:ILE:CB	2.59	0.50
1:E:125:VAL:HG13	1:E:126:ASP:N	2.26	0.50
1:A:172:HIS:ND1	1:B:147:PRO:CB	2.74	0.50
1:A:552:GLU:O	1:A:556:SER:HB3	2.11	0.50
1:B:216:TYR:O	1:B:216:TYR:HD1	1.95	0.50
1:C:146:ILE:CG2	1:C:147:PRO:CD	2.87	0.50
1:C:216:TYR:HD1	1:C:216:TYR:O	1.94	0.50
1:C:261:GLU:HG2	1:D:151:LEU:HD12	1.92	0.50
1:E:39:LYS:HD3	1:E:39:LYS:C	2.36	0.50
1:E:100:LEU:HA	1:E:112:LEU:HG	1.93	0.50
1:E:281:VAL:HG21	1:E:319:MET:CE	2.41	0.50
1:E:435:THR:HG23	1:E:475:THR:HB	1.93	0.50
1:F:46:GLN:HE21	1:F:46:GLN:CA	2.22	0.50
1:F:407:LYS:HB2	1:F:408:PRO:HD3	1.92	0.50
1:F:789:MET:CG	1:G:789:MET:CE	2.89	0.50
1:G:635:GLU:HG2	1:G:636:TYR:CE2	2.47	0.50
1:A:65:GLU:C	1:A:67:GLY:H	2.18	0.50
1:A:786:TYR:O	1:D:789:MET:HE1	2.10	0.50
1:C:164:ARG:HD2	1:D:262:ALA:HB1	1.93	0.50
1:D:103:ASN:HB3	1:D:106:ALA:CB	2.38	0.50
1:G:545:LYS:HD3	1:G:545:LYS:N	2.20	0.50
1:H:292:GLN:OE1	1:H:356:VAL:HA	2.11	0.50
1:A:35:ARG:HH12	1:A:86:VAL:HB	1.77	0.50
1:A:682:VAL:HG13	1:A:749:ILE:CD1	2.37	0.50
1:B:100:LEU:O	1:B:112:LEU:HD12	2.12	0.50
1:C:320:LEU:CD2	1:C:332:PRO:HG3	2.42	0.50
1:D:677:PHE:HB3	4:D:904[B]:NH:O4	2.12	0.50
1:E:772:TRP:CH2	1:E:776:SER:HB3	2.46	0.50
1:F:677:PHE:CE2	1:F:702:ILE:HD11	2.47	0.50
1:A:53:PHE:HA	1:A:57:PRO:HG2	1.93	0.50
1:A:83:PRO:O	1:A:85:TRP:N	2.45	0.50
1:A:85:TRP:CD2	1:A:101:ARG:HD2	2.46	0.50
1:A:472:MET:HG2	1:A:514:ILE:HD13	1.94	0.50
1:B:789:MET:CE	1:C:789:MET:CB	2.73	0.50
1:C:48:GLN:O	1:C:51:ALA:N	2.44	0.50
1:C:176:SER:O	1:C:179:PRO:HD2	2.12	0.50
1:C:338:THR:HG23	1:C:366:ARG:CG	2.42	0.50
1:C:617:SER:HB3	1:C:623:LYS:HG3	1.93	0.50
1:D:103:ASN:ND2	1:D:108:VAL:CG1	2.74	0.50
1:F:264:ASP:OD1	1:F:267:THR:HB	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:717:GLY:O	1:G:720:ALA:HB3	2.11	0.50
1:A:284:LEU:HD13	1:A:337:LEU:HB2	1.94	0.50
1:A:417:ASP:O	1:A:421:VAL:HG23	2.11	0.50
1:C:536:TYR:HH	1:C:738:TRP:HZ3	1.58	0.50
1:G:56:LEU:HD13	1:G:63:LYS:HG2	1.94	0.50
1:G:212:LYS:HE2	1:G:232:LYS:HZ1	1.73	0.50
1:A:82:LEU:HB3	1:A:83:PRO:CD	2.38	0.50
1:A:419:ASN:HB3	1:A:471:ALA:CB	2.42	0.50
1:E:53:PHE:O	1:E:57:PRO:CG	2.47	0.50
1:G:35:ARG:HD3	1:G:102:VAL:CG1	2.42	0.50
1:H:435:THR:HG23	1:H:475:THR:CB	2.41	0.50
1:A:420:LEU:C	1:A:420:LEU:CD1	2.84	0.50
1:B:613:ARG:CG	1:B:626:MET:HE2	2.42	0.50
1:C:171:PHE:CD1	1:C:263:PRO:HD2	2.46	0.50
1:C:573:PRO:HD2	1:C:603:LEU:O	2.12	0.50
1:C:726:ASP:O	1:C:730:LYS:HG3	2.12	0.50
1:D:83:PRO:CB	1:D:84:PRO:HD3	2.42	0.50
1:D:657:LEU:O	1:D:661:ILE:HG12	2.12	0.50
1:E:78:GLU:OE2	1:E:121:LYS:CE	2.59	0.50
1:F:65:GLU:O	1:F:68:PRO:CD	2.59	0.50
1:F:158:GLY:HA3	1:F:519:PRO:O	2.11	0.50
1:F:580:ARG:NH1	2:F:901:UDP:O1B	2.45	0.50
1:F:790:PHE:O	1:F:794:LYS:HB3	2.11	0.50
1:G:48:GLN:HE22	1:G:52:GLU:CB	2.24	0.50
1:G:70:PHE:O	1:G:73:LEU:N	2.44	0.50
1:G:124:LEU:HD23	1:G:124:LEU:C	2.35	0.50
1:G:477:PHE:HA	1:G:520:LYS:HB2	1.94	0.50
1:H:794:LYS:HD3	1:H:794:LYS:C	2.36	0.50
1:A:118:LEU:O	1:A:122:GLU:HG3	2.12	0.50
1:B:232:LYS:O	1:B:235:GLU:HB2	2.12	0.50
1:D:327:GLY:C	1:D:328:LEU:HD23	2.37	0.50
1:D:451:TYR:HB3	1:D:454:LYS:HE2	1.92	0.50
1:D:544:THR:HG22	1:D:547:HIS:CE1	2.46	0.50
1:D:590:LEU:HB2	1:D:671:PRO:HG3	1.93	0.50
1:E:486:ILE:HG22	1:E:516:VAL:CG2	2.38	0.50
1:E:518:ASP:OD1	1:E:520:LYS:HG2	2.12	0.50
1:F:85:TRP:CE3	1:F:101:ARG:CD	2.95	0.50
1:G:176:SER:O	1:G:179:PRO:HD2	2.12	0.50
1:G:443:THR:HG21	1:G:495:GLN:HA	1.93	0.50
1:C:146:ILE:HG22	1:C:147:PRO:N	2.27	0.49
1:C:181:LEU:HD13	1:C:206:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:719:GLN:HG3	5:D:913:SO4:O4	2.12	0.49
1:B:56:LEU:CB	1:B:57:PRO:HD2	2.41	0.49
1:B:76:THR:N	1:B:90:VAL:HG13	2.26	0.49
1:B:407:LYS:HB2	1:B:408:PRO:HD2	1.93	0.49
1:B:407:LYS:HB2	1:B:408:PRO:CD	2.42	0.49
1:C:131:GLY:HA3	1:C:134:THR:CG2	2.42	0.49
1:C:420:LEU:C	1:C:420:LEU:HD13	2.37	0.49
1:C:692:PHE:N	1:C:692:PHE:CD1	2.81	0.49
1:D:131:GLY:CA	1:D:134:THR:HG23	2.42	0.49
1:D:491:GLU:CD	1:D:491:GLU:H	2.20	0.49
1:F:59:GLN:CG	1:F:60:THR:H	2.23	0.49
1:F:437:ALA:O	1:F:438:HIS:HB2	2.12	0.49
1:H:386:TRP:N	1:H:387:PRO:HD2	2.27	0.49
1:H:468:ASP:O	1:H:472:MET:HB2	2.11	0.49
1:H:748:ARG:HH12	1:H:752:LYS:HE3	1.76	0.49
1:A:719:GLN:HG3	5:A:913:SO4:O2	2.12	0.49
1:B:225:LEU:O	1:B:228:GLU:HG2	2.12	0.49
1:B:565:CYS:SG	1:B:633:ILE:HD13	2.52	0.49
1:E:583:ARG:HG2	1:E:583:ARG:HH11	1.77	0.49
1:G:83:PRO:C	1:G:85:TRP:N	2.70	0.49
1:G:575:LEU:HD21	1:G:724:LEU:HD13	1.94	0.49
1:G:756:GLN:HG2	1:G:757:ILE:N	2.27	0.49
1:A:65:GLU:OE2	1:A:65:GLU:CA	2.60	0.49
1:A:435:THR:HG23	1:A:475:THR:HB	1.93	0.49
1:B:445:TYR:O	1:B:448:SER:HB3	2.13	0.49
1:B:613:ARG:HG3	1:B:626:MET:HE2	1.95	0.49
1:C:688:GLY:O	1:C:690:PRO:HD3	2.12	0.49
1:D:292:GLN:OE1	1:D:356:VAL:HA	2.12	0.49
1:D:616:GLU:HA	1:D:616:GLU:OE1	2.12	0.49
1:E:35:ARG:HD2	1:E:104:LEU:CA	2.35	0.49
1:F:54:GLU:O	1:F:55:ALA:HB3	2.12	0.49
1:F:242:TRP:HB2	1:F:249:VAL:HG13	1.95	0.49
1:H:39:LYS:CA	1:H:104:LEU:HD22	2.43	0.49
1:B:716:HIS:HB3	5:B:913:SO4:S	2.52	0.49
1:C:56:LEU:HB3	1:C:57:PRO:CD	2.42	0.49
1:E:35:ARG:O	1:E:39:LYS:N	2.34	0.49
1:E:135:LEU:CD1	1:H:789:MET:HG3	2.42	0.49
1:F:682:VAL:HG13	1:F:749:ILE:HD12	1.95	0.49
1:F:770:GLY:O	1:F:773:LYS:HB2	2.13	0.49
1:H:65:GLU:HA	1:H:65:GLU:OE2	2.11	0.49
1:H:174:LYS:CD	1:H:174:LYS:H	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:LEU:HB2	1:B:671:PRO:HG3	1.95	0.49
1:D:48:GLN:O	1:D:51:ALA:HB3	2.12	0.49
1:E:85:TRP:HA	1:E:104:LEU:H	1.77	0.49
1:H:45:GLN:CD	1:H:80:ILE:HG22	2.37	0.49
1:H:76:THR:O	1:H:77:GLN:CB	2.61	0.49
1:H:76:THR:O	1:H:77:GLN:HB2	2.13	0.49
1:H:441:GLU:OE1	1:H:441:GLU:HA	2.11	0.49
1:H:582:ASP:HB2	1:H:621:GLU:OE1	2.12	0.49
1:A:60:THR:CG2	1:A:62:LYS:CB	2.87	0.49
1:A:211:ARG:HH22	1:B:151:LEU:HD23	1.77	0.49
1:C:104:LEU:H	1:C:104:LEU:CD2	2.25	0.49
1:C:534:PHE:O	1:C:687:CYS:HA	2.13	0.49
1:E:28:GLU:O	1:E:32:LEU:HB2	2.12	0.49
1:G:543:LEU:HB3	1:G:545:LYS:CE	2.25	0.49
1:H:46:GLN:HG3	1:H:50:ILE:HB	1.94	0.49
1:A:45:GLN:HE22	1:A:80:ILE:HD12	1.77	0.49
1:B:155:ILE:HB	1:B:483:PHE:CE2	2.48	0.49
1:C:216:TYR:CD2	1:C:232:LYS:HG2	2.47	0.49
1:D:32:LEU:HD21	1:D:105:HIS:HA	1.94	0.49
1:D:84:PRO:HB2	1:D:85:TRP:CD1	2.48	0.49
1:E:483:PHE:CE1	1:E:487:ALA:HB3	2.48	0.49
1:E:762:LEU:HD12	1:E:762:LEU:C	2.37	0.49
1:G:679:LEU:HB2	2:G:901:UDP:O2A	2.13	0.49
1:A:713:ASP:OD1	1:A:715:TYR:N	2.42	0.49
1:B:131:GLY:N	1:B:134:THR:CG2	2.76	0.49
1:C:105:HIS:O	1:C:106:ALA:CB	2.60	0.49
1:C:188:SER:HB2	1:C:192:LYS:O	2.12	0.49
1:D:479:ILE:HD11	1:D:762:LEU:HD13	1.94	0.49
1:E:590:LEU:HB2	1:E:671:PRO:HG3	1.95	0.49
1:A:73:LEU:HD23	1:A:73:LEU:C	2.37	0.49
1:A:518:ASP:OD1	1:A:520:LYS:HG2	2.12	0.49
1:A:673:LEU:HD23	1:A:714:PRO:HB2	1.95	0.49
1:D:318:GLU:CD	1:D:760:GLN:HG2	2.38	0.49
1:D:748:ARG:NH1	1:D:752:LYS:HE3	2.28	0.49
1:E:387:PRO:HD3	1:E:802:VAL:HB	1.94	0.49
1:H:131:GLY:O	1:H:132:ASN:C	2.56	0.49
1:A:69:PHE:HE1	1:A:73:LEU:HD12	1.78	0.48
1:B:56:LEU:O	1:B:58:GLU:O	2.31	0.48
1:D:242:TRP:O	1:D:252:MET:HG3	2.12	0.48
1:G:31:ALA:CB	1:G:35:ARG:NH2	2.70	0.48
1:G:117:PHE:O	1:G:120:PHE:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:711:HIS:HE1	5:G:912:SO4:O3	1.96	0.48
1:H:437:ALA:C	1:H:439:ALA:H	2.20	0.48
1:H:679:LEU:N	2:H:901:UDP:O1A	2.46	0.48
1:A:30:LEU:HD22	1:A:30:LEU:N	2.28	0.48
1:A:49:ILE:CG2	1:A:50:ILE:N	2.76	0.48
1:B:59:GLN:O	1:B:60:THR:HG22	2.13	0.48
1:B:75:SER:C	1:B:77:GLN:H	2.22	0.48
1:B:216:TYR:HD1	1:B:216:TYR:C	2.22	0.48
1:C:420:LEU:HD23	1:C:467:ALA:HB2	1.94	0.48
1:C:434:CYS:HB2	1:C:477:PHE:CZ	2.48	0.48
1:D:216:TYR:HD2	1:D:232:LYS:HE2	1.77	0.48
1:D:249:VAL:O	1:D:253:ILE:HG13	2.13	0.48
1:D:564:LEU:HD22	1:D:613:ARG:NH2	2.28	0.48
1:F:52:GLU:C	1:F:52:GLU:CD	2.81	0.48
1:F:230:GLU:OE1	1:F:240:ARG:NH1	2.46	0.48
1:H:174:LYS:HD2	1:H:174:LYS:H	1.77	0.48
1:C:34:SER:HA	1:C:59:GLN:NE2	2.25	0.48
1:E:105:HIS:O	1:E:106:ALA:CB	2.61	0.48
1:E:565:CYS:C	1:E:566:VAL:HG23	2.38	0.48
1:H:338:THR:CG2	1:H:366:ARG:HG2	2.40	0.48
1:A:59:GLN:HG3	1:A:60:THR:N	2.12	0.48
1:B:82:LEU:HD13	1:B:82:LEU:H	1.76	0.48
1:B:210:LEU:CD2	1:B:253:ILE:HG23	2.35	0.48
1:C:437:ALA:C	1:C:439:ALA:H	2.21	0.48
1:F:69:PHE:CD1	1:F:70:PHE:N	2.82	0.48
1:F:414:ASN:O	1:F:418:GLY:HA3	2.13	0.48
1:G:56:LEU:HG	1:G:70:PHE:HE1	1.78	0.48
1:G:62:LYS:O	1:G:63:LYS:C	2.55	0.48
1:G:125:VAL:CG1	1:G:126:ASP:N	2.75	0.48
1:A:524:VAL:HG12	1:A:758:TYR:CD2	2.48	0.48
1:B:90:VAL:CG1	1:B:91:ARG:H	2.27	0.48
1:B:231:ALA:O	1:B:235:GLU:HG3	2.13	0.48
1:D:55:ALA:O	1:D:59:GLN:CB	2.62	0.48
1:D:137:LEU:HD11	1:D:790:PHE:CZ	2.49	0.48
1:E:400:LEU:HD12	1:E:401:SER:N	2.29	0.48
1:E:434:CYS:HA	1:E:477:PHE:O	2.14	0.48
1:F:56:LEU:O	1:F:63:LYS:HE2	2.13	0.48
1:F:308:ILE:HG22	1:F:336:ILE:HD13	1.95	0.48
1:H:290:PHE:O	1:H:366:ARG:NH1	2.46	0.48
1:H:491:GLU:H	1:H:491:GLU:CD	2.19	0.48
1:C:518:ASP:CG	1:C:520:LYS:HG2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ILE:HG12	1:D:121:LYS:HG2	1.96	0.48
1:D:82:LEU:C	1:D:82:LEU:CD1	2.86	0.48
1:D:245:ASN:O	1:D:249:VAL:HG23	2.14	0.48
1:D:312:VAL:HG23	1:D:313:ARG:N	2.29	0.48
1:E:298:TYR:HE1	1:E:649:MET:HE1	1.78	0.48
1:F:566:VAL:HA	8:F:874:HOH:O	2.13	0.48
1:G:146:ILE:HD11	1:G:162:LEU:CD1	2.44	0.48
1:H:33:LEU:C	1:H:36:VAL:H	2.21	0.48
1:H:60:THR:O	1:H:63:LYS:HG3	2.13	0.48
1:A:88:LEU:HB2	1:A:100:LEU:HD23	1.95	0.48
1:A:680:THR:HG23	2:A:901:UDP:O2A	2.12	0.48
1:B:348:THR:O	1:B:351:GLU:HG2	2.14	0.48
1:B:594:TYR:CE1	1:B:601:ARG:HG2	2.49	0.48
1:B:784:ARG:O	1:B:788:GLU:HG3	2.14	0.48
1:D:60:THR:C	1:D:62:LYS:N	2.72	0.48
1:D:91:ARG:HD2	1:D:97:TRP:CZ2	2.48	0.48
1:D:435:THR:HG23	1:D:475:THR:CB	2.43	0.48
1:E:61:ARG:C	1:E:63:LYS:N	2.72	0.48
1:E:536:TYR:CE1	1:E:537:THR:HG23	2.49	0.48
1:F:82:LEU:O	1:F:85:TRP:O	2.31	0.48
1:F:86:VAL:HG13	1:F:86:VAL:O	2.12	0.48
1:G:63:LYS:C	1:G:65:GLU:HG2	2.39	0.48
1:G:284:LEU:HD13	1:G:337:LEU:HB2	1.96	0.48
1:A:82:LEU:CB	1:A:83:PRO:HD2	2.42	0.48
1:A:677:PHE:HB3	3:A:903[A]:LCN:O4	2.14	0.48
1:B:124:LEU:HD23	1:B:124:LEU:C	2.38	0.48
1:B:716:HIS:HB3	5:B:913:SO4:O4	2.13	0.48
1:C:80:ILE:HD13	1:C:121:LYS:CG	2.43	0.48
1:C:794:LYS:HE2	1:C:794:LYS:HA	1.94	0.48
1:D:27:ASN:HB2	1:D:30:LEU:CD2	2.40	0.48
1:D:547:HIS:O	1:D:551:GLU:CG	2.61	0.48
1:E:171:PHE:CD1	1:E:263:PRO:HD2	2.49	0.48
1:F:140:GLU:N	1:F:141:PRO:CD	2.77	0.48
1:F:726:ASP:O	1:F:730:LYS:HG3	2.13	0.48
1:A:65:GLU:C	1:A:67:GLY:N	2.72	0.48
1:A:153:LYS:HD3	1:A:154:TYR:CE2	2.48	0.48
1:A:717:GLY:O	1:A:720:ALA:HB3	2.13	0.48
1:E:348:THR:O	1:E:351:GLU:HG2	2.13	0.48
1:F:419:ASN:OD1	1:F:435:THR:HB	2.14	0.48
1:F:704:VAL:HA	5:F:912:SO4:O1	2.14	0.48
1:H:125:VAL:HG21	1:H:450:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD12	1:B:261:GLU:CB	2.44	0.48
1:C:33:LEU:O	1:C:36:VAL:HB	2.13	0.48
1:C:43:ILE:O	1:C:43:ILE:HG22	2.14	0.48
1:C:143:ASN:ND2	1:C:780:ARG:HH22	2.11	0.48
1:E:328:LEU:HD23	1:E:328:LEU:N	2.28	0.48
1:F:189:HIS:CE1	1:F:190:GLN:HG3	2.48	0.48
1:G:84:PRO:HB2	1:G:103:ASN:ND2	2.29	0.48
1:A:30:LEU:H	1:A:30:LEU:CD2	2.27	0.47
1:B:89:ALA:HA	1:B:99:TYR:HA	1.96	0.47
1:B:217:LEU:HA	1:B:220:LEU:HD12	1.96	0.47
1:B:248:ARG:HB3	1:B:248:ARG:NH1	2.24	0.47
1:B:525:SER:HB3	1:B:753:TYR:HD1	1.79	0.47
1:D:790:PHE:O	1:D:794:LYS:HB3	2.14	0.47
1:E:44:LEU:HA	1:E:124:LEU:CD1	2.43	0.47
1:E:772:TRP:CZ2	1:E:776:SER:HB3	2.49	0.47
1:E:790:PHE:O	1:E:794:LYS:HB3	2.14	0.47
1:F:298:TYR:HE1	1:F:649:MET:HE1	1.79	0.47
1:H:407:LYS:CB	1:H:408:PRO:CD	2.91	0.47
1:B:230:GLU:O	1:B:234:GLU:CG	2.62	0.47
1:B:442:LYS:HD2	1:B:449:ASP:HB3	1.96	0.47
1:C:348:THR:O	1:C:351:GLU:HG2	2.13	0.47
1:D:547:HIS:O	1:D:551:GLU:HG3	2.14	0.47
1:E:45:GLN:HB3	1:E:80:ILE:HD13	1.96	0.47
1:E:770:GLY:O	1:E:773:LYS:HB2	2.13	0.47
1:F:65:GLU:HA	1:F:68:PRO:HG2	1.94	0.47
1:F:477:PHE:HA	1:F:520:LYS:HB2	1.94	0.47
1:F:547:HIS:O	1:F:551:GLU:CG	2.61	0.47
1:H:189:HIS:CE1	1:H:279:PHE:HB2	2.49	0.47
1:C:169:LYS:HG2	1:C:176:SER:OG	2.14	0.47
1:E:407:LYS:HB2	1:E:408:PRO:CD	2.44	0.47
1:F:143:ASN:HA	1:F:780:ARG:HH12	1.78	0.47
1:F:452:TRP:CD1	1:F:504:LEU:HB3	2.49	0.47
1:H:76:THR:O	1:H:89:ALA:O	2.33	0.47
1:H:146:ILE:CG2	1:H:147:PRO:O	2.53	0.47
1:A:259:LEU:CD2	1:A:267:THR:HG22	2.44	0.47
1:A:417:ASP:OD1	1:A:417:ASP:N	2.45	0.47
1:A:789:MET:CE	1:D:789:MET:CG	2.92	0.47
1:B:291:ALA:HB3	1:B:295:VAL:HG11	1.97	0.47
1:C:564:LEU:HD13	1:C:613:ARG:NH2	2.26	0.47
1:D:39:LYS:NZ	1:D:104:LEU:HB3	2.28	0.47
1:D:56:LEU:O	1:D:63:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:GLU:HG3	1:E:29:VAL:HG23	1.97	0.47
1:E:44:LEU:HD11	1:E:451:TYR:OH	2.15	0.47
1:G:30:LEU:N	1:G:30:LEU:HD12	2.29	0.47
1:B:155:ILE:HB	1:B:483:PHE:HE2	1.78	0.47
1:C:46:GLN:HB3	1:C:50:ILE:HG12	1.96	0.47
1:C:47:ASN:O	1:C:48:GLN:C	2.58	0.47
1:G:140:GLU:N	1:G:141:PRO:HD2	2.30	0.47
1:G:216:TYR:HD1	1:G:216:TYR:O	1.98	0.47
1:G:264:ASP:OD1	1:G:267:THR:HB	2.14	0.47
2:H:901:UDP:O1B	4:H:904[B]:NHF:H1	2.14	0.47
1:A:52:GLU:O	1:A:57:PRO:HD2	2.14	0.47
1:A:565:CYS:C	1:A:566:VAL:HG23	2.38	0.47
1:A:651:ARG:HA	1:A:654:ASN:HB2	1.97	0.47
1:B:146:ILE:HG22	1:B:147:PRO:N	2.30	0.47
1:E:435:THR:HG23	1:E:475:THR:CB	2.44	0.47
1:E:793:LEU:HD11	1:H:135:LEU:CD2	2.44	0.47
1:F:106:ALA:O	1:F:107:LEU:C	2.57	0.47
1:G:679:LEU:N	2:G:901:UDP:O2A	2.47	0.47
1:H:303:GLY:H	2:H:901:UDP:H5'1	1.80	0.47
1:A:82:LEU:C	1:A:83:PRO:O	2.53	0.47
1:A:212:LYS:HE2	1:A:232:LYS:NZ	2.29	0.47
1:A:542:ARG:HD2	1:A:659:ARG:HD2	1.96	0.47
1:A:657:LEU:O	1:A:661:ILE:HG12	2.15	0.47
1:B:82:LEU:C	1:B:84:PRO:CD	2.86	0.47
1:B:216:TYR:CD1	1:B:216:TYR:C	2.92	0.47
1:C:125:VAL:HG21	1:C:450:ILE:HG12	1.95	0.47
1:C:131:GLY:H	1:C:134:THR:HG21	1.79	0.47
1:C:151:LEU:HD23	1:D:211:ARG:HH22	1.80	0.47
1:D:131:GLY:O	1:D:134:THR:HG23	2.14	0.47
1:D:386:TRP:N	1:D:387:PRO:HD2	2.29	0.47
1:D:438:HIS:ND1	4:D:904[B]:NHF:H6A	2.29	0.47
1:E:52:GLU:O	1:E:57:PRO:HD2	2.14	0.47
1:E:315:LEU:HG	1:E:319:MET:HE3	1.90	0.47
1:E:784:ARG:O	1:E:788:GLU:HG3	2.14	0.47
1:F:407:LYS:CB	1:F:408:PRO:CD	2.90	0.47
1:F:677:PHE:HB3	3:F:903[A]:LCN:O4	2.15	0.47
1:G:31:ALA:HB3	1:G:35:ARG:NH2	2.30	0.47
1:G:83:PRO:C	1:G:85:TRP:H	2.23	0.47
1:G:148:ARG:HG3	1:G:148:ARG:NH1	2.28	0.47
1:G:415:TYR:CG	1:G:416:SER:N	2.83	0.47
1:G:609:VAL:HG22	1:G:645:ILE:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:43:ILE:HG23	1:H:43:ILE:O	2.14	0.47
1:H:659:ARG:O	1:H:662:CYS:HB2	2.14	0.47
1:A:221:LYS:HB3	1:A:221:LYS:HE2	1.65	0.47
1:A:271:PHE:O	1:A:275:VAL:HG23	2.15	0.47
1:B:566:VAL:CG1	1:B:567:LEU:N	2.78	0.47
1:E:125:VAL:HG13	1:E:126:ASP:H	1.78	0.47
1:F:44:LEU:CD1	1:F:451:TYR:OH	2.63	0.47
1:A:61:ARG:C	1:A:63:LYS:H	2.22	0.47
1:A:789:MET:CG	1:D:789:MET:CE	2.92	0.47
1:B:575:LEU:O	1:B:606:LEU:HD12	2.14	0.47
1:C:414:ASN:O	1:C:418:GLY:HA3	2.14	0.47
1:F:32:LEU:O	1:F:36:VAL:HG23	2.14	0.47
1:F:242:TRP:HA	1:F:252:MET:HE3	1.97	0.47
1:F:242:TRP:CB	1:F:249:VAL:HG13	2.45	0.47
1:F:415:TYR:CG	1:F:416:SER:N	2.83	0.47
1:H:160:ASP:O	1:H:164:ARG:HG3	2.15	0.47
1:H:561:LYS:HD3	1:H:613:ARG:O	2.15	0.47
1:A:545:LYS:HD3	1:A:545:LYS:N	2.23	0.47
1:B:52:GLU:C	1:B:56:LEU:CB	2.88	0.47
1:B:60:THR:CG2	1:B:61:ARG:H	2.06	0.47
1:B:93:ARG:HB2	1:B:96:VAL:HG21	1.97	0.47
1:B:131:GLY:CA	1:B:134:THR:HG23	2.45	0.47
1:B:135:LEU:HD11	1:C:789:MET:HG3	1.96	0.47
1:C:60:THR:O	1:C:63:LYS:CD	2.63	0.47
1:C:484:GLN:HG3	1:C:485:GLU:N	2.29	0.47
1:F:583:ARG:HG2	1:F:583:ARG:HH11	1.79	0.47
1:A:105:HIS:O	1:A:106:ALA:HB2	2.15	0.46
1:A:135:LEU:HD22	1:D:793:LEU:HD11	1.97	0.46
1:B:56:LEU:O	1:B:58:GLU:N	2.48	0.46
1:B:216:TYR:CE2	1:B:232:LYS:HG2	2.51	0.46
1:C:524:VAL:HG12	1:C:758:TYR:CD2	2.51	0.46
1:E:45:GLN:HG2	1:E:80:ILE:CD1	2.45	0.46
1:H:483:PHE:CZ	1:H:487:ALA:HB3	2.50	0.46
1:B:113:GLN:CG	1:B:114:PRO:HD2	2.38	0.46
1:B:212:LYS:HE2	1:B:232:LYS:NZ	2.30	0.46
1:B:230:GLU:O	1:B:234:GLU:HG3	2.15	0.46
1:C:158:GLY:HA3	1:C:519:PRO:O	2.15	0.46
1:C:705:HIS:HB2	1:C:711:HIS:ND1	2.30	0.46
1:F:35:ARG:HD3	1:F:104:LEU:HD23	1.97	0.46
1:F:216:TYR:HE1	1:F:220:LEU:HD11	1.80	0.46
1:H:315:LEU:O	1:H:319:MET:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:CD2	1:A:90:VAL:HG11	2.40	0.46
1:A:711:HIS:CE1	5:A:912:SO4:O1	2.67	0.46
1:A:790:PHE:O	1:A:794:LYS:HB3	2.15	0.46
1:B:207:GLN:HG3	1:B:211:ARG:HH21	1.76	0.46
1:D:54:GLU:O	1:D:58:GLU:CB	2.63	0.46
1:D:312:VAL:HG11	1:D:336:ILE:HD11	1.96	0.46
1:F:35:ARG:CG	1:F:104:LEU:HA	2.45	0.46
1:F:245:ASN:OD1	1:F:248:ARG:HG3	2.16	0.46
1:F:417:ASP:N	1:F:417:ASP:OD1	2.48	0.46
1:F:445:TYR:O	1:F:448:SER:HB3	2.16	0.46
1:G:124:LEU:C	1:G:124:LEU:CD2	2.89	0.46
1:G:259:LEU:O	1:G:263:PRO:HG3	2.15	0.46
1:H:46:GLN:N	1:H:79:ALA:O	2.48	0.46
1:A:772:TRP:CE2	1:A:776:SER:HB3	2.51	0.46
1:C:30:LEU:O	1:C:33:LEU:HG	2.15	0.46
1:C:56:LEU:HG	1:C:70:PHE:HE1	1.80	0.46
1:D:230:GLU:OE1	1:D:240:ARG:NH1	2.49	0.46
1:D:376:VAL:HG21	1:D:388:TYR:CE2	2.51	0.46
1:F:420:LEU:C	1:F:420:LEU:CD1	2.89	0.46
1:G:63:LYS:O	1:G:64:LEU:C	2.56	0.46
1:B:128:VAL:HG22	1:B:129:LYS:N	2.28	0.46
1:B:659:ARG:O	1:B:662:CYS:HB2	2.16	0.46
1:C:56:LEU:HD13	1:C:63:LYS:HG2	1.98	0.46
1:C:207:GLN:HA	1:C:207:GLN:HE21	1.79	0.46
1:C:442:LYS:HG3	1:C:465:PHE:CZ	2.50	0.46
1:D:514:ILE:HG13	1:D:515:ASP:N	2.31	0.46
1:E:174:LYS:HD2	1:E:174:LYS:N	2.31	0.46
1:F:162:LEU:HD21	1:F:772:TRP:CG	2.50	0.46
1:F:393:THR:HG23	1:F:425:LEU:HG	1.97	0.46
1:G:29:VAL:O	1:G:29:VAL:HG12	2.15	0.46
1:H:32:LEU:CD2	1:H:35:ARG:NH1	2.78	0.46
1:H:87:ALA:HB2	1:H:120:PHE:CD2	2.51	0.46
1:A:28:GLU:O	1:A:32:LEU:HG	2.15	0.46
1:A:512:HIS:HE1	1:A:515:ASP:HB2	1.78	0.46
2:A:901:UDP:O2B	4:A:904[B]:NHF:H1	2.15	0.46
1:C:39:LYS:HZ1	1:C:105:HIS:CE1	2.33	0.46
1:C:582:ASP:HB2	1:C:621:GLU:OE1	2.15	0.46
1:C:792:ALA:HA	1:C:796:ARG:HG3	1.97	0.46
1:D:284:LEU:N	1:D:284:LEU:CD2	2.78	0.46
1:F:248:ARG:HB3	1:F:248:ARG:NH1	2.31	0.46
1:H:565:CYS:HB3	1:H:639:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:573:PRO:HD2	1:H:603:LEU:O	2.15	0.46
1:A:298:TYR:CE1	1:A:649:MET:CE	2.98	0.46
1:A:353:LEU:HD13	1:A:365:LEU:HD13	1.98	0.46
1:B:207:GLN:CG	1:B:211:ARG:NH2	2.77	0.46
1:C:86:VAL:HG13	1:C:102:VAL:HG22	1.96	0.46
1:D:468:ASP:O	1:D:472:MET:HB2	2.15	0.46
1:E:757:ILE:HG22	1:E:761:ARG:HG2	1.96	0.46
1:H:483:PHE:CE1	1:H:487:ALA:HB3	2.50	0.46
1:A:61:ARG:C	1:A:63:LYS:N	2.73	0.46
1:B:525:SER:HB3	1:B:753:TYR:CD1	2.51	0.46
1:C:80:ILE:HD11	1:C:121:LYS:CE	2.46	0.46
1:C:131:GLY:CA	1:C:134:THR:CG2	2.93	0.46
1:D:80:ILE:HD11	1:D:121:LYS:HE2	1.98	0.46
1:E:60:THR:O	1:E:63:LYS:CD	2.63	0.46
1:G:581:LEU:HG	1:G:625:GLU:HG2	1.98	0.46
1:H:35:ARG:HB3	1:H:104:LEU:O	2.15	0.46
1:H:566:VAL:O	1:H:640:GLY:HA2	2.15	0.46
1:A:185:ARG:HD2	1:A:198:GLU:OE2	2.15	0.46
1:B:131:GLY:C	1:B:134:THR:HG23	2.41	0.46
1:B:337:LEU:HD12	1:B:396:ALA:HB1	1.98	0.46
1:C:46:GLN:HB2	1:C:50:ILE:CG1	2.46	0.46
1:D:105:HIS:O	1:D:106:ALA:HB2	2.16	0.46
1:D:283:ILE:C	1:D:284:LEU:HD22	2.41	0.46
1:E:63:LYS:O	1:E:64:LEU:C	2.59	0.46
1:E:100:LEU:HD12	1:E:100:LEU:O	2.16	0.46
1:E:304:GLN:O	1:E:308:ILE:HG13	2.16	0.46
1:E:789:MET:HE1	1:H:790:PHE:N	2.31	0.46
1:F:705:HIS:N	5:F:912:SO4:O1	2.39	0.46
1:G:193:ASN:HB3	1:G:239:GLU:HG3	1.98	0.46
1:H:143:ASN:C	1:H:145:SER:N	2.74	0.46
1:H:295:VAL:N	1:H:649:MET:HG2	2.31	0.46
1:H:677:PHE:HB3	4:H:904[B]:NHF:O4	2.16	0.46
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.74	0.46
1:C:65:GLU:C	1:C:67:GLY:H	2.24	0.46
1:C:118:LEU:O	1:C:122:GLU:HG3	2.16	0.46
1:C:790:PHE:O	1:C:794:LYS:HB3	2.16	0.46
1:D:216:TYR:HD1	1:D:216:TYR:O	1.99	0.46
1:F:625:GLU:O	1:F:629:MET:HG2	2.15	0.46
1:F:791:TYR:CE1	1:F:795:TYR:CD2	3.04	0.46
1:G:82:LEU:CG	1:G:83:PRO:HD3	2.45	0.46
1:G:160:ASP:O	1:G:164:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:564:LEU:HD12	1:G:564:LEU:HA	1.69	0.46
1:H:163:ASN:O	1:H:167:SER:HB2	2.16	0.46
1:H:173:ASP:HB3	1:H:176:SER:CB	2.44	0.46
1:B:133:PHE:CD1	1:C:424:LEU:HD22	2.51	0.45
1:B:290:PHE:HB3	1:B:338:THR:HG21	1.97	0.45
1:B:318:GLU:HG3	1:B:763:LEU:HD12	1.98	0.45
1:B:414:ASN:O	1:B:418:GLY:HA3	2.16	0.45
1:E:534:PHE:HB2	1:E:535:PRO:HD2	1.96	0.45
1:F:81:VAL:CG1	1:F:86:VAL:HG23	2.45	0.45
1:F:160:ASP:O	1:F:164:ARG:HG3	2.16	0.45
1:F:723:THR:HG23	6:F:921:MLA:O3A	2.16	0.45
1:G:83:PRO:CB	1:G:84:PRO:CD	2.93	0.45
1:G:226:TYR:CE2	1:G:240:ARG:HG2	2.51	0.45
1:C:142:PHE:O	1:C:780:ARG:NH1	2.50	0.45
1:C:796:ARG:HB2	1:C:797:PRO:CD	2.40	0.45
1:D:582:ASP:HB2	1:D:621:GLU:OE1	2.16	0.45
1:E:85:TRP:CD1	1:E:85:TRP:N	2.83	0.45
1:E:447:ASP:O	1:E:451:TYR:HB2	2.16	0.45
1:E:588:SER:HB3	1:E:625:GLU:OE2	2.15	0.45
1:G:80:ILE:HG23	1:G:124:LEU:HD12	1.98	0.45
1:H:433:GLN:O	1:H:476:ASP:HB2	2.17	0.45
1:B:82:LEU:CD1	1:B:120:PHE:CZ	3.00	0.45
1:B:445:TYR:O	1:B:448:SER:CB	2.65	0.45
1:C:171:PHE:HD1	1:C:263:PRO:HD2	1.81	0.45
1:D:76:THR:O	1:D:76:THR:HG22	2.15	0.45
1:D:103:ASN:ND2	1:D:108:VAL:HG11	2.32	0.45
1:D:131:GLY:C	1:D:134:THR:HG23	2.41	0.45
1:D:440:LEU:HD12	1:D:495:GLN:HB3	1.97	0.45
1:F:777:ASN:OD1	1:F:778:LEU:HD12	2.16	0.45
1:H:293:ASP:O	1:H:295:VAL:HG13	2.16	0.45
1:A:63:LYS:O	1:A:64:LEU:C	2.59	0.45
1:B:44:LEU:C	1:B:45:GLN:HG3	2.41	0.45
1:D:104:LEU:HA	1:D:104:LEU:HD23	1.73	0.45
1:D:472:MET:HG2	1:D:514:ILE:HD13	1.98	0.45
1:D:716:HIS:HB3	5:D:913:SO4:O4	2.15	0.45
1:E:232:LYS:O	1:E:235:GLU:HB2	2.17	0.45
1:F:35:ARG:HG3	1:F:104:LEU:HD22	1.99	0.45
1:H:225:LEU:O	1:H:228:GLU:HG2	2.17	0.45
1:A:146:ILE:HG22	1:A:147:PRO:N	2.32	0.45
1:A:479:ILE:HD11	1:A:762:LEU:HD13	1.98	0.45
1:C:155:ILE:HB	1:C:483:PHE:HE2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LEU:HB2	1:D:83:PRO:CD	2.46	0.45
1:D:135:LEU:HD12	1:D:136:GLU:N	2.32	0.45
1:E:60:THR:HG23	1:E:62:LYS:CB	2.47	0.45
1:E:154:TYR:OH	1:F:262:ALA:HB3	2.16	0.45
1:F:65:GLU:C	1:F:68:PRO:CD	2.87	0.45
1:H:688:GLY:O	1:H:690:PRO:HD3	2.16	0.45
1:A:46:GLN:HG3	1:A:51:ALA:CB	2.47	0.45
1:A:54:GLU:O	1:A:58:GLU:CB	2.65	0.45
1:B:146:ILE:CG2	1:B:147:PRO:CD	2.73	0.45
1:C:69:PHE:CE1	1:C:73:LEU:HD11	2.51	0.45
1:F:748:ARG:HH12	1:F:752:LYS:HE3	1.82	0.45
1:A:82:LEU:HD12	1:A:120:PHE:CE1	2.52	0.45
1:E:60:THR:O	1:E:63:LYS:HG3	2.17	0.45
1:E:156:GLY:HA3	1:E:523:ILE:HG13	1.98	0.45
1:E:561:LYS:HD3	1:E:613:ARG:O	2.17	0.45
1:F:585:LYS:HD2	8:F:856:HOH:O	2.15	0.45
1:H:279:PHE:CE1	1:H:330:ILE:HD12	2.52	0.45
1:A:74:LYS:HE3	1:A:74:LYS:HB2	1.68	0.45
1:A:789:MET:CE	1:D:790:PHE:N	2.80	0.45
1:B:793:LEU:HB3	1:C:793:LEU:HB3	1.99	0.45
1:D:119:HIS:CE1	1:D:129:LYS:CB	2.99	0.45
1:E:670:GLN:HG3	1:E:670:GLN:O	2.16	0.45
1:E:789:MET:CE	1:H:789:MET:CE	2.79	0.45
1:G:148:ARG:HH11	1:G:148:ARG:CG	2.29	0.45
1:H:34:SER:OG	1:H:55:ALA:CB	2.58	0.45
1:H:39:LYS:HD3	1:H:39:LYS:C	2.41	0.45
1:H:353:LEU:CD1	1:H:365:LEU:HD13	2.47	0.45
1:H:438:HIS:ND1	4:H:904[B]:NH:F:H6	2.30	0.45
1:A:151:LEU:HB3	1:A:153:LYS:HG2	1.98	0.45
1:A:702:ILE:HA	1:A:753:TYR:OH	2.17	0.45
1:C:86:VAL:HG13	1:C:86:VAL:O	2.16	0.45
1:D:52:GLU:C	1:D:57:PRO:HD2	2.41	0.45
1:D:63:LYS:O	1:D:64:LEU:C	2.60	0.45
1:F:435:THR:CG2	1:F:475:THR:HB	2.47	0.45
1:F:794:LYS:HE2	1:F:794:LYS:HA	1.99	0.45
1:G:565:CYS:C	1:G:566:VAL:HG23	2.42	0.45
1:H:692:PHE:CD1	1:H:692:PHE:N	2.85	0.45
1:A:35:ARG:NH2	1:A:102:VAL:CB	2.76	0.45
1:A:226:TYR:CE2	1:A:240:ARG:HG2	2.51	0.45
1:B:43:ILE:CG1	1:B:44:LEU:H	2.29	0.45
1:B:136:GLU:HG2	1:B:511:VAL:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:PHE:CD1	1:B:290:PHE:C	2.93	0.45
1:B:490:LYS:HB3	1:B:491:GLU:OE2	2.17	0.45
1:C:441:GLU:OE1	1:C:444:LYS:HE2	2.17	0.45
1:D:44:LEU:HA	1:D:44:LEU:HD13	1.87	0.45
1:D:52:GLU:HG2	1:D:57:PRO:HD2	1.99	0.45
1:D:80:ILE:HD12	1:D:80:ILE:N	2.32	0.45
1:D:552:GLU:O	1:D:556:SER:HB3	2.17	0.45
1:E:85:TRP:HB2	1:E:102:VAL:O	2.17	0.45
1:E:583:ARG:HG2	1:E:583:ARG:NH1	2.32	0.45
1:F:290:PHE:O	1:F:366:ARG:NH1	2.48	0.45
1:F:441:GLU:OE1	1:F:441:GLU:HA	2.16	0.45
1:G:61:ARG:C	1:G:63:LYS:H	2.25	0.45
1:H:39:LYS:CG	1:H:104:LEU:CG	2.92	0.45
1:A:762:LEU:HD12	1:A:762:LEU:C	2.42	0.44
1:B:50:ILE:C	1:B:52:GLU:N	2.73	0.44
1:B:56:LEU:CB	1:B:57:PRO:HD3	2.47	0.44
1:C:65:GLU:OE2	1:C:65:GLU:CA	2.59	0.44
1:C:252:MET:HG2	1:C:274:ARG:HD2	1.99	0.44
1:C:443:THR:HG21	1:C:495:GLN:HA	1.98	0.44
1:D:170:LEU:HD22	1:D:177:LEU:HD23	1.98	0.44
1:E:400:LEU:HD12	1:E:400:LEU:C	2.42	0.44
1:H:46:GLN:HB3	1:H:79:ALA:HB3	1.95	0.44
1:H:82:LEU:HD21	1:H:120:PHE:CZ	2.52	0.44
1:H:99:TYR:CD2	1:H:99:TYR:N	2.83	0.44
1:A:46:GLN:CB	1:A:79:ALA:O	2.61	0.44
1:F:187:HIS:NE2	1:F:276:PRO:O	2.50	0.44
1:F:230:GLU:O	1:F:234:GLU:HG3	2.17	0.44
1:H:259:LEU:O	1:H:263:PRO:HG3	2.16	0.44
1:C:174:LYS:HD2	1:C:174:LYS:N	2.32	0.44
1:C:276:PRO:HG3	1:C:326:GLN:CB	2.47	0.44
1:C:713:ASP:OD1	1:C:715:TYR:HB2	2.16	0.44
1:D:60:THR:C	1:D:62:LYS:H	2.24	0.44
1:F:178:LEU:N	1:F:179:PRO:CD	2.80	0.44
1:F:483:PHE:CZ	1:F:487:ALA:HB3	2.52	0.44
1:G:63:LYS:O	1:G:65:GLU:CG	2.63	0.44
1:G:154:TYR:OH	1:H:262:ALA:HB3	2.17	0.44
1:H:39:LYS:CG	1:H:104:LEU:HB3	2.47	0.44
1:H:39:LYS:HG3	1:H:104:LEU:CB	2.46	0.44
1:H:438:HIS:O	1:H:439:ALA:HB2	2.18	0.44
1:A:46:GLN:O	1:A:78:GLU:HA	2.17	0.44
1:A:547:HIS:O	1:A:551:GLU:CG	2.62	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:TRP:CG	1:B:453:LYS:N	2.85	0.44
1:B:792:ALA:HA	1:B:796:ARG:HG3	2.00	0.44
1:C:63:LYS:O	1:C:64:LEU:C	2.60	0.44
1:C:706:GLY:HA2	1:C:710:PHE:CE2	2.52	0.44
1:E:793:LEU:HB3	1:H:793:LEU:HB3	2.00	0.44
1:G:43:ILE:HG12	1:G:82:LEU:HA	1.98	0.44
1:G:565:CYS:C	1:G:566:VAL:CG2	2.91	0.44
1:H:485:GLU:O	1:H:495:GLN:HB2	2.18	0.44
1:A:83:PRO:CB	1:A:84:PRO:CD	2.89	0.44
1:A:564:LEU:HD12	1:A:564:LEU:HA	1.84	0.44
1:B:96:VAL:HG23	1:B:96:VAL:O	2.17	0.44
1:D:355:ARG:HD2	1:D:359:SER:O	2.18	0.44
1:D:493:VAL:HG23	1:D:497:GLU:HG2	1.98	0.44
1:E:45:GLN:HG3	1:E:124:LEU:CD2	2.48	0.44
1:F:290:PHE:CD2	1:F:305:VAL:HG22	2.53	0.44
1:F:538:GLU:OE1	1:F:541:ARG:HD3	2.17	0.44
1:F:748:ARG:NH1	1:F:752:LYS:HE3	2.33	0.44
1:G:525:SER:HB3	1:G:753:TYR:HD1	1.83	0.44
1:H:56:LEU:HG	1:H:70:PHE:CE1	2.51	0.44
1:H:119:HIS:HE1	1:H:129:LYS:CB	2.27	0.44
1:H:414:ASN:O	1:H:418:GLY:HA3	2.17	0.44
1:H:415:TYR:CG	1:H:416:SER:N	2.78	0.44
1:A:73:LEU:C	1:A:73:LEU:CD2	2.90	0.44
1:B:90:VAL:CG1	1:B:91:ARG:N	2.81	0.44
1:B:420:LEU:C	1:B:420:LEU:HD13	2.43	0.44
1:C:48:GLN:O	1:C:49:ILE:C	2.60	0.44
1:C:69:PHE:HE1	1:C:73:LEU:CD1	2.31	0.44
1:C:662:CYS:SG	1:C:689:LEU:HB2	2.57	0.44
1:G:518:ASP:HA	1:G:519:PRO:HD3	1.83	0.44
1:G:641:GLN:CD	1:G:641:GLN:N	2.76	0.44
1:A:35:ARG:HH11	1:A:104:LEU:HA	1.82	0.44
1:C:69:PHE:O	1:C:69:PHE:CD1	2.71	0.44
1:D:48:GLN:HB3	1:D:76:THR:O	2.17	0.44
1:D:780:ARG:HA	1:D:780:ARG:HD2	1.73	0.44
1:F:44:LEU:HB3	1:F:45:GLN:H	1.41	0.44
1:A:43:ILE:HD11	1:A:83:PRO:HD3	2.00	0.44
1:C:103:ASN:ND2	1:C:105:HIS:O	2.51	0.44
1:C:151:LEU:HD23	1:D:211:ARG:NH2	2.33	0.44
1:C:437:ALA:O	1:C:438:HIS:HB2	2.18	0.44
1:F:251:ASP:O	1:F:255:LEU:HG	2.18	0.44
1:G:592:GLU:CG	1:G:596:LYS:HE3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:582:ASP:C	1:H:582:ASP:OD1	2.60	0.44
1:A:449:ASP:O	1:A:452:TRP:HD1	2.00	0.44
1:A:681:VAL:HG13	1:A:691:THR:HG21	2.00	0.44
1:A:784:ARG:O	1:A:788:GLU:HG3	2.18	0.44
1:B:103:ASN:C	1:B:105:HIS:N	2.75	0.44
1:B:130:ASN:HD21	1:B:506:GLY:H	1.65	0.44
1:B:588:SER:HB3	1:B:625:GLU:OE2	2.18	0.44
1:B:761:ARG:NE	1:B:761:ARG:HA	2.33	0.44
1:C:69:PHE:CE1	1:C:73:LEU:HG	2.53	0.44
1:C:367:VAL:HG22	1:C:399:GLU:HG3	1.98	0.44
1:C:784:ARG:O	1:C:788:GLU:HG3	2.18	0.44
1:D:41:LYS:HE3	1:D:54:GLU:HG3	1.97	0.44
1:D:420:LEU:HD13	1:D:420:LEU:C	2.43	0.44
1:D:795:TYR:O	1:D:796:ARG:C	2.61	0.44
1:E:41:LYS:HE2	1:E:54:GLU:CD	2.43	0.44
1:F:565:CYS:C	1:F:566:VAL:HG23	2.42	0.44
1:H:420:LEU:C	1:H:420:LEU:CD1	2.91	0.44
1:B:491:GLU:H	1:B:491:GLU:CD	2.25	0.43
1:C:61:ARG:C	1:C:63:LYS:H	2.25	0.43
1:E:147:PRO:HB2	1:F:172:HIS:ND1	2.33	0.43
1:F:713:ASP:C	1:F:713:ASP:OD1	2.61	0.43
1:H:146:ILE:CD1	1:H:772:TRP:CZ2	3.01	0.43
1:H:146:ILE:HD11	1:H:772:TRP:CH2	2.53	0.43
1:H:216:TYR:CE1	1:H:220:LEU:HD11	2.53	0.43
1:C:319:MET:HE3	1:C:334:ILE:HD11	1.98	0.43
1:E:83:PRO:C	1:E:85:TRP:H	2.26	0.43
1:E:221:LYS:HE2	1:E:221:LYS:HB3	1.87	0.43
1:E:410:LEU:HD12	1:E:411:ILE:H	1.83	0.43
1:A:578:MET:HG3	1:A:609:VAL:HB	2.00	0.43
1:B:438:HIS:O	1:B:439:ALA:HB2	2.18	0.43
1:B:794:LYS:O	1:B:794:LYS:HD3	2.18	0.43
1:D:512:HIS:CE1	1:D:515:ASP:HB2	2.53	0.43
1:E:61:ARG:C	1:E:63:LYS:H	2.26	0.43
1:E:82:LEU:H	1:E:82:LEU:CD2	2.18	0.43
1:F:172:HIS:NE2	1:F:261:GLU:O	2.51	0.43
1:G:54:GLU:OE2	1:G:55:ALA:HA	2.17	0.43
1:G:150:THR:N	1:H:261:GLU:OE1	2.49	0.43
1:G:259:LEU:HD21	1:G:267:THR:HG22	2.00	0.43
1:G:617:SER:O	1:G:623:LYS:HD2	2.18	0.43
1:G:657:LEU:O	1:G:661:ILE:HG12	2.17	0.43
1:A:91:ARG:NH2	1:A:94:PRO:HA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLU:HG2	1:B:511:VAL:CG2	2.48	0.43
1:C:48:GLN:O	1:C:52:GLU:N	2.41	0.43
1:D:411:ILE:HG13	1:D:431:VAL:CG1	2.49	0.43
1:D:434:CYS:HB2	1:D:477:PHE:CZ	2.53	0.43
1:D:469:ILE:HD13	1:D:469:ILE:HA	1.78	0.43
1:E:131:GLY:HA3	1:E:134:THR:CG2	2.48	0.43
1:G:67:GLY:N	1:G:68:PRO:HD2	2.30	0.43
1:G:178:LEU:N	1:G:179:PRO:CD	2.81	0.43
1:A:206:LEU:HD12	1:A:206:LEU:C	2.43	0.43
1:B:146:ILE:HG23	1:B:147:PRO:HD2	1.90	0.43
1:B:171:PHE:HD1	1:B:263:PRO:HD2	1.83	0.43
1:C:486:ILE:HG22	1:C:516:VAL:HG22	1.99	0.43
1:D:43:ILE:O	1:D:43:ILE:HG13	2.18	0.43
1:D:680:THR:HG23	2:D:901:UDP:O1A	2.19	0.43
1:E:162:LEU:HD11	1:E:772:TRP:CD2	2.54	0.43
1:F:565:CYS:HB2	1:F:642:PHE:O	2.18	0.43
1:G:52:GLU:O	1:G:57:PRO:HD2	2.19	0.43
1:H:339:ARG:HH12	1:H:380:ILE:HG13	1.83	0.43
1:H:407:LYS:HB2	1:H:408:PRO:HD2	1.99	0.43
1:A:52:GLU:CD	1:A:53:PHE:N	2.76	0.43
1:A:60:THR:C	1:A:62:LYS:H	2.26	0.43
1:A:789:MET:CE	1:D:789:MET:HG2	2.49	0.43
1:B:400:LEU:C	1:B:400:LEU:HD12	2.43	0.43
1:C:143:ASN:HD22	1:C:780:ARG:HH22	1.65	0.43
1:C:176:SER:C	1:C:179:PRO:HD2	2.44	0.43
1:D:63:LYS:HE2	1:D:63:LYS:HB2	1.70	0.43
1:E:156:GLY:O	1:E:522:ASN:HA	2.19	0.43
1:E:585:LYS:HD3	1:E:585:LYS:HA	1.74	0.43
1:F:407:LYS:HB2	1:F:408:PRO:HD2	2.00	0.43
1:H:46:GLN:HB2	1:H:79:ALA:O	2.19	0.43
1:H:259:LEU:HD21	1:H:268:LEU:HA	2.00	0.43
1:A:582:ASP:C	1:A:582:ASP:OD1	2.61	0.43
1:B:67:GLY:HA2	1:B:68:PRO:HD3	1.81	0.43
1:B:130:ASN:ND2	1:B:506:GLY:H	2.17	0.43
1:C:512:HIS:CE1	1:C:515:ASP:HB2	2.53	0.43
1:C:683:GLU:OE2	2:C:901:UDP:O3'	2.32	0.43
1:D:27:ASN:N	1:D:27:ASN:ND2	2.67	0.43
1:D:493:VAL:HG23	1:D:497:GLU:CG	2.48	0.43
1:E:143:ASN:CB	1:E:148:ARG:NH2	2.66	0.43
1:F:177:LEU:HD22	1:F:260:LEU:HD23	2.01	0.43
1:G:437:ALA:O	1:G:438:HIS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:TYR:CE1	1:B:649:MET:CE	2.98	0.43
1:C:112:LEU:HD12	1:C:112:LEU:HA	1.87	0.43
1:C:163:ASN:O	1:C:167:SER:HB2	2.19	0.43
1:D:60:THR:O	1:D:63:LYS:CD	2.60	0.43
1:D:81:VAL:CG2	1:D:86:VAL:HG23	2.48	0.43
1:E:194:LEU:HD22	1:E:328:LEU:HD11	2.00	0.43
1:E:580:ARG:O	1:E:585:LYS:HG3	2.19	0.43
1:F:420:LEU:HD13	1:F:420:LEU:O	2.17	0.43
1:G:82:LEU:CB	1:G:83:PRO:CD	2.96	0.43
1:G:131:GLY:O	1:G:134:THR:HG23	2.18	0.43
1:H:243:GLY:HA2	1:H:326:GLN:HA	2.00	0.43
1:H:271:PHE:O	1:H:275:VAL:HG23	2.18	0.43
1:H:435:THR:CG2	1:H:475:THR:HB	2.49	0.43
1:A:69:PHE:O	1:A:73:LEU:HB2	2.19	0.43
1:A:580:ARG:HD3	2:A:901:UDP:O1B	2.18	0.43
1:B:249:VAL:O	1:B:253:ILE:HG13	2.19	0.43
1:C:65:GLU:O	1:C:70:PHE:HB2	2.18	0.43
1:C:216:TYR:HD2	1:C:232:LYS:HE2	1.83	0.43
1:E:86:VAL:O	1:E:102:VAL:HG12	2.18	0.43
1:E:438:HIS:O	1:E:439:ALA:HB2	2.19	0.43
1:E:730:LYS:HE3	6:E:921:MLA:HC22	2.00	0.43
1:F:116:GLU:HA	1:F:119:HIS:CD2	2.51	0.43
1:H:46:GLN:HB2	1:H:79:ALA:CB	2.37	0.43
1:H:437:ALA:O	1:H:438:HIS:HB2	2.19	0.43
1:H:479:ILE:HD11	1:H:762:LEU:HD13	2.01	0.43
1:A:72:LEU:C	1:A:72:LEU:CD1	2.92	0.43
1:A:146:ILE:HD11	1:A:162:LEU:HD13	2.00	0.43
1:C:564:LEU:HD12	1:C:564:LEU:HA	1.87	0.43
1:E:72:LEU:C	1:E:72:LEU:CD1	2.92	0.43
1:F:126:ASP:C	1:F:128:VAL:H	2.26	0.43
1:F:442:LYS:HD2	1:F:449:ASP:HB3	2.01	0.43
1:H:130:ASN:C	1:H:134:THR:HG21	2.44	0.43
1:A:348:THR:O	1:A:351:GLU:HG2	2.18	0.42
1:C:518:ASP:HA	1:C:519:PRO:HD3	1.86	0.42
1:D:310:ASP:HB3	1:D:755:TRP:CE2	2.54	0.42
1:D:443:THR:HG21	1:D:495:GLN:HA	2.00	0.42
1:E:355:ARG:HD2	1:E:359:SER:O	2.19	0.42
1:F:154:TYR:HA	1:F:157:ASN:HB2	2.01	0.42
1:F:281:VAL:HG21	1:F:319:MET:CE	2.33	0.42
1:F:386:TRP:N	1:F:387:PRO:HD2	2.34	0.42
1:F:491:GLU:CD	1:F:491:GLU:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:56:LEU:CD1	1:G:63:LYS:HG2	2.48	0.42
1:H:438:HIS:ND1	4:H:904[B]:NHF:C6	2.82	0.42
1:H:713:ASP:HA	1:H:714:PRO:HD2	1.83	0.42
1:A:156:GLY:HA3	1:A:523:ILE:HG13	2.00	0.42
1:A:449:ASP:HB2	1:A:504:LEU:HD23	2.00	0.42
1:C:239:GLU:HA	1:C:239:GLU:OE2	2.19	0.42
1:C:419:ASN:HB3	1:C:471:ALA:CB	2.49	0.42
1:C:536:TYR:OH	1:C:738:TRP:HZ3	2.02	0.42
1:D:694:THR:HG23	1:D:694:THR:O	2.19	0.42
1:E:453:LYS:HB2	1:E:453:LYS:HE2	1.78	0.42
1:E:782:GLU:HG3	1:H:141:PRO:HB2	2.01	0.42
1:F:313:ARG:HD3	1:F:357:TYR:O	2.19	0.42
1:H:407:LYS:HB2	1:H:408:PRO:HD3	2.02	0.42
1:H:778:LEU:HD12	1:H:778:LEU:HA	1.87	0.42
1:A:756:GLN:HG2	1:A:757:ILE:H	1.81	0.42
1:C:46:GLN:CB	1:C:50:ILE:CG1	2.97	0.42
1:D:103:ASN:CB	1:D:106:ALA:CB	2.81	0.42
1:D:163:ASN:O	1:D:167:SER:HB2	2.18	0.42
1:E:189:HIS:CE1	1:E:190:GLN:NE2	2.87	0.42
1:F:65:GLU:CA	1:F:68:PRO:CG	2.92	0.42
1:F:283:ILE:HG23	1:F:414:ASN:HD21	1.84	0.42
1:F:315:LEU:CG	1:F:319:MET:HE3	2.34	0.42
1:F:419:ASN:CG	1:F:435:THR:HB	2.44	0.42
1:F:437:ALA:C	1:F:439:ALA:N	2.77	0.42
1:G:41:LYS:CB	1:G:41:LYS:NZ	2.82	0.42
1:G:83:PRO:HB2	1:G:85:TRP:HB2	2.01	0.42
1:H:315:LEU:HG	1:H:319:MET:HE3	1.91	0.42
1:A:590:LEU:HB2	1:A:671:PRO:HG3	2.02	0.42
1:B:54:GLU:O	1:B:58:GLU:C	2.63	0.42
1:B:518:ASP:HA	1:B:519:PRO:HD3	1.93	0.42
1:D:148:ARG:HH11	1:D:148:ARG:CG	2.28	0.42
1:E:588:SER:CB	1:E:625:GLU:OE2	2.68	0.42
1:E:790:PHE:H	1:H:789:MET:HE1	1.85	0.42
1:F:83:PRO:CG	1:F:84:PRO:CD	2.96	0.42
1:G:80:ILE:HD13	1:G:117:PHE:CE2	2.54	0.42
1:H:31:ALA:CA	1:H:33:LEU:HD23	2.27	0.42
1:H:56:LEU:HB3	1:H:57:PRO:HD3	2.00	0.42
1:B:167:SER:OG	1:B:264:ASP:CA	2.67	0.42
1:B:394:GLU:O	1:B:397:ALA:HB3	2.19	0.42
1:C:315:LEU:HD13	1:C:762:LEU:HD23	2.02	0.42
2:D:901:UDP:O2A	4:D:904[B]:NHF:H3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:173:ASP:HB3	1:F:176:SER:HB2	1.96	0.42
1:F:410:LEU:HD12	1:F:411:ILE:H	1.84	0.42
1:G:149:PRO:HG2	1:G:517:PHE:O	2.19	0.42
1:G:315:LEU:C	1:G:319:MET:HE3	2.44	0.42
1:H:341:LEU:HA	1:H:342:PRO:HD3	1.89	0.42
1:A:279:PHE:HB2	1:A:409:ASP:OD2	2.19	0.42
1:B:518:ASP:CG	1:B:520:LYS:HG2	2.44	0.42
1:B:794:LYS:HD3	1:B:794:LYS:C	2.43	0.42
1:C:178:LEU:HB2	1:C:179:PRO:HD3	2.01	0.42
1:C:320:LEU:HD21	1:C:332:PRO:HG3	2.02	0.42
1:C:386:TRP:N	1:C:387:PRO:HD2	2.34	0.42
1:C:400:LEU:C	1:C:400:LEU:CD1	2.92	0.42
1:C:542:ARG:CZ	1:C:659:ARG:HB3	2.50	0.42
1:C:566:VAL:CG1	1:C:567:LEU:N	2.83	0.42
1:C:756:GLN:HG2	1:C:757:ILE:HD13	2.01	0.42
1:D:125:VAL:CG1	1:D:126:ASP:N	2.82	0.42
1:F:43:ILE:HG23	1:F:44:LEU:CD2	2.48	0.42
1:F:68:PRO:C	1:F:70:PHE:H	2.27	0.42
1:F:665:LYS:HD3	1:F:665:LYS:HA	1.69	0.42
1:F:796:ARG:HB2	1:F:797:PRO:HD3	2.01	0.42
1:G:35:ARG:O	1:G:38:ALA:HB3	2.20	0.42
1:G:692:PHE:CD1	1:G:692:PHE:N	2.87	0.42
1:H:544:THR:HA	1:H:547:HIS:ND1	2.35	0.42
1:A:128:VAL:HG23	1:A:129:LYS:O	2.19	0.42
1:A:565:CYS:HB2	1:A:642:PHE:O	2.19	0.42
1:B:320:LEU:CD2	1:B:332:PRO:HG3	2.50	0.42
1:C:34:SER:N	1:C:59:GLN:HE22	2.18	0.42
1:C:49:ILE:HD13	1:C:49:ILE:H	1.84	0.42
1:C:130:ASN:HB3	1:C:134:THR:OG1	2.19	0.42
1:C:162:LEU:HD11	1:C:772:TRP:CD2	2.54	0.42
1:C:514:ILE:HG13	1:C:515:ASP:N	2.34	0.42
1:C:756:GLN:HG2	1:C:757:ILE:H	1.81	0.42
1:E:65:GLU:O	1:E:66:GLY:C	2.59	0.42
1:F:176:SER:O	1:F:179:PRO:HD2	2.20	0.42
1:F:284:LEU:N	1:F:284:LEU:HD22	2.35	0.42
1:G:80:ILE:CD1	1:G:117:PHE:CZ	3.03	0.42
1:G:83:PRO:CG	1:G:85:TRP:HB2	2.50	0.42
1:H:137:LEU:HD11	1:H:790:PHE:CZ	2.54	0.42
1:H:303:GLY:N	2:H:901:UDP:H5'1	2.35	0.42
1:C:50:ILE:O	1:C:54:GLU:CB	2.63	0.42
1:C:170:LEU:HD22	1:C:177:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ALA:HB3	1:C:295:VAL:HG11	2.01	0.42
1:C:315:LEU:HG	1:C:319:MET:HE2	2.00	0.42
1:D:373:LYS:HB2	1:D:373:LYS:HE3	1.85	0.42
1:D:577:THR:HG22	1:D:608:VAL:HG22	2.02	0.42
1:E:290:PHE:CD1	1:E:290:PHE:C	2.98	0.42
1:F:195:MET:HE1	1:F:252:MET:HE1	2.02	0.42
1:F:400:LEU:C	1:F:400:LEU:CD1	2.92	0.42
1:F:461:PHE:HB3	1:F:465:PHE:CE2	2.54	0.42
1:G:780:ARG:HD2	1:G:780:ARG:HA	1.79	0.42
1:B:641:GLN:N	1:B:641:GLN:CD	2.77	0.42
1:C:45:GLN:HB2	1:C:80:ILE:HA	2.01	0.42
1:C:440:LEU:HD12	1:C:495:GLN:HB3	2.02	0.42
1:C:796:ARG:O	1:C:800:GLN:HG3	2.20	0.42
1:D:570:LYS:O	1:D:570:LYS:HG2	2.19	0.42
1:E:160:ASP:O	1:E:164:ARG:HG3	2.20	0.42
1:E:763:LEU:HD23	1:E:763:LEU:HA	1.83	0.42
1:F:83:PRO:HG2	1:F:84:PRO:HD2	2.02	0.42
1:F:632:LEU:HD23	1:F:632:LEU:HA	1.86	0.42
1:G:41:LYS:H	1:G:41:LYS:HG2	1.54	0.42
1:G:43:ILE:O	1:G:44:LEU:CB	2.68	0.42
1:G:81:VAL:HG22	1:G:86:VAL:CB	2.49	0.42
1:G:585:LYS:NZ	2:G:901:UDP:O1B	2.36	0.42
1:H:83:PRO:CB	1:H:84:PRO:CD	2.86	0.42
1:H:221:LYS:HE2	1:H:221:LYS:HB3	1.82	0.42
1:H:242:TRP:HA	1:H:252:MET:CE	2.50	0.42
1:B:484:GLN:HG2	1:B:698:GLY:HA2	2.02	0.42
1:B:583:ARG:HG2	1:B:583:ARG:HH11	1.85	0.42
1:C:150:THR:N	1:D:261:GLU:OE1	2.53	0.42
1:C:441:GLU:HG2	1:C:464:GLN:NE2	2.34	0.42
1:D:103:ASN:HD22	1:D:108:VAL:HG11	1.85	0.42
1:E:45:GLN:CB	1:E:79:ALA:O	2.68	0.42
1:E:56:LEU:HB3	1:E:57:PRO:CD	2.50	0.42
1:E:566:VAL:HG12	1:E:567:LEU:N	2.35	0.42
1:F:43:ILE:CG2	1:F:44:LEU:HD23	2.49	0.42
1:F:466:THR:HG23	1:F:790:PHE:CZ	2.55	0.42
1:A:793:LEU:HB3	1:D:793:LEU:HB3	2.02	0.41
1:B:284:LEU:O	1:B:414:ASN:HB2	2.19	0.41
1:C:49:ILE:O	1:C:53:PHE:N	2.48	0.41
1:C:217:LEU:HD11	1:C:249:VAL:HG11	2.01	0.41
1:C:692:PHE:HZ	1:C:727:PHE:CG	2.38	0.41
1:D:65:GLU:O	1:D:66:GLY:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:HIS:ND1	1:D:129:LYS:CB	2.83	0.41
1:D:146:ILE:CG1	1:D:772:TRP:CZ2	3.03	0.41
1:D:181:LEU:HD12	1:D:196:LEU:CD1	2.50	0.41
1:D:688:GLY:O	1:D:690:PRO:HD3	2.20	0.41
1:E:146:ILE:HG22	1:E:147:PRO:N	2.35	0.41
1:E:665:LYS:HD3	1:E:665:LYS:HA	1.82	0.41
1:G:81:VAL:CG2	1:G:86:VAL:HG23	2.47	0.41
1:G:125:VAL:HG13	1:G:126:ASP:OD1	2.19	0.41
1:G:387:PRO:HD3	1:G:802:VAL:HB	2.02	0.41
1:G:420:LEU:HD13	1:G:420:LEU:C	2.44	0.41
1:A:35:ARG:HE	1:A:102:VAL:CB	2.32	0.41
1:A:514:ILE:HG13	1:A:515:ASP:N	2.35	0.41
1:A:789:MET:HE2	1:D:789:MET:CG	2.49	0.41
1:D:125:VAL:CG1	1:D:126:ASP:H	2.33	0.41
1:E:462:SER:HB2	1:E:507:LEU:HD21	2.02	0.41
1:E:789:MET:HG3	1:H:135:LEU:HD21	2.01	0.41
1:F:716:HIS:HB3	5:F:913:SO4:O4	2.20	0.41
1:F:789:MET:HE1	1:G:786:TYR:O	2.21	0.41
1:G:125:VAL:HG13	1:G:126:ASP:N	2.34	0.41
1:G:195:MET:HE2	1:G:275:VAL:HG22	2.01	0.41
1:H:564:LEU:HD12	1:H:564:LEU:HA	1.82	0.41
1:A:636:TYR:O	1:A:637:LYS:C	2.63	0.41
1:B:178:LEU:N	1:B:179:PRO:HD2	2.35	0.41
1:B:257:LEU:HA	1:B:260:LEU:HD12	2.02	0.41
1:B:772:TRP:CZ2	1:B:776:SER:HB3	2.55	0.41
1:C:410:LEU:HD12	1:C:411:ILE:H	1.85	0.41
1:C:574:ILE:O	1:C:666:GLY:HA3	2.20	0.41
1:C:682:VAL:HG13	1:C:749:ILE:HD12	2.02	0.41
1:C:794:LYS:O	1:C:794:LYS:HD3	2.21	0.41
1:E:102:VAL:O	1:E:102:VAL:HG13	2.20	0.41
1:E:338:THR:CG2	1:E:366:ARG:HG2	2.49	0.41
1:F:68:PRO:C	1:F:70:PHE:N	2.78	0.41
1:G:146:ILE:HD11	1:G:772:TRP:CZ2	2.55	0.41
1:G:673:LEU:HD23	1:G:714:PRO:HB2	2.03	0.41
1:A:37:GLU:OE2	1:A:59:GLN:NE2	2.54	0.41
1:A:80:ILE:O	1:A:86:VAL:HG22	2.21	0.41
1:A:677:PHE:HB3	4:A:904[B]:NHF:O4	2.20	0.41
1:C:339:ARG:O	1:C:366:ARG:HG2	2.20	0.41
1:D:50:ILE:O	1:D:53:PHE:CB	2.69	0.41
1:E:113:GLN:HB3	1:E:114:PRO:CD	2.51	0.41
1:E:259:LEU:O	1:E:263:PRO:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:ALA:O	1:F:56:LEU:C	2.62	0.41
1:F:91:ARG:HD2	1:F:97:TRP:CZ2	2.55	0.41
1:F:415:TYR:HA	1:F:437:ALA:O	2.20	0.41
1:F:633:ILE:HA	1:F:638:LEU:HD12	2.02	0.41
1:G:438:HIS:O	1:G:439:ALA:HB2	2.20	0.41
1:G:462:SER:HB2	1:G:507:LEU:HD21	2.02	0.41
1:H:46:GLN:NE2	1:H:50:ILE:HG21	2.35	0.41
1:B:178:LEU:N	1:B:179:PRO:CD	2.84	0.41
1:C:72:LEU:HD13	1:C:73:LEU:N	2.36	0.41
1:C:221:LYS:HE2	1:C:221:LYS:HB3	1.85	0.41
1:E:560:ASN:OD1	1:E:562:GLU:HB2	2.20	0.41
1:G:660:TYR:O	1:G:663:ASP:HB2	2.21	0.41
1:A:534:PHE:HB2	1:A:535:PRO:HD2	2.03	0.41
1:B:143:ASN:CB	1:B:780:ARG:NH1	2.83	0.41
1:B:756:GLN:NE2	1:B:757:ILE:HD11	2.35	0.41
1:C:157:ASN:O	1:C:160:ASP:HB2	2.20	0.41
1:D:290:PHE:CD1	1:D:290:PHE:C	2.99	0.41
1:D:387:PRO:HD3	1:D:802:VAL:HB	2.01	0.41
1:E:386:TRP:CH2	1:E:464:GLN:HG3	2.55	0.41
1:E:386:TRP:CZ2	1:E:464:GLN:HG3	2.56	0.41
1:E:622:GLU:O	1:E:626:MET:HG3	2.21	0.41
1:E:772:TRP:CZ2	1:E:776:SER:CB	3.03	0.41
1:F:276:PRO:HG3	1:F:326:GLN:CG	2.44	0.41
1:G:290:PHE:HB3	1:G:338:THR:HG21	2.01	0.41
1:G:442:LYS:HD2	1:G:449:ASP:HB3	2.02	0.41
1:H:130:ASN:HD21	1:H:506:GLY:N	2.00	0.41
1:H:415:TYR:HA	1:H:437:ALA:O	2.20	0.41
1:A:794:LYS:C	1:A:797:PRO:HD2	2.45	0.41
1:B:609:VAL:HA	1:B:645:ILE:O	2.20	0.41
1:C:420:LEU:C	1:C:420:LEU:CD1	2.94	0.41
1:E:43:ILE:HA	1:E:81:VAL:O	2.20	0.41
1:E:56:LEU:HD22	1:E:56:LEU:HA	1.86	0.41
1:E:546:PHE:CG	1:E:653:ARG:HG3	2.56	0.41
1:F:128:VAL:HG13	1:F:129:LYS:O	2.21	0.41
1:F:419:ASN:HB3	1:F:471:ALA:HB1	2.03	0.41
1:G:333:ARG:HG2	1:G:333:ARG:HH11	1.85	0.41
1:H:400:LEU:HD13	1:H:404:LEU:HD12	2.01	0.41
1:H:415:TYR:O	1:H:419:ASN:ND2	2.54	0.41
1:H:534:PHE:HB2	1:H:535:PRO:HD2	2.03	0.41
1:H:534:PHE:O	1:H:687:CYS:HA	2.20	0.41
1:A:85:TRP:CG	1:A:101:ARG:HD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HD11	1:A:772:TRP:CE3	2.56	0.41
1:A:320:LEU:CD2	1:A:332:PRO:HG3	2.51	0.41
1:A:581:LEU:HG	1:A:625:GLU:HG2	2.03	0.41
1:A:777:ASN:OD1	1:A:778:LEU:HD12	2.21	0.41
1:B:93:ARG:HB2	1:B:96:VAL:CG2	2.51	0.41
1:C:65:GLU:C	1:C:67:GLY:N	2.79	0.41
1:C:534:PHE:CB	1:C:535:PRO:CD	2.93	0.41
1:D:612:ASP:OD1	1:D:614:ARG:NH1	2.54	0.41
1:F:216:TYR:HE2	1:F:232:LYS:HG2	1.82	0.41
1:F:276:PRO:HG3	1:F:326:GLN:CB	2.51	0.41
1:G:195:MET:O	1:G:239:GLU:N	2.53	0.41
1:H:49:ILE:HD11	1:H:696:LYS:HZ3	1.84	0.41
1:H:82:LEU:HD21	1:H:120:PHE:HZ	1.84	0.41
1:H:277:MET:HE2	1:H:277:MET:HB3	1.84	0.41
1:H:772:TRP:CZ2	1:H:776:SER:HB3	2.56	0.41
1:A:69:PHE:O	1:A:69:PHE:CD1	2.74	0.41
1:A:142:PHE:O	1:A:780:ARG:NH1	2.54	0.41
1:A:437:ALA:O	1:A:438:HIS:HB2	2.21	0.41
1:B:87:ALA:HB2	1:B:120:PHE:CD2	2.50	0.41
1:B:212:LYS:HE2	1:B:232:LYS:HZ1	1.86	0.41
1:B:292:GLN:OE1	1:B:357:TYR:N	2.46	0.41
1:B:518:ASP:OD1	1:B:519:PRO:HD2	2.21	0.41
1:C:69:PHE:HE1	1:C:73:LEU:CG	2.34	0.41
1:C:159:VAL:HG21	1:C:765:LEU:HD23	2.03	0.41
1:C:719:GLN:HG3	5:C:913:SO4:O1	2.21	0.41
1:D:69:PHE:CD1	1:D:69:PHE:O	2.74	0.41
1:D:166:LEU:HA	1:D:166:LEU:HD23	1.77	0.41
1:D:565:CYS:HB2	1:D:642:PHE:O	2.21	0.41
1:E:30:LEU:HD23	1:E:30:LEU:HA	1.94	0.41
1:E:178:LEU:N	1:E:179:PRO:HD2	2.35	0.41
1:F:63:LYS:O	1:F:64:LEU:C	2.64	0.41
1:F:469:ILE:HD13	1:F:469:ILE:HA	1.93	0.41
1:G:86:VAL:HG12	1:G:104:LEU:CD2	2.51	0.41
1:G:407:LYS:CB	1:G:408:PRO:CD	2.91	0.41
1:G:469:ILE:HD13	1:G:469:ILE:HA	1.89	0.41
1:A:172:HIS:CE1	1:B:147:PRO:HB2	2.56	0.41
1:C:538:GLU:OE1	1:C:541:ARG:HD3	2.21	0.41
1:D:455:LEU:HA	1:D:455:LEU:HD23	1.83	0.41
1:D:564:LEU:HD12	1:D:564:LEU:HA	1.80	0.41
1:E:61:ARG:HH11	1:E:61:ARG:HG3	1.86	0.41
1:F:194:LEU:HD22	1:F:328:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:716:HIS:HB3	5:F:913:SO4:O2	2.21	0.41
1:F:789:MET:HE3	1:G:789:MET:CG	2.51	0.41
1:G:341:LEU:HA	1:G:342:PRO:HD3	1.87	0.41
1:H:77:GLN:O	1:H:78:GLU:CB	2.67	0.41
1:H:195:MET:HE1	1:H:252:MET:HE1	2.02	0.41
1:H:252:MET:HE3	1:H:252:MET:HB3	1.97	0.41
1:H:796:ARG:O	1:H:800:GLN:HG3	2.21	0.41
1:A:60:THR:OG1	1:A:61:ARG:N	2.54	0.40
1:B:137:LEU:HD11	1:B:790:PHE:CE1	2.55	0.40
1:B:174:LYS:N	1:B:174:LYS:CD	2.84	0.40
1:C:536:TYR:CD1	1:C:662:CYS:HB3	2.56	0.40
1:D:80:ILE:HG23	1:D:124:LEU:HD22	2.03	0.40
1:D:514:ILE:HG13	1:D:515:ASP:H	1.85	0.40
1:E:547:HIS:O	1:E:551:GLU:HG3	2.21	0.40
1:G:80:ILE:HD13	1:G:117:PHE:CZ	2.56	0.40
1:G:261:GLU:HG2	1:H:151:LEU:HD12	2.03	0.40
1:G:518:ASP:CG	1:G:520:LYS:HG2	2.46	0.40
1:G:574:ILE:O	1:G:666:GLY:HA3	2.20	0.40
1:H:178:LEU:N	1:H:179:PRO:HD2	2.36	0.40
1:A:135:LEU:HD13	1:D:789:MET:HA	2.03	0.40
1:B:415:TYR:CG	1:B:416:SER:N	2.88	0.40
1:D:52:GLU:O	1:D:53:PHE:C	2.63	0.40
1:D:113:GLN:HG3	1:D:114:PRO:HD2	2.02	0.40
1:D:146:ILE:HG22	1:D:147:PRO:N	2.36	0.40
1:D:178:LEU:HD23	1:D:178:LEU:HA	1.91	0.40
1:D:284:LEU:HD13	1:D:337:LEU:HB2	2.02	0.40
1:D:692:PHE:CG	1:D:724:LEU:HD21	2.57	0.40
1:E:30:LEU:HD23	1:E:33:LEU:HD12	2.03	0.40
1:E:394:GLU:OE2	1:H:132:ASN:CG	2.65	0.40
1:F:243:GLY:HA2	1:F:326:GLN:HA	2.02	0.40
1:G:159:VAL:HG13	1:G:160:ASP:N	2.36	0.40
1:G:677:PHE:HB3	4:G:904[B]:NHF:H4	2.02	0.40
1:G:781:LEU:HD12	1:G:781:LEU:HA	1.75	0.40
1:H:146:ILE:HD11	1:H:165:HIS:CD2	2.57	0.40
1:H:322:ARG:HD2	1:H:763:LEU:HD12	2.02	0.40
1:B:171:PHE:CD1	1:B:263:PRO:HD2	2.57	0.40
1:B:438:HIS:HB3	4:B:904[B]:NHF:O5	2.21	0.40
1:B:789:MET:CB	1:C:789:MET:CE	2.85	0.40
1:C:32:LEU:HD13	1:C:32:LEU:C	2.47	0.40
1:C:46:GLN:CB	1:C:50:ILE:HG12	2.51	0.40
1:C:342:PRO:HB2	1:C:377:ARG:NH2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:ASP:CG	1:C:377:ARG:HE	2.29	0.40
1:C:483:PHE:CZ	1:C:487:ALA:HB3	2.55	0.40
1:C:630:TYR:O	1:C:633:ILE:HB	2.21	0.40
1:D:230:GLU:O	1:D:234:GLU:HG3	2.20	0.40
1:F:65:GLU:C	1:F:68:PRO:HG2	2.46	0.40
1:F:174:LYS:H	1:F:174:LYS:HD2	1.86	0.40
1:G:81:VAL:HG22	1:G:86:VAL:HB	2.04	0.40
1:G:221:LYS:HB3	1:G:221:LYS:HE2	1.66	0.40
1:G:702:ILE:HG23	1:G:753:TYR:CE2	2.56	0.40
1:H:484:GLN:HG3	1:H:485:GLU:N	2.36	0.40
1:A:156:GLY:O	1:A:522:ASN:HA	2.20	0.40
1:A:172:HIS:ND1	1:B:147:PRO:CG	2.85	0.40
1:A:419:ASN:HB3	1:A:471:ALA:HB1	2.03	0.40
1:A:435:THR:HG23	1:A:475:THR:CB	2.52	0.40
1:B:243:GLY:HA2	1:B:326:GLN:HA	2.03	0.40
1:B:283:ILE:C	1:B:284:LEU:HD22	2.46	0.40
1:B:778:LEU:HA	1:B:778:LEU:HD12	1.73	0.40
1:C:544:THR:O	1:C:547:HIS:HB2	2.20	0.40
1:C:565:CYS:C	1:C:566:VAL:HG23	2.46	0.40
1:C:616:GLU:HA	1:C:616:GLU:OE1	2.21	0.40
1:D:140:GLU:N	1:D:141:PRO:CD	2.85	0.40
1:D:210:LEU:HB2	1:D:257:LEU:HD21	2.04	0.40
1:E:298:TYR:CE1	1:E:649:MET:HE1	2.55	0.40
1:G:82:LEU:H	1:G:82:LEU:HG	1.68	0.40
1:H:425:LEU:HD23	1:H:425:LEU:HA	1.76	0.40
1:H:543:LEU:CA	1:H:545:LYS:HE3	2.41	0.40
1:A:472:MET:HE3	1:A:472:MET:HB2	1.88	0.40
1:B:657:LEU:O	1:B:661:ILE:HG12	2.21	0.40
1:C:178:LEU:N	1:C:179:PRO:HD2	2.36	0.40
1:C:212:LYS:HE2	1:C:232:LYS:NZ	2.36	0.40
1:C:284:LEU:HD13	1:C:337:LEU:HB2	2.04	0.40
1:C:597:ASN:OD1	1:C:597:ASN:C	2.64	0.40
1:C:717:GLY:O	1:C:720:ALA:HB3	2.21	0.40
1:C:758:TYR:CD1	1:C:758:TYR:C	3.00	0.40
1:D:348:THR:O	1:D:351:GLU:HG2	2.20	0.40
1:D:518:ASP:CG	1:D:520:LYS:HG2	2.46	0.40
1:E:30:LEU:HD21	1:E:62:LYS:CB	2.51	0.40
1:F:482:THR:HB	1:F:701:GLU:CD	2.46	0.40
1:H:59:GLN:HG2	1:H:60:THR:N	2.36	0.40
1:H:578:MET:O	1:H:579:ALA:HB2	2.21	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	779/816 (96%)	741 (95%)	37 (5%)	1 (0%)	48	77
1	B	778/816 (95%)	724 (93%)	52 (7%)	2 (0%)	36	66
1	C	779/816 (96%)	739 (95%)	40 (5%)	0	100	100
1	D	779/816 (96%)	741 (95%)	38 (5%)	0	100	100
1	E	779/816 (96%)	742 (95%)	35 (4%)	2 (0%)	36	66
1	F	779/816 (96%)	737 (95%)	39 (5%)	3 (0%)	30	60
1	G	779/816 (96%)	743 (95%)	36 (5%)	0	100	100
1	H	778/816 (95%)	736 (95%)	40 (5%)	2 (0%)	36	66
All	All	6230/6528 (95%)	5903 (95%)	317 (5%)	10 (0%)	43	72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	29	VAL
1	B	56	LEU
1	F	63	LYS
1	A	83	PRO
1	E	63	LYS
1	F	43	ILE
1	B	108	VAL
1	E	43	ILE
1	H	83	PRO
1	F	49	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	670/718 (93%)	636 (95%)	34 (5%)	21	54
1	B	635/718 (88%)	601 (95%)	34 (5%)	20	51
1	C	673/718 (94%)	641 (95%)	32 (5%)	23	56
1	D	671/718 (94%)	632 (94%)	39 (6%)	18	49
1	E	668/718 (93%)	634 (95%)	34 (5%)	21	54
1	F	672/718 (94%)	639 (95%)	33 (5%)	22	55
1	G	674/718 (94%)	642 (95%)	32 (5%)	23	57
1	H	658/718 (92%)	615 (94%)	43 (6%)	15	43
All	All	5321/5744 (93%)	5040 (95%)	281 (5%)	20	52

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	46	GLN
1	A	49	ILE
1	A	54	GLU
1	A	59	GLN
1	A	65	GLU
1	A	72	LEU
1	A	86	VAL
1	A	100	LEU
1	A	140	GLU
1	A	148	ARG
1	A	174	LYS
1	A	216	TYR
1	A	253	ILE
1	A	258	ASP
1	A	285	SER
1	A	322	ARG
1	A	345	VAL
1	A	358	ASP
1	A	375	ILE
1	A	420	LEU
1	A	484	GLN
1	A	491	GLU
1	A	493	VAL

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Mol	Chain	Res	Type
1	A	516	VAL
1	A	545	LYS
1	A	556	SER
1	A	572	LYS
1	A	602	GLU
1	A	670	GLN
1	A	759	SER
1	A	777	ASN
1	A	781	LEU
1	A	794	LYS
1	B	43	ILE
1	B	45	GLN
1	B	46	GLN
1	B	60	THR
1	B	82	LEU
1	B	99	TYR
1	B	125	VAL
1	B	140	GLU
1	B	143	ASN
1	B	148	ARG
1	B	167	SER
1	B	248	ARG
1	B	251	ASP
1	B	252	MET
1	B	258	ASP
1	B	285	SER
1	B	337	LEU
1	B	450	ILE
1	B	484	GLN
1	B	493	VAL
1	B	498	SER
1	B	516	VAL
1	B	545	LYS
1	B	556	SER
1	B	572	LYS
1	B	602	GLU
1	B	623	LYS
1	B	712	ILE
1	B	722	ASP
1	B	743	LYS
1	B	759	SER
1	B	773	LYS

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Mol	Chain	Res	Type
1	B	777	ASN
1	B	778	LEU
1	C	39	LYS
1	C	43	ILE
1	C	45	GLN
1	C	46	GLN
1	C	49	ILE
1	C	50	ILE
1	C	56	LEU
1	C	65	GLU
1	C	72	LEU
1	C	75	SER
1	C	119	HIS
1	C	128	VAL
1	C	148	ARG
1	C	174	LYS
1	C	252	MET
1	C	258	ASP
1	C	322	ARG
1	C	345	VAL
1	C	375	ILE
1	C	420	LEU
1	C	484	GLN
1	C	491	GLU
1	C	493	VAL
1	C	516	VAL
1	C	545	LYS
1	C	556	SER
1	C	646	SER
1	C	692	PHE
1	C	702	ILE
1	C	756	GLN
1	C	759	SER
1	C	778	LEU
1	D	27	ASN
1	D	30	LEU
1	D	32	LEU
1	D	39	LYS
1	D	44	LEU
1	D	52	GLU
1	D	63	LYS
1	D	72	LEU

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Mol	Chain	Res	Type
1	D	76	THR
1	D	105	HIS
1	D	111	GLU
1	D	119	HIS
1	D	120	PHE
1	D	140	GLU
1	D	148	ARG
1	D	174	LYS
1	D	216	TYR
1	D	258	ASP
1	D	284	LEU
1	D	285	SER
1	D	322	ARG
1	D	340	LEU
1	D	345	VAL
1	D	358	ASP
1	D	412	ILE
1	D	484	GLN
1	D	491	GLU
1	D	516	VAL
1	D	545	LYS
1	D	556	SER
1	D	563	HIS
1	D	564	LEU
1	D	572	LYS
1	D	602	GLU
1	D	623	LYS
1	D	708	SER
1	D	759	SER
1	D	773	LYS
1	D	778	LEU
1	E	30	LEU
1	E	32	LEU
1	E	44	LEU
1	E	45	GLN
1	E	50	ILE
1	E	54	GLU
1	E	56	LEU
1	E	59	GLN
1	E	72	LEU
1	E	82	LEU
1	E	112	LEU

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Mol	Chain	Res	Type
1	E	119	HIS
1	E	132	ASN
1	E	136	GLU
1	E	140	GLU
1	E	148	ARG
1	E	167	SER
1	E	174	LYS
1	E	178	LEU
1	E	285	SER
1	E	322	ARG
1	E	328	LEU
1	E	358	ASP
1	E	375	ILE
1	E	463	CYS
1	E	484	GLN
1	E	491	GLU
1	E	516	VAL
1	E	545	LYS
1	E	572	LYS
1	E	664	THR
1	E	759	SER
1	E	773	LYS
1	E	778	LEU
1	F	32	LEU
1	F	46	GLN
1	F	52	GLU
1	F	54	GLU
1	F	56	LEU
1	F	60	THR
1	F	69	PHE
1	F	70	PHE
1	F	74	LYS
1	F	80	ILE
1	F	105	HIS
1	F	128	VAL
1	F	140	GLU
1	F	148	ARG
1	F	174	LYS
1	F	252	MET
1	F	253	ILE
1	F	258	ASP
1	F	322	ARG

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Mol	Chain	Res	Type
1	F	340	LEU
1	F	345	VAL
1	F	375	ILE
1	F	412	ILE
1	F	420	LEU
1	F	436	ILE
1	F	484	GLN
1	F	516	VAL
1	F	545	LYS
1	F	572	LYS
1	F	708	SER
1	F	759	SER
1	F	773	LYS
1	F	781	LEU
1	G	32	LEU
1	G	41	LYS
1	G	45	GLN
1	G	49	ILE
1	G	50	ILE
1	G	54	GLU
1	G	82	LEU
1	G	90	VAL
1	G	125	VAL
1	G	148	ARG
1	G	174	LYS
1	G	205	THR
1	G	216	TYR
1	G	258	ASP
1	G	322	ARG
1	G	340	LEU
1	G	345	VAL
1	G	358	ASP
1	G	375	ILE
1	G	420	LEU
1	G	484	GLN
1	G	491	GLU
1	G	493	VAL
1	G	516	VAL
1	G	545	LYS
1	G	556	SER
1	G	563	HIS
1	G	664	THR

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Mol	Chain	Res	Type
1	G	708	SER
1	G	759	SER
1	G	773	LYS
1	G	781	LEU
1	H	32	LEU
1	H	34	SER
1	H	45	GLN
1	H	46	GLN
1	H	56	LEU
1	H	72	LEU
1	H	73	LEU
1	H	99	TYR
1	H	112	LEU
1	H	125	VAL
1	H	134	THR
1	H	145	SER
1	H	146	ILE
1	H	148	ARG
1	H	178	LEU
1	H	251	ASP
1	H	252	MET
1	H	337	LEU
1	H	358	ASP
1	H	375	ILE
1	H	420	LEU
1	H	425	LEU
1	H	450	ILE
1	H	484	GLN
1	H	491	GLU
1	H	493	VAL
1	H	516	VAL
1	H	545	LYS
1	H	556	SER
1	H	561	LYS
1	H	563	HIS
1	H	565	CYS
1	H	572	LYS
1	H	649	MET
1	H	708	SER
1	H	722	ASP
1	H	743	LYS
1	H	750	GLU

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Mol	Chain	Res	Type
1	H	757	ILE
1	H	759	SER
1	H	777	ASN
1	H	778	LEU
1	H	781	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	59	GLN
1	A	189	HIS
1	A	190	GLN
1	A	405	ASN
1	A	460	HIS
1	A	484	GLN
1	A	495	GLN
1	A	512	HIS
1	A	563	HIS
1	A	711	HIS
1	A	774	HIS
1	B	130	ASN
1	B	132	ASN
1	B	163	ASN
1	B	207	GLN
1	B	287	HIS
1	B	294	ASN
1	B	427	HIS
1	B	433	GLN
1	B	605	ASN
1	B	670	GLN
1	B	774	HIS
1	B	777	ASN
1	C	45	GLN
1	C	47	ASN
1	C	59	GLN
1	C	119	HIS
1	C	132	ASN
1	C	143	ASN
1	C	189	HIS
1	C	190	GLN
1	C	287	HIS

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Mol	Chain	Res	Type
1	C	292	GLN
1	C	464	GLN
1	C	512	HIS
1	C	737	HIS
1	C	777	ASN
1	D	46	GLN
1	D	48	GLN
1	D	103	ASN
1	D	105	HIS
1	D	143	ASN
1	D	208	HIS
1	D	287	HIS
1	D	460	HIS
1	D	512	HIS
1	D	547	HIS
1	E	59	GLN
1	E	77	GLN
1	E	143	ASN
1	E	189	HIS
1	E	190	GLN
1	E	512	HIS
1	F	46	GLN
1	F	48	GLN
1	F	59	GLN
1	F	119	HIS
1	F	157	ASN
1	F	190	GLN
1	F	294	ASN
1	F	414	ASN
1	F	484	GLN
1	F	495	GLN
1	F	512	HIS
1	F	711	HIS
1	G	45	GLN
1	G	46	GLN
1	G	48	GLN
1	G	59	GLN
1	G	103	ASN
1	G	105	HIS
1	G	119	HIS
1	G	143	ASN
1	G	157	ASN

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Mol	Chain	Res	Type
1	G	165	HIS
1	G	189	HIS
1	G	460	HIS
1	G	484	GLN
1	G	495	GLN
1	G	605	ASN
1	G	705	HIS
1	G	711	HIS
1	G	716	HIS
1	G	774	HIS
1	H	46	GLN
1	H	119	HIS
1	H	130	ASN
1	H	460	HIS
1	H	512	HIS
1	H	605	ASN
1	H	777	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](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 64 ligands modelled in this entry, 8 are monoatomic - leaving 56 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
5	SO4	D	913	-	4,4,4	0.30	0	6,6,6	0.13	0
5	SO4	D	911	-	4,4,4	0.34	0	6,6,6	0.25	0
5	SO4	B	912	-	4,4,4	0.26	0	6,6,6	0.16	0
6	MLA	C	921	-	6,6,6	1.25	0	7,7,7	1.41	1 (14%)
2	UDP	C	901	-	25,26,26	0.97	0	38,40,40	1.57	5 (13%)
6	MLA	G	921	-	6,6,6	1.20	0	7,7,7	1.26	0
5	SO4	D	912	-	4,4,4	0.26	0	6,6,6	0.23	0
6	MLA	F	921	-	6,6,6	1.12	0	7,7,7	1.51	1 (14%)
6	MLA	B	921	-	6,6,6	1.31	0	7,7,7	1.26	0
5	SO4	H	911	-	4,4,4	0.28	0	6,6,6	0.20	0
6	MLA	H	921	-	6,6,6	1.14	0	7,7,7	1.46	0
3	LCN	A	903[A]	-	11,11,11	2.08	2 (18%)	11,15,15	2.45	3 (27%)
4	NHF	C	904[B]	-	11,11,11	1.86	4 (36%)	11,15,15	0.70	0
2	UDP	D	901	-	25,26,26	1.04	0	38,40,40	1.94	8 (21%)
4	NHF	A	904[B]	-	11,11,11	1.70	4 (36%)	11,15,15	0.93	0
2	UDP	H	901	-	25,26,26	1.03	1 (4%)	38,40,40	1.82	6 (15%)
5	SO4	E	912	-	4,4,4	0.30	0	6,6,6	0.07	0
2	UDP	G	901	-	25,26,26	1.04	1 (4%)	38,40,40	1.52	6 (15%)
5	SO4	F	912	-	4,4,4	0.28	0	6,6,6	0.21	0
2	UDP	A	901	-	25,26,26	0.98	0	38,40,40	1.71	6 (15%)
4	NHF	F	904[B]	-	11,11,11	1.87	4 (36%)	11,15,15	0.74	0
5	SO4	C	913	-	4,4,4	0.30	0	6,6,6	0.06	0
6	MLA	E	921	-	6,6,6	1.33	0	7,7,7	0.95	0
3	LCN	D	903[A]	-	11,11,11	2.05	4 (36%)	11,15,15	2.32	3 (27%)
3	LCN	C	903[A]	-	11,11,11	2.08	3 (27%)	11,15,15	2.75	3 (27%)
3	LCN	B	903[A]	-	11,11,11	1.97	3 (27%)	11,15,15	2.79	2 (18%)
5	SO4	F	911	-	4,4,4	0.29	0	6,6,6	0.30	0
5	SO4	E	911	-	4,4,4	0.32	0	6,6,6	0.36	0
5	SO4	A	913	-	4,4,4	0.33	0	6,6,6	0.10	0
5	SO4	A	911	-	4,4,4	0.30	0	6,6,6	0.26	0
6	MLA	D	921	-	6,6,6	1.31	0	7,7,7	1.12	0
5	SO4	G	913	-	4,4,4	0.27	0	6,6,6	0.16	0
4	NHF	D	904[B]	-	11,11,11	1.80	4 (36%)	11,15,15	1.66	1 (9%)
5	SO4	F	913	-	4,4,4	0.31	0	6,6,6	0.17	0
5	SO4	H	912	-	4,4,4	0.33	0	6,6,6	0.06	0
5	SO4	E	913	-	4,4,4	0.30	0	6,6,6	0.13	0
3	LCN	F	903[A]	-	11,11,11	2.01	3 (27%)	11,15,15	2.93	3 (27%)
4	NHF	B	904[B]	-	11,11,11	1.90	5 (45%)	11,15,15	1.01	1 (9%)
5	SO4	G	912	-	4,4,4	0.30	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NHF	G	904[B]	-	11,11,11	1.87	4 (36%)	11,15,15	0.62	0
5	SO4	G	911	-	4,4,4	0.36	0	6,6,6	0.14	0
2	UDP	E	901	-	25,26,26	0.99	1 (4%)	38,40,40	1.67	7 (18%)
3	LCN	E	903[A]	-	11,11,11	1.98	1 (9%)	11,15,15	2.91	2 (18%)
5	SO4	A	912	-	4,4,4	0.29	0	6,6,6	0.20	0
2	UDP	B	901	-	25,26,26	0.99	1 (4%)	38,40,40	1.87	7 (18%)
4	NHF	E	904[B]	-	11,11,11	1.82	3 (27%)	11,15,15	0.68	0
2	UDP	F	901	-	25,26,26	1.03	1 (4%)	38,40,40	1.69	6 (15%)
5	SO4	H	913	-	4,4,4	0.32	0	6,6,6	0.10	0
6	MLA	A	921	-	6,6,6	1.15	0	7,7,7	1.32	0
3	LCN	H	903[A]	-	11,11,11	2.01	3 (27%)	11,15,15	2.53	2 (18%)
5	SO4	B	913	-	4,4,4	0.31	0	6,6,6	0.23	0
5	SO4	B	911	-	4,4,4	0.41	0	6,6,6	0.21	0
5	SO4	C	911	-	4,4,4	0.25	0	6,6,6	0.25	0
4	NHF	H	904[B]	-	11,11,11	1.76	3 (27%)	11,15,15	0.81	1 (9%)
5	SO4	C	912	-	4,4,4	0.28	0	6,6,6	0.13	0
3	LCN	G	903[A]	-	11,11,11	2.03	3 (27%)	11,15,15	2.78	2 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MLA	C	921	-	-	2/4/4/4	-
2	UDP	C	901	-	-	5/16/32/32	0/2/2/2
6	MLA	G	921	-	-	0/4/4/4	-
6	MLA	F	921	-	-	4/4/4/4	-
6	MLA	B	921	-	-	0/4/4/4	-
6	MLA	H	921	-	-	1/4/4/4	-
3	LCN	A	903[A]	-	-	0/2/19/19	0/1/1/1
4	NHF	C	904[B]	-	-	2/2/19/19	0/1/1/1
2	UDP	D	901	-	-	5/16/32/32	0/2/2/2
4	NHF	A	904[B]	-	-	2/2/19/19	0/1/1/1
2	UDP	H	901	-	-	2/16/32/32	0/2/2/2
2	UDP	G	901	-	-	1/16/32/32	0/2/2/2
2	UDP	A	901	-	-	5/16/32/32	0/2/2/2
4	NHF	F	904[B]	-	-	2/2/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MLA	E	921	-	-	0/4/4/4	-
3	LCN	D	903[A]	-	-	2/2/19/19	0/1/1/1
3	LCN	C	903[A]	-	-	1/2/19/19	0/1/1/1
3	LCN	B	903[A]	-	-	0/2/19/19	0/1/1/1
6	MLA	D	921	-	-	2/4/4/4	-
4	NHF	D	904[B]	-	-	1/2/19/19	0/1/1/1
3	LCN	F	903[A]	-	-	0/2/19/19	0/1/1/1
4	NHF	B	904[B]	-	-	1/2/19/19	0/1/1/1
4	NHF	G	904[B]	-	-	0/2/19/19	0/1/1/1
2	UDP	E	901	-	-	3/16/32/32	0/2/2/2
3	LCN	E	903[A]	-	-	1/2/19/19	0/1/1/1
2	UDP	B	901	-	-	4/16/32/32	0/2/2/2
4	NHF	E	904[B]	-	-	1/2/19/19	0/1/1/1
2	UDP	F	901	-	-	4/16/32/32	0/2/2/2
6	MLA	A	921	-	-	2/4/4/4	-
3	LCN	H	903[A]	-	-	0/2/19/19	0/1/1/1
4	NHF	H	904[B]	-	-	1/2/19/19	0/1/1/1
3	LCN	G	903[A]	-	-	0/2/19/19	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903[A]	LCN	O5-C5	-5.12	1.39	1.44
3	C	903[A]	LCN	O5-C5	-4.98	1.39	1.44
3	E	903[A]	LCN	O5-C5	-4.96	1.39	1.44
3	G	903[A]	LCN	O5-C5	-4.93	1.39	1.44
3	H	903[A]	LCN	O5-C5	-4.90	1.39	1.44
3	D	903[A]	LCN	O5-C5	-4.75	1.39	1.44
3	F	903[A]	LCN	O5-C5	-4.69	1.39	1.44
3	B	903[A]	LCN	O5-C5	-4.48	1.39	1.44
4	B	904[B]	NHF	C4-C3	-2.88	1.49	1.53
4	G	904[B]	NHF	O5-C5	-2.85	1.37	1.43
4	E	904[B]	NHF	O5-C5	-2.75	1.38	1.43
4	F	904[B]	NHF	O5-C5	-2.72	1.38	1.43
4	D	904[B]	NHF	C4-C3	-2.72	1.49	1.53
4	F	904[B]	NHF	C4-C3	-2.68	1.49	1.53
4	H	904[B]	NHF	O5-C5	-2.67	1.38	1.43
4	C	904[B]	NHF	O5-C5	-2.63	1.38	1.43
4	A	904[B]	NHF	O5-C5	-2.63	1.38	1.43
3	F	903[A]	LCN	C4-C3	-2.59	1.49	1.53
3	B	903[A]	LCN	C4-C3	-2.55	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	904[B]	NHF	C4-C3	-2.54	1.49	1.53
4	C	904[B]	NHF	C4-C3	-2.52	1.49	1.53
4	B	904[B]	NHF	O5-C5	-2.50	1.38	1.43
4	B	904[B]	NHF	O5-C1	-2.44	1.37	1.43
4	C	904[B]	NHF	O5-C1	-2.37	1.38	1.43
4	E	904[B]	NHF	O5-C1	-2.34	1.38	1.43
4	E	904[B]	NHF	C4-C3	-2.34	1.49	1.53
4	F	904[B]	NHF	O5-C1	-2.34	1.38	1.43
4	H	904[B]	NHF	C4-C3	-2.34	1.49	1.53
4	G	904[B]	NHF	O5-C1	-2.33	1.38	1.43
4	A	904[B]	NHF	O5-C1	-2.30	1.38	1.43
4	D	904[B]	NHF	O5-C5	-2.29	1.39	1.43
4	D	904[B]	NHF	O5-C1	-2.27	1.38	1.43
3	C	903[A]	LCN	O4-C4	-2.27	1.37	1.43
3	D	903[A]	LCN	O4-C4	-2.26	1.37	1.43
4	H	904[B]	NHF	O5-C1	-2.25	1.38	1.43
3	F	903[A]	LCN	O4-C4	-2.24	1.37	1.43
2	G	901	UDP	C5-C4	-2.23	1.38	1.43
3	A	903[A]	LCN	O4-C4	-2.22	1.37	1.43
3	G	903[A]	LCN	C4-C3	-2.21	1.50	1.53
3	B	903[A]	LCN	O4-C4	-2.19	1.37	1.43
2	E	901	UDP	C5-C4	-2.19	1.39	1.43
4	A	904[B]	NHF	C4-C3	-2.11	1.50	1.53
4	D	904[B]	NHF	C1-C2	-2.11	1.49	1.51
2	F	901	UDP	O4'-C4'	-2.11	1.40	1.45
2	H	901	UDP	PA-O3A	2.09	1.61	1.59
3	H	903[A]	LCN	O4-C4	-2.09	1.37	1.43
3	G	903[A]	LCN	O4-C4	-2.07	1.37	1.43
4	B	904[B]	NHF	C3-C2	-2.07	1.49	1.52
3	D	903[A]	LCN	O5-C1	2.07	1.39	1.35
4	F	904[B]	NHF	O3-C3	-2.07	1.38	1.42
4	C	904[B]	NHF	O3-C3	-2.05	1.38	1.42
3	C	903[A]	LCN	C4-C3	-2.05	1.50	1.53
4	G	904[B]	NHF	O3-C3	-2.05	1.38	1.42
4	B	904[B]	NHF	O3-C3	-2.04	1.38	1.42
3	H	903[A]	LCN	C3-C2	2.03	1.52	1.50
3	D	903[A]	LCN	C3-C2	2.03	1.52	1.50
2	B	901	UDP	C5-C4	-2.01	1.39	1.43
4	A	904[B]	NHF	O3-C3	-2.01	1.38	1.42

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	903[A]	LCN	O5-C1-C2	-8.53	117.21	125.57
2	D	901	UDP	C4-N3-C2	-7.20	117.67	126.61
3	F	903[A]	LCN	O5-C1-C2	-7.10	118.62	125.57
3	C	903[A]	LCN	O5-C1-C2	-6.81	118.90	125.57
3	G	903[A]	LCN	O5-C1-C2	-6.73	118.97	125.57
2	B	901	UDP	C4-N3-C2	-6.69	118.31	126.61
2	H	901	UDP	C4-N3-C2	-6.64	118.37	126.61
3	H	903[A]	LCN	O5-C1-C2	-6.42	119.28	125.57
2	A	901	UDP	C4-N3-C2	-6.28	118.81	126.61
2	F	901	UDP	C4-N3-C2	-6.23	118.87	126.61
3	B	903[A]	LCN	O5-C1-C2	-6.16	119.54	125.57
3	B	903[A]	LCN	C5-O5-C1	5.86	124.66	115.62
3	A	903[A]	LCN	O5-C1-C2	-5.84	119.85	125.57
2	E	901	UDP	C4-N3-C2	-5.81	119.40	126.61
2	C	901	UDP	C4-N3-C2	-5.70	119.53	126.61
3	F	903[A]	LCN	C5-O5-C1	5.58	124.23	115.62
3	G	903[A]	LCN	C5-O5-C1	5.49	124.10	115.62
3	C	903[A]	LCN	C5-O5-C1	5.28	123.78	115.62
2	G	901	UDP	C4-N3-C2	-5.22	120.14	126.61
3	D	903[A]	LCN	O5-C1-C2	-5.19	120.48	125.57
2	B	901	UDP	N3-C2-N1	5.01	121.42	114.89
3	A	903[A]	LCN	C5-O5-C1	4.94	123.25	115.62
2	A	901	UDP	N3-C2-N1	4.89	121.25	114.89
2	D	901	UDP	N3-C2-N1	4.81	121.15	114.89
2	D	901	UDP	C5-C4-N3	4.78	121.50	114.80
2	F	901	UDP	N3-C2-N1	4.73	121.05	114.89
3	H	903[A]	LCN	C5-O5-C1	4.66	122.81	115.62
3	D	903[A]	LCN	C5-O5-C1	4.44	122.47	115.62
2	H	901	UDP	N3-C2-N1	4.41	120.63	114.89
2	C	901	UDP	N3-C2-N1	4.33	120.52	114.89
2	F	901	UDP	C5-C4-N3	4.23	120.72	114.80
4	D	904[B]	NHF	C1-O5-C5	4.18	117.54	111.67
2	H	901	UDP	C5-C4-N3	4.00	120.41	114.80
2	G	901	UDP	N3-C2-N1	3.98	120.07	114.89
2	E	901	UDP	N3-C2-N1	3.98	120.07	114.89
2	B	901	UDP	C5-C4-N3	3.93	120.30	114.80
2	A	901	UDP	C5-C4-N3	3.67	119.94	114.80
2	E	901	UDP	C5-C4-N3	3.61	119.85	114.80
3	E	903[A]	LCN	C5-O5-C1	3.59	121.17	115.62
2	C	901	UDP	C5-C4-N3	3.58	119.81	114.80
2	B	901	UDP	O4-C4-C5	-3.44	119.23	125.16
2	G	901	UDP	C5-C4-N3	3.35	119.49	114.80
2	H	901	UDP	O4-C4-C5	-3.32	119.43	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	901	UDP	O2-C2-N1	-3.07	118.80	122.80
2	D	901	UDP	O4-C4-C5	-3.07	119.87	125.16
2	G	901	UDP	O4-C4-C5	-2.88	120.20	125.16
2	D	901	UDP	O2A-PA-O3A	2.87	115.04	107.27
2	E	901	UDP	O2-C2-N1	-2.87	119.06	122.80
2	E	901	UDP	O4-C4-C5	-2.83	120.28	125.16
3	D	903[A]	LCN	O5-C5-C6	2.73	111.47	107.01
2	A	901	UDP	O2-C2-N1	-2.72	119.25	122.80
2	A	901	UDP	O4-C4-C5	-2.65	120.59	125.16
2	C	901	UDP	O4-C4-C5	-2.63	120.62	125.16
2	E	901	UDP	O2B-PB-O3A	2.57	113.24	104.64
2	D	901	UDP	O2-C2-N1	-2.52	119.52	122.80
2	H	901	UDP	O2A-PA-O3A	2.51	114.05	107.27
2	B	901	UDP	C1'-N1-C2	2.49	122.06	117.59
4	B	904[B]	NHF	C1-O5-C5	2.29	114.89	111.67
2	B	901	UDP	O2-C2-N1	-2.29	119.82	122.80
2	D	901	UDP	C5-C6-N1	-2.25	118.18	121.84
2	G	901	UDP	O2-C2-N1	-2.24	119.88	122.80
2	F	901	UDP	O4-C4-C5	-2.22	121.33	125.16
2	F	901	UDP	O2B-PB-O3A	2.22	112.07	104.64
6	C	921	MLA	O3B-C3-C2	2.12	121.09	114.51
2	G	901	UDP	O3B-PB-O3A	2.12	111.75	104.64
2	C	901	UDP	O2-C2-N1	-2.11	120.06	122.80
2	B	901	UDP	O3B-PB-O3A	2.08	111.62	104.64
2	E	901	UDP	C5-C6-N1	-2.06	118.48	121.84
2	F	901	UDP	C5-C6-N1	-2.05	118.50	121.84
2	A	901	UDP	O2B-PB-O3A	2.05	111.52	104.64
3	F	903[A]	LCN	O4-C4-C3	-2.05	105.58	109.64
6	F	921	MLA	O1A-C1-C2	2.05	120.85	114.51
3	A	903[A]	LCN	O5-C5-C6	2.04	110.34	107.01
2	D	901	UDP	O2B-PB-O3A	2.03	111.43	104.64
3	C	903[A]	LCN	O5-C5-C6	2.01	110.29	107.01
4	H	904[B]	NHF	C1-O5-C5	2.00	114.48	111.67

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	UDP	PA-O3A-PB-O2B
2	A	901	UDP	PA-O3A-PB-O3B
2	D	901	UDP	PA-O3A-PB-O2B
3	D	903[A]	LCN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	904[B]	NHF	O5-C5-C6-O6
3	D	903[A]	LCN	C4-C5-C6-O6
2	E	901	UDP	O4'-C4'-C5'-O5'
4	C	904[B]	NHF	C4-C5-C6-O6
4	A	904[B]	NHF	O5-C5-C6-O6
4	F	904[B]	NHF	C4-C5-C6-O6
2	E	901	UDP	C3'-C4'-C5'-O5'
4	D	904[B]	NHF	O5-C5-C6-O6
4	A	904[B]	NHF	C4-C5-C6-O6
2	A	901	UDP	C3'-C4'-C5'-O5'
2	B	901	UDP	C3'-C4'-C5'-O5'
2	B	901	UDP	O4'-C4'-C5'-O5'
4	E	904[B]	NHF	O5-C5-C6-O6
2	A	901	UDP	O4'-C4'-C5'-O5'
2	C	901	UDP	O4'-C4'-C5'-O5'
4	B	904[B]	NHF	O5-C5-C6-O6
2	C	901	UDP	C3'-C4'-C5'-O5'
4	H	904[B]	NHF	O5-C5-C6-O6
2	D	901	UDP	O4'-C4'-C5'-O5'
4	F	904[B]	NHF	O5-C5-C6-O6
2	D	901	UDP	C3'-C4'-C5'-O5'
2	F	901	UDP	C3'-C4'-C5'-O5'
2	F	901	UDP	O4'-C4'-C5'-O5'
6	D	921	MLA	O1A-C1-C2-C3
2	A	901	UDP	PB-O3A-PA-O5'
2	B	901	UDP	PB-O3A-PA-O5'
2	E	901	UDP	PB-O3A-PA-O5'
6	D	921	MLA	O1B-C1-C2-C3
2	C	901	UDP	PA-O3A-PB-O1B
2	F	901	UDP	PA-O3A-PB-O2B
2	F	901	UDP	PA-O3A-PB-O3B
3	C	903[A]	LCN	C4-C5-C6-O6
6	A	921	MLA	O1B-C1-C2-C3
6	F	921	MLA	O1B-C1-C2-C3
6	A	921	MLA	O1A-C1-C2-C3
6	C	921	MLA	O1A-C1-C2-C3
3	E	903[A]	LCN	C4-C5-C6-O6
2	B	901	UDP	PA-O3A-PB-O1B
2	H	901	UDP	PB-O3A-PA-O1A
6	C	921	MLA	O1B-C1-C2-C3
6	F	921	MLA	O1A-C1-C2-C3
2	D	901	UDP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	C	901	UDP	PA-O3A-PB-O2B
2	C	901	UDP	PA-O3A-PB-O3B
2	D	901	UDP	PA-O3A-PB-O3B
2	H	901	UDP	PB-O3A-PA-O2A
6	F	921	MLA	C1-C2-C3-O3A
6	H	921	MLA	O1B-C1-C2-C3
6	F	921	MLA	C1-C2-C3-O3B
2	G	901	UDP	PB-O3A-PA-O2A

There are no ring outliers.

33 monomers are involved in 57 short contacts:

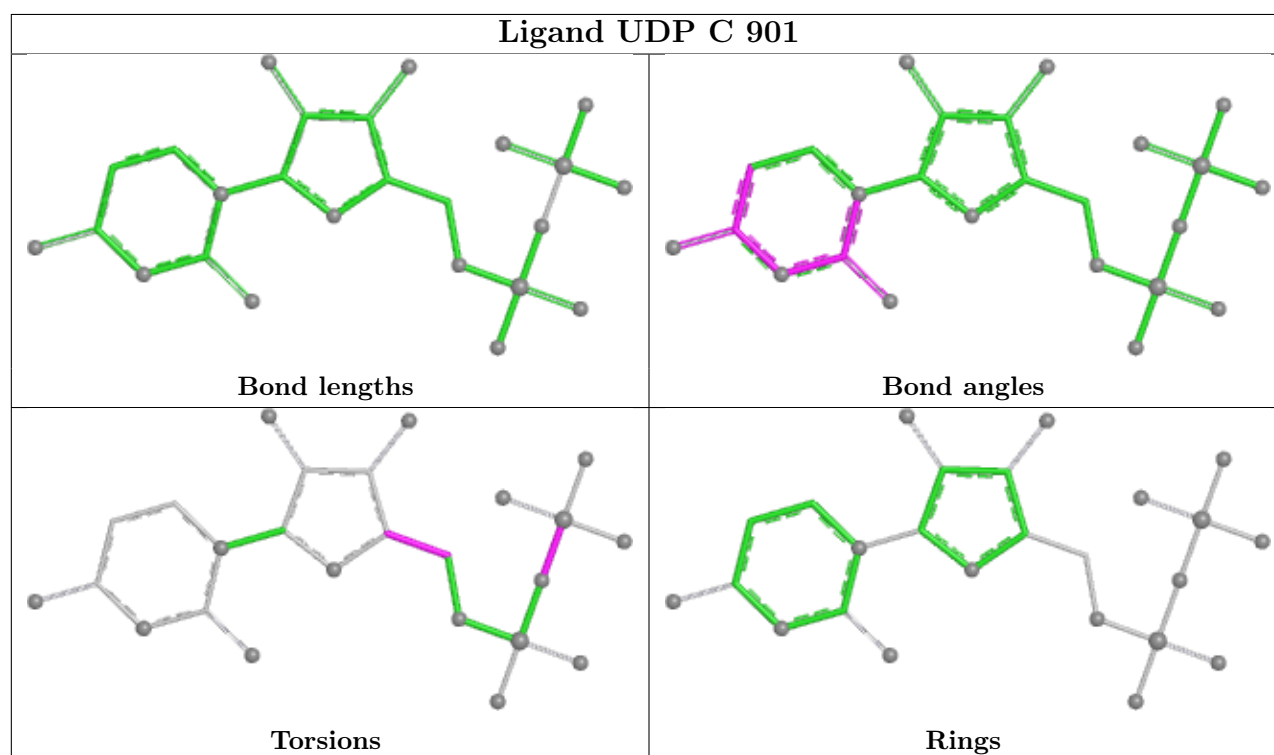
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	913	SO4	2	0
5	B	912	SO4	1	0
2	C	901	UDP	1	0
6	F	921	MLA	1	0
3	A	903[A]	LCN	1	0
4	C	904[B]	NHF	1	0
2	D	901	UDP	4	0
4	A	904[B]	NHF	2	0
2	H	901	UDP	4	0
5	E	912	SO4	1	0
2	G	901	UDP	4	0
5	F	912	SO4	2	0
2	A	901	UDP	3	0
5	C	913	SO4	1	0
6	E	921	MLA	1	0
3	D	903[A]	LCN	1	0
5	A	913	SO4	1	0
5	G	913	SO4	1	0
4	D	904[B]	NHF	6	0
5	F	913	SO4	3	0
3	F	903[A]	LCN	1	0
4	B	904[B]	NHF	2	0
5	G	912	SO4	1	0
4	G	904[B]	NHF	1	0
2	E	901	UDP	1	0
5	A	912	SO4	2	0
2	B	901	UDP	1	0
4	E	904[B]	NHF	2	0
2	F	901	UDP	1	0

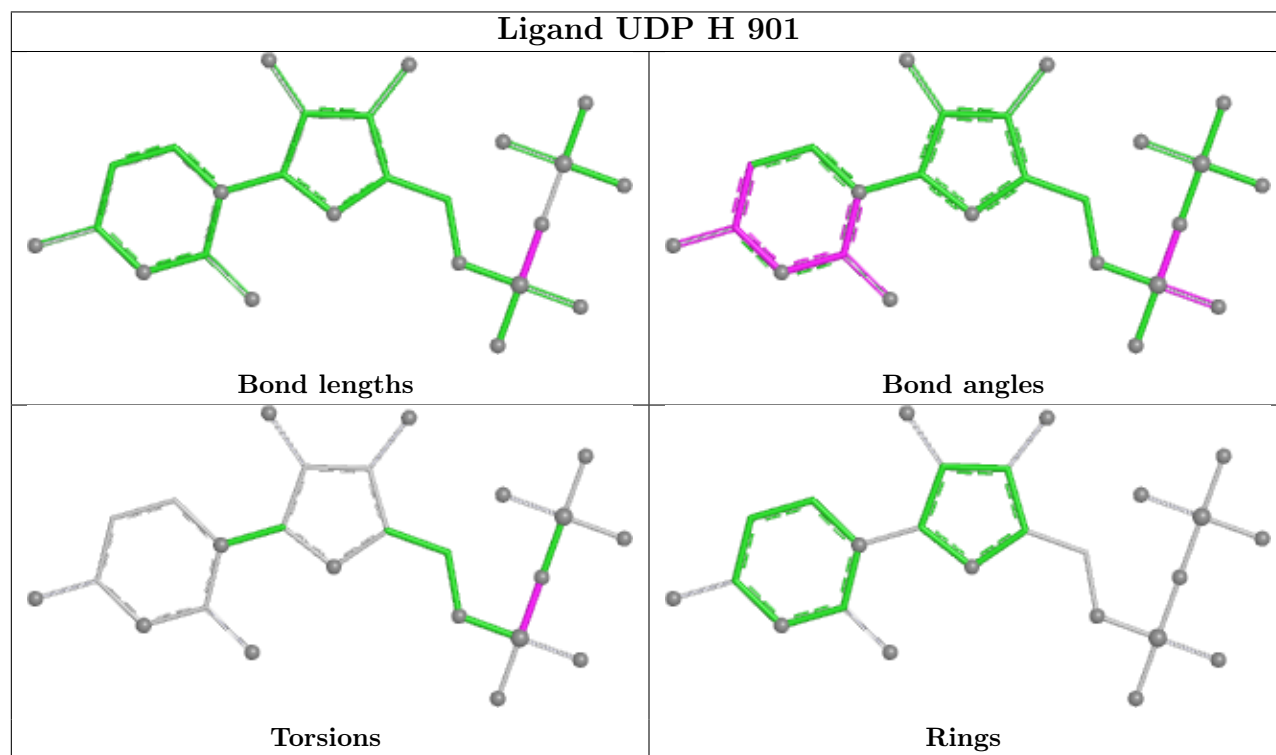
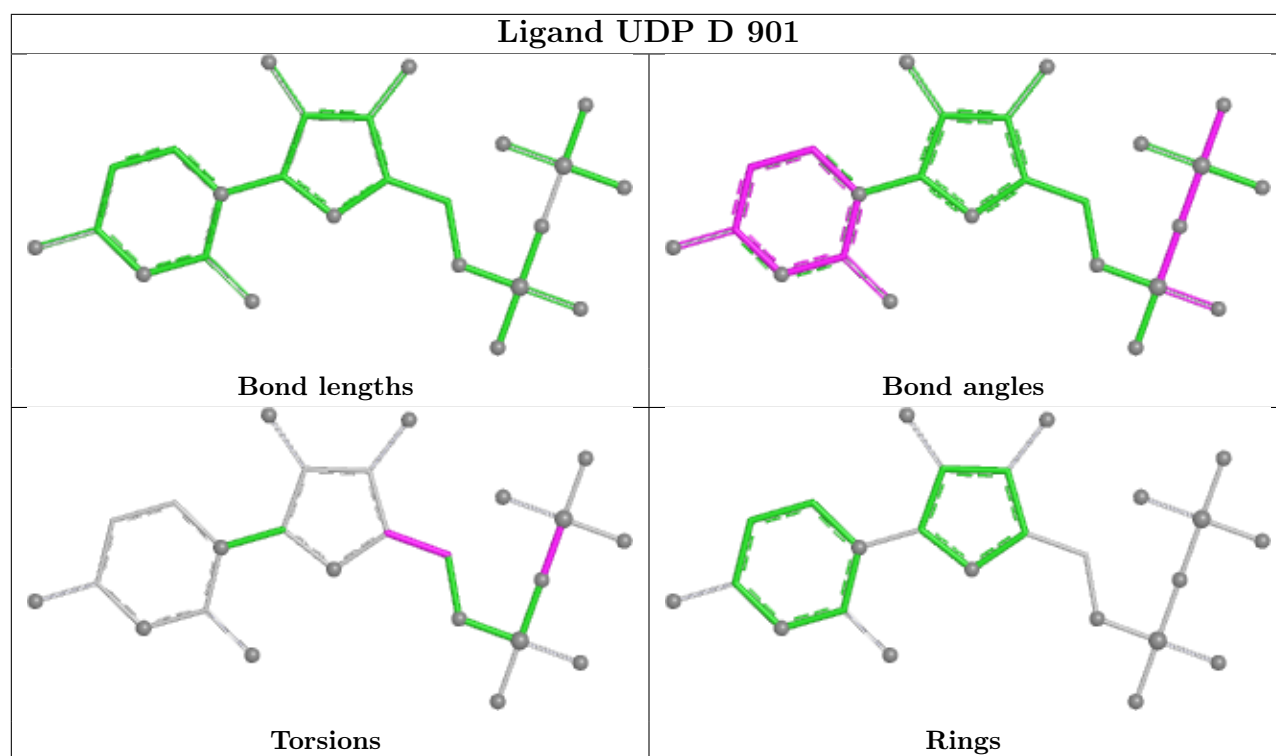
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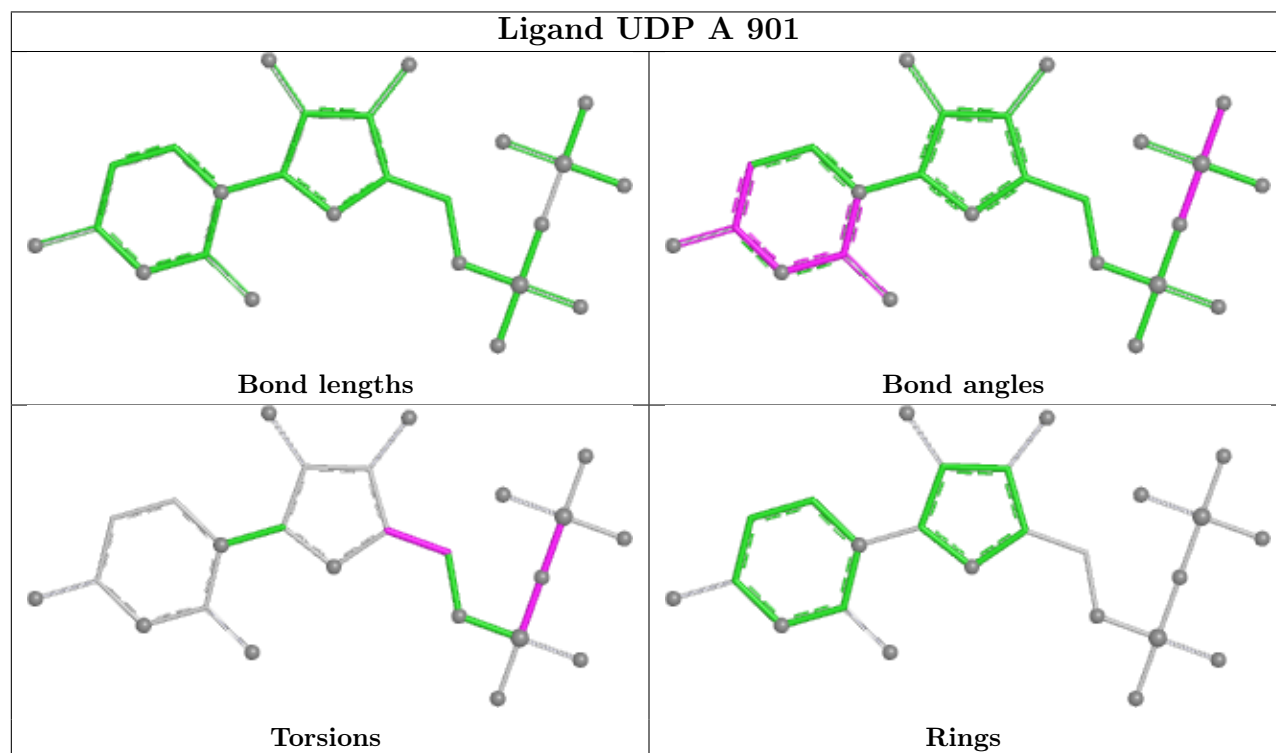
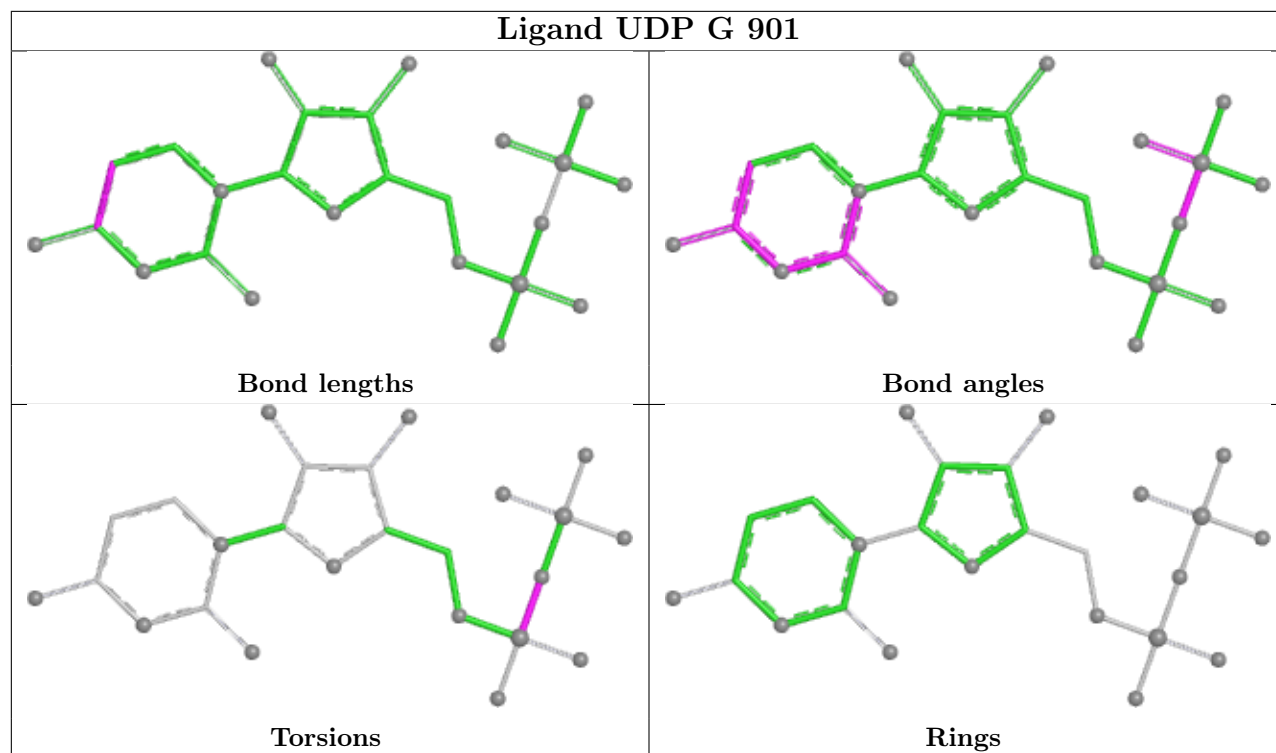
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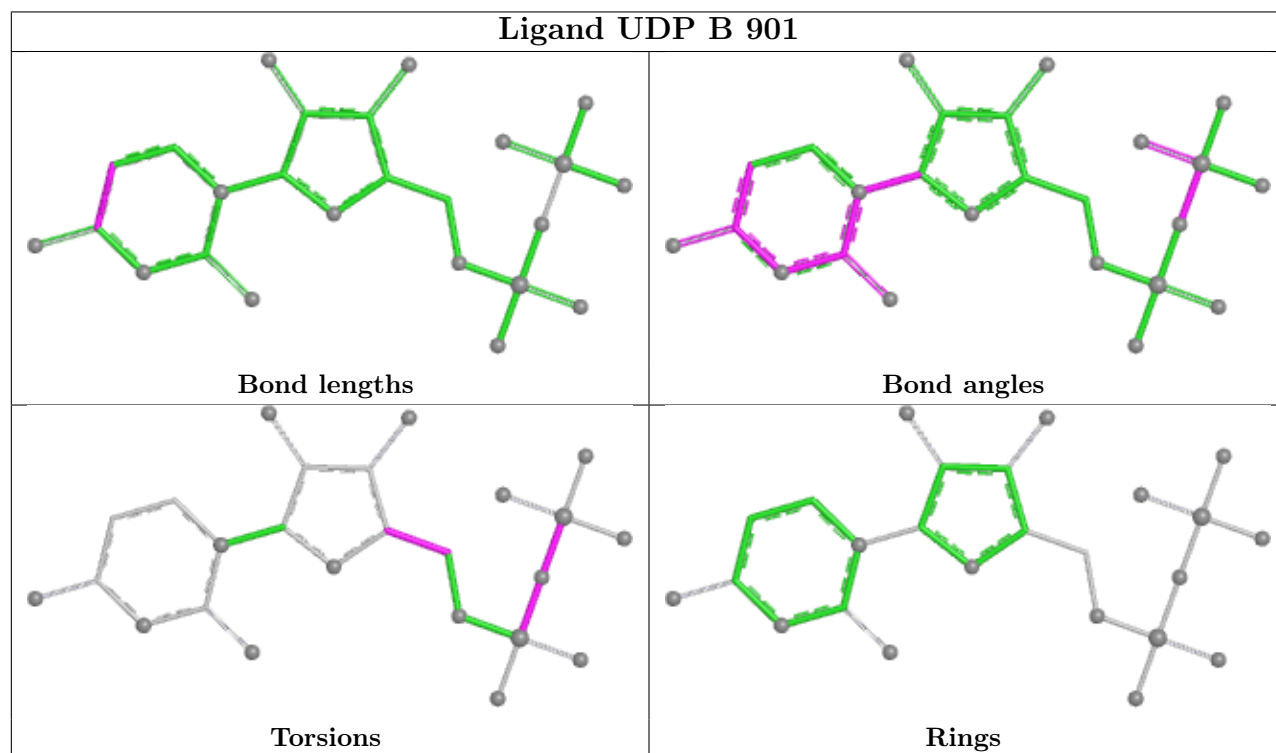
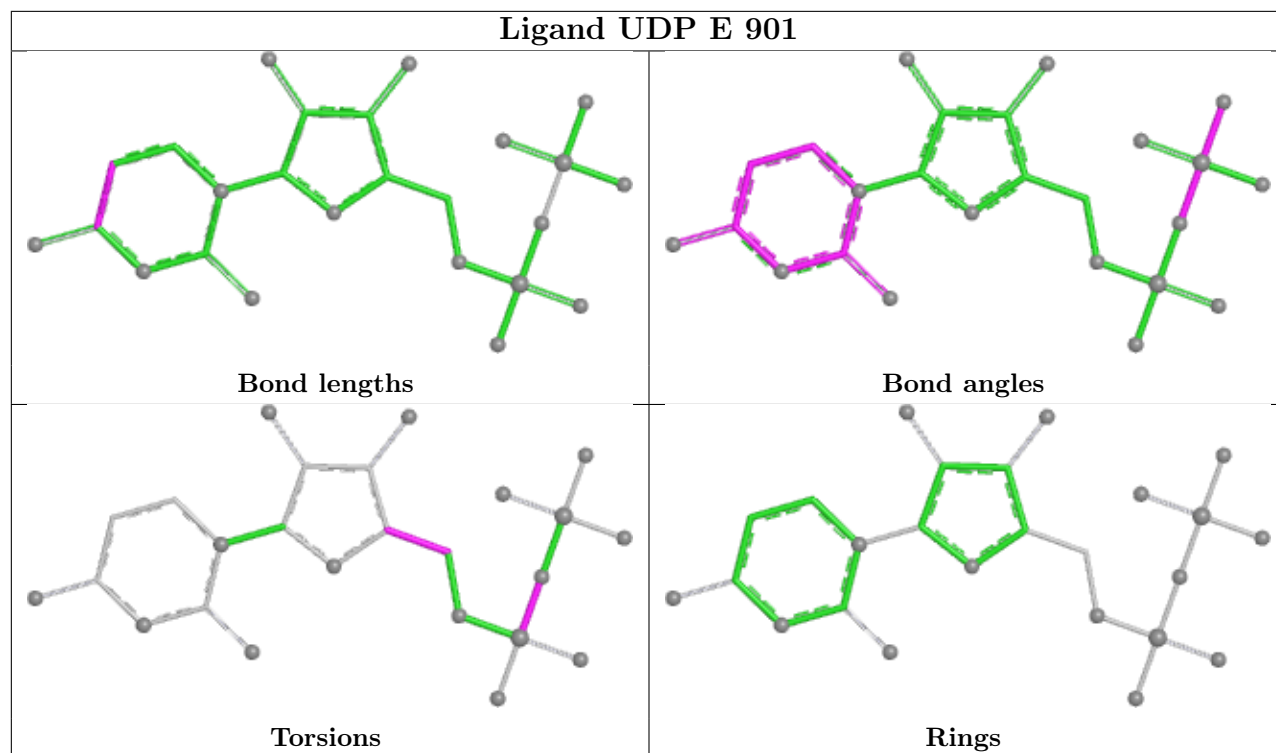
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	913	SO4	1	0
5	B	913	SO4	4	0
4	H	904[B]	NHF	4	0
3	G	903[A]	LCN	1	0

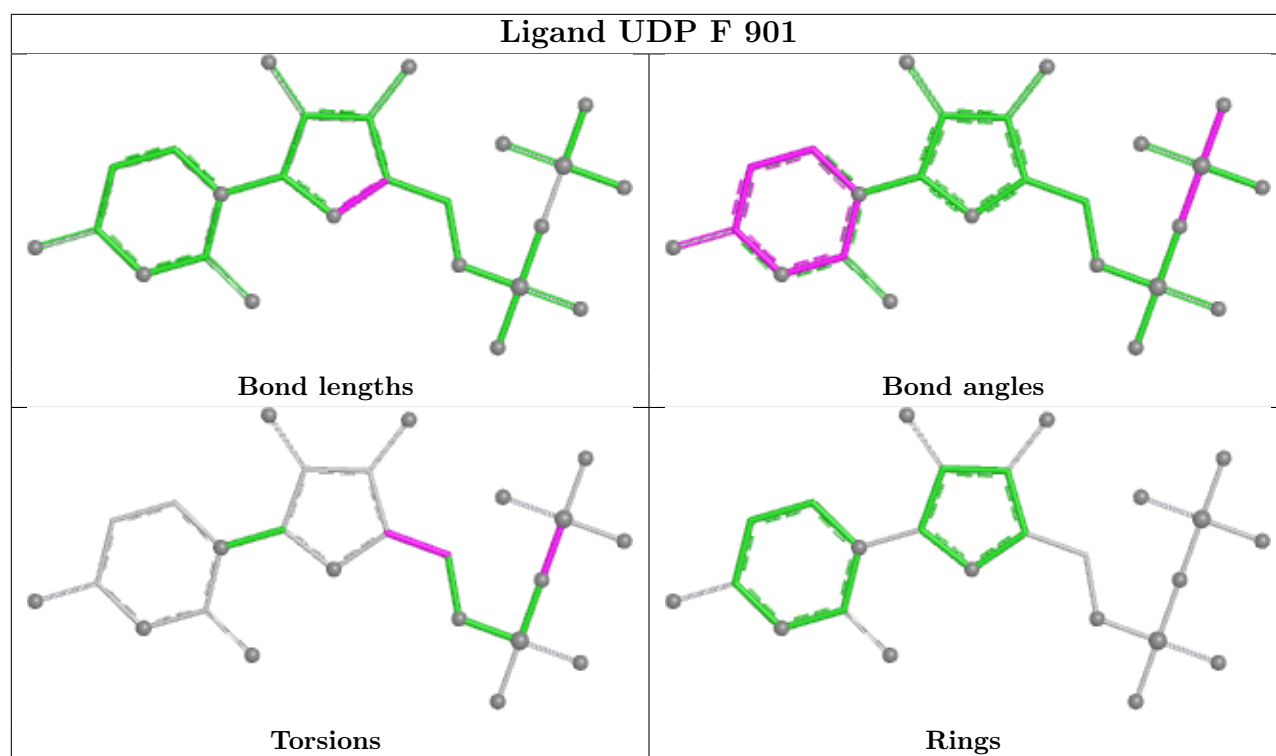
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	781/816 (95%)	-0.32	41 (5%) 33 25	19, 34, 105, 147	0
1	B	780/816 (95%)	0.04	74 (9%) 14 10	23, 43, 130, 171	0
1	C	781/816 (95%)	0.01	35 (4%) 38 30	30, 52, 101, 141	0
1	D	781/816 (95%)	-0.36	30 (3%) 44 35	22, 35, 92, 136	0
1	E	781/816 (95%)	-0.21	43 (5%) 30 23	23, 39, 116, 147	0
1	F	781/816 (95%)	-0.38	32 (4%) 41 33	17, 33, 84, 128	0
1	G	781/816 (95%)	-0.32	18 (2%) 61 51	22, 39, 81, 126	0
1	H	780/816 (95%)	0.02	78 (10%) 12 9	26, 43, 127, 156	0
All	All	6246/6528 (95%)	-0.19	351 (5%) 30 23	17, 41, 105, 171	0

All (351) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	103	ASN	7.1
1	H	51	ALA	7.0
1	B	57	PRO	6.7
1	H	73	LEU	6.4
1	H	56	LEU	6.2
1	B	51	ALA	6.1
1	B	38	ALA	6.0
1	H	72	LEU	6.0
1	B	54	GLU	5.9
1	H	34	SER	5.8
1	H	83	PRO	5.8
1	B	77	GLN	5.8
1	B	58	GLU	5.7
1	H	68	PRO	5.6
1	H	59	GLN	5.6
1	H	55	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	H	84	PRO	5.2
1	H	85	TRP	5.2
1	E	33	LEU	5.2
1	A	30	LEU	5.2
1	G	29	VAL	5.2
1	E	35	ARG	5.1
1	E	172	HIS	5.1
1	B	63	LYS	5.1
1	C	129	LYS	5.1
1	H	70	PHE	5.0
1	F	29	VAL	5.0
1	B	69	PHE	4.9
1	E	175	GLU	4.9
1	B	87	ALA	4.8
1	C	106	ALA	4.8
1	H	104	LEU	4.8
1	B	80	ILE	4.7
1	H	108	VAL	4.7
1	H	74	LYS	4.7
1	H	102	VAL	4.7
1	B	60	THR	4.7
1	H	86	VAL	4.7
1	B	62	LYS	4.6
1	D	49	ILE	4.6
1	C	29	VAL	4.6
1	B	30	LEU	4.6
1	E	29	VAL	4.6
1	A	44	LEU	4.6
1	E	62	LYS	4.5
1	B	83	PRO	4.5
1	B	67	GLY	4.4
1	C	44	LEU	4.4
1	H	57	PRO	4.4
1	B	68	PRO	4.4
1	B	85	TRP	4.4
1	D	29	VAL	4.4
1	H	49	ILE	4.4
1	B	86	VAL	4.3
1	H	60	THR	4.3
1	A	29	VAL	4.3
1	H	52	GLU	4.3
1	B	43	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
1	E	49	ILE	4.3
1	H	50	ILE	4.3
1	B	35	ARG	4.2
1	B	101	ARG	4.2
1	H	71	ASP	4.2
1	B	61	ARG	4.2
1	H	129	LYS	4.2
1	H	105	HIS	4.1
1	B	55	ALA	4.1
1	H	43	ILE	4.1
1	A	31	ALA	4.1
1	E	44	LEU	4.1
1	H	28	GLU	4.1
1	B	84	PRO	4.1
1	H	90	VAL	4.0
1	A	68	PRO	4.0
1	H	98	GLU	4.0
1	G	69	PHE	4.0
1	B	49	ILE	4.0
1	B	64	LEU	4.0
1	H	30	LEU	4.0
1	H	62	LYS	4.0
1	H	88	LEU	3.9
1	D	57	PRO	3.9
1	F	33	LEU	3.8
1	H	64	LEU	3.8
1	H	75	SER	3.8
1	B	42	GLY	3.8
1	H	53	PHE	3.8
1	H	79	ALA	3.8
1	B	65	GLU	3.7
1	H	89	ALA	3.7
1	A	35	ARG	3.7
1	B	53	PHE	3.7
1	H	130	ASN	3.7
1	A	34	SER	3.7
1	F	175	GLU	3.7
1	E	56	LEU	3.6
1	E	36	VAL	3.6
1	H	107	LEU	3.6
1	A	59	GLN	3.6
1	C	32	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	32	LEU	3.6
1	E	31	ALA	3.6
1	B	70	PHE	3.6
1	A	32	LEU	3.5
1	A	56	LEU	3.5
1	H	65	GLU	3.5
1	B	47	ASN	3.5
1	B	172	HIS	3.5
1	B	31	ALA	3.5
1	H	32	LEU	3.5
1	H	82	LEU	3.5
1	H	172	HIS	3.5
1	B	59	GLN	3.4
1	B	191	GLY	3.4
1	H	58	GLU	3.4
1	H	33	LEU	3.4
1	B	82	LEU	3.4
1	A	49	ILE	3.3
1	E	43	ILE	3.3
1	A	82	LEU	3.3
1	E	59	GLN	3.3
1	G	30	LEU	3.3
1	H	99	TYR	3.3
1	H	106	ALA	3.3
1	B	90	VAL	3.3
1	F	145	SER	3.3
1	A	51	ALA	3.2
1	A	33	LEU	3.2
1	C	128	VAL	3.2
1	A	64	LEU	3.2
1	A	41	LYS	3.2
1	E	85	TRP	3.2
1	H	69	PHE	3.2
1	B	108	VAL	3.2
1	F	66	GLY	3.2
1	C	28	GLU	3.2
1	C	68	PRO	3.2
1	F	64	LEU	3.1
1	D	46	GLN	3.1
1	E	50	ILE	3.1
1	B	32	LEU	3.1
1	H	128	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	101	ARG	3.1
1	H	81	VAL	3.1
1	E	778	LEU	3.1
1	D	128	VAL	3.1
1	E	66	GLY	3.1
1	F	44	LEU	3.1
1	B	76	THR	3.1
1	F	172	HIS	3.0
1	B	75	SER	3.0
1	D	83	PRO	3.0
1	A	69	PHE	3.0
1	A	62	LYS	3.0
1	C	57	PRO	3.0
1	B	120	PHE	3.0
1	G	129	LYS	3.0
1	E	68	PRO	3.0
1	C	38	ALA	3.0
1	E	144	ALA	3.0
1	A	63	LYS	3.0
1	H	66	GLY	3.0
1	A	144	ALA	3.0
1	B	79	ALA	3.0
1	B	106	ALA	3.0
1	C	172	HIS	3.0
1	B	107	LEU	2.9
1	H	61	ARG	2.9
1	D	30	LEU	2.9
1	B	48	GLN	2.9
1	B	630	TYR	2.9
1	D	51	ALA	2.9
1	F	34	SER	2.9
1	C	60	THR	2.9
1	C	64	LEU	2.9
1	D	82	LEU	2.9
1	B	110	GLU	2.9
1	E	30	LEU	2.9
1	F	30	LEU	2.9
1	B	74	LYS	2.8
1	C	634	GLU	2.8
1	B	71	ASP	2.8
1	A	84	PRO	2.8
1	C	190	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	106	ALA	2.8
1	A	66	GLY	2.8
1	F	191	GLY	2.8
1	B	81	VAL	2.8
1	C	43	ILE	2.8
1	C	49	ILE	2.8
1	G	778	LEU	2.8
1	B	66	GLY	2.8
1	B	190	GLN	2.7
1	E	128	VAL	2.7
1	B	779	ASP	2.7
1	E	34	SER	2.7
1	F	83	PRO	2.7
1	D	36	VAL	2.7
1	B	104	LEU	2.7
1	B	144	ALA	2.7
1	G	35	ARG	2.7
1	H	126	ASP	2.7
1	E	64	LEU	2.7
1	E	57	PRO	2.7
1	D	65	GLU	2.7
1	E	52	GLU	2.7
1	D	64	LEU	2.7
1	F	49	ILE	2.6
1	A	57	PRO	2.6
1	C	130	ASN	2.6
1	B	41	LYS	2.6
1	B	78	GLU	2.6
1	C	62	LYS	2.6
1	H	44	LEU	2.6
1	A	143	ASN	2.6
1	E	104	LEU	2.6
1	F	190	GLN	2.6
1	H	109	VAL	2.6
1	A	108	VAL	2.6
1	B	102	VAL	2.6
1	H	100	LEU	2.6
1	A	46	GLN	2.6
1	B	72	LEU	2.6
1	G	64	LEU	2.6
1	D	69	PHE	2.6
1	A	60	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	46	GLN	2.5
1	H	134	THR	2.5
1	G	33	LEU	2.5
1	H	131	GLY	2.5
1	H	630	TYR	2.5
1	H	54	GLU	2.5
1	C	69	PHE	2.5
1	E	190	GLN	2.5
1	F	144	ALA	2.5
1	F	68	PRO	2.5
1	A	65	GLU	2.5
1	B	98	GLU	2.5
1	F	31	ALA	2.5
1	G	106	ALA	2.5
1	H	76	THR	2.5
1	E	145	SER	2.5
1	E	70	PHE	2.5
1	B	109	VAL	2.4
1	D	34	SER	2.4
1	A	129	LYS	2.4
1	C	59	GLN	2.4
1	D	55	ALA	2.4
1	D	172	HIS	2.4
1	A	104	LEU	2.4
1	G	67	GLY	2.4
1	H	29	VAL	2.4
1	C	58	GLU	2.4
1	G	38	ALA	2.4
1	H	38	ALA	2.4
1	D	630	TYR	2.4
1	D	32	LEU	2.4
1	H	31	ALA	2.4
1	A	73	LEU	2.4
1	G	82	LEU	2.4
1	A	50	ILE	2.4
1	B	36	VAL	2.4
1	A	39	LYS	2.4
1	A	71	ASP	2.4
1	E	63	LYS	2.4
1	B	28	GLU	2.4
1	B	111	GLU	2.4
1	D	56	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	32	LEU	2.4
1	F	43	ILE	2.4
1	F	61	ARG	2.3
1	H	35	ARG	2.3
1	E	69	PHE	2.3
1	H	120	PHE	2.3
1	B	37	GLU	2.3
1	A	72	LEU	2.3
1	G	630	TYR	2.3
1	B	34	SER	2.3
1	E	82	LEU	2.3
1	D	60	THR	2.3
1	E	60	THR	2.3
1	A	128	VAL	2.3
1	H	67	GLY	2.3
1	F	27	ASN	2.3
1	C	31	ALA	2.3
1	E	51	ALA	2.3
1	C	56	LEU	2.3
1	G	56	LEU	2.3
1	E	61	ARG	2.3
1	E	38	ALA	2.3
1	F	779	ASP	2.3
1	G	201	GLN	2.3
1	H	48	GLN	2.3
1	C	63	LYS	2.3
1	B	128	VAL	2.3
1	F	147	PRO	2.3
1	A	70	PHE	2.2
1	D	31	ALA	2.2
1	H	80	ILE	2.2
1	C	614	ARG	2.2
1	A	83	PRO	2.2
1	H	133	PHE	2.2
1	D	28	GLU	2.2
1	H	110	GLU	2.2
1	A	103	ASN	2.2
1	C	61	ARG	2.2
1	D	68	PRO	2.2
1	F	56	LEU	2.2
1	G	51	ALA	2.2
1	H	87	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	27	ASN	2.2
1	F	193	ASN	2.2
1	E	71	ASP	2.2
1	F	57	PRO	2.2
1	A	53	PHE	2.2
1	E	108	VAL	2.2
1	C	127	GLY	2.2
1	C	191	GLY	2.2
1	F	63	LYS	2.2
1	B	73	LEU	2.2
1	A	106	ALA	2.2
1	D	50	ILE	2.1
1	B	105	HIS	2.1
1	F	53	PHE	2.1
1	F	69	PHE	2.1
1	F	28	GLU	2.1
1	H	78	GLU	2.1
1	B	103	ASN	2.1
1	C	66	GLY	2.1
1	B	88	LEU	2.1
1	H	112	LEU	2.1
1	H	111	GLU	2.1
1	H	113	GLN	2.1
1	C	83	PRO	2.1
1	E	103	ASN	2.1
1	D	73	LEU	2.1
1	E	127	GLY	2.1
1	B	506	GLY	2.1
1	C	51	ALA	2.1
1	G	59	GLN	2.0
1	D	84	PRO	2.0
1	D	132	ASN	2.0
1	F	192	LYS	2.0
1	B	145	SER	2.0
1	D	45	GLN	2.0
1	C	778	LEU	2.0
1	D	44	LEU	2.0
1	F	405	ASN	2.0
1	D	53	PHE	2.0
1	C	65	GLU	2.0
1	C	660	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

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
5	SO4	C	912	5/5	0.65	0.25	84,89,106,115	0
5	SO4	H	912	5/5	0.78	0.22	70,77,86,105	0
5	SO4	H	913	5/5	0.79	0.29	81,87,102,115	0
5	SO4	D	912	5/5	0.81	0.18	59,77,86,101	0
5	SO4	C	913	5/5	0.83	0.19	81,84,103,107	0
7	K	E	931	1/1	0.83	0.10	73,73,73,73	0
3	LCN	D	903[A]	11/11	0.84	0.16	24,27,32,32	21
5	SO4	B	913	5/5	0.84	0.26	68,71,80,95	0
5	SO4	B	912	5/5	0.85	0.16	70,76,90,106	0
5	SO4	G	912	5/5	0.88	0.20	59,69,86,94	0
5	SO4	A	912	5/5	0.88	0.17	51,56,69,85	0
6	MLA	C	921	7/7	0.89	0.13	70,73,87,91	0
6	MLA	G	921	7/7	0.89	0.13	58,62,74,74	0
4	NHF	C	904[B]	11/11	0.89	0.16	37,38,45,47	21
5	SO4	B	911	5/5	0.90	0.17	45,47,65,81	0
4	NHF	F	904[B]	11/11	0.91	0.15	24,25,30,32	21
5	SO4	E	913	5/5	0.91	0.20	56,63,79,86	0
7	K	F	931	1/1	0.91	0.11	82,82,82,82	0
4	NHF	H	904[B]	11/11	0.92	0.18	32,34,40,41	21
5	SO4	F	912	5/5	0.92	0.17	55,58,68,85	0
6	MLA	E	921	7/7	0.92	0.12	42,50,55,56	0
4	NHF	E	904[B]	11/11	0.92	0.17	27,29,34,35	21
5	SO4	G	913	5/5	0.92	0.16	59,63,84,96	0
5	SO4	E	911	5/5	0.92	0.19	44,48,60,65	0
7	K	G	931	1/1	0.92	0.14	74,74,74,74	0
4	NHF	B	904[B]	11/11	0.93	0.10	29,32,37,38	21
5	SO4	E	912	5/5	0.93	0.17	57,62,70,86	0

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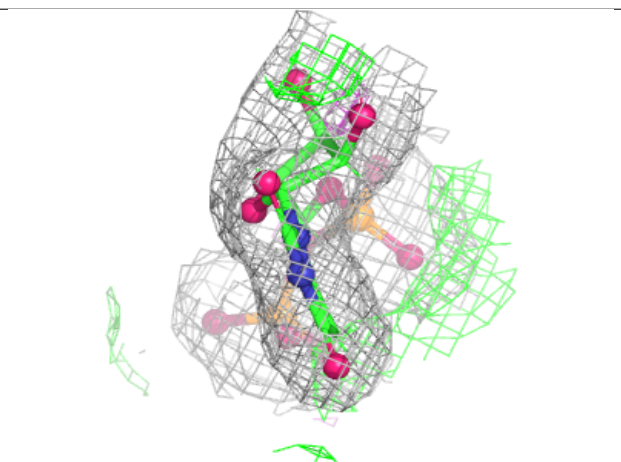
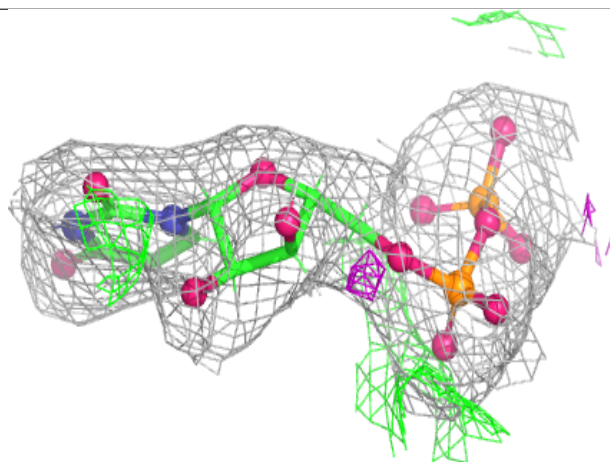
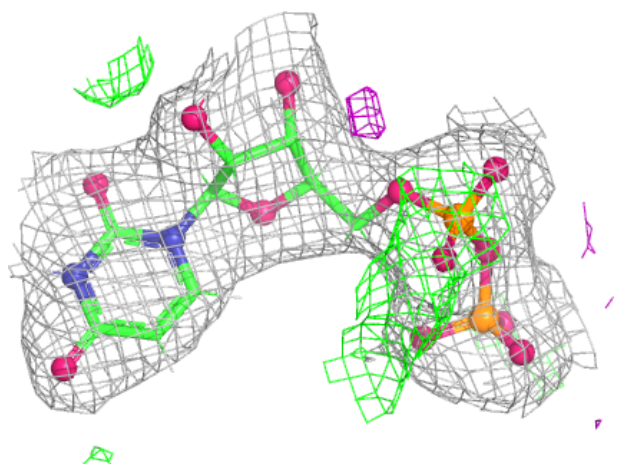
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MLA	H	921	7/7	0.93	0.12	52,61,68,70	0
7	K	B	931	1/1	0.93	0.11	83,83,83,83	0
5	SO4	D	911	5/5	0.93	0.22	43,47,64,77	0
5	SO4	F	911	5/5	0.93	0.19	42,42,63,71	0
4	NHF	G	904[B]	11/11	0.93	0.09	26,27,32,33	21
5	SO4	D	913	5/5	0.94	0.17	46,47,69,73	0
3	LCN	E	903[A]	11/11	0.94	0.14	26,30,35,36	21
7	K	D	931	1/1	0.94	0.15	72,72,72,72	0
3	LCN	H	903[A]	11/11	0.94	0.16	32,34,41,41	21
4	NHF	D	904[B]	11/11	0.94	0.10	24,27,32,32	21
5	SO4	H	911	5/5	0.94	0.19	44,47,65,70	0
7	K	H	931	1/1	0.94	0.07	69,69,69,69	0
5	SO4	F	913	5/5	0.95	0.18	49,51,53,70	0
5	SO4	A	911	5/5	0.95	0.19	35,43,59,63	0
5	SO4	C	911	5/5	0.95	0.14	48,51,70,71	0
3	LCN	G	903[A]	11/11	0.95	0.08	25,28,33,34	21
5	SO4	A	913	5/5	0.95	0.20	44,50,74,74	0
3	LCN	A	903[A]	11/11	0.95	0.13	23,25,29,30	21
6	MLA	B	921	7/7	0.95	0.10	51,58,61,61	0
3	LCN	B	903[A]	11/11	0.95	0.09	29,32,37,39	21
6	MLA	D	921	7/7	0.95	0.10	33,40,44,46	0
5	SO4	G	911	5/5	0.96	0.14	35,41,56,61	0
3	LCN	F	903[A]	11/11	0.96	0.09	23,27,31,33	21
3	LCN	C	903[A]	11/11	0.97	0.10	36,39,46,48	21
7	K	C	931	1/1	0.97	0.12	81,81,81,81	0
6	MLA	A	921	7/7	0.97	0.09	31,38,42,42	0
6	MLA	F	921	7/7	0.97	0.09	33,38,42,43	0
2	UDP	H	901	25/25	0.97	0.06	28,34,41,44	0
4	NHF	A	904[B]	11/11	0.97	0.10	23,25,29,30	21
7	K	A	931	1/1	0.97	0.07	61,61,61,61	0
2	UDP	D	901	25/25	0.98	0.05	22,28,34,39	0
2	UDP	E	901	25/25	0.98	0.05	21,27,35,38	0
2	UDP	G	901	25/25	0.98	0.05	20,28,34,41	0
2	UDP	B	901	25/25	0.98	0.04	23,31,37,43	0
2	UDP	C	901	25/25	0.98	0.06	32,41,49,54	0
2	UDP	A	901	25/25	0.99	0.04	18,23,29,32	0
2	UDP	F	901	25/25	0.99	0.04	16,23,29,34	0

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

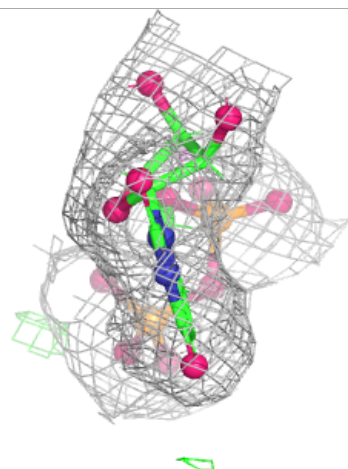
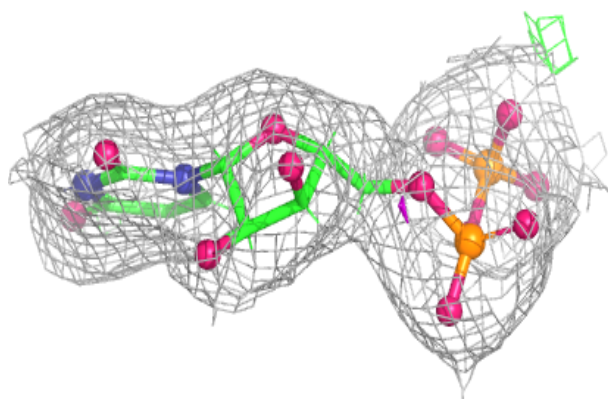
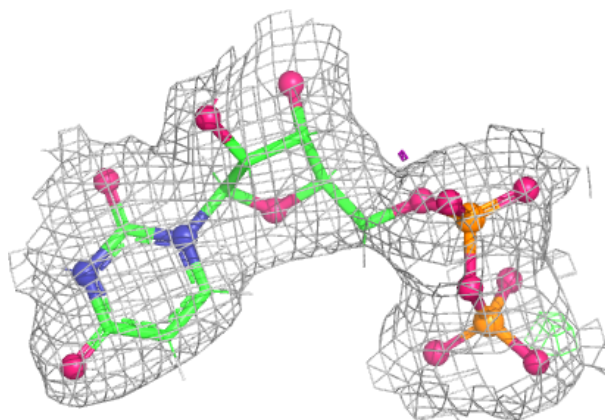
Electron density around UDP H 901:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



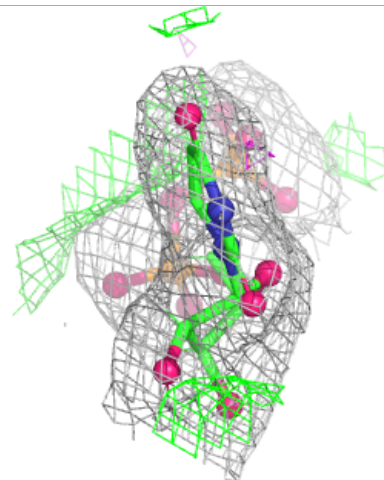
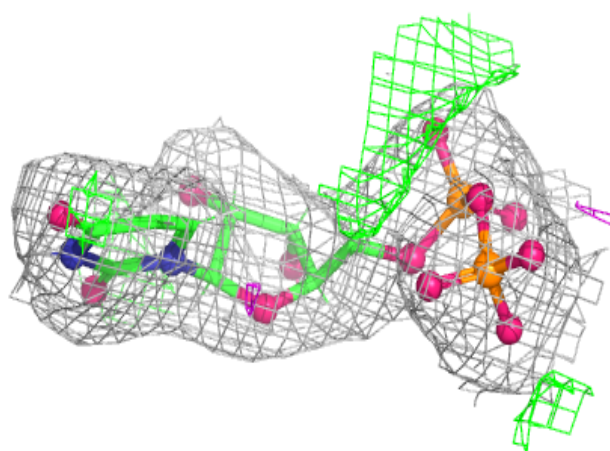
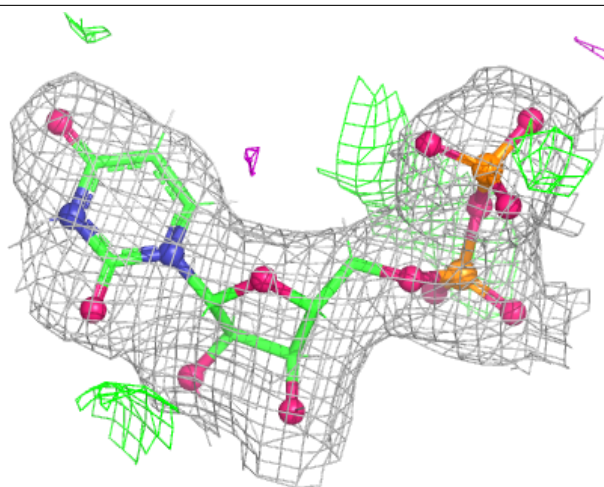
Electron density around UDP D 901:

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



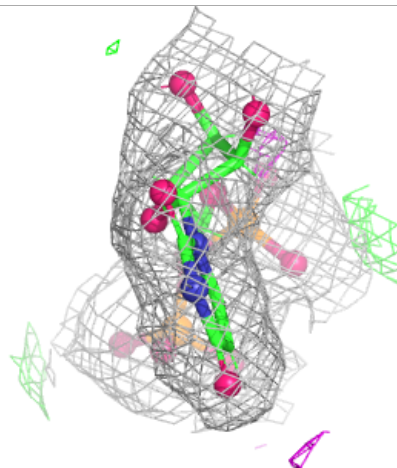
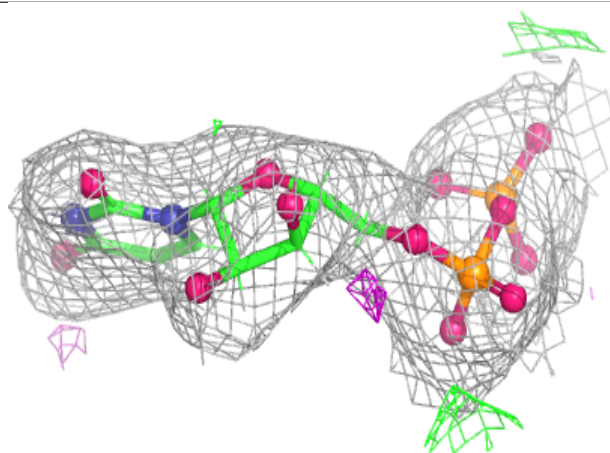
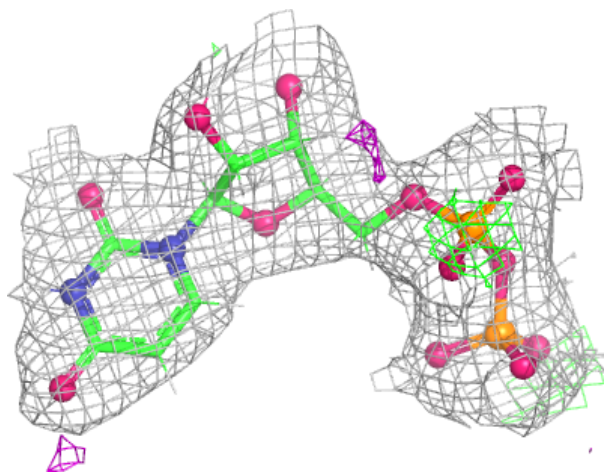
Electron density around UDP E 901:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



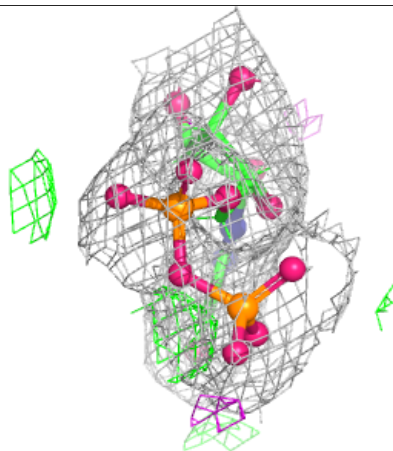
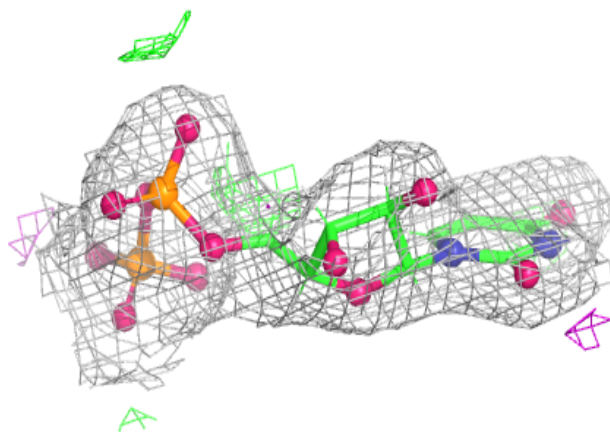
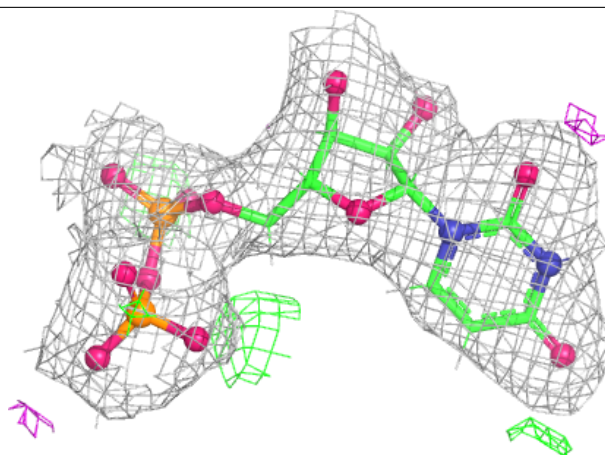
Electron density around UDP G 901:

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



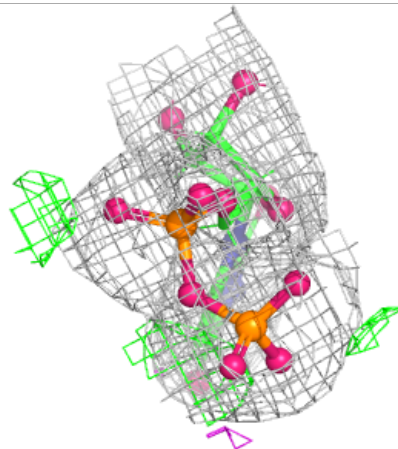
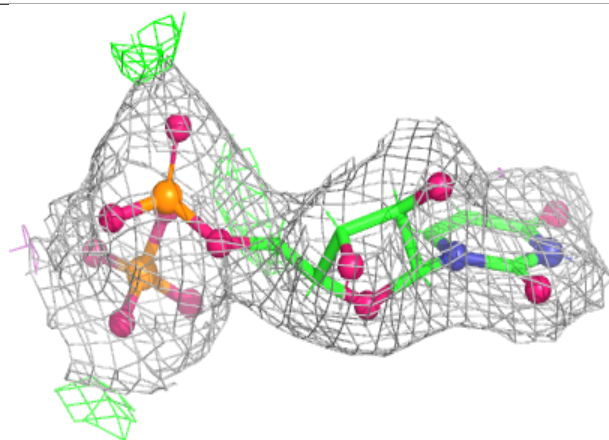
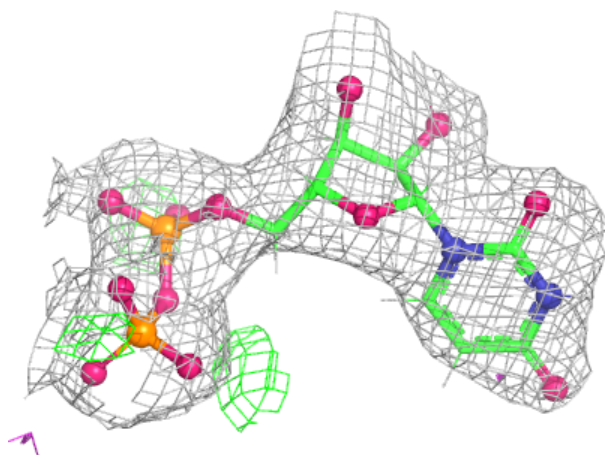
Electron density around UDP B 901:

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



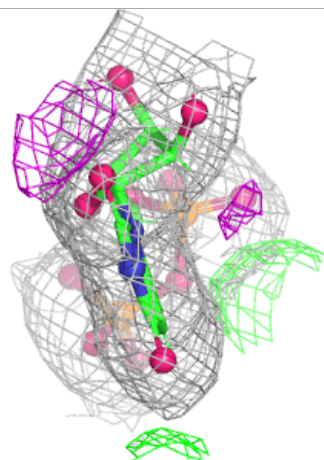
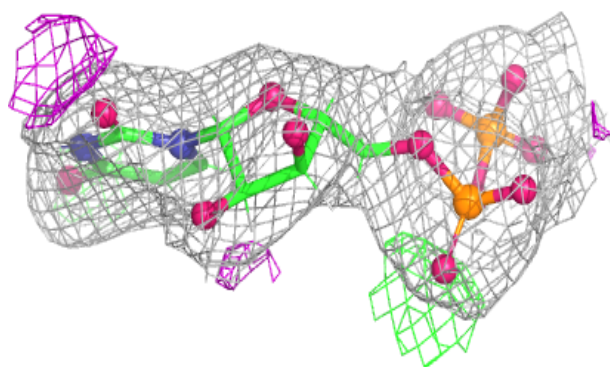
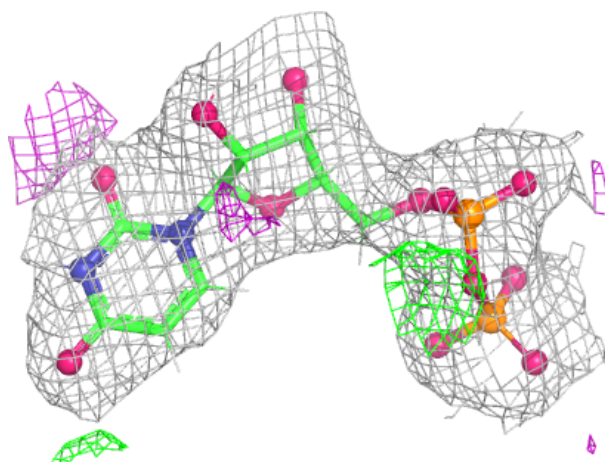
Electron density around UDP C 901:

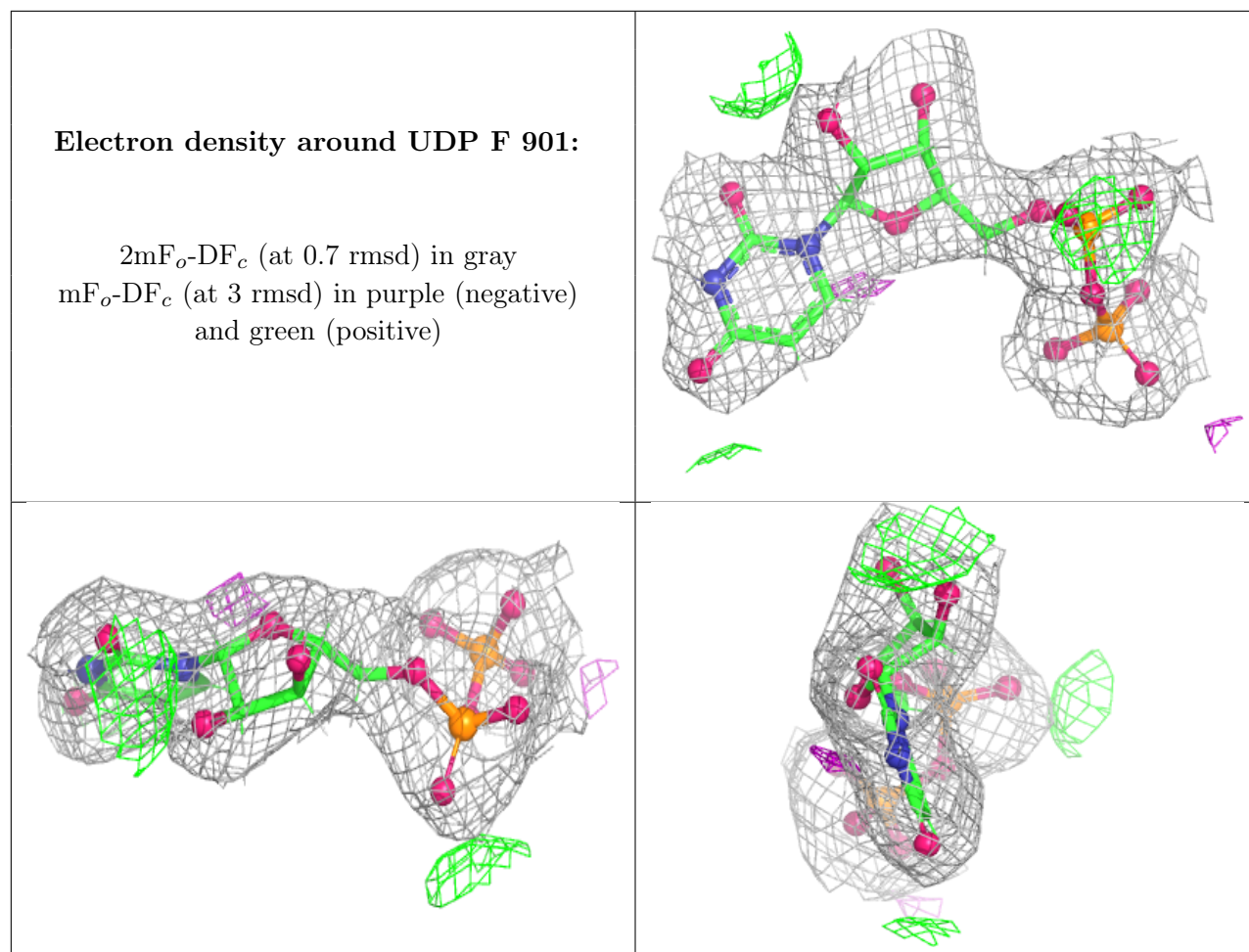
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around UDP A 901:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.