



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:41 AM BST

PDB ID : 3O8O
Title : Structure of phosphofructokinase from *Saccharomyces cerevisiae*
Authors : Banaszak, K.; Mechin, I.; Kopperschlager, G.; Rypniewski, W.
Deposited on : 2010-08-03
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

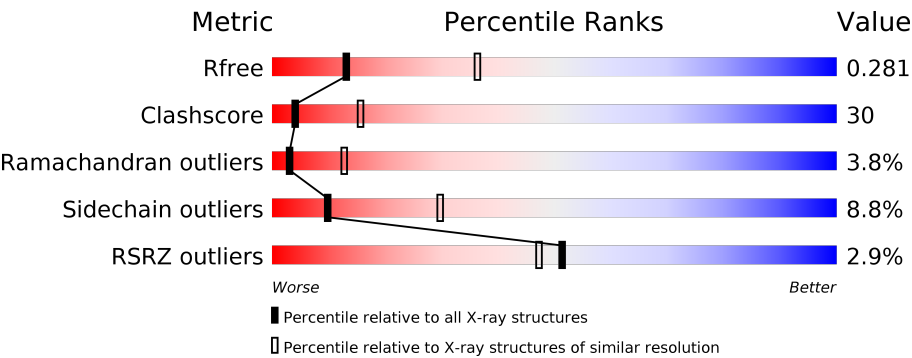
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	787	<div><div>3%</div><div><div></div><div>52%</div><div>37%</div><div>6%</div><div>5%</div></div></div>
1	C	787	<div><div>4%</div><div><div></div><div>51%</div><div>38%</div><div>5%</div><div>5%</div></div></div>
1	E	787	<div><div>3%</div><div><div></div><div>53%</div><div>35%</div><div>6%</div><div></div></div></div>
1	G	787	<div><div>3%</div><div><div></div><div>53%</div><div>34%</div><div>6%</div><div>5%</div></div></div>
2	B	766	<div><div>3%</div><div><div></div><div>53%</div><div>39%</div><div>7%</div><div></div></div></div>
2	D	766	<div><div>2%</div><div><div></div><div>53%</div><div>39%</div><div>6%</div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	766	<div> <div style="width: 3%;"></div> <div style="width: 53%; background-color: #00ff00;"></div> <div style="width: 39%; background-color: #ffff00;"></div> <div style="width: 7%; background-color: #ffa500;"></div> <div style="width: 1%; background-color: #ff0000;"></div> </div> <p>3% 53% 39% 7%</p>
2	H	766	<div> <div style="width: 0.5%;"></div> <div style="width: 54%; background-color: #00ff00;"></div> <div style="width: 39%; background-color: #ffff00;"></div> <div style="width: 6%; background-color: #ffa500;"></div> <div style="width: 0.5%; background-color: #ff0000;"></div> </div> <p>% 54% 39% 6%</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 46645 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

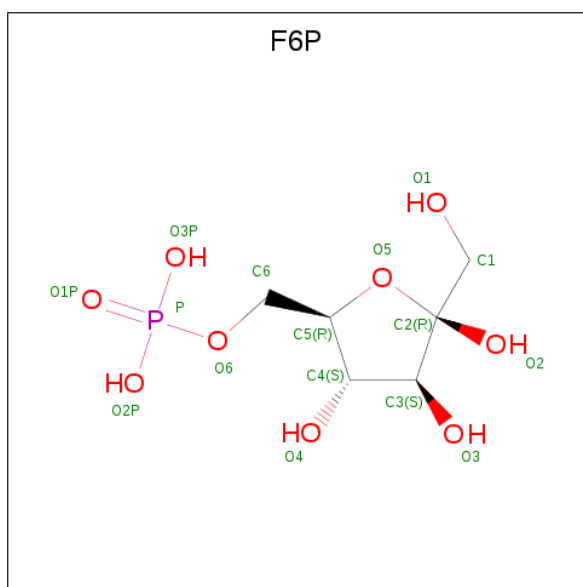
- Molecule 1 is a protein called 6-phosphofructokinase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	273	0	0
			5759	3620	1019	1098	22			
1	C	750	Total	C	N	O	S	196	0	0
			5759	3620	1019	1098	22			
1	E	752	Total	C	N	O	S	260	0	0
			5777	3631	1023	1101	22			
1	G	746	Total	C	N	O	S	289	0	0
			5733	3604	1015	1092	22			

- Molecule 2 is a protein called 6-phosphofructokinase subunit beta.

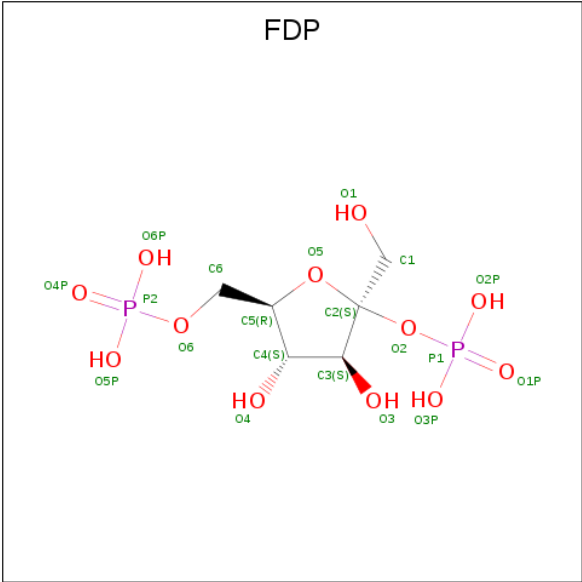
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	763	Total	C	N	O	S	364	0	0
			5834	3652	1034	1118	30			
2	D	763	Total	C	N	O	S	266	0	0
			5834	3652	1034	1118	30			
2	F	762	Total	C	N	O	S	279	0	0
			5827	3647	1033	1117	30			
2	H	763	Total	C	N	O	S	173	0	0
			5834	3652	1034	1118	30			

- Molecule 3 is 6-O-phosphono-beta-D-fructofuranose (three-letter code: F6P) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		
3	C	1	Total	C	O	P	0	0
			16	6	9	1		
3	D	1	Total	C	O	P	0	0
			16	6	9	1		
3	E	1	Total	C	O	P	0	0
			16	6	9	1		
3	F	1	Total	C	O	P	0	0
			16	6	9	1		
3	G	1	Total	C	O	P	0	0
			16	6	9	1		
3	H	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is 2,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FDP) (formula: $C_6H_{14}O_{12}P_2$).

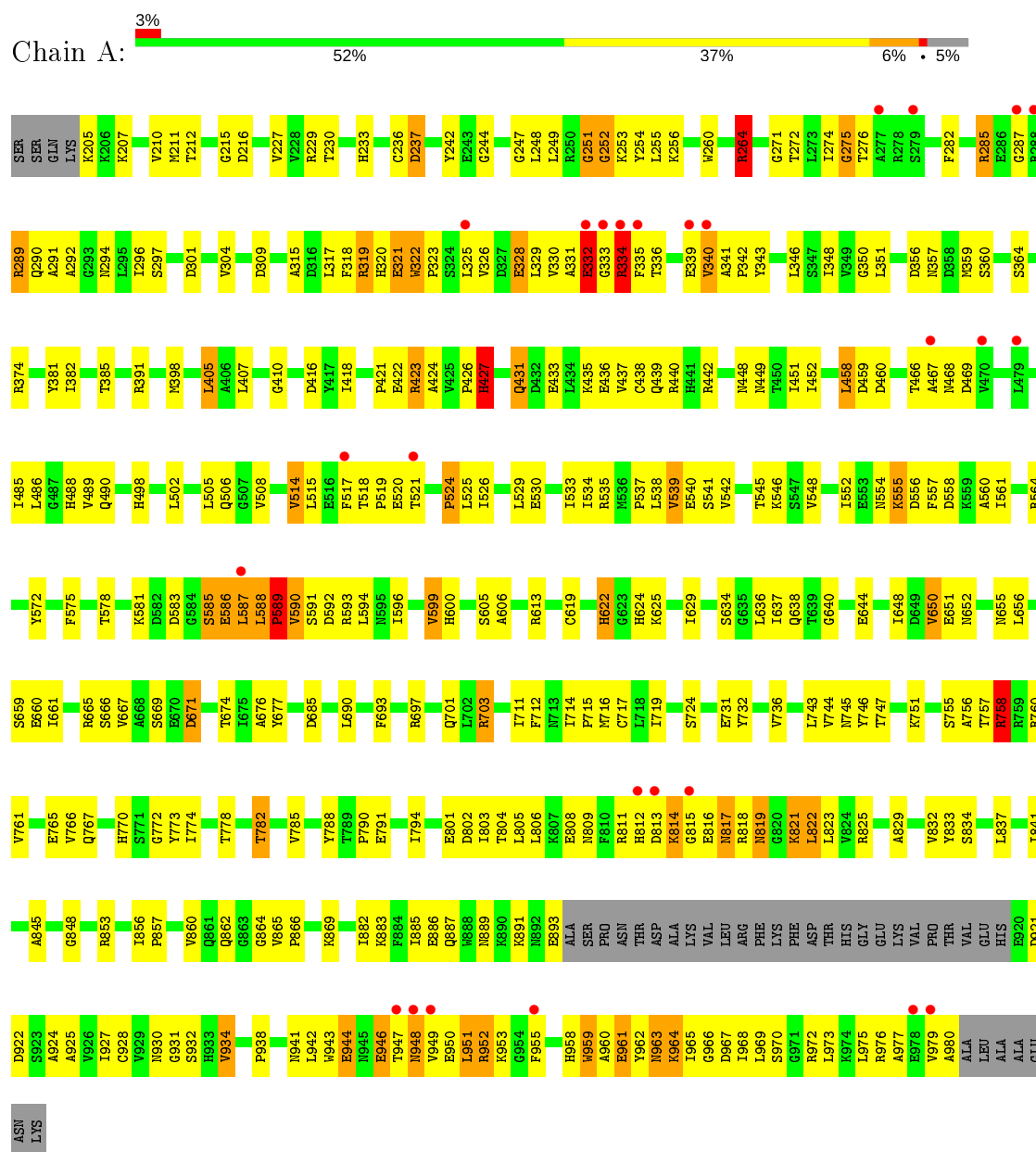


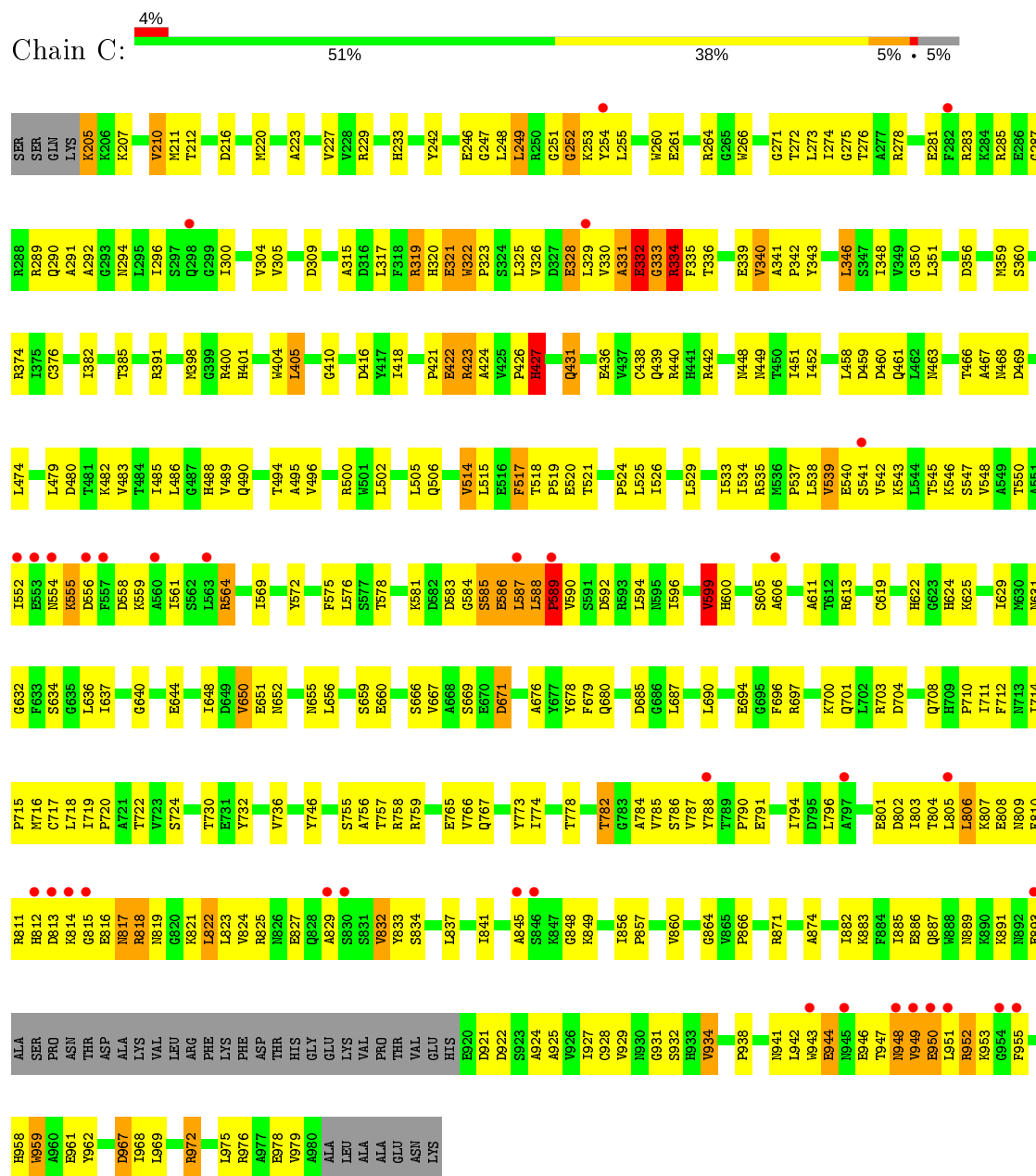
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		
4	E	1	Total	C	O	P	0	0
			20	6	12	2		
4	F	1	Total	C	O	P	0	0
			20	6	12	2		
4	G	1	Total	C	O	P	0	0
			20	6	12	2		
4	H	1	Total	C	O	P	0	0
			20	6	12	2		

3 Residue-property plots

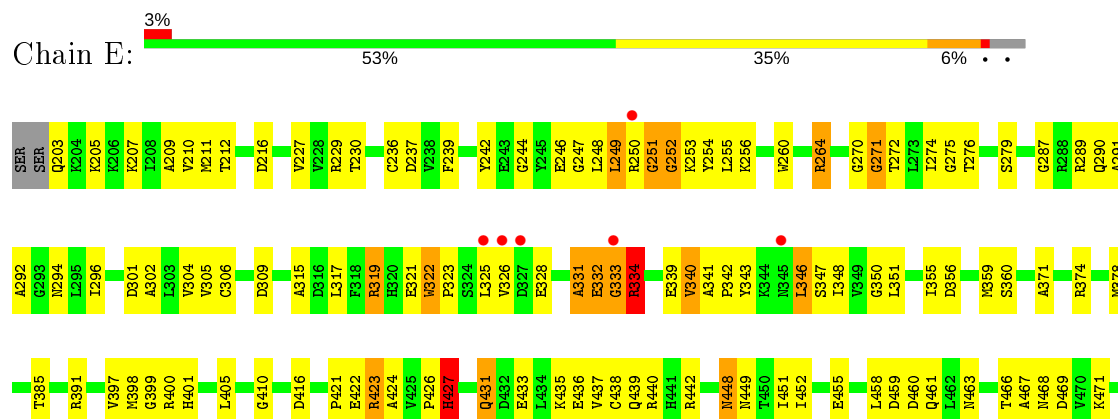
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

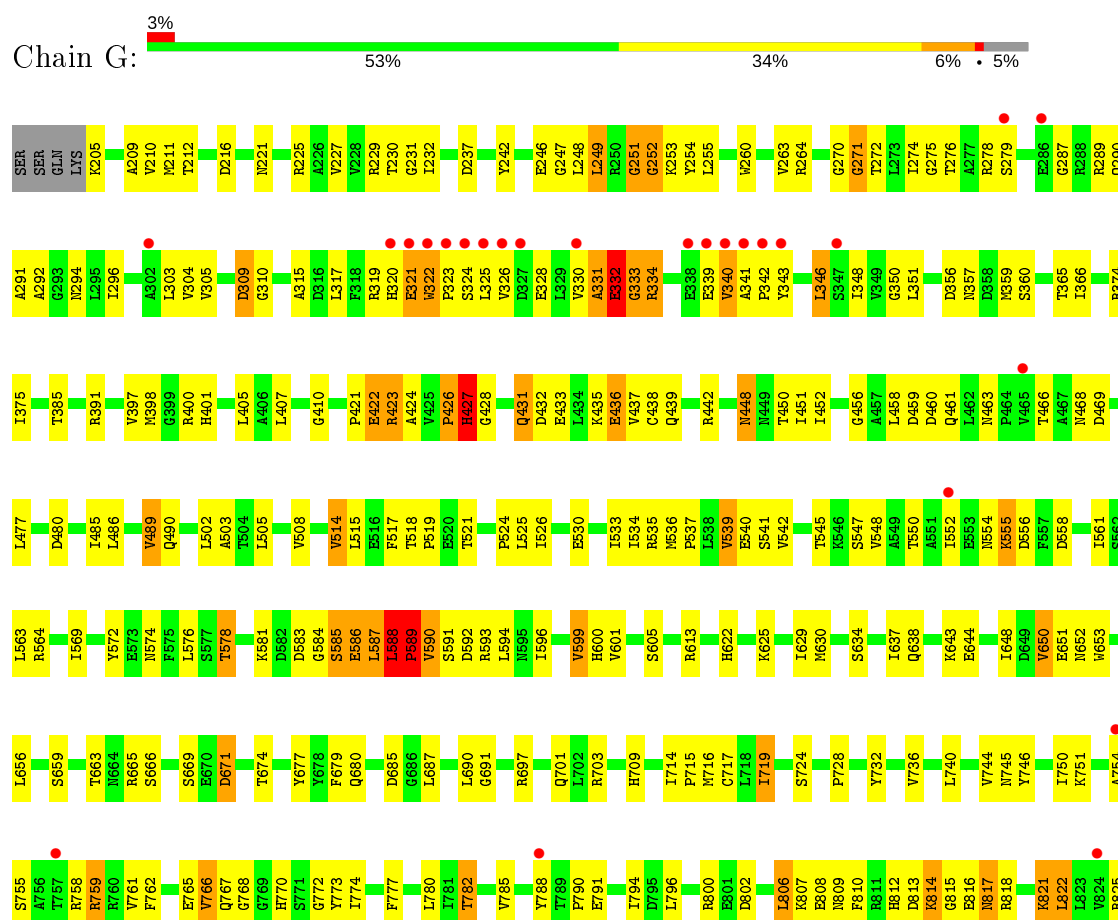
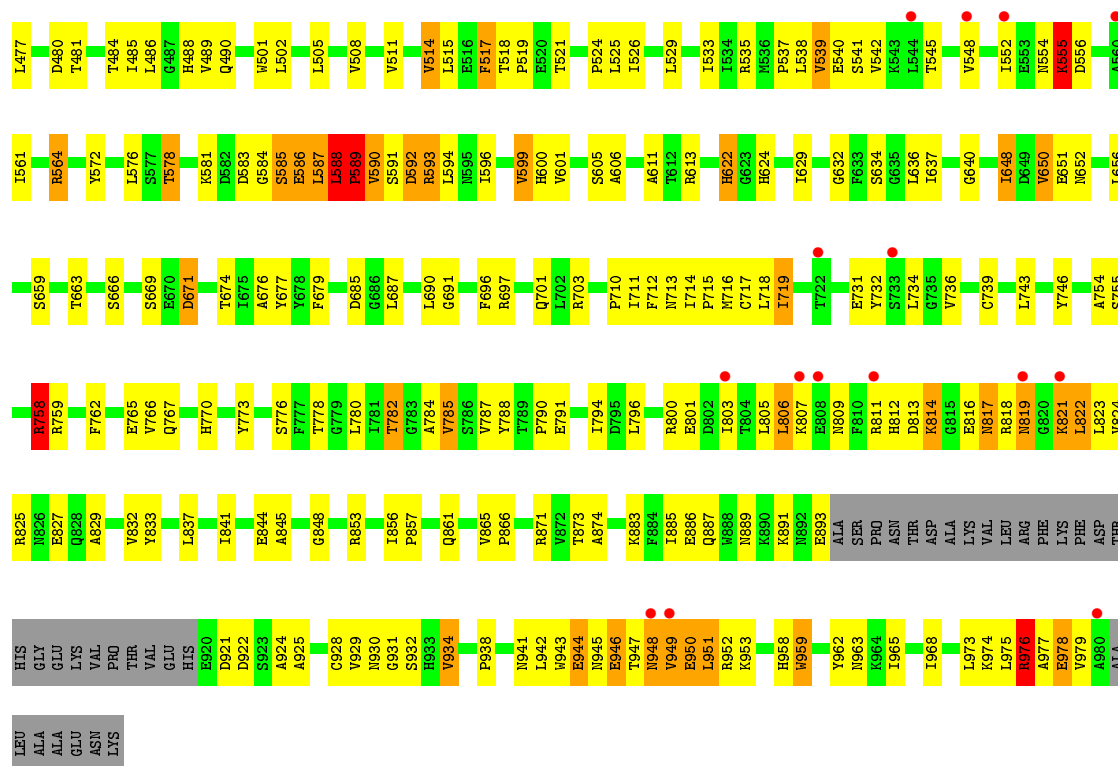
- Molecule 1: 6-phosphofructokinase subunit alpha

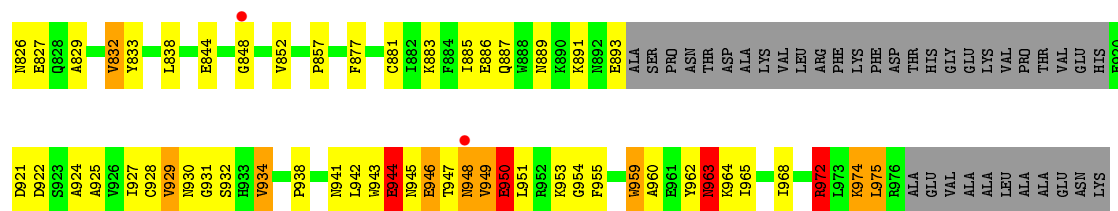




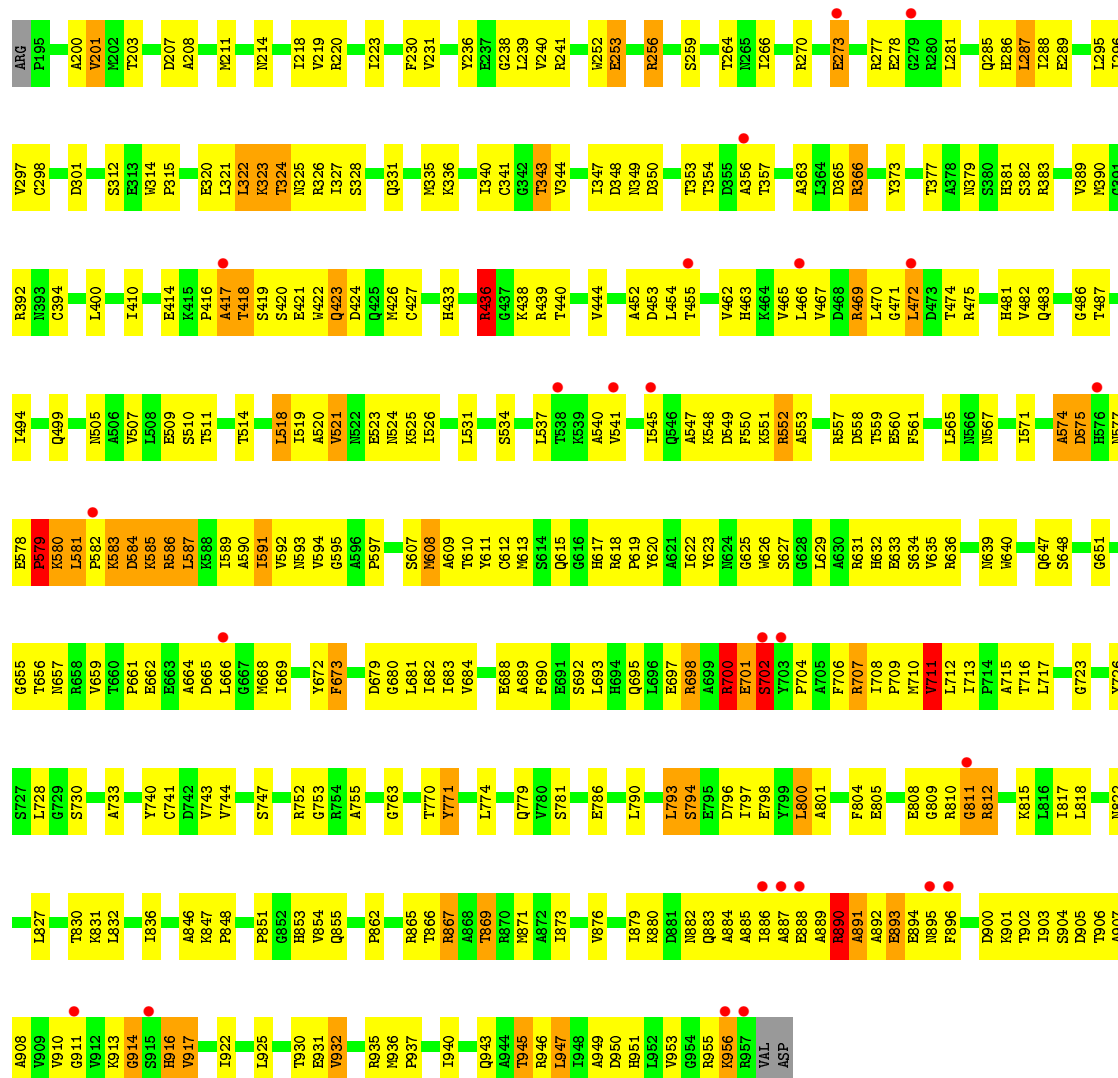
• Molecule 1: 6-phosphofructokinase subunit alpha







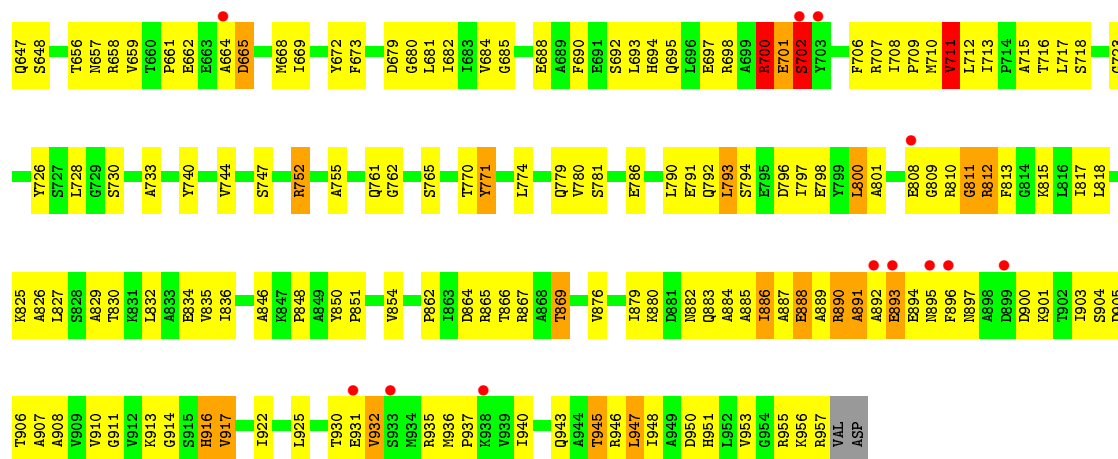
• Molecule 2: 6-phosphofructokinase subunit beta



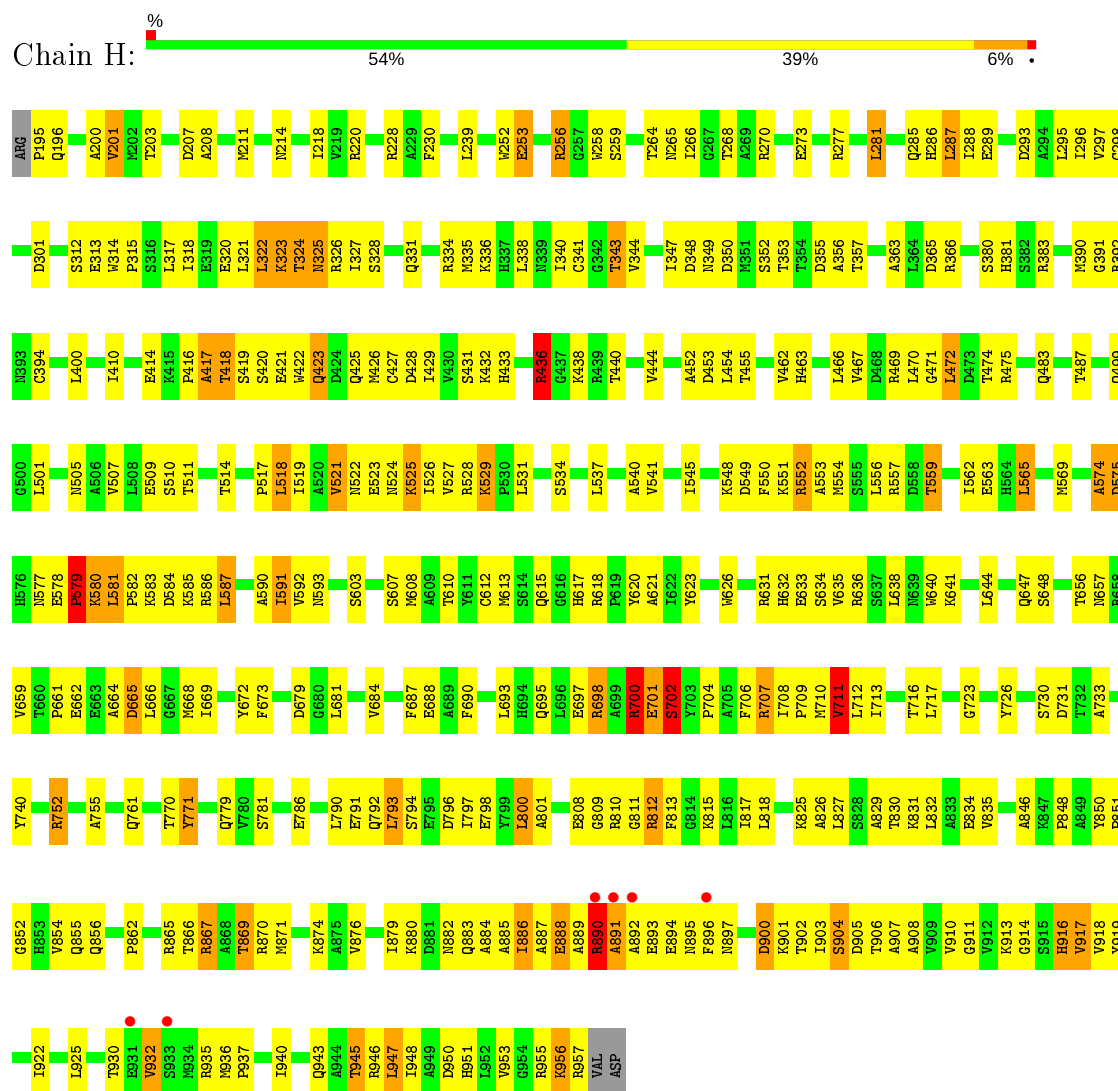
• Molecule 2: 6-phosphofructokinase subunit beta







• Molecule 2: 6-phosphofructokinase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	180.05Å 186.21Å 236.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.90 34.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.90) 98.4 (34.97-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.309 0.236 , 0.281	Depositor DCC
R_{free} test set	3446 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	46645	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FDP, F6P

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	0.53	0/5860	0.80	13/7925 (0.2%)
1	C	0.58	1/5860 (0.0%)	0.83	11/7925 (0.1%)
1	E	0.57	0/5878	0.82	17/7948 (0.2%)
1	G	0.59	1/5834 (0.0%)	0.80	9/7889 (0.1%)
2	B	0.52	1/5940 (0.0%)	0.79	14/8038 (0.2%)
2	D	0.55	1/5940 (0.0%)	0.83	20/8038 (0.2%)
2	F	0.51	0/5932	0.80	17/8027 (0.2%)
2	H	0.59	0/5940	0.84	19/8038 (0.2%)
All	All	0.56	4/47184 (0.0%)	0.81	120/63828 (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
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	376	CYS	CB-SG	-7.40	1.69	1.82
2	B	741	CYS	CB-SG	-5.75	1.72	1.81
2	D	760	CYS	CB-SG	-5.12	1.73	1.81
1	G	881	CYS	CB-SG	-5.10	1.73	1.81

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	759	ARG	NE-CZ-NH1	-9.97	115.32	120.30
1	C	283	ARG	NE-CZ-NH2	9.78	125.19	120.30
2	H	436	ARG	NE-CZ-NH1	-9.71	115.44	120.30
1	A	289	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	C	283	ARG	NE-CZ-NH1	-9.64	115.48	120.30
1	E	759	ARG	NE-CZ-NH2	9.21	124.91	120.30
1	A	289	ARG	NE-CZ-NH2	9.11	124.86	120.30
2	D	334	ARG	NE-CZ-NH1	-8.87	115.87	120.30
1	G	264	ARG	NE-CZ-NH2	-8.32	116.14	120.30
2	H	631	ARG	NE-CZ-NH1	-8.28	116.16	120.30
2	F	636	ARG	NE-CZ-NH2	8.13	124.36	120.30
1	C	818	ARG	NE-CZ-NH1	-8.10	116.25	120.30
2	D	334	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	A	264	ARG	NE-CZ-NH2	7.96	124.28	120.30
2	F	636	ARG	NE-CZ-NH1	-7.86	116.37	120.30
2	D	326	ARG	NE-CZ-NH1	-7.72	116.44	120.30
2	H	631	ARG	NE-CZ-NH2	7.71	124.15	120.30
1	C	264	ARG	NE-CZ-NH2	-7.69	116.45	120.30
2	D	923	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	C	818	ARG	NE-CZ-NH2	7.66	124.13	120.30
2	D	923	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	E	758	ARG	NE-CZ-NH1	-7.58	116.51	120.30
2	H	436	ARG	NE-CZ-NH2	7.55	124.07	120.30
2	B	698	ARG	NE-CZ-NH2	7.55	124.07	120.30
2	F	698	ARG	NE-CZ-NH2	-7.50	116.55	120.30
2	D	812	ARG	NE-CZ-NH2	-7.34	116.63	120.30
2	D	326	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	G	264	ARG	NE-CZ-NH1	7.32	123.96	120.30
2	H	270	ARG	NE-CZ-NH2	-7.32	116.64	120.30
2	B	698	ARG	NE-CZ-NH1	-7.32	116.64	120.30
2	F	812	ARG	NE-CZ-NH2	-7.30	116.65	120.30
2	F	698	ARG	NE-CZ-NH1	7.29	123.94	120.30
2	H	812	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	A	319	ARG	NE-CZ-NH2	7.07	123.83	120.30
2	H	270	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	D	698	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	E	264	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	E	319	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	C	592	ASP	N-CA-C	-6.84	92.53	111.00
2	B	812	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	E	758	ARG	NE-CZ-NH2	6.82	123.71	120.30
2	H	698	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	H	812	ARG	NE-CZ-NH2	6.77	123.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ARG	NE-CZ-NH1	-6.77	116.92	120.30
1	E	264	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	A	264	ARG	NE-CZ-NH1	-6.70	116.95	120.30
2	F	270	ARG	NE-CZ-NH1	-6.67	116.96	120.30
2	D	270	ARG	NE-CZ-NH2	-6.67	116.97	120.30
2	D	698	ARG	NE-CZ-NH2	6.63	123.61	120.30
2	D	812	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	A	334	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	C	334	ARG	NE-CZ-NH2	-6.58	117.01	120.30
2	B	812	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	G	334	ARG	NE-CZ-NH2	-6.56	117.02	120.30
2	D	277	ARG	NE-CZ-NH2	6.55	123.58	120.30
2	B	270	ARG	NE-CZ-NH1	-6.51	117.04	120.30
2	H	277	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	C	264	ARG	NE-CZ-NH1	6.49	123.55	120.30
2	B	277	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	E	334	ARG	NE-CZ-NH1	-6.48	117.06	120.30
2	B	277	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	H	698	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	E	592	ASP	N-CA-C	-6.38	93.76	111.00
2	D	270	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	285	ARG	NE-CZ-NH2	6.35	123.48	120.30
2	H	277	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	F	812	ARG	NE-CZ-NH1	6.33	123.47	120.30
2	D	277	ARG	NE-CZ-NH1	-6.33	117.14	120.30
2	F	618	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	285	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	G	592	ASP	N-CA-C	-6.28	94.04	111.00
2	D	436	ARG	NE-CZ-NH2	-6.27	117.16	120.30
2	H	811	GLY	N-CA-C	6.21	128.62	113.10
1	E	334	ARG	NE-CZ-NH2	6.20	123.40	120.30
2	D	618	ARG	NE-CZ-NH1	-6.17	117.22	120.30
2	B	436	ARG	NE-CZ-NH2	-6.14	117.23	120.30
2	D	811	GLY	N-CA-C	6.13	128.42	113.10
1	C	599	VAL	CB-CA-C	-6.13	99.76	111.40
2	B	811	GLY	N-CA-C	6.11	128.38	113.10
2	F	270	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	A	334	ARG	NE-CZ-NH2	6.07	123.33	120.30
2	B	270	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	592	ASP	N-CA-C	-6.06	94.65	111.00
2	D	618	ARG	NE-CZ-NH2	6.04	123.32	120.30
2	B	618	ARG	NE-CZ-NH1	-6.03	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	618	ARG	NE-CZ-NH2	6.01	123.30	120.30
1	E	811	ARG	NE-CZ-NH2	-5.99	117.31	120.30
2	H	618	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	D	436	ARG	NE-CZ-NH1	5.89	123.24	120.30
2	F	436	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	F	890	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	G	334	ARG	NE-CZ-NH1	5.75	123.17	120.30
2	H	890	ARG	NE-CZ-NH2	5.74	123.17	120.30
2	F	811	GLY	N-CA-C	5.72	127.41	113.10
1	E	319	ARG	NE-CZ-NH2	-5.71	117.45	120.30
2	F	277	ARG	NE-CZ-NH1	-5.67	117.47	120.30
2	F	277	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	811	ARG	NE-CZ-NH2	5.58	123.09	120.30
2	F	618	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	H	890	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	G	319	ARG	NE-CZ-NH1	-5.54	117.53	120.30
2	H	618	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	H	731	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	972	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	B	890	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	B	585	LYS	N-CA-C	-5.30	96.68	111.00
2	H	352	SER	N-CA-C	5.29	125.28	111.00
1	E	719	ILE	N-CA-C	-5.22	96.89	111.00
1	G	945	ASN	N-CA-C	-5.21	96.92	111.00
1	G	588	LEU	N-CA-C	-5.20	96.97	111.00
1	A	811	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	E	811	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	E	588	LEU	N-CA-C	-5.15	97.09	111.00
1	C	811	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	E	205	LYS	N-CA-C	5.08	124.73	111.00
2	F	352	SER	N-CA-C	5.07	124.69	111.00
2	D	585	LYS	N-CA-C	-5.07	97.32	111.00
1	E	593	ARG	N-CA-C	-5.07	97.32	111.00
1	G	719	ILE	N-CA-C	-5.05	97.36	111.00
2	F	436	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	771	TYR	Sidechain
2	D	771	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	F	771	TYR	Sidechain
2	H	771	TYR	Sidechain

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	5759	0	5758	334	0
1	C	5759	0	5758	326	0
1	E	5777	0	5779	323	0
1	G	5733	0	5733	306	0
2	B	5834	0	5799	366	0
2	D	5834	0	5799	349	0
2	F	5827	0	5791	327	1
2	H	5834	0	5799	373	1
3	A	16	0	11	4	0
3	B	16	0	11	4	0
3	C	16	0	11	1	0
3	D	16	0	11	3	0
3	E	16	0	11	2	0
3	F	16	0	11	4	0
3	G	16	0	11	2	0
3	H	16	0	11	5	0
4	A	20	0	10	6	0
4	B	20	0	10	3	0
4	C	20	0	10	1	0
4	D	20	0	10	2	0
4	E	20	0	10	0	0
4	F	20	0	10	3	0
4	G	20	0	10	0	0
4	H	20	0	10	2	0
All	All	46645	0	46384	2612	1

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 30.

All (2612) 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:C:427:HIS:HB3	1:C:460:ASP:HB2	1.33	1.10
1:A:665:ARG:HH21	4:A:1:FDP:H62	1.12	1.07
1:A:427:HIS:HB3	1:A:460:ASP:HB2	1.35	1.06
2:H:874:LYS:HD3	2:H:917:VAL:HG11	1.34	1.06
1:G:427:HIS:HB3	1:G:460:ASP:HB2	1.40	1.03
1:E:427:HIS:HB3	1:E:460:ASP:HB2	1.40	1.02
2:B:416:PRO:O	2:B:418:THR:HG22	1.60	1.02
2:H:416:PRO:O	2:H:418:THR:HG22	1.61	0.99
2:H:578:GLU:O	2:H:580:LYS:N	1.95	0.99
2:D:416:PRO:O	2:D:418:THR:HG22	1.60	0.98
2:H:214:ASN:ND2	2:H:343:THR:HG21	1.78	0.98
2:B:418:THR:HA	2:B:421:GLU:HB2	1.44	0.98
2:D:874:LYS:HD3	2:D:917:VAL:HG11	1.43	0.98
1:C:518:THR:OG1	1:C:521:THR:HG23	1.64	0.97
1:E:599:VAL:HG13	1:E:629:ILE:HB	1.46	0.97
2:B:418:THR:HG23	2:B:419:SER:H	1.28	0.97
2:D:418:THR:HG23	2:D:419:SER:H	1.26	0.97
2:B:635:VAL:O	2:B:636:ARG:HD2	1.64	0.97
1:C:804:THR:CG2	1:C:979:VAL:HG21	1.95	0.97
1:A:665:ARG:NH2	4:A:1:FDP:H62	1.79	0.96
1:A:599:VAL:HG13	1:A:629:ILE:HB	1.48	0.96
1:G:599:VAL:HG13	1:G:629:ILE:HB	1.44	0.96
2:F:416:PRO:O	2:F:418:THR:HG22	1.65	0.96
2:B:711:VAL:HA	2:B:908:ALA:O	1.66	0.95
1:E:821:LYS:HZ2	1:E:821:LYS:HB2	1.31	0.95
1:A:319:ARG:HB2	1:A:348:ILE:HD12	1.48	0.95
2:H:578:GLU:O	2:H:580:LYS:HG3	1.66	0.95
2:B:578:GLU:O	2:B:580:LYS:HG3	1.66	0.94
1:C:669:SER:H	1:C:701:GLN:HE22	1.14	0.94
2:F:418:THR:HG23	2:F:419:SER:H	1.31	0.94
2:F:701:GLU:O	2:F:702:SER:HB2	1.68	0.94
1:G:581:LYS:HB3	1:G:586:GLU:HB3	1.49	0.94
2:H:577:ASN:HB3	2:H:579:PRO:HG2	1.46	0.94
2:D:578:GLU:O	2:D:580:LYS:N	2.01	0.94
2:F:578:GLU:O	2:F:580:LYS:N	2.01	0.93
1:C:466:THR:HG22	1:C:468:ASN:H	1.33	0.93
2:D:577:ASN:HB3	2:D:579:PRO:HG2	1.51	0.93
2:B:577:ASN:HB3	2:B:579:PRO:HG2	1.51	0.93
2:D:882:ASN:HD22	2:D:906:THR:HG22	1.34	0.93
2:B:701:GLU:O	2:B:702:SER:HB2	1.69	0.93
2:H:418:THR:HG23	2:H:419:SER:H	1.32	0.93
1:A:466:THR:HG22	1:A:468:ASN:H	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:ASN:HD22	2:B:906:THR:HG22	1.34	0.93
1:E:466:THR:HG22	1:E:468:ASN:H	1.29	0.93
1:A:669:SER:H	1:A:701:GLN:HE22	1.13	0.92
1:E:581:LYS:HB3	1:E:586:GLU:HB3	1.51	0.92
2:B:913:LYS:O	2:B:916:HIS:HB2	1.70	0.92
2:B:578:GLU:O	2:B:580:LYS:N	2.03	0.92
1:E:431:GLN:HE21	1:E:431:GLN:H	1.15	0.91
1:E:431:GLN:NE2	1:E:431:GLN:H	1.66	0.91
2:B:790:LEU:HD11	1:C:841:ILE:CG2	2.00	0.91
2:D:635:VAL:O	2:D:636:ARG:HD2	1.71	0.90
1:G:212:THR:HG21	1:G:272:THR:OG1	1.70	0.90
1:C:431:GLN:H	1:C:431:GLN:NE2	1.68	0.90
2:F:607:SER:OG	2:F:869:THR:HB	1.69	0.90
2:B:214:ASN:ND2	2:B:343:THR:HG21	1.86	0.90
2:H:701:GLU:O	2:H:702:SER:HB2	1.71	0.90
2:D:711:VAL:HA	2:D:908:ALA:O	1.72	0.90
2:F:214:ASN:ND2	2:F:343:THR:HG21	1.86	0.90
1:G:669:SER:H	1:G:701:GLN:HE22	1.13	0.90
2:H:792:GLN:HE22	2:H:957:ARG:CB	1.85	0.89
1:G:825:ARG:NH1	1:G:829:ALA:HB3	1.87	0.89
2:F:711:VAL:HA	2:F:908:ALA:O	1.70	0.89
2:F:882:ASN:HD22	2:F:906:THR:HG22	1.37	0.89
2:D:701:GLU:O	2:D:702:SER:HB2	1.71	0.89
2:F:577:ASN:C	2:F:579:PRO:HD2	1.93	0.89
1:E:212:THR:HG21	1:E:272:THR:OG1	1.73	0.88
2:B:577:ASN:C	2:B:579:PRO:HD2	1.93	0.88
1:A:356:ASP:OD2	3:A:988:F6P:H11	1.73	0.88
2:H:214:ASN:HD21	2:H:343:THR:HG21	1.37	0.87
1:G:466:THR:HB	1:G:469:ASP:OD1	1.74	0.87
1:A:328:GLU:O	1:A:332:GLU:HG3	1.75	0.87
2:D:913:LYS:O	2:D:916:HIS:HB2	1.75	0.87
1:E:947:THR:HG22	1:E:953:LYS:H	1.38	0.87
2:F:578:GLU:O	2:F:580:LYS:HG3	1.74	0.87
2:H:711:VAL:HA	2:H:908:ALA:O	1.74	0.86
1:A:809:ASN:HB2	1:A:975:LEU:HD11	1.57	0.86
2:B:793:LEU:O	2:B:797:ILE:HG13	1.76	0.86
1:A:431:GLN:NE2	1:A:431:GLN:H	1.73	0.86
1:G:466:THR:HG22	1:G:468:ASN:H	1.37	0.86
2:D:582:PRO:HD2	2:D:615:GLN:O	1.75	0.86
1:G:974:LYS:HG2	1:G:975:LEU:HD13	1.58	0.86
1:E:319:ARG:HB2	1:E:348:ILE:HD12	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:348:ASP:OD2	3:H:986:F6P:H11	1.74	0.86
2:H:577:ASN:C	2:H:579:PRO:HD2	1.96	0.85
2:F:348:ASP:OD2	3:F:984:F6P:H11	1.77	0.85
2:F:577:ASN:HB3	2:F:579:PRO:HG2	1.58	0.85
1:G:505:LEU:HB3	1:G:533:ILE:HD11	1.58	0.85
2:B:790:LEU:HD11	1:C:841:ILE:HG21	1.57	0.85
2:D:577:ASN:C	2:D:579:PRO:HD2	1.96	0.85
1:E:949:VAL:O	1:E:951:LEU:N	2.10	0.84
2:F:582:PRO:HD2	2:F:615:GLN:O	1.77	0.84
2:B:936:MET:HB2	2:B:937:PRO:HD2	1.59	0.84
1:G:975:LEU:H	1:G:975:LEU:HD22	1.40	0.84
1:G:505:LEU:HB3	1:G:533:ILE:CD1	2.08	0.84
2:D:381:HIS:HB2	2:D:383:ARG:HG3	1.60	0.84
2:D:214:ASN:ND2	2:D:343:THR:HG21	1.93	0.83
2:D:578:GLU:N	2:D:579:PRO:HD2	1.93	0.83
1:E:669:SER:H	1:E:701:GLN:HE22	1.22	0.83
2:B:427:CYS:SG	2:B:470:LEU:HD23	2.19	0.83
2:F:554:MET:HG2	2:F:562:ILE:HG12	1.58	0.83
1:A:336:THR:OG1	1:A:339:GLU:HG3	1.78	0.83
1:C:431:GLN:H	1:C:431:GLN:HE21	1.23	0.83
2:B:582:PRO:HD2	2:B:615:GLN:O	1.79	0.83
2:D:575:ASP:HB3	2:D:613:MET:HB3	1.60	0.83
1:E:583:ASP:HB3	1:E:585:SER:OG	1.78	0.83
1:E:588:LEU:HD13	1:E:593:ARG:HH12	1.43	0.83
1:C:587:LEU:O	1:C:622:HIS:HA	1.79	0.83
1:E:844:GLU:OE2	2:H:826:ALA:N	2.12	0.83
2:D:607:SER:OG	2:D:869:THR:HB	1.79	0.82
1:A:505:LEU:HB3	1:A:533:ILE:HD11	1.60	0.82
2:H:936:MET:HB2	2:H:937:PRO:HD2	1.59	0.82
2:H:792:GLN:HE22	2:H:957:ARG:HB2	1.43	0.82
1:G:583:ASP:HB3	1:G:585:SER:OG	1.78	0.82
1:G:782:THR:HG21	1:G:822:LEU:HD11	1.60	0.82
2:F:381:HIS:HB2	2:F:383:ARG:HG3	1.60	0.82
2:F:936:MET:HB2	2:F:937:PRO:HD2	1.62	0.82
1:E:466:THR:HB	1:E:469:ASP:OD1	1.79	0.81
1:E:822:LEU:O	1:E:822:LEU:HD12	1.80	0.81
1:A:212:THR:HG21	1:A:272:THR:OG1	1.80	0.81
1:A:466:THR:HB	1:A:469:ASP:OD1	1.80	0.81
1:C:212:THR:HG21	1:C:272:THR:OG1	1.80	0.81
1:G:963:ASN:ND2	1:G:963:ASN:H	1.76	0.81
2:H:578:GLU:N	2:H:579:PRO:HD2	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:HB3	1:A:533:ILE:CD1	2.09	0.81
2:F:214:ASN:HD21	2:F:343:THR:HG21	1.44	0.81
1:G:703:ARG:HD3	1:G:921:ASP:OD1	1.79	0.81
1:C:466:THR:HG22	1:C:468:ASN:N	1.95	0.81
2:H:882:ASN:HD22	2:H:906:THR:HG22	1.46	0.81
2:H:587:LEU:H	2:H:617:HIS:HD1	1.28	0.81
1:A:947:THR:HG22	1:A:953:LYS:H	1.45	0.81
1:A:669:SER:H	1:A:701:GLN:NE2	1.78	0.81
1:G:770:HIS:O	1:G:953:LYS:HD2	1.80	0.81
1:G:431:GLN:NE2	1:G:431:GLN:H	1.80	0.80
1:A:289:ARG:HB2	1:A:325:LEU:HD22	1.63	0.80
1:A:518:THR:OG1	1:A:521:THR:HG23	1.82	0.80
2:H:664:ALA:O	2:H:665:ASP:HB3	1.81	0.80
2:B:710:MET:O	2:B:711:VAL:HG12	1.82	0.80
2:H:418:THR:HA	2:H:421:GLU:HB2	1.63	0.80
1:G:518:THR:OG1	1:G:521:THR:HG23	1.82	0.80
2:F:664:ALA:O	2:F:665:ASP:HB3	1.82	0.79
2:D:554:MET:HG2	2:D:562:ILE:HG12	1.65	0.79
1:E:466:THR:HG22	1:E:468:ASN:N	1.97	0.79
1:E:796:LEU:HD22	2:H:790:LEU:HD22	1.63	0.79
2:F:418:THR:HA	2:F:421:GLU:HB2	1.63	0.79
2:D:467:VAL:O	2:D:471:GLY:HA2	1.81	0.79
2:H:195:PRO:HG2	2:H:334:ARG:HH11	1.45	0.79
2:H:575:ASP:HB3	2:H:613:MET:HB3	1.65	0.79
1:C:427:HIS:CB	1:C:460:ASP:HB2	2.12	0.79
2:F:826:ALA:N	1:G:844:GLU:OE2	2.16	0.79
1:G:588:LEU:HD13	1:G:593:ARG:HH12	1.46	0.79
1:G:669:SER:H	1:G:701:GLN:NE2	1.80	0.79
1:E:813:ASP:CG	1:E:814:LYS:H	1.84	0.78
2:H:582:PRO:HD2	2:H:615:GLN:O	1.82	0.78
2:B:467:VAL:O	2:B:471:GLY:HA2	1.82	0.78
2:B:900:ASP:H	2:B:903:ILE:HD11	1.48	0.78
1:C:505:LEU:HB3	1:C:533:ILE:CD1	2.14	0.78
2:D:587:LEU:N	2:D:587:LEU:HD12	1.98	0.78
2:H:381:HIS:HB2	2:H:383:ARG:HG3	1.65	0.78
2:H:581:LEU:HB2	2:H:582:PRO:HD3	1.65	0.78
1:G:782:THR:CG2	1:G:822:LEU:HD11	2.13	0.78
2:B:578:GLU:N	2:B:579:PRO:HD2	1.99	0.78
2:B:886:ILE:O	2:B:890:ARG:HB2	1.83	0.78
2:H:390:MET:HG3	2:H:483:GLN:NE2	1.99	0.78
1:A:427:HIS:CB	1:A:460:ASP:HB2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:319:ARG:HD2	1:E:346:LEU:O	1.84	0.77
2:H:913:LYS:O	2:H:916:HIS:HB2	1.84	0.77
2:B:587:LEU:H	2:B:617:HIS:HD1	1.32	0.77
1:E:541:SER:O	1:E:545:THR:HG23	1.83	0.77
1:E:950:GLU:O	1:E:951:LEU:HB2	1.85	0.77
1:G:466:THR:HG22	1:G:468:ASN:N	1.98	0.77
1:A:770:HIS:CD2	1:A:951:LEU:HA	2.20	0.77
2:B:575:ASP:HB3	2:B:613:MET:HB3	1.65	0.77
2:D:664:ALA:O	2:D:665:ASP:HB3	1.83	0.77
1:C:328:GLU:O	1:C:332:GLU:HG3	1.84	0.77
2:D:348:ASP:OD2	3:D:982:F6P:H11	1.84	0.77
2:F:436:ARG:NH2	2:F:575:ASP:OD1	2.16	0.77
2:F:946:ARG:HG3	2:F:946:ARG:HH21	1.49	0.77
1:C:947:THR:HG22	1:C:953:LYS:H	1.50	0.77
1:A:431:GLN:HE21	1:A:431:GLN:H	1.28	0.77
1:A:466:THR:HG22	1:A:468:ASN:N	1.99	0.77
1:C:289:ARG:HG2	1:C:329:LEU:HD21	1.66	0.77
2:B:390:MET:HG3	2:B:483:GLN:NE2	1.99	0.77
1:A:947:THR:HG21	1:A:951:LEU:HB2	1.64	0.77
2:F:467:VAL:O	2:F:471:GLY:HA2	1.85	0.77
2:B:935:ARG:HH12	4:B:2:FDP:P1	2.07	0.76
2:H:418:THR:HG23	2:H:419:SER:N	1.99	0.76
1:A:587:LEU:O	1:A:622:HIS:HA	1.85	0.76
1:A:782:THR:HG21	1:A:822:LEU:HD11	1.66	0.76
1:C:669:SER:H	1:C:701:GLN:NE2	1.82	0.76
1:E:590:VAL:HG23	1:E:591:SER:H	1.50	0.76
1:G:974:LYS:HG2	1:G:975:LEU:N	1.99	0.76
1:C:466:THR:HB	1:C:469:ASP:OD1	1.85	0.76
2:B:581:LEU:HB2	2:B:582:PRO:HD3	1.67	0.76
1:C:319:ARG:HD3	1:C:346:LEU:O	1.86	0.76
2:D:900:ASP:H	2:D:903:ILE:HD11	1.51	0.76
1:E:587:LEU:O	1:E:622:HIS:HA	1.86	0.76
2:F:578:GLU:N	2:F:579:PRO:HD2	2.01	0.76
1:G:422:GLU:O	1:G:423:ARG:HD2	1.85	0.76
2:B:505:ASN:O	2:B:509:GLU:HG2	1.86	0.76
1:C:356:ASP:OD2	3:C:988:F6P:H11	1.85	0.76
1:C:825:ARG:NH1	1:C:829:ALA:HB3	2.00	0.76
1:A:583:ASP:HB3	1:A:585:SER:OG	1.86	0.76
2:D:418:THR:HG23	2:D:419:SER:N	2.00	0.76
1:A:813:ASP:CG	1:A:814:LYS:H	1.89	0.76
2:B:418:THR:HG23	2:B:419:SER:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:913:LYS:O	2:F:916:HIS:HB2	1.86	0.76
2:H:903:ILE:HD12	2:H:904:SER:N	2.01	0.76
1:G:326:VAL:HG13	1:G:340:VAL:HG21	1.66	0.75
2:D:793:LEU:O	2:D:797:ILE:HG13	1.87	0.75
1:A:326:VAL:O	1:A:330:VAL:HG23	1.85	0.75
1:E:782:THR:HG21	1:E:822:LEU:HD11	1.66	0.75
2:F:427:CYS:SG	2:F:470:LEU:HD23	2.26	0.75
2:H:710:MET:O	2:H:711:VAL:HG12	1.85	0.75
1:C:276:THR:HG23	1:C:276:THR:O	1.86	0.75
1:C:287:GLY:O	1:C:290:GLN:HB3	1.85	0.75
1:C:613:ARG:HA	1:C:650:VAL:HG21	1.69	0.75
2:H:583:LYS:O	2:H:585:LYS:N	2.19	0.75
1:C:505:LEU:HB3	1:C:533:ILE:HD11	1.69	0.75
1:G:431:GLN:HE21	1:G:431:GLN:H	1.35	0.75
1:G:822:LEU:HD12	1:G:822:LEU:O	1.86	0.74
2:H:418:THR:CG2	2:H:419:SER:H	1.91	0.74
1:E:800:ARG:HD2	2:H:790:LEU:HB3	1.68	0.74
2:H:607:SER:OG	2:H:869:THR:HB	1.87	0.74
2:B:381:HIS:HB2	2:B:383:ARG:HG3	1.68	0.74
2:D:946:ARG:HH21	2:D:946:ARG:HG3	1.52	0.74
2:H:946:ARG:HH21	2:H:946:ARG:HG3	1.53	0.74
1:A:348:ILE:O	1:A:524:PRO:HD2	1.86	0.74
2:B:607:SER:OG	2:B:869:THR:HB	1.88	0.74
2:B:214:ASN:HD21	2:B:343:THR:HG21	1.50	0.74
1:E:669:SER:H	1:E:701:GLN:NE2	1.86	0.74
2:B:903:ILE:HD12	2:B:904:SER:N	2.03	0.74
1:G:360:SER:N	1:G:545:THR:HG22	2.03	0.74
2:B:414:GLU:OE1	2:B:557:ARG:NH1	2.20	0.74
2:D:587:LEU:H	2:D:617:HIS:HD1	1.35	0.74
2:F:903:ILE:HD12	2:F:904:SER:N	2.02	0.74
1:G:589:PRO:HD2	1:G:622:HIS:O	1.87	0.74
2:F:505:ASN:O	2:F:509:GLU:HG2	1.87	0.74
2:F:418:THR:HG23	2:F:419:SER:N	2.03	0.73
1:A:330:VAL:HA	1:A:335:PHE:O	1.87	0.73
2:B:946:ARG:HG3	2:B:946:ARG:HH21	1.51	0.73
1:C:205:LYS:O	1:C:207:LYS:HD2	1.88	0.73
1:E:505:LEU:HB3	1:E:533:ILE:CD1	2.17	0.73
1:C:804:THR:HG23	1:C:979:VAL:HG21	1.69	0.73
1:G:587:LEU:O	1:G:622:HIS:HA	1.88	0.73
1:G:770:HIS:CB	1:G:951:LEU:HB3	2.19	0.73
1:A:782:THR:CG2	1:A:822:LEU:HD11	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:ARG:HG3	1:C:335:PHE:CD1	2.23	0.73
2:D:892:ALA:HB3	2:D:894:GLU:HG2	1.71	0.73
2:F:203:THR:OG1	2:F:264:THR:HG21	1.88	0.73
2:B:633:GLU:HB2	2:B:672:TYR:CZ	2.24	0.73
1:C:599:VAL:HG13	1:C:629:ILE:HB	1.68	0.73
1:E:613:ARG:HD2	1:E:650:VAL:O	1.89	0.73
1:C:326:VAL:O	1:C:330:VAL:HG23	1.86	0.73
2:F:285:GLN:O	2:F:289:GLU:HG3	1.88	0.73
2:B:392:ARG:HH21	3:B:980:F6P:H12	1.52	0.73
2:F:889:ALA:C	2:F:891:ALA:H	1.92	0.73
1:G:486:LEU:O	1:G:489:VAL:HG22	1.89	0.73
1:G:590:VAL:HG23	1:G:591:SER:H	1.53	0.73
1:E:832:VAL:O	2:H:831:LYS:NZ	2.20	0.72
1:E:703:ARG:HD3	1:E:921:ASP:OD1	1.87	0.72
2:F:900:ASP:H	2:F:903:ILE:HD11	1.53	0.72
2:H:554:MET:HG2	2:H:562:ILE:HG12	1.70	0.72
2:D:327:ILE:HA	2:D:331:GLN:HE22	1.52	0.72
1:A:336:THR:HG1	1:A:339:GLU:HG3	1.52	0.72
1:A:825:ARG:NH1	1:A:829:ALA:HB3	2.04	0.72
2:F:392:ARG:HH21	3:F:984:F6P:H12	1.54	0.72
2:B:956:LYS:NZ	2:B:956:LYS:HA	2.03	0.72
1:C:594:LEU:HD21	1:C:889:ASN:ND2	2.04	0.72
1:A:289:ARG:HD2	1:A:328:GLU:HB3	1.72	0.72
2:B:285:GLN:O	2:B:289:GLU:HG3	1.88	0.72
2:D:264:THR:HG22	2:D:266:ILE:H	1.54	0.72
2:D:936:MET:HB2	2:D:937:PRO:HD2	1.72	0.72
2:H:323:LYS:O	2:H:324:THR:HB	1.88	0.72
1:G:292:ALA:O	1:G:296:ILE:HG13	1.90	0.72
2:H:467:VAL:O	2:H:471:GLY:HA2	1.89	0.72
2:H:889:ALA:C	2:H:891:ALA:H	1.92	0.72
1:A:685:ASP:O	1:A:714:ILE:HB	1.89	0.72
2:H:701:GLU:HB3	2:H:897:ASN:HD22	1.53	0.72
1:E:287:GLY:O	1:E:290:GLN:HB3	1.89	0.71
1:G:448:ASN:HD22	1:G:448:ASN:H	1.35	0.71
2:B:900:ASP:N	2:B:903:ILE:HD11	2.04	0.71
1:E:782:THR:CG2	1:E:822:LEU:HD11	2.19	0.71
2:D:583:LYS:O	2:D:585:LYS:N	2.23	0.71
1:G:613:ARG:HA	1:G:650:VAL:HG21	1.71	0.71
2:H:414:GLU:OE1	2:H:557:ARG:NH1	2.22	0.71
2:B:587:LEU:N	2:B:587:LEU:HD12	2.05	0.71
1:E:385:THR:HA	2:F:207:ASP:OD2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:537:PRO:HG2	1:C:540:GLU:HB2	1.71	0.71
1:C:782:THR:HG21	1:C:822:LEU:HD11	1.72	0.71
2:D:418:THR:CG2	2:D:419:SER:H	1.91	0.71
1:E:518:THR:OG1	1:E:521:THR:HG23	1.90	0.71
1:G:360:SER:H	1:G:545:THR:HG22	1.54	0.71
2:H:285:GLN:O	2:H:289:GLU:HG3	1.90	0.71
1:A:287:GLY:O	1:A:290:GLN:HB3	1.91	0.71
1:C:422:GLU:HG2	1:C:564:ARG:HD2	1.71	0.71
1:G:505:LEU:CB	1:G:533:ILE:HD11	2.20	0.71
2:H:428:ASP:OD1	2:H:432:LYS:NZ	2.23	0.71
2:B:348:ASP:OD2	3:B:980:F6P:H11	1.90	0.71
1:A:946:GLU:O	1:A:955:PHE:CZ	2.44	0.71
1:C:285:ARG:NH2	1:C:328:GLU:OE2	2.24	0.71
2:D:587:LEU:HD23	2:D:883:GLN:NE2	2.05	0.71
1:A:336:THR:HG23	1:A:339:GLU:CD	2.10	0.70
2:F:201:VAL:HG11	2:F:218:ILE:HD13	1.72	0.70
1:A:613:ARG:HA	1:A:650:VAL:HG21	1.73	0.70
2:B:956:LYS:HZ3	2:B:956:LYS:HA	1.56	0.70
1:G:427:HIS:CB	1:G:460:ASP:HB2	2.16	0.70
1:A:822:LEU:O	1:A:822:LEU:HD12	1.91	0.70
1:A:216:ASP:OD2	2:B:377:THR:HA	1.90	0.70
1:C:541:SER:O	1:C:545:THR:HG23	1.91	0.70
1:E:844:GLU:OE2	2:H:825:LYS:N	2.24	0.70
1:E:832:VAL:HG22	2:H:834:GLU:HB3	1.72	0.70
1:A:703:ARG:HD3	1:A:921:ASP:OD1	1.91	0.70
2:F:522:ASN:ND2	2:F:527:VAL:HG21	2.05	0.70
1:G:326:VAL:HG13	1:G:340:VAL:CG2	2.21	0.70
2:H:203:THR:OG1	2:H:264:THR:HG21	1.92	0.70
1:A:767:GLN:NE2	4:A:1:FDP:H3	2.06	0.70
2:D:710:MET:O	2:D:711:VAL:HG12	1.91	0.70
1:G:326:VAL:O	1:G:330:VAL:HG23	1.91	0.70
1:C:587:LEU:HB3	1:C:622:HIS:CE1	2.27	0.70
2:F:418:THR:HG1	2:F:422:TRP:HD1	1.31	0.70
2:F:900:ASP:N	2:F:903:ILE:HD11	2.06	0.70
1:E:356:ASP:OD2	3:E:988:F6P:H11	1.91	0.70
1:E:427:HIS:CB	1:E:460:ASP:HB2	2.20	0.70
2:F:827:LEU:HB3	2:F:832:LEU:HD13	1.72	0.70
1:G:947:THR:HG22	1:G:953:LYS:H	1.56	0.70
1:A:588:LEU:HD13	1:A:593:ARG:HH12	1.55	0.70
1:G:541:SER:O	1:G:545:THR:HG23	1.92	0.70
2:D:704:PRO:HA	2:D:707:ARG:HG2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:822:LEU:C	1:E:822:LEU:HD12	2.12	0.69
2:F:288:ILE:HA	2:F:335:MET:HE1	1.72	0.69
2:F:621:ALA:HB2	2:F:638:LEU:HD11	1.74	0.69
2:H:281:LEU:HD23	2:H:326:ARG:NH2	2.07	0.69
2:H:704:PRO:HA	2:H:707:ARG:HG2	1.74	0.69
1:A:594:LEU:HD21	1:A:889:ASN:ND2	2.07	0.69
2:D:505:ASN:O	2:D:509:GLU:HG2	1.92	0.69
2:F:575:ASP:HB3	2:F:613:MET:HB3	1.72	0.69
2:H:792:GLN:HE22	2:H:957:ARG:HB3	1.55	0.69
1:C:249:LEU:HD21	1:C:281:GLU:HB3	1.73	0.69
1:E:796:LEU:HD11	2:H:793:LEU:HD13	1.73	0.69
2:F:327:ILE:HA	2:F:331:GLN:HE22	1.58	0.69
2:D:328:SER:H	2:D:331:GLN:NE2	1.89	0.69
1:G:594:LEU:HD21	1:G:889:ASN:ND2	2.07	0.69
2:B:930:THR:HG22	2:B:932:VAL:N	2.08	0.69
1:E:947:THR:HG23	1:E:947:THR:O	1.91	0.69
1:A:505:LEU:CB	1:A:533:ILE:HD11	2.21	0.69
2:B:664:ALA:O	2:B:665:ASP:HB3	1.91	0.69
2:F:581:LEU:HB2	2:F:582:PRO:HD3	1.73	0.69
1:G:637:ILE:HD13	1:G:671:ASP:HB3	1.73	0.69
2:B:889:ALA:C	2:B:891:ALA:H	1.95	0.69
1:C:212:THR:O	1:C:212:THR:HG23	1.91	0.69
1:C:600:HIS:HD2	1:C:659:SER:OG	1.75	0.69
1:C:613:ARG:HD2	1:C:650:VAL:O	1.93	0.69
2:D:323:LYS:O	2:D:324:THR:HB	1.93	0.69
2:B:418:THR:CG2	2:B:419:SER:H	1.93	0.69
2:D:903:ILE:HD12	2:D:904:SER:N	2.07	0.69
1:G:422:GLU:HG2	1:G:564:ARG:HD2	1.74	0.69
1:E:589:PRO:HD2	1:E:622:HIS:O	1.94	0.68
1:C:931:GLY:O	1:C:932:SER:HB3	1.92	0.68
1:G:287:GLY:O	1:G:290:GLN:HB3	1.93	0.68
1:C:703:ARG:HD3	1:C:921:ASP:OD1	1.94	0.68
2:F:583:LYS:O	2:F:585:LYS:N	2.26	0.68
2:F:834:GLU:HB3	1:G:832:VAL:HG22	1.75	0.68
1:G:814:LYS:NZ	1:G:814:LYS:HA	2.08	0.68
2:B:288:ILE:HA	2:B:335:MET:HE1	1.75	0.68
2:D:889:ALA:C	2:D:891:ALA:H	1.97	0.68
2:B:583:LYS:O	2:B:585:LYS:N	2.27	0.68
1:A:422:GLU:O	1:A:423:ARG:HD2	1.93	0.68
1:C:319:ARG:HG2	1:C:346:LEU:HB3	1.75	0.68
2:B:201:VAL:HG11	2:B:218:ILE:HD13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:ILE:HA	2:B:331:GLN:HE22	1.59	0.68
2:D:907:ALA:O	2:D:922:ILE:HG22	1.94	0.68
2:D:930:THR:HG22	2:D:932:VAL:N	2.07	0.68
2:F:323:LYS:O	2:F:324:THR:HB	1.94	0.68
2:H:418:THR:HG1	2:H:422:TRP:HD1	1.39	0.68
2:H:579:PRO:O	2:H:580:LYS:C	2.31	0.68
2:D:589:ILE:HD13	2:D:879:ILE:HG21	1.74	0.68
1:C:637:ILE:HD13	1:C:671:ASP:HB3	1.75	0.68
2:H:681:LEU:O	2:H:710:MET:O	2.10	0.68
2:B:323:LYS:O	2:B:324:THR:HB	1.92	0.68
2:B:436:ARG:NH2	2:B:575:ASP:OD1	2.22	0.68
2:D:591:ILE:HD13	2:D:592:VAL:H	1.59	0.68
1:E:210:VAL:CG1	1:E:227:VAL:HG11	2.24	0.68
1:C:505:LEU:CB	1:C:533:ILE:HD11	2.24	0.67
2:F:201:VAL:CG1	2:F:218:ILE:HD13	2.24	0.67
2:F:633:GLU:HB2	2:F:672:TYR:CZ	2.27	0.67
1:G:947:THR:O	1:G:947:THR:HG23	1.94	0.67
1:A:746:TYR:CD1	2:B:854:VAL:HG11	2.29	0.67
2:B:595:GLY:O	2:B:656:THR:OG1	2.12	0.67
1:C:326:VAL:HG13	1:C:340:VAL:HG21	1.76	0.67
2:D:317:LEU:O	2:D:321:LEU:HD23	1.94	0.67
2:D:930:THR:HG22	2:D:932:VAL:H	1.57	0.67
1:E:637:ILE:HD13	1:E:671:ASP:HB3	1.77	0.67
2:F:341:CYS:HB2	2:F:507:VAL:HG13	1.75	0.67
1:G:770:HIS:HB2	1:G:951:LEU:HB3	1.74	0.67
2:B:462:VAL:O	2:B:466:LEU:HD23	1.95	0.67
2:H:525:LYS:NZ	2:H:525:LYS:HB2	2.09	0.67
1:A:732:TYR:CE1	1:A:736:VAL:HB	2.30	0.67
1:E:814:LYS:O	1:E:816:GLU:HG3	1.93	0.67
1:E:947:THR:O	1:E:948:ASN:C	2.32	0.67
2:H:591:ILE:HD13	2:H:592:VAL:H	1.60	0.67
2:B:950:ASP:OD1	2:B:955:ARG:HD3	1.94	0.67
2:D:827:LEU:HB3	2:D:832:LEU:HD13	1.76	0.67
1:E:825:ARG:NH1	1:E:829:ALA:HB3	2.09	0.67
1:E:776:SER:HB3	1:E:963:ASN:HD21	1.59	0.67
2:F:950:ASP:OD1	2:F:955:ARG:HD3	1.94	0.67
2:H:196:GLN:NE2	2:H:228:ARG:HD3	2.10	0.67
1:E:587:LEU:C	1:E:589:PRO:HD3	2.14	0.67
1:E:600:HIS:HD2	1:E:659:SER:OG	1.77	0.67
2:H:264:THR:CG2	2:H:266:ILE:HG12	2.25	0.67
1:C:249:LEU:CD1	1:C:290:GLN:HG2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:325:ASN:O	2:F:327:ILE:N	2.23	0.67
2:B:240:VAL:HG21	2:B:273:GLU:HB2	1.77	0.67
1:C:326:VAL:HG13	1:C:340:VAL:CG2	2.25	0.67
2:H:317:LEU:O	2:H:321:LEU:HD23	1.94	0.67
2:D:400:LEU:HD12	2:D:866:THR:HG21	1.77	0.67
2:H:579:PRO:O	2:H:581:LEU:N	2.28	0.67
1:A:724:SER:OG	4:A:1:FDP:H12	1.95	0.66
2:D:203:THR:OG1	2:D:264:THR:HG21	1.95	0.66
2:F:244:PRO:O	2:F:245:GLU:HB3	1.95	0.66
1:C:697:ARG:HH22	1:C:949:VAL:HG22	1.60	0.66
1:C:746:TYR:CD1	2:D:854:VAL:HG11	2.29	0.66
2:F:710:MET:O	2:F:711:VAL:HG12	1.94	0.66
2:H:264:THR:HG22	2:H:266:ILE:H	1.59	0.66
2:H:894:GLU:C	2:H:896:PHE:H	1.98	0.66
1:A:599:VAL:CG1	1:A:629:ILE:HB	2.25	0.66
1:A:961:GLU:O	1:A:964:LYS:HG2	1.95	0.66
2:D:587:LEU:H	2:D:587:LEU:HD12	1.60	0.66
1:E:505:LEU:HB3	1:E:533:ILE:HD11	1.77	0.66
1:E:755:SER:HB3	1:E:817:ASN:O	1.96	0.66
2:F:256:ARG:HD2	2:F:812:ARG:O	1.95	0.66
2:F:579:PRO:O	2:F:580:LYS:C	2.33	0.66
1:G:581:LYS:HD2	1:G:586:GLU:HB2	1.75	0.66
1:C:319:ARG:HB2	1:C:348:ILE:HD12	1.76	0.66
1:G:356:ASP:OD2	3:G:988:F6P:H11	1.96	0.66
2:H:635:VAL:O	2:H:636:ARG:HD2	1.96	0.66
1:C:212:THR:HG22	1:C:274:ILE:HG13	1.77	0.66
2:D:240:VAL:HG21	2:D:273:GLU:HB2	1.77	0.66
2:D:575:ASP:CB	2:D:613:MET:HB3	2.25	0.66
1:G:400:ARG:HH11	1:G:400:ARG:HG2	1.60	0.66
1:A:427:HIS:HA	1:A:459:ASP:HB2	1.77	0.66
1:A:693:PHE:CD2	1:A:952:ARG:HB3	2.31	0.66
2:H:325:ASN:O	2:H:327:ILE:N	2.27	0.66
1:E:212:THR:HG23	1:E:212:THR:O	1.95	0.66
1:E:800:ARG:NH2	2:H:791:GLU:HG3	2.11	0.66
1:A:816:GLU:O	1:A:818:ARG:N	2.28	0.66
1:C:400:ARG:HG2	1:C:400:ARG:HH11	1.59	0.66
1:C:816:GLU:O	1:C:818:ARG:N	2.29	0.66
2:D:201:VAL:HG11	2:D:218:ILE:HD13	1.76	0.66
1:E:505:LEU:CB	1:E:533:ILE:HD11	2.26	0.66
2:H:827:LEU:HB3	2:H:832:LEU:HD13	1.77	0.66
2:D:256:ARG:HD2	2:D:812:ARG:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:ALA:O	2:D:211:MET:HG3	1.96	0.65
1:A:212:THR:HG22	1:A:274:ILE:HG13	1.77	0.65
2:B:579:PRO:O	2:B:580:LYS:C	2.34	0.65
1:C:427:HIS:HA	1:C:459:ASP:HB2	1.77	0.65
1:C:587:LEU:C	1:C:589:PRO:HD3	2.15	0.65
2:D:552:ARG:C	2:D:552:ARG:HD3	2.16	0.65
1:C:778:THR:O	1:C:782:THR:HB	1.96	0.65
2:D:214:ASN:HD21	2:D:343:THR:HG21	1.60	0.65
1:E:253:LYS:C	1:E:255:LEU:H	1.98	0.65
2:B:681:LEU:O	2:B:710:MET:O	2.15	0.65
1:C:360:SER:N	1:C:545:THR:HG22	2.11	0.65
2:F:681:LEU:O	2:F:710:MET:O	2.15	0.65
1:A:587:LEU:C	1:A:589:PRO:HD3	2.17	0.65
2:B:579:PRO:O	2:B:581:LEU:N	2.30	0.65
1:E:360:SER:N	1:E:545:THR:HG22	2.11	0.65
2:B:201:VAL:CG1	2:B:218:ILE:HD13	2.27	0.65
1:C:253:LYS:C	1:C:255:LEU:H	2.00	0.65
2:D:201:VAL:CG1	2:D:218:ILE:HD13	2.26	0.65
2:H:522:ASN:ND2	2:H:527:VAL:HG21	2.11	0.65
1:C:360:SER:H	1:C:545:THR:HG22	1.62	0.65
2:D:701:GLU:HB2	2:D:897:ASN:HD22	1.62	0.65
2:F:579:PRO:O	2:F:581:LEU:N	2.30	0.65
2:B:453:ASP:CG	2:B:455:THR:HG23	2.17	0.65
2:D:549:ASP:OD2	2:D:552:ARG:HB2	1.97	0.65
1:G:773:TYR:HA	1:G:959:TRP:CD2	2.32	0.65
2:H:793:LEU:O	2:H:797:ILE:HG13	1.96	0.65
2:B:827:LEU:HB3	2:B:832:LEU:HD13	1.78	0.65
1:C:330:VAL:HA	1:C:335:PHE:O	1.97	0.65
1:A:251:GLY:O	1:A:252:GLY:O	2.15	0.64
1:A:360:SER:N	1:A:545:THR:HG22	2.12	0.64
2:B:693:LEU:CD2	2:B:922:ILE:HB	2.27	0.64
2:F:591:ILE:HD13	2:F:592:VAL:H	1.62	0.64
2:D:390:MET:HG3	2:D:483:GLN:NE2	2.13	0.64
2:D:418:THR:HG1	2:D:422:TRP:HD1	1.36	0.64
2:D:950:ASP:OD1	2:D:955:ARG:HD3	1.97	0.64
1:G:802:ASP:OD1	1:G:972:ARG:NH2	2.28	0.64
1:A:947:THR:CG2	1:A:951:LEU:HB2	2.26	0.64
2:D:462:VAL:O	2:D:466:LEU:HD23	1.98	0.64
2:D:681:LEU:O	2:D:710:MET:O	2.16	0.64
1:A:210:VAL:CG1	1:A:227:VAL:HG11	2.28	0.64
1:E:289:ARG:HB2	1:E:325:LEU:HD22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:264:THR:HG22	2:F:266:ILE:H	1.62	0.64
1:A:212:THR:HG23	1:A:212:THR:O	1.97	0.64
1:E:581:LYS:HD2	1:E:586:GLU:HB2	1.80	0.64
2:H:876:VAL:HG12	2:H:880:LYS:HE3	1.79	0.64
2:H:935:ARG:HH12	4:H:8:FDP:P1	2.19	0.64
2:D:900:ASP:N	2:D:903:ILE:HD11	2.12	0.64
2:F:436:ARG:HG3	2:F:436:ARG:O	1.97	0.64
2:F:930:THR:HG22	2:F:932:VAL:N	2.12	0.64
2:B:203:THR:OG1	2:B:264:THR:HG21	1.96	0.64
2:B:392:ARG:NH2	3:B:980:F6P:H12	2.11	0.64
2:F:320:GLU:O	2:F:324:THR:HG22	1.97	0.64
2:H:321:LEU:O	2:H:325:ASN:O	2.16	0.64
2:B:575:ASP:CB	2:B:613:MET:HB3	2.28	0.64
1:E:292:ALA:O	1:E:296:ILE:HG13	1.98	0.64
2:F:522:ASN:HD22	2:F:527:VAL:HG21	1.61	0.64
2:F:907:ALA:O	2:F:922:ILE:HG22	1.97	0.64
1:G:581:LYS:HB3	1:G:586:GLU:CB	2.27	0.64
1:G:587:LEU:C	1:G:589:PRO:HD3	2.17	0.64
1:G:685:ASP:O	1:G:714:ILE:HB	1.97	0.64
1:A:537:PRO:HG2	1:A:540:GLU:HB2	1.79	0.64
1:A:541:SER:O	1:A:545:THR:HG23	1.97	0.64
1:C:289:ARG:HB2	1:C:325:LEU:HD22	1.79	0.64
1:A:253:LYS:C	1:A:255:LEU:H	2.00	0.63
1:A:809:ASN:HB2	1:A:975:LEU:CD1	2.27	0.63
2:D:801:ALA:O	2:D:805:GLU:HG3	1.97	0.63
2:B:591:ILE:HD13	2:B:592:VAL:H	1.62	0.63
1:E:931:GLY:O	1:E:932:SER:HB3	1.98	0.63
2:F:220:ARG:HD2	2:F:252:TRP:CE2	2.33	0.63
1:A:947:THR:HG23	1:A:947:THR:O	1.98	0.63
2:B:511:THR:OG1	2:B:514:THR:HG23	1.99	0.63
2:B:752:ARG:HD2	2:B:809:GLY:O	1.98	0.63
2:H:327:ILE:HA	2:H:331:GLN:HE22	1.63	0.63
1:E:427:HIS:HA	1:E:459:ASP:HB2	1.80	0.63
2:F:793:LEU:O	2:F:797:ILE:HG13	1.97	0.63
1:A:947:THR:O	1:A:948:ASN:C	2.36	0.63
1:C:329:LEU:HD22	1:C:334:ARG:HG2	1.81	0.63
1:C:941:ASN:O	1:C:944:GLU:HG3	1.99	0.63
1:C:216:ASP:OD2	2:D:377:THR:HA	1.99	0.63
2:D:433:HIS:ND1	2:D:640:TRP:CZ2	2.67	0.63
1:E:950:GLU:O	1:E:950:GLU:HG2	1.98	0.63
1:A:703:ARG:HH11	1:A:921:ASP:CG	2.01	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:298:CYS:SG	2:B:343:THR:HG22	2.38	0.63
1:C:336:THR:OG1	1:C:339:GLU:HG3	1.98	0.63
2:D:633:GLU:HB2	2:D:672:TYR:CZ	2.33	0.63
2:B:436:ARG:HG3	2:B:436:ARG:O	1.97	0.63
1:C:422:GLU:CG	1:C:564:ARG:HD2	2.28	0.63
1:G:613:ARG:HD2	1:G:650:VAL:O	1.98	0.63
1:A:341:ALA:HB3	1:A:342:PRO:CD	2.28	0.63
1:A:398:MET:HE3	1:A:488:HIS:HA	1.80	0.63
2:B:201:VAL:HG11	2:B:218:ILE:CD1	2.28	0.63
1:A:757:THR:HG23	2:B:597:PRO:HD3	1.81	0.63
1:C:805:LEU:HD21	1:C:976:ARG:HG2	1.80	0.63
2:F:281:LEU:HD23	2:F:326:ARG:NH2	2.14	0.63
1:C:622:HIS:HD2	1:C:886:GLU:OE1	1.82	0.63
2:D:463:HIS:HD2	2:D:474:THR:HG22	1.64	0.63
1:G:276:THR:O	1:G:276:THR:HG23	1.98	0.63
1:G:746:TYR:CE1	2:H:854:VAL:CG1	2.82	0.63
2:H:436:ARG:HH12	2:H:575:ASP:CG	2.02	0.63
2:H:466:LEU:HD12	2:H:472:LEU:HD11	1.81	0.63
2:H:950:ASP:OD1	2:H:955:ARG:HD3	1.97	0.63
1:A:341:ALA:HB3	1:A:342:PRO:HD3	1.81	0.62
2:D:641:LYS:O	2:D:644:LEU:HD12	1.99	0.62
2:F:701:GLU:HB3	2:F:897:ASN:HD22	1.62	0.62
2:F:494:ILE:HG23	2:F:774:LEU:HD23	1.80	0.62
2:B:577:ASN:C	2:B:579:PRO:CD	2.67	0.62
1:C:348:ILE:O	1:C:524:PRO:HD2	2.00	0.62
1:E:360:SER:H	1:E:545:THR:HG22	1.64	0.62
1:G:410:GLY:HA2	1:G:452:ILE:HD12	1.80	0.62
2:H:930:THR:HG22	2:H:932:VAL:N	2.14	0.62
1:E:249:LEU:CD1	1:E:290:GLN:HG2	2.29	0.62
2:F:433:HIS:ND1	2:F:640:TRP:CZ2	2.67	0.62
1:G:348:ILE:O	1:G:524:PRO:HD2	1.99	0.62
1:A:542:VAL:O	1:A:546:LYS:HB2	1.99	0.62
1:A:613:ARG:HD2	1:A:650:VAL:O	1.98	0.62
2:B:704:PRO:HA	2:B:707:ARG:HG2	1.79	0.62
1:C:710:PRO:HG2	1:G:674:THR:HA	1.81	0.62
1:G:212:THR:HG23	1:G:212:THR:O	1.98	0.62
2:H:892:ALA:O	2:H:894:GLU:N	2.30	0.62
1:E:485:ILE:HD12	1:E:485:ILE:N	2.14	0.62
1:E:508:VAL:HG11	1:E:965:ILE:HD12	1.82	0.62
1:G:788:TYR:HB3	1:G:794:ILE:HD11	1.81	0.62
2:H:505:ASN:O	2:H:509:GLU:HG2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:552:ARG:HD3	2:H:552:ARG:C	2.19	0.62
2:H:577:ASN:C	2:H:579:PRO:CD	2.68	0.62
1:C:251:GLY:O	1:C:252:GLY:O	2.17	0.62
1:C:216:ASP:H	2:D:381:HIS:HE1	1.48	0.62
2:D:704:PRO:HA	2:D:707:ARG:HH11	1.64	0.62
2:D:779:GLN:HA	2:D:953:VAL:HG21	1.80	0.62
2:F:641:LYS:O	2:F:644:LEU:HD12	1.99	0.62
2:B:341:CYS:HB2	2:B:507:VAL:HG13	1.82	0.62
1:C:422:GLU:O	1:C:423:ARG:HD2	2.00	0.62
1:E:594:LEU:HD21	1:E:889:ASN:ND2	2.14	0.62
1:G:451:ILE:HD12	1:G:451:ILE:N	2.15	0.62
2:B:264:THR:CG2	2:B:266:ILE:HG12	2.29	0.62
2:D:436:ARG:O	2:D:436:ARG:HG3	1.99	0.62
2:F:201:VAL:HG11	2:F:218:ILE:CD1	2.28	0.62
1:C:613:ARG:HA	1:C:650:VAL:CG2	2.30	0.62
2:D:591:ILE:HD13	2:D:592:VAL:N	2.15	0.62
2:D:717:LEU:HB2	2:D:733:ALA:CB	2.29	0.62
1:E:276:THR:HG23	1:E:276:THR:O	2.00	0.62
1:E:711:ILE:O	1:E:714:ILE:HG23	2.00	0.62
1:E:801:GLU:OE1	1:E:976:ARG:HD3	1.99	0.62
2:F:786:GLU:OE2	2:F:946:ARG:NH2	2.24	0.62
1:A:590:VAL:HG23	1:A:591:SER:H	1.63	0.62
1:E:348:ILE:O	1:E:524:PRO:HD2	2.00	0.62
2:F:418:THR:CG2	2:F:419:SER:H	1.95	0.62
1:A:422:GLU:HG2	1:A:564:ARG:HD2	1.81	0.61
2:D:665:ASP:O	2:D:669:ILE:HG12	2.00	0.61
2:D:392:ARG:HH21	3:D:982:F6P:H12	1.65	0.61
1:G:427:HIS:HA	1:G:459:ASP:HB2	1.81	0.61
1:G:822:LEU:HD12	1:G:822:LEU:C	2.19	0.61
1:A:822:LEU:C	1:A:822:LEU:HD12	2.20	0.61
1:C:461:GLN:HB2	1:C:463:ASN:ND2	2.14	0.61
2:H:256:ARG:HD2	2:H:812:ARG:O	1.99	0.61
2:H:239:LEU:O	2:H:286:HIS:HD2	1.82	0.61
2:H:341:CYS:HB2	2:H:507:VAL:HG13	1.82	0.61
1:A:596:ILE:HD12	1:A:885:ILE:HG21	1.82	0.61
2:F:587:LEU:H	2:F:617:HIS:HD1	1.47	0.61
2:F:892:ALA:O	2:F:894:GLU:N	2.30	0.61
2:D:579:PRO:O	2:D:581:LEU:N	2.33	0.61
1:E:400:ARG:HG3	1:E:401:HIS:N	2.15	0.61
1:E:400:ARG:HG3	1:E:401:HIS:H	1.64	0.61
2:B:704:PRO:HA	2:B:707:ARG:HH11	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:ARG:O	1:C:448:ASN:HA	2.00	0.61
1:C:589:PRO:HD2	1:C:622:HIS:O	2.01	0.61
2:F:577:ASN:C	2:F:579:PRO:CD	2.68	0.61
2:H:940:ILE:HD12	2:H:943:GLN:NE2	2.15	0.61
1:C:822:LEU:O	1:C:822:LEU:HD12	2.00	0.61
2:D:298:CYS:HA	2:D:343:THR:O	2.00	0.61
2:H:892:ALA:C	2:H:894:GLU:H	2.03	0.61
1:C:832:VAL:HG12	1:C:833:TYR:CD1	2.36	0.61
2:D:322:LEU:O	2:D:324:THR:N	2.32	0.61
2:D:786:GLU:OE2	2:D:946:ARG:NH2	2.23	0.61
1:E:816:GLU:O	1:E:818:ARG:N	2.33	0.61
2:F:781:SER:HA	2:F:818:LEU:O	2.01	0.61
2:H:889:ALA:O	2:H:891:ALA:N	2.33	0.61
1:C:669:SER:N	1:C:701:GLN:NE2	2.49	0.61
2:H:256:ARG:NH1	2:H:813:PHE:CE1	2.68	0.61
2:H:701:GLU:HB3	2:H:897:ASN:ND2	2.16	0.61
1:A:242:TYR:O	1:A:247:GLY:HA3	2.01	0.61
1:A:600:HIS:HD2	1:A:659:SER:OG	1.83	0.61
2:H:587:LEU:HD23	2:H:883:GLN:NE2	2.16	0.61
2:H:647:GLN:HE22	2:H:869:THR:CG2	2.14	0.61
1:A:801:GLU:OE1	1:A:976:ARG:NE	2.34	0.61
2:B:463:HIS:HD2	2:B:474:THR:HG22	1.66	0.61
1:E:588:LEU:HD13	1:E:593:ARG:NH1	2.14	0.61
1:G:247:GLY:HA2	1:G:254:TYR:HD2	1.66	0.61
2:H:400:LEU:HD12	2:H:866:THR:HG21	1.81	0.61
2:D:578:GLU:N	2:D:579:PRO:CD	2.64	0.60
1:A:276:THR:O	1:A:276:THR:HG23	2.00	0.60
1:C:805:LEU:HD11	1:C:972:ARG:HG3	1.83	0.60
2:H:591:ILE:HD13	2:H:592:VAL:N	2.16	0.60
2:B:587:LEU:HD21	2:B:883:GLN:CG	2.31	0.60
2:D:436:ARG:NH2	2:D:575:ASP:OD1	2.32	0.60
1:C:619:CYS:SG	1:C:882:ILE:HD12	2.41	0.60
2:D:321:LEU:O	2:D:325:ASN:O	2.20	0.60
2:D:414:GLU:OE1	2:D:557:ARG:NH1	2.34	0.60
2:D:577:ASN:HB3	2:D:579:PRO:CG	2.30	0.60
1:E:422:GLU:HG2	1:E:564:ARG:HD2	1.82	0.60
1:G:448:ASN:H	1:G:448:ASN:ND2	1.99	0.60
2:B:633:GLU:HB2	2:B:672:TYR:OH	2.01	0.60
2:B:935:ARG:NH1	4:B:2:FDP:O3P	2.34	0.60
1:C:822:LEU:C	1:C:822:LEU:HD12	2.22	0.60
2:D:792:GLN:HE22	2:D:957:ARG:C	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:TRP:O	1:A:960:ALA:C	2.39	0.60
1:C:400:ARG:HG3	1:C:401:HIS:H	1.65	0.60
1:C:791:GLU:OE1	1:C:791:GLU:N	2.28	0.60
2:D:314:TRP:HB3	2:D:315:PRO:HD3	1.83	0.60
1:E:788:TYR:HB3	1:E:794:ILE:HD11	1.84	0.60
1:E:813:ASP:CG	1:E:814:LYS:N	2.55	0.60
1:G:599:VAL:CG1	1:G:629:ILE:HB	2.25	0.60
2:F:521:VAL:HG13	2:F:526:ILE:HD13	1.82	0.60
1:G:622:HIS:HD2	1:G:886:GLU:OE1	1.85	0.60
2:B:591:ILE:HD13	2:B:592:VAL:N	2.16	0.60
1:C:794:ILE:O	1:C:794:ILE:HG22	2.02	0.60
2:H:324:THR:HG23	2:H:326:ARG:HG3	1.82	0.60
2:H:770:THR:CG2	2:H:946:ARG:HD2	2.32	0.60
1:E:210:VAL:HG12	1:E:304:VAL:HB	1.83	0.60
1:E:422:GLU:O	1:E:423:ARG:HD2	2.01	0.60
2:F:288:ILE:HA	2:F:335:MET:CE	2.32	0.60
1:G:599:VAL:HG13	1:G:629:ILE:CB	2.26	0.60
1:G:669:SER:N	1:G:701:GLN:NE2	2.50	0.60
2:B:930:THR:HG22	2:B:932:VAL:H	1.65	0.60
2:D:220:ARG:HD2	2:D:252:TRP:CZ2	2.37	0.60
2:D:587:LEU:HD21	2:D:883:GLN:CG	2.32	0.60
1:A:947:THR:CG2	1:A:953:LYS:H	2.14	0.59
1:E:341:ALA:HB3	1:E:342:PRO:CD	2.32	0.59
1:G:613:ARG:HA	1:G:650:VAL:CG2	2.32	0.59
4:A:1:FDP:O4P	2:B:847:LYS:NZ	2.34	0.59
2:F:591:ILE:HD13	2:F:592:VAL:N	2.17	0.59
1:G:400:ARG:HG3	1:G:401:HIS:H	1.66	0.59
1:G:590:VAL:HG23	1:G:591:SER:N	2.18	0.59
1:G:974:LYS:CG	1:G:975:LEU:HD13	2.30	0.59
2:H:900:ASP:H	2:H:903:ILE:HD11	1.66	0.59
1:A:690:LEU:HD23	1:A:719:ILE:HB	1.83	0.59
2:B:288:ILE:HA	2:B:335:MET:CE	2.32	0.59
1:G:341:ALA:HB3	1:G:342:PRO:CD	2.32	0.59
2:H:195:PRO:HG2	2:H:334:ARG:NH1	2.15	0.59
2:H:798:GLU:O	2:H:801:ALA:HB3	2.03	0.59
1:E:821:LYS:CB	1:E:821:LYS:HZ2	2.08	0.59
1:A:439:GLN:HA	1:A:439:GLN:OE1	2.02	0.59
2:B:256:ARG:HD2	2:B:812:ARG:O	2.03	0.59
2:F:414:GLU:OE1	2:F:557:ARG:NH1	2.35	0.59
2:B:321:LEU:O	2:B:325:ASN:O	2.20	0.59
2:B:577:ASN:HB3	2:B:579:PRO:CG	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:HIS:C	1:C:427:HIS:ND1	2.56	0.59
1:A:841:ILE:CG2	2:D:790:LEU:HD11	2.32	0.59
1:E:594:LEU:N	1:E:624:HIS:ND1	2.48	0.59
1:A:634:SER:HB3	1:A:666:SER:CB	2.32	0.59
2:B:892:ALA:O	2:B:894:GLU:N	2.32	0.59
2:D:320:GLU:O	2:D:324:THR:HG22	2.03	0.59
2:D:704:PRO:HA	2:D:707:ARG:NH1	2.18	0.59
2:F:554:MET:HG2	2:F:562:ILE:CG1	2.29	0.59
1:G:679:PHE:CE2	1:G:687:LEU:HD22	2.38	0.59
2:H:587:LEU:HD12	2:H:587:LEU:N	2.18	0.59
1:A:613:ARG:HA	1:A:650:VAL:CG2	2.33	0.59
2:F:328:SER:H	2:F:331:GLN:NE2	2.00	0.59
1:G:537:PRO:HG2	1:G:540:GLU:HB2	1.84	0.59
2:H:621:ALA:HB2	2:H:638:LEU:HD11	1.83	0.59
2:B:661:PRO:HD2	2:B:695:GLN:NE2	2.17	0.59
1:C:782:THR:CG2	1:C:822:LEU:HD11	2.32	0.59
2:D:577:ASN:C	2:D:579:PRO:CD	2.70	0.59
1:A:756:ALA:HB1	2:B:597:PRO:HB3	1.85	0.59
1:C:972:ARG:HD3	1:C:976:ARG:HH21	1.67	0.59
2:F:417:ALA:O	2:F:418:THR:HB	2.02	0.59
1:G:697:ARG:NH1	1:G:943:TRP:HH2	2.01	0.59
1:G:773:TYR:HD1	1:G:959:TRP:CD1	2.21	0.59
2:H:436:ARG:NH1	2:H:575:ASP:OD2	2.34	0.59
1:A:968:ILE:HD13	1:A:973:LEU:HD12	1.84	0.58
2:B:264:THR:HG22	2:B:266:ILE:H	1.67	0.58
1:E:319:ARG:NH1	1:E:517:PHE:HE2	2.00	0.58
1:G:949:VAL:O	1:G:950:GLU:O	2.21	0.58
1:C:438:CYS:O	1:C:442:ARG:HG3	2.02	0.58
2:D:615:GLN:OE1	2:D:880:LYS:NZ	2.36	0.58
1:E:636:LEU:HD12	1:E:640:GLY:HA2	1.84	0.58
2:F:344:VAL:HG22	2:F:357:THR:HG22	1.85	0.58
2:H:900:ASP:N	2:H:903:ILE:HD11	2.18	0.58
1:C:685:ASP:O	1:C:714:ILE:HB	2.04	0.58
2:D:200:ALA:HA	2:D:230:PHE:O	2.02	0.58
2:F:264:THR:CG2	2:F:266:ILE:HG12	2.33	0.58
2:H:907:ALA:O	2:H:922:ILE:HG22	2.02	0.58
1:A:518:THR:HB	1:A:519:PRO:HD2	1.85	0.58
2:B:647:GLN:HE22	2:B:869:THR:CG2	2.16	0.58
1:C:466:THR:CG2	1:C:468:ASN:H	2.12	0.58
1:C:809:ASN:HB2	1:C:975:LEU:CD1	2.33	0.58
2:F:903:ILE:HD12	2:F:904:SER:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:VAL:HG13	1:A:629:ILE:CB	2.28	0.58
2:B:587:LEU:HD23	2:B:883:GLN:NE2	2.19	0.58
1:C:336:THR:HG23	1:C:339:GLU:CD	2.24	0.58
1:C:439:GLN:HA	1:C:439:GLN:OE1	2.04	0.58
1:C:766:VAL:HG11	1:C:774:ILE:HG22	1.84	0.58
2:D:579:PRO:O	2:D:580:LYS:C	2.41	0.58
1:E:539:VAL:O	1:E:542:VAL:HG22	2.03	0.58
2:F:317:LEU:O	2:F:321:LEU:HD23	2.03	0.58
2:F:575:ASP:CB	2:F:613:MET:HB3	2.33	0.58
1:G:539:VAL:O	1:G:542:VAL:HG22	2.04	0.58
1:A:976:ARG:O	1:A:979:VAL:HB	2.03	0.58
1:C:703:ARG:HH11	1:C:921:ASP:CG	2.06	0.58
1:C:947:THR:HG22	1:C:953:LYS:N	2.17	0.58
1:E:703:ARG:HH11	1:E:921:ASP:CG	2.06	0.58
1:G:253:LYS:C	1:G:255:LEU:H	2.06	0.58
2:H:575:ASP:CB	2:H:613:MET:HB3	2.33	0.58
2:H:578:GLU:N	2:H:579:PRO:CD	2.64	0.58
1:A:766:VAL:HG11	1:A:774:ILE:HG22	1.84	0.58
2:B:298:CYS:HA	2:B:343:THR:O	2.04	0.58
1:G:583:ASP:C	1:G:585:SER:H	2.07	0.58
1:A:651:GLU:HG3	1:A:652:ASN:ND2	2.18	0.58
1:A:216:ASP:H	2:B:381:HIS:HE1	1.52	0.58
1:C:424:ALA:HB1	1:C:459:ASP:C	2.24	0.58
2:D:661:PRO:HD2	2:D:695:GLN:NE2	2.18	0.58
1:E:947:THR:CG2	1:E:953:LYS:H	2.14	0.58
1:G:928:CYS:O	1:G:934:VAL:HA	2.04	0.58
1:A:291:ALA:O	1:A:294:ASN:N	2.37	0.58
1:A:669:SER:N	1:A:701:GLN:NE2	2.48	0.58
2:B:679:ASP:O	2:B:708:ILE:HB	2.04	0.58
2:B:903:ILE:HD12	2:B:904:SER:H	1.67	0.58
2:D:325:ASN:O	2:D:327:ILE:N	2.31	0.58
2:F:418:THR:CG2	2:F:419:SER:N	2.66	0.58
1:G:400:ARG:HG3	1:G:401:HIS:N	2.19	0.58
2:H:709:PRO:HB2	2:H:879:ILE:HD13	1.86	0.58
2:B:327:ILE:HB	2:B:331:GLN:HE21	1.69	0.57
2:D:285:GLN:O	2:D:289:GLU:HG3	2.03	0.57
2:D:327:ILE:HA	2:D:331:GLN:NE2	2.19	0.57
2:D:522:ASN:ND2	2:D:527:VAL:HG21	2.19	0.57
1:E:438:CYS:O	1:E:442:ARG:HG3	2.04	0.57
1:G:448:ASN:HD22	1:G:448:ASN:N	1.99	0.57
1:G:941:ASN:O	1:G:944:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:963:ASN:ND2	1:G:963:ASN:N	2.51	0.57
2:H:320:GLU:O	2:H:324:THR:HG22	2.03	0.57
2:F:327:ILE:HA	2:F:331:GLN:NE2	2.18	0.57
2:H:288:ILE:HA	2:H:335:MET:CE	2.34	0.57
1:C:967:ASP:OD2	1:C:972:ARG:HD2	2.05	0.57
2:D:632:HIS:O	2:D:633:GLU:C	2.42	0.57
2:D:752:ARG:HD2	2:D:809:GLY:O	2.04	0.57
2:F:793:LEU:HD13	1:G:796:LEU:HD11	1.84	0.57
1:A:485:ILE:N	1:A:485:ILE:HD12	2.18	0.57
1:A:360:SER:H	1:A:545:THR:HG22	1.67	0.57
2:B:324:THR:HG23	2:B:326:ARG:HG3	1.86	0.57
2:D:264:THR:HG22	2:D:266:ILE:N	2.18	0.57
1:E:251:GLY:O	1:E:252:GLY:O	2.22	0.57
1:E:211:MET:HE3	1:E:305:VAL:HG22	1.86	0.57
2:F:792:GLN:HE22	2:F:957:ARG:HB3	1.68	0.57
1:G:427:HIS:ND1	1:G:427:HIS:C	2.57	0.57
2:H:786:GLU:OE2	2:H:946:ARG:NH2	2.23	0.57
1:A:589:PRO:HD2	1:A:622:HIS:O	2.04	0.57
1:C:400:ARG:HG3	1:C:401:HIS:N	2.19	0.57
2:D:244:PRO:O	2:D:245:GLU:HB3	2.04	0.57
2:D:587:LEU:CD2	2:D:883:GLN:NE2	2.68	0.57
2:F:414:GLU:OE2	2:F:414:GLU:N	2.35	0.57
2:H:418:THR:OG1	2:H:419:SER:N	2.35	0.57
2:B:422:TRP:CH2	2:B:465:VAL:HG21	2.39	0.57
2:B:693:LEU:HD23	2:B:922:ILE:HB	1.86	0.57
2:D:892:ALA:C	2:D:894:GLU:H	2.08	0.57
1:E:350:GLY:O	1:E:351:LEU:HD23	2.05	0.57
1:E:427:HIS:ND1	1:E:427:HIS:C	2.58	0.57
1:E:590:VAL:HG23	1:E:591:SER:N	2.17	0.57
2:B:892:ALA:C	2:B:894:GLU:H	2.06	0.57
1:C:320:HIS:O	1:C:321:GLU:HB2	2.05	0.57
1:E:949:VAL:O	1:E:952:ARG:N	2.38	0.57
1:A:424:ALA:HB1	1:A:459:ASP:C	2.25	0.57
2:B:890:ARG:HG2	2:B:890:ARG:O	2.05	0.57
2:F:889:ALA:O	2:F:891:ALA:N	2.35	0.57
1:G:251:GLY:O	1:G:252:GLY:O	2.22	0.57
2:F:790:LEU:HD22	1:G:796:LEU:HD22	1.87	0.57
2:H:416:PRO:HG2	2:H:550:PHE:CZ	2.40	0.57
2:H:874:LYS:HD2	2:H:917:VAL:HG21	1.87	0.57
2:B:894:GLU:C	2:B:896:PHE:H	2.07	0.57
1:C:341:ALA:HB3	1:C:342:PRO:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:832:VAL:HG12	1:C:833:TYR:N	2.19	0.57
2:F:511:THR:OG1	2:F:514:THR:HG23	2.05	0.57
1:G:270:GLY:O	1:G:271:GLY:O	2.22	0.57
1:G:317:LEU:HD12	1:G:317:LEU:N	2.20	0.57
2:H:501:LEU:O	2:H:501:LEU:HD12	2.04	0.57
1:E:431:GLN:O	1:E:435:LYS:HG3	2.05	0.57
1:E:486:LEU:O	1:E:489:VAL:HG22	2.05	0.57
2:H:752:ARG:HD2	2:H:809:GLY:O	2.05	0.57
1:A:210:VAL:HG12	1:A:304:VAL:HB	1.86	0.56
1:A:329:LEU:O	1:A:334:ARG:HB3	2.05	0.56
2:B:417:ALA:O	2:B:418:THR:HB	2.04	0.56
1:C:421:PRO:C	1:C:423:ARG:H	2.08	0.56
2:D:709:PRO:HB2	2:D:879:ILE:HD13	1.87	0.56
1:E:212:THR:HG22	1:E:274:ILE:HG13	1.87	0.56
2:F:220:ARG:HD2	2:F:252:TRP:CZ2	2.40	0.56
2:F:537:LEU:O	2:F:540:ALA:HB3	2.05	0.56
2:F:577:ASN:HB3	2:F:579:PRO:CG	2.33	0.56
2:F:894:GLU:C	2:F:896:PHE:H	2.08	0.56
2:F:701:GLU:HB3	2:F:897:ASN:ND2	2.20	0.56
2:F:779:GLN:HA	2:F:953:VAL:HG21	1.87	0.56
1:G:703:ARG:HH11	1:G:921:ASP:CG	2.08	0.56
1:A:794:ILE:HD11	1:A:829:ALA:HB1	1.87	0.56
1:A:841:ILE:HG21	2:D:790:LEU:HD11	1.87	0.56
1:A:860:VAL:HG11	2:B:740:TYR:CD1	2.39	0.56
2:F:940:ILE:HD12	2:F:943:GLN:NE2	2.19	0.56
1:G:422:GLU:CG	1:G:564:ARG:HD2	2.35	0.56
2:H:201:VAL:HG13	2:H:218:ILE:HG21	1.87	0.56
2:H:298:CYS:HA	2:H:343:THR:O	2.05	0.56
1:A:964:LYS:H	1:A:964:LYS:HD2	1.69	0.56
2:B:322:LEU:O	2:B:324:THR:N	2.34	0.56
1:E:977:ALA:C	1:E:979:VAL:H	2.07	0.56
2:F:281:LEU:HD12	2:F:317:LEU:CD2	2.36	0.56
2:H:633:GLU:HB2	2:H:672:TYR:CZ	2.40	0.56
1:A:385:THR:HA	2:B:207:ASP:OD2	2.05	0.56
2:B:704:PRO:HA	2:B:707:ARG:NH1	2.21	0.56
2:F:347:ILE:HB	2:F:363:ALA:HB2	1.87	0.56
2:H:554:MET:HG2	2:H:562:ILE:CG1	2.34	0.56
1:E:451:ILE:HD12	1:E:451:ILE:N	2.20	0.56
1:E:928:CYS:O	1:E:934:VAL:HA	2.05	0.56
1:G:249:LEU:CD1	1:G:290:GLN:HG2	2.35	0.56
1:A:778:THR:O	1:A:782:THR:HB	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:418:THR:HG1	2:B:422:TRP:HD1	1.43	0.56
1:C:331:ALA:O	1:C:332:GLU:C	2.43	0.56
1:C:804:THR:HG22	1:C:979:VAL:HG21	1.83	0.56
2:D:565:LEU:O	2:D:569:MET:HG2	2.05	0.56
2:D:770:THR:CG2	2:D:946:ARG:HD2	2.35	0.56
2:H:522:ASN:HD22	2:H:527:VAL:HG21	1.70	0.56
2:H:521:VAL:HG13	2:H:526:ILE:HD13	1.87	0.56
2:H:704:PRO:HA	2:H:707:ARG:HH11	1.70	0.56
1:A:941:ASN:O	1:A:944:GLU:HG3	2.06	0.56
1:C:249:LEU:HD21	1:C:281:GLU:CB	2.36	0.56
1:C:634:SER:HB3	1:C:666:SER:CB	2.36	0.56
1:C:802:ASP:OD1	1:C:972:ARG:NH2	2.23	0.56
2:D:657:ASN:OD1	2:D:659:VAL:HG23	2.06	0.56
2:D:874:LYS:CD	2:D:917:VAL:HG11	2.28	0.56
2:H:657:ASN:OD1	2:H:659:VAL:HG23	2.05	0.56
2:F:578:GLU:N	2:F:579:PRO:CD	2.68	0.56
1:G:814:LYS:HZ2	1:G:814:LYS:HA	1.69	0.56
1:G:385:THR:HA	2:H:207:ASP:OD2	2.06	0.56
1:C:539:VAL:O	1:C:542:VAL:HG22	2.06	0.56
1:C:948:ASN:O	1:C:950:GLU:N	2.33	0.56
1:E:583:ASP:C	1:E:585:SER:H	2.08	0.56
2:F:752:ARG:HD2	2:F:809:GLY:O	2.05	0.56
2:B:420:SER:HA	2:B:423:GLN:NE2	2.21	0.56
1:C:746:TYR:CE1	2:D:854:VAL:CG1	2.88	0.56
2:D:704:PRO:HA	2:D:707:ARG:CG	2.35	0.56
2:F:208:ALA:O	2:F:211:MET:HG3	2.04	0.56
1:G:883:LYS:O	1:G:887:GLN:HG3	2.06	0.56
2:B:350:ASP:HB3	2:B:394:CYS:HB2	1.87	0.56
1:C:801:GLU:OE1	1:C:976:ARG:HD3	2.06	0.56
1:E:537:PRO:HG2	1:E:540:GLU:HB2	1.86	0.56
1:E:949:VAL:O	1:E:950:GLU:C	2.41	0.56
1:G:211:MET:HE3	1:G:305:VAL:HG22	1.88	0.56
1:G:331:ALA:O	1:G:332:GLU:C	2.43	0.56
2:B:886:ILE:HD12	2:B:887:ALA:N	2.20	0.55
2:D:347:ILE:HB	2:D:363:ALA:HB2	1.87	0.55
2:D:892:ALA:O	2:D:894:GLU:N	2.33	0.55
1:E:968:ILE:HG12	1:E:973:LEU:HD12	1.88	0.55
2:F:770:THR:CG2	2:F:946:ARG:HD2	2.36	0.55
1:G:210:VAL:CG1	1:G:227:VAL:HG11	2.36	0.55
1:G:350:GLY:O	1:G:351:LEU:HD23	2.05	0.55
2:H:537:LEU:O	2:H:540:ALA:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:549:ASP:OD2	2:H:552:ARG:HB2	2.07	0.55
2:H:577:ASN:HB3	2:H:579:PRO:CG	2.28	0.55
1:A:431:GLN:O	1:A:435:LYS:HG3	2.06	0.55
1:C:331:ALA:O	1:C:333:GLY:N	2.39	0.55
2:D:328:SER:N	2:D:331:GLN:NE2	2.54	0.55
1:E:341:ALA:HB3	1:E:342:PRO:HD3	1.88	0.55
1:G:690:LEU:HD23	1:G:719:ILE:HB	1.87	0.55
1:A:391:ARG:O	1:A:448:ASN:HA	2.06	0.55
2:B:665:ASP:O	2:B:669:ILE:HG12	2.05	0.55
1:C:812:HIS:N	1:C:812:HIS:CD2	2.74	0.55
2:D:679:ASP:O	2:D:708:ILE:HB	2.05	0.55
1:E:572:TYR:CE2	1:E:576:LEU:HD11	2.41	0.55
1:E:679:PHE:CE2	1:E:687:LEU:HD22	2.41	0.55
2:F:324:THR:HG23	2:F:326:ARG:HG3	1.87	0.55
1:G:893:GLU:HA	1:G:893:GLU:OE2	2.06	0.55
1:G:963:ASN:H	1:G:963:ASN:HD22	1.52	0.55
2:H:392:ARG:HH21	3:H:986:F6P:H12	1.72	0.55
1:A:422:GLU:CG	1:A:564:ARG:HD2	2.36	0.55
1:E:589:PRO:O	1:E:593:ARG:NH1	2.39	0.55
2:F:589:ILE:HD13	2:F:879:ILE:HG21	1.89	0.55
2:F:876:VAL:HG12	2:F:880:LYS:HE3	1.89	0.55
1:C:421:PRO:O	1:C:423:ARG:N	2.40	0.55
1:E:822:LEU:C	1:E:822:LEU:CD1	2.74	0.55
2:F:886:ILE:HD12	2:F:887:ALA:N	2.21	0.55
2:H:704:PRO:HA	2:H:707:ARG:CG	2.37	0.55
1:A:322:TRP:HB3	1:A:323:PRO:HD3	1.89	0.55
1:A:809:ASN:CA	1:A:975:LEU:HD21	2.37	0.55
2:B:578:GLU:N	2:B:579:PRO:CD	2.68	0.55
2:D:587:LEU:N	2:D:587:LEU:CD1	2.68	0.55
1:G:755:SER:HB3	1:G:817:ASN:O	2.06	0.55
2:H:264:THR:HG22	2:H:266:ILE:HG12	1.88	0.55
2:B:418:THR:HA	2:B:421:GLU:CB	2.28	0.55
1:C:210:VAL:CG1	1:C:227:VAL:HG11	2.37	0.55
1:C:320:HIS:O	1:C:321:GLU:CB	2.54	0.55
1:C:893:GLU:OE2	1:C:893:GLU:HA	2.07	0.55
1:A:813:ASP:CG	1:A:814:LYS:N	2.60	0.55
2:B:632:HIS:O	2:B:633:GLU:C	2.45	0.55
2:B:701:GLU:O	2:B:701:GLU:CD	2.45	0.55
1:C:556:ASP:OD2	1:C:559:LYS:HB2	2.07	0.55
2:D:554:MET:HG2	2:D:562:ILE:CG1	2.37	0.55
2:D:647:GLN:HE22	2:D:869:THR:CG2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:239:LEU:HD22	2:F:287:LEU:HD22	1.88	0.55
1:G:391:ARG:HG2	1:G:480:ASP:HB3	1.89	0.55
1:G:548:VAL:O	1:G:552:ILE:HG12	2.07	0.55
1:A:946:GLU:CD	1:A:946:GLU:O	2.45	0.55
2:B:578:GLU:C	2:B:580:LYS:H	2.10	0.55
2:B:587:LEU:HD21	2:B:883:GLN:HG3	1.88	0.55
1:C:583:ASP:C	1:C:585:SER:H	2.09	0.55
2:D:851:PRO:O	2:D:854:VAL:HG22	2.07	0.55
1:E:669:SER:N	1:E:701:GLN:NE2	2.54	0.55
1:E:717:CYS:HA	1:E:925:ALA:O	2.07	0.55
1:E:893:GLU:OE2	1:E:893:GLU:HA	2.06	0.55
2:F:662:GLU:H	2:F:695:GLN:HE22	1.53	0.55
1:G:424:ALA:HB1	1:G:459:ASP:C	2.27	0.55
1:G:922:ASP:HA	1:G:938:PRO:HG3	1.88	0.55
2:H:587:LEU:HD21	2:H:883:GLN:CG	2.37	0.55
1:A:637:ILE:HD13	1:A:671:ASP:HB3	1.89	0.55
1:A:922:ASP:HA	1:A:938:PRO:HG3	1.89	0.55
1:A:946:GLU:CD	1:A:946:GLU:C	2.65	0.55
2:B:239:LEU:O	2:B:286:HIS:HD2	1.89	0.55
2:B:314:TRP:HB3	2:B:315:PRO:HD3	1.88	0.55
2:B:900:ASP:O	2:B:903:ILE:HG13	2.08	0.55
1:C:599:VAL:CG1	1:C:629:ILE:HB	2.37	0.55
1:E:613:ARG:HA	1:E:650:VAL:HG21	1.87	0.55
1:G:825:ARG:HH11	1:G:829:ALA:HB3	1.69	0.55
1:A:519:PRO:HG2	1:A:520:GLU:H	1.72	0.54
2:D:770:THR:HG23	2:D:946:ARG:HD2	1.90	0.54
1:E:697:ARG:NH1	1:E:943:TRP:HH2	2.04	0.54
1:C:229:ARG:HD3	1:C:260:TRP:CZ2	2.42	0.54
1:C:291:ALA:O	1:C:294:ASN:N	2.40	0.54
1:C:594:LEU:N	1:C:624:HIS:ND1	2.52	0.54
2:F:889:ALA:C	2:F:891:ALA:N	2.61	0.54
1:G:423:ARG:CD	1:G:561:ILE:HD12	2.37	0.54
1:G:581:LYS:C	1:G:583:ASP:H	2.10	0.54
1:G:816:GLU:O	1:G:818:ARG:N	2.40	0.54
2:H:220:ARG:HD2	2:H:252:TRP:CZ2	2.42	0.54
1:E:837:LEU:HD22	2:H:831:LYS:HD2	1.88	0.54
1:A:438:CYS:O	1:A:442:ARG:HG3	2.06	0.54
1:A:398:MET:HB3	3:A:988:F6P:O3	2.07	0.54
2:B:320:GLU:O	2:B:324:THR:HG22	2.07	0.54
2:B:582:PRO:O	2:B:586:ARG:NH1	2.37	0.54
1:C:790:PRO:HD2	1:C:791:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:578:GLU:C	2:D:580:LYS:H	2.09	0.54
1:E:424:ALA:HB1	1:E:459:ASP:C	2.28	0.54
2:F:416:PRO:O	2:F:417:ALA:C	2.45	0.54
2:F:780:VAL:HG12	2:F:781:SER:N	2.23	0.54
1:G:586:GLU:O	1:G:587:LEU:C	2.46	0.54
2:B:278:GLU:HA	2:B:278:GLU:OE1	2.07	0.54
2:D:680:GLY:HA3	2:D:879:ILE:HD12	1.88	0.54
2:F:575:ASP:OD1	2:F:575:ASP:C	2.45	0.54
2:F:582:PRO:O	2:F:586:ARG:NH1	2.37	0.54
1:G:438:CYS:O	1:G:442:ARG:HG3	2.08	0.54
2:H:417:ALA:O	2:H:418:THR:HB	2.08	0.54
1:A:360:SER:HB3	1:A:545:THR:HG22	1.90	0.54
2:B:325:ASN:O	2:B:327:ILE:N	2.31	0.54
1:E:806:LEU:O	1:E:807:LYS:C	2.45	0.54
1:G:697:ARG:O	1:G:701:GLN:HG3	2.08	0.54
2:H:541:VAL:O	2:H:545:ILE:HG12	2.08	0.54
1:G:554:ASN:O	1:G:556:ASP:N	2.41	0.54
2:H:431:SER:OG	2:H:470:LEU:HD11	2.07	0.54
2:H:704:PRO:HA	2:H:707:ARG:NH1	2.23	0.54
2:H:894:GLU:O	2:H:896:PHE:N	2.41	0.54
1:A:931:GLY:O	1:A:932:SER:HB3	2.07	0.54
2:B:889:ALA:O	2:B:891:ALA:N	2.41	0.54
2:D:220:ARG:HD2	2:D:252:TRP:CE2	2.42	0.54
1:E:378:MET:HE3	2:F:482:VAL:HG21	1.88	0.54
1:E:813:ASP:OD1	1:E:814:LYS:N	2.17	0.54
2:F:946:ARG:CG	2:F:946:ARG:HH21	2.21	0.54
1:C:599:VAL:HG13	1:C:629:ILE:CB	2.38	0.54
2:D:201:VAL:HG11	2:D:218:ILE:CD1	2.36	0.54
1:E:315:ALA:O	1:E:348:ILE:HD13	2.08	0.54
1:G:341:ALA:HB3	1:G:342:PRO:HD3	1.89	0.54
1:G:634:SER:HB3	1:G:666:SER:CB	2.38	0.54
2:H:348:ASP:OD2	3:H:986:F6P:C1	2.52	0.54
2:H:416:PRO:HD2	2:H:550:PHE:CD1	2.42	0.54
1:A:596:ILE:CD1	1:A:885:ILE:HG21	2.38	0.54
2:B:740:TYR:CE1	2:B:851:PRO:HB3	2.43	0.54
2:B:709:PRO:HB2	2:B:879:ILE:HD13	1.90	0.54
1:C:801:GLU:O	1:C:805:LEU:HG	2.08	0.54
2:D:522:ASN:HD21	2:D:529:LYS:CE	2.21	0.54
1:E:466:THR:CG2	1:E:468:ASN:H	2.11	0.54
2:F:350:ASP:HB3	2:F:394:CYS:HB2	1.90	0.54
2:F:418:THR:OG1	2:F:419:SER:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:248:LEU:HG	1:G:291:ALA:HB1	1.89	0.54
1:G:320:HIS:O	1:G:321:GLU:HB2	2.07	0.54
1:G:518:THR:HB	1:G:519:PRO:HD2	1.90	0.54
2:H:341:CYS:SG	2:H:519:ILE:CD1	2.96	0.54
2:B:418:THR:CA	2:B:421:GLU:HB2	2.29	0.54
2:B:798:GLU:O	2:B:801:ALA:HB3	2.08	0.54
1:C:329:LEU:O	1:C:334:ARG:HB3	2.08	0.54
2:D:239:LEU:O	2:D:286:HIS:HD2	1.90	0.54
2:D:381:HIS:CD2	2:D:383:ARG:HH21	2.26	0.54
1:E:319:ARG:HB2	1:E:348:ILE:CD1	2.34	0.54
1:E:685:ASP:O	1:E:715:PRO:HD2	2.07	0.54
1:E:596:ILE:HD12	1:E:885:ILE:HG21	1.90	0.54
1:E:946:GLU:C	1:E:946:GLU:CD	2.66	0.54
1:G:210:VAL:HG12	1:G:304:VAL:HB	1.90	0.54
1:G:398:MET:HB3	3:G:988:F6P:O3	2.08	0.54
1:G:931:GLY:O	1:G:932:SER:HB3	2.08	0.54
2:B:453:ASP:OD2	2:B:455:THR:HG23	2.07	0.53
2:D:889:ALA:O	2:D:891:ALA:N	2.41	0.53
1:E:289:ARG:HA	1:E:325:LEU:HD13	1.89	0.53
1:E:809:ASN:OD1	1:E:809:ASN:C	2.46	0.53
1:E:948:ASN:O	1:E:950:GLU:N	2.40	0.53
2:F:466:LEU:HD12	2:F:472:LEU:HD11	1.89	0.53
2:F:518:LEU:HD23	2:F:518:LEU:C	2.28	0.53
2:F:752:ARG:CZ	2:F:811:GLY:HA2	2.38	0.53
2:F:829:ALA:HB3	2:F:850:TYR:CZ	2.43	0.53
1:G:767:GLN:HG2	1:G:827:GLU:OE2	2.08	0.53
2:H:324:THR:O	2:H:325:ASN:HB2	2.08	0.53
1:A:289:ARG:CD	1:A:328:GLU:HB3	2.38	0.53
1:A:636:LEU:HD12	1:A:640:GLY:HA2	1.90	0.53
2:B:541:VAL:O	2:B:545:ILE:HG12	2.08	0.53
2:B:779:GLN:HA	2:B:953:VAL:HG21	1.91	0.53
1:C:596:ILE:HD12	1:C:885:ILE:HG21	1.90	0.53
2:D:466:LEU:HD12	2:D:472:LEU:HD11	1.89	0.53
2:D:522:ASN:HD21	2:D:529:LYS:NZ	2.06	0.53
1:E:958:HIS:CD2	1:E:958:HIS:H	2.26	0.53
2:H:886:ILE:HD12	2:H:887:ALA:N	2.23	0.53
1:A:947:THR:HG22	1:A:953:LYS:O	2.07	0.53
2:D:591:ILE:HB	2:D:608:MET:CE	2.39	0.53
2:D:931:GLU:HG3	2:D:931:GLU:O	2.08	0.53
1:E:554:ASN:O	1:E:556:ASP:N	2.40	0.53
2:F:463:HIS:HD2	2:F:474:THR:HG22	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:208:ALA:O	2:H:211:MET:HG3	2.08	0.53
1:A:350:GLY:O	1:A:351:LEU:HD23	2.08	0.53
2:B:680:GLY:HA3	2:B:879:ILE:HD12	1.89	0.53
2:F:341:CYS:CB	2:F:507:VAL:HG13	2.38	0.53
2:H:281:LEU:HD12	2:H:317:LEU:CD2	2.39	0.53
2:H:327:ILE:HA	2:H:331:GLN:NE2	2.23	0.53
1:G:216:ASP:H	2:H:381:HIS:HE1	1.54	0.53
1:A:685:ASP:O	1:A:715:PRO:HD2	2.09	0.53
1:A:802:ASP:OD1	1:A:972:ARG:NH2	2.36	0.53
2:H:883:GLN:O	2:H:887:ALA:HB2	2.09	0.53
2:B:366:ARG:HG2	2:B:482:VAL:O	2.09	0.53
2:B:589:ILE:HD13	2:B:879:ILE:HG21	1.91	0.53
2:D:541:VAL:O	2:D:545:ILE:HG12	2.08	0.53
2:H:641:LYS:O	2:H:644:LEU:HD12	2.08	0.53
1:A:248:LEU:HG	1:A:291:ALA:HB1	1.91	0.53
1:A:212:THR:HG23	1:A:275:GLY:O	2.08	0.53
2:B:907:ALA:O	2:B:922:ILE:HG22	2.08	0.53
1:C:276:THR:HG21	2:D:381:HIS:CE1	2.43	0.53
2:F:353:THR:CG2	2:F:534:SER:HA	2.38	0.53
2:H:314:TRP:HB3	2:H:315:PRO:HD3	1.91	0.53
2:H:903:ILE:HD12	2:H:904:SER:H	1.70	0.53
1:A:285:ARG:NH2	1:A:328:GLU:OE2	2.42	0.53
2:B:208:ALA:O	2:B:211:MET:HG3	2.09	0.53
1:C:422:GLU:OE1	1:C:564:ARG:NH1	2.34	0.53
1:C:685:ASP:O	1:C:715:PRO:HD2	2.09	0.53
2:D:528:ARG:O	2:D:529:LYS:HD2	2.09	0.53
1:E:525:LEU:HD23	1:E:525:LEU:C	2.28	0.53
1:E:599:VAL:CG1	1:E:629:ILE:HB	2.29	0.53
1:G:770:HIS:CG	1:G:951:LEU:HB3	2.43	0.53
2:H:201:VAL:CG1	2:H:218:ILE:HD13	2.39	0.53
2:H:889:ALA:C	2:H:891:ALA:N	2.61	0.53
2:B:794:SER:OG	1:C:796:LEU:HD12	2.08	0.53
2:D:264:THR:CG2	2:D:266:ILE:HG12	2.39	0.53
2:H:426:MET:CE	2:H:466:LEU:HD22	2.39	0.53
1:A:619:CYS:SG	1:A:882:ILE:HD12	2.49	0.53
2:B:353:THR:CG2	2:B:534:SER:HA	2.38	0.53
2:B:353:THR:HG21	2:B:534:SER:HA	1.90	0.53
2:B:753:GLY:HA2	2:B:804:PHE:CD2	2.44	0.53
1:C:767:GLN:HG2	1:C:827:GLU:OE2	2.09	0.53
2:D:353:THR:CG2	2:D:534:SER:HA	2.39	0.53
2:D:350:ASP:HB3	2:D:394:CYS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:522:ASN:HD22	2:D:527:VAL:HG21	1.74	0.53
2:D:353:THR:HG21	2:D:534:SER:HA	1.91	0.53
2:D:779:GLN:OE1	2:D:953:VAL:HG22	2.09	0.53
1:E:778:THR:O	1:E:782:THR:HB	2.09	0.53
1:E:977:ALA:C	1:E:979:VAL:N	2.62	0.53
2:F:648:SER:HA	2:F:865:ARG:HD3	1.89	0.53
2:F:770:THR:HG23	2:F:946:ARG:HD2	1.89	0.53
2:H:350:ASP:HB3	2:H:394:CYS:HB2	1.91	0.53
1:A:230:THR:OG1	1:A:508:VAL:HG22	2.09	0.52
2:B:717:LEU:HB2	2:B:733:ALA:CB	2.39	0.52
2:B:779:GLN:OE1	2:B:953:VAL:HG22	2.08	0.52
1:C:803:ILE:HD13	1:C:845:ALA:CB	2.39	0.52
1:G:317:LEU:CD1	1:G:317:LEU:H	2.22	0.52
2:H:717:LEU:C	2:H:717:LEU:HD12	2.29	0.52
2:B:327:ILE:HA	2:B:331:GLN:NE2	2.23	0.52
2:B:381:HIS:CD2	2:B:383:ARG:HH21	2.28	0.52
2:B:801:ALA:O	2:B:805:GLU:HG3	2.09	0.52
2:D:522:ASN:HD21	2:D:529:LYS:HE3	1.74	0.52
2:D:626:TRP:NE1	2:D:661:PRO:HG3	2.24	0.52
2:D:697:GLU:O	2:D:700:ARG:HB2	2.08	0.52
1:E:461:GLN:HB2	1:E:463:ASN:ND2	2.24	0.52
1:E:770:HIS:CD2	1:E:951:LEU:HA	2.44	0.52
1:E:944:GLU:HA	1:E:946:GLU:OE1	2.09	0.52
2:F:892:ALA:C	2:F:894:GLU:H	2.09	0.52
2:H:322:LEU:O	2:H:324:THR:N	2.37	0.52
2:H:327:ILE:HB	2:H:331:GLN:HE21	1.73	0.52
1:A:301:ASP:OD1	1:A:301:ASP:N	2.43	0.52
1:A:236:CYS:SG	1:A:515:LEU:HD21	2.49	0.52
1:A:374:ARG:HD2	2:B:373:TYR:CZ	2.45	0.52
2:B:704:PRO:HA	2:B:707:ARG:CG	2.38	0.52
2:D:886:ILE:HD12	2:D:887:ALA:N	2.24	0.52
2:F:697:GLU:O	2:F:700:ARG:HB2	2.08	0.52
2:H:664:ALA:O	2:H:665:ASP:CB	2.57	0.52
1:A:205:LYS:HE3	1:A:237:ASP:CG	2.29	0.52
2:B:547:ALA:O	2:B:549:ASP:N	2.43	0.52
2:B:697:GLU:O	2:B:700:ARG:HB2	2.09	0.52
1:C:717:CYS:HA	1:C:925:ALA:O	2.09	0.52
1:C:813:ASP:O	1:C:815:GLY:N	2.40	0.52
1:C:958:HIS:C	1:C:959:TRP:CD1	2.82	0.52
1:G:331:ALA:O	1:G:333:GLY:N	2.42	0.52
2:H:665:ASP:O	2:H:669:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:CD2	1:A:968:ILE:HD12	2.44	0.52
1:A:320:HIS:O	1:A:321:GLU:HB2	2.10	0.52
2:B:662:GLU:H	2:B:695:GLN:HE22	1.56	0.52
1:C:972:ARG:HH11	1:C:976:ARG:HH21	1.58	0.52
2:F:462:VAL:O	2:F:466:LEU:HD23	2.09	0.52
1:G:951:LEU:HD22	1:G:951:LEU:N	2.25	0.52
1:A:323:PRO:O	1:A:326:VAL:HB	2.09	0.52
2:B:328:SER:H	2:B:331:GLN:NE2	2.06	0.52
2:B:365:ASP:HA	2:B:862:PRO:HG2	1.92	0.52
2:B:771:TYR:OH	2:B:945:THR:HG21	2.10	0.52
2:D:537:LEU:O	2:D:540:ALA:HB3	2.08	0.52
2:F:701:GLU:CD	2:F:701:GLU:O	2.48	0.52
2:H:701:GLU:O	2:H:702:SER:CB	2.53	0.52
1:A:289:ARG:HA	1:A:325:LEU:HD13	1.92	0.52
1:A:292:ALA:O	1:A:296:ILE:HG13	2.09	0.52
1:A:865:VAL:HG13	1:A:866:PRO:HD2	1.92	0.52
2:B:312:SER:O	2:B:315:PRO:HD2	2.10	0.52
1:C:805:LEU:O	1:C:975:LEU:HD13	2.10	0.52
1:G:317:LEU:HD12	1:G:317:LEU:H	1.74	0.52
1:C:947:THR:HG23	1:C:952:ARG:N	2.25	0.52
2:D:293:ASP:HB3	2:D:335:MET:HE3	1.92	0.52
2:D:343:THR:HG22	2:D:343:THR:O	2.09	0.52
1:E:581:LYS:HB3	1:E:586:GLU:CB	2.30	0.52
1:E:812:HIS:N	1:E:812:HIS:CD2	2.78	0.52
2:F:578:GLU:C	2:F:580:LYS:H	2.13	0.52
2:F:883:GLN:O	2:F:887:ALA:HB2	2.09	0.52
2:H:298:CYS:SG	2:H:343:THR:HG22	2.50	0.52
2:H:522:ASN:HD21	2:H:529:LYS:CE	2.23	0.52
1:C:322:TRP:CZ3	1:C:343:TYR:O	2.63	0.52
2:D:587:LEU:HD21	2:D:883:GLN:HG3	1.92	0.52
1:E:319:ARG:HG3	1:E:346:LEU:HB3	1.91	0.52
1:E:946:GLU:CD	1:E:946:GLU:O	2.49	0.52
2:F:945:THR:HA	2:F:948:ILE:HG12	1.92	0.52
1:G:466:THR:CG2	1:G:468:ASN:H	2.15	0.52
1:G:525:LEU:HD23	1:G:525:LEU:C	2.30	0.52
1:C:782:THR:HG22	1:C:784:ALA:H	1.75	0.51
1:C:825:ARG:HH11	1:C:829:ALA:HB3	1.75	0.51
1:C:809:ASN:HB2	1:C:975:LEU:HD11	1.91	0.51
2:F:264:THR:HG22	2:F:266:ILE:HG12	1.93	0.51
2:F:665:ASP:O	2:F:669:ILE:HG12	2.10	0.51
2:F:717:LEU:HD12	2:F:717:LEU:C	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:716:MET:O	1:G:924:ALA:HA	2.10	0.51
1:A:320:HIS:O	1:A:321:GLU:CB	2.57	0.51
1:A:823:LEU:N	1:A:823:LEU:HD12	2.25	0.51
1:C:518:THR:HB	1:C:519:PRO:HD2	1.92	0.51
2:D:903:ILE:HD12	2:D:904:SER:H	1.74	0.51
1:E:800:ARG:HG3	2:H:790:LEU:HD13	1.93	0.51
1:E:841:ILE:HD11	2:H:827:LEU:HD21	1.92	0.51
2:F:341:CYS:HB2	2:F:507:VAL:CG1	2.40	0.51
1:G:439:GLN:HA	1:G:439:GLN:OE1	2.10	0.51
2:H:522:ASN:HD21	2:H:529:LYS:NZ	2.08	0.51
1:A:289:ARG:NH2	1:A:328:GLU:HG2	2.25	0.51
1:A:928:CYS:O	1:A:934:VAL:HA	2.10	0.51
2:B:673:PHE:HZ	2:B:681:LEU:HD22	1.74	0.51
1:C:276:THR:CG2	1:C:276:THR:O	2.57	0.51
1:C:805:LEU:HD13	1:C:972:ARG:HA	1.91	0.51
2:D:288:ILE:HA	2:D:335:MET:HE1	1.91	0.51
2:D:416:PRO:HD2	2:D:550:PHE:CD1	2.45	0.51
1:C:746:TYR:CE1	2:D:854:VAL:HG13	2.45	0.51
2:D:771:TYR:OH	2:D:945:THR:HG21	2.10	0.51
2:F:327:ILE:HB	2:F:331:GLN:HE21	1.74	0.51
2:F:615:GLN:OE1	2:F:880:LYS:NZ	2.43	0.51
1:G:322:TRP:HB3	1:G:323:PRO:HD3	1.91	0.51
1:G:421:PRO:C	1:G:423:ARG:H	2.12	0.51
1:G:572:TYR:CE2	1:G:576:LEU:HD11	2.45	0.51
1:A:381:TYR:CE2	2:B:366:ARG:HD2	2.46	0.51
1:A:963:ASN:O	1:A:967:ASP:N	2.41	0.51
1:A:966:GLY:O	1:A:970:SER:HB3	2.10	0.51
2:B:433:HIS:ND1	2:B:640:TRP:CZ2	2.78	0.51
2:B:657:ASN:OD1	2:B:659:VAL:HG23	2.10	0.51
2:B:715:ALA:HB2	2:B:728:LEU:HB2	1.90	0.51
1:C:558:ASP:O	1:C:561:ILE:HG22	2.11	0.51
2:D:754:ARG:NH2	2:D:847:LYS:HE3	2.25	0.51
1:E:518:THR:HB	1:E:519:PRO:HD2	1.92	0.51
2:F:239:LEU:HD22	2:F:287:LEU:CD2	2.40	0.51
2:F:392:ARG:NH2	3:F:984:F6P:H12	2.23	0.51
1:G:596:ILE:HD12	1:G:885:ILE:HG21	1.93	0.51
2:H:911:GLY:O	2:H:917:VAL:HA	2.09	0.51
2:B:683:ILE:O	2:B:712:LEU:HD12	2.11	0.51
2:B:797:ILE:HD13	2:B:836:ILE:HA	1.93	0.51
2:B:916:HIS:O	2:B:917:VAL:HG23	2.11	0.51
1:C:697:ARG:NH2	1:C:949:VAL:HG22	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:776:SER:CB	1:E:963:ASN:HD21	2.23	0.51
1:G:291:ALA:O	1:G:294:ASN:N	2.44	0.51
1:G:583:ASP:O	1:G:583:ASP:OD2	2.29	0.51
1:G:947:THR:HG22	1:G:953:LYS:O	2.11	0.51
2:H:852:GLY:O	2:H:855:GLN:HG3	2.10	0.51
1:A:600:HIS:CE1	1:A:661:ILE:HD11	2.45	0.51
1:A:860:VAL:HG11	2:B:740:TYR:CE1	2.46	0.51
2:B:349:ASN:OD1	2:B:356:ALA:HA	2.11	0.51
2:B:587:LEU:N	2:B:587:LEU:CD1	2.74	0.51
1:C:398:MET:HG3	1:C:490:GLN:NE2	2.25	0.51
1:E:391:ARG:HG2	1:E:480:ASP:HB3	1.93	0.51
1:E:400:ARG:HG2	1:E:400:ARG:HH11	1.76	0.51
1:E:431:GLN:N	1:E:431:GLN:HE21	1.98	0.51
2:H:578:GLU:C	2:H:580:LYS:H	2.09	0.51
1:A:229:ARG:HD3	1:A:260:TRP:CZ2	2.45	0.51
1:A:951:LEU:N	1:A:951:LEU:HD23	2.25	0.51
1:C:676:ALA:HB2	1:C:712:PHE:CZ	2.46	0.51
2:D:563:GLU:OE2	2:D:870:ARG:NE	2.32	0.51
2:D:935:ARG:O	2:D:936:MET:HB3	2.10	0.51
1:E:767:GLN:HG2	1:E:827:GLU:OE2	2.11	0.51
2:F:298:CYS:CB	2:F:343:THR:HG22	2.40	0.51
1:G:732:TYR:CE1	1:G:736:VAL:HB	2.46	0.51
2:H:418:THR:O	2:H:419:SER:HB2	2.10	0.51
2:H:438:LYS:HG2	2:H:440:THR:O	2.10	0.51
1:C:542:VAL:O	1:C:546:LYS:HB2	2.10	0.51
2:D:797:ILE:HD13	2:D:836:ILE:HA	1.93	0.51
1:E:883:LYS:O	1:E:887:GLN:HG3	2.09	0.51
2:F:344:VAL:CG2	2:F:357:THR:HG22	2.40	0.51
2:F:541:VAL:O	2:F:545:ILE:HG12	2.11	0.51
1:G:212:THR:HG22	1:G:274:ILE:HG13	1.93	0.51
1:G:588:LEU:HD13	1:G:593:ARG:NH1	2.21	0.51
1:A:812:HIS:N	1:A:812:HIS:CD2	2.77	0.51
2:B:201:VAL:HG13	2:B:218:ILE:HG21	1.93	0.51
1:A:758:ARG:NH1	2:B:655:GLY:CA	2.73	0.51
1:E:229:ARG:HD3	1:E:260:TRP:CZ2	2.46	0.51
1:E:790:PRO:HD2	1:E:791:GLU:OE1	2.11	0.51
2:F:347:ILE:HB	2:F:363:ALA:CB	2.40	0.51
2:H:453:ASP:O	2:H:454:LEU:HB2	2.10	0.51
2:H:603:SER:HB3	2:H:647:GLN:OE1	2.11	0.51
1:A:809:ASN:HA	1:A:975:LEU:HD21	1.92	0.51
1:C:495:ALA:HB3	1:C:500:ARG:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:809:ASN:HB2	1:C:975:LEU:CD2	2.40	0.51
2:D:798:GLU:O	2:D:801:ALA:HB3	2.11	0.51
1:E:791:GLU:CD	1:E:959:TRP:HH2	2.15	0.51
2:H:436:ARG:HG3	2:H:436:ARG:O	2.10	0.51
2:H:679:ASP:O	2:H:708:ILE:HB	2.10	0.51
1:C:249:LEU:HD13	1:C:290:GLN:HG2	1.93	0.50
1:C:252:GLY:O	1:C:253:LYS:HB3	2.10	0.50
2:D:633:GLU:HB2	2:D:672:TYR:OH	2.12	0.50
1:E:391:ARG:O	1:E:448:ASN:HA	2.10	0.50
1:E:423:ARG:CD	1:E:561:ILE:HD12	2.41	0.50
2:F:494:ILE:HD13	2:F:771:TYR:HD2	1.76	0.50
2:F:565:LEU:O	2:F:569:MET:HG2	2.11	0.50
1:G:246:GLU:O	1:G:249:LEU:HB3	2.11	0.50
1:G:330:VAL:HG22	1:G:340:VAL:HG11	1.93	0.50
2:H:662:GLU:H	2:H:695:GLN:HE22	1.59	0.50
2:H:697:GLU:O	2:H:700:ARG:HB2	2.12	0.50
1:A:381:TYR:HD2	2:B:486:GLY:CA	2.24	0.50
1:A:590:VAL:HG23	1:A:591:SER:N	2.27	0.50
2:D:416:PRO:HG2	2:D:550:PHE:CZ	2.46	0.50
1:E:322:TRP:CZ3	1:E:343:TYR:O	2.65	0.50
1:E:538:LEU:HD23	1:E:538:LEU:C	2.31	0.50
2:F:239:LEU:O	2:F:286:HIS:HD2	1.95	0.50
2:F:381:HIS:CB	2:F:383:ARG:HG3	2.36	0.50
1:G:242:TYR:O	1:G:247:GLY:HA3	2.10	0.50
1:G:600:HIS:HD2	1:G:659:SER:OG	1.93	0.50
1:C:276:THR:CG2	2:D:381:HIS:CE1	2.95	0.50
1:C:538:LEU:C	1:C:538:LEU:HD23	2.31	0.50
2:D:256:ARG:NH1	2:D:813:PHE:CE1	2.79	0.50
2:D:587:LEU:H	2:D:587:LEU:CD1	2.23	0.50
2:F:726:TYR:OH	2:F:864:ASP:OD2	2.23	0.50
1:G:754:ALA:HB2	1:G:762:PHE:CE1	2.45	0.50
2:H:201:VAL:CG1	2:H:218:ILE:HG21	2.42	0.50
2:H:528:ARG:O	2:H:529:LYS:HD2	2.12	0.50
1:A:427:HIS:ND1	1:A:427:HIS:C	2.65	0.50
1:A:962:TYR:O	1:A:965:ILE:N	2.44	0.50
1:C:525:LEU:C	1:C:525:LEU:HD23	2.31	0.50
1:C:860:VAL:HG11	2:D:740:TYR:CD1	2.46	0.50
1:C:233:HIS:CE1	1:C:968:ILE:HD13	2.47	0.50
2:D:341:CYS:HB2	2:D:507:VAL:HG13	1.93	0.50
2:F:390:MET:HG3	2:F:483:GLN:NE2	2.25	0.50
1:G:320:HIS:O	1:G:321:GLU:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:638:GLN:O	1:G:638:GLN:HG3	2.10	0.50
2:H:328:SER:H	2:H:331:GLN:NE2	2.09	0.50
2:H:463:HIS:HD2	2:H:474:THR:HG22	1.76	0.50
2:H:717:LEU:HB2	2:H:733:ALA:CB	2.41	0.50
2:B:545:ILE:HD11	2:B:553:ALA:CB	2.41	0.50
1:C:431:GLN:N	1:C:431:GLN:NE2	2.50	0.50
2:D:744:VAL:O	2:D:747:SER:HB3	2.12	0.50
2:D:889:ALA:C	2:D:891:ALA:N	2.64	0.50
2:F:298:CYS:HA	2:F:343:THR:O	2.12	0.50
2:F:522:ASN:HD21	2:F:529:LYS:CE	2.24	0.50
1:G:717:CYS:HA	1:G:925:ALA:O	2.12	0.50
2:H:201:VAL:HG11	2:H:218:ILE:HD13	1.93	0.50
1:A:622:HIS:HD2	1:A:886:GLU:OE1	1.95	0.50
2:B:626:TRP:NE1	2:B:661:PRO:HG3	2.26	0.50
1:C:342:PRO:HG2	1:C:343:TYR:CD1	2.46	0.50
1:C:708:GLN:O	1:G:709:HIS:HE1	1.94	0.50
1:E:410:GLY:HA2	1:E:452:ILE:HD12	1.94	0.50
2:H:253:GLU:O	2:H:256:ARG:HB3	2.12	0.50
2:H:416:PRO:O	2:H:417:ALA:C	2.49	0.50
2:H:565:LEU:O	2:H:569:MET:HG2	2.12	0.50
1:A:790:PRO:HD2	1:A:791:GLU:OE1	2.11	0.50
2:D:420:SER:HA	2:D:423:GLN:NE2	2.26	0.50
2:D:582:PRO:O	2:D:586:ARG:NH1	2.41	0.50
2:D:761:GLN:HG3	2:D:855:GLN:NE2	2.27	0.50
2:F:428:ASP:OD2	2:F:432:LYS:NZ	2.45	0.50
2:F:930:THR:HG22	2:F:932:VAL:H	1.76	0.50
2:F:947:LEU:HD22	2:F:951:HIS:CE1	2.46	0.50
2:H:427:CYS:SG	2:H:470:LEU:HD23	2.52	0.50
2:H:781:SER:HA	2:H:818:LEU:O	2.11	0.50
1:C:667:VAL:HG11	1:C:697:ARG:HD3	1.93	0.50
1:C:942:LEU:C	1:C:944:GLU:H	2.16	0.50
2:D:422:TRP:CH2	2:D:465:VAL:HG21	2.46	0.50
1:G:485:ILE:HD12	1:G:485:ILE:N	2.26	0.50
2:H:347:ILE:HB	2:H:363:ALA:HB2	1.93	0.50
2:H:525:LYS:HB2	2:H:525:LYS:HZ3	1.74	0.50
2:H:711:VAL:CG2	2:H:910:VAL:HG22	2.41	0.50
1:A:539:VAL:O	1:A:542:VAL:HG22	2.11	0.50
2:B:201:VAL:CG1	2:B:218:ILE:HG21	2.42	0.50
2:B:253:GLU:O	2:B:256:ARG:HB3	2.12	0.50
2:D:298:CYS:SG	2:D:343:THR:HG22	2.51	0.50
2:D:327:ILE:CA	2:D:331:GLN:NE2	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:935:ARG:NH1	4:D:4:FDP:O3P	2.45	0.50
2:D:662:GLU:H	2:D:695:GLN:HE22	1.59	0.50
1:C:660:GLU:C	2:D:752:ARG:HH22	2.14	0.50
2:D:883:GLN:O	2:D:887:ALA:HB2	2.11	0.50
1:E:248:LEU:HG	1:E:291:ALA:HB1	1.94	0.50
2:F:726:TYR:CE1	2:F:730:SER:HB3	2.46	0.50
2:H:453:ASP:CG	2:H:455:THR:HG23	2.32	0.50
1:A:594:LEU:N	1:A:624:HIS:ND1	2.55	0.49
2:B:574:ALA:CB	2:B:610:THR:HB	2.41	0.49
2:B:580:LYS:HD2	2:B:586:ARG:NH2	2.27	0.49
2:B:851:PRO:O	2:B:854:VAL:HG22	2.12	0.49
1:C:212:THR:O	1:C:212:THR:CG2	2.59	0.49
2:D:354:THR:CB	2:D:520:ALA:HB1	2.42	0.49
2:D:416:PRO:O	2:D:417:ALA:C	2.50	0.49
1:G:291:ALA:HA	1:G:294:ASN:ND2	2.27	0.49
2:H:894:GLU:C	2:H:896:PHE:N	2.65	0.49
1:A:339:GLU:C	1:A:341:ALA:H	2.15	0.49
1:A:883:LYS:O	1:A:887:GLN:HG3	2.11	0.49
2:B:264:THR:HG22	2:B:266:ILE:N	2.26	0.49
2:B:400:LEU:HD12	2:B:866:THR:HG21	1.94	0.49
2:B:418:THR:HG21	2:B:422:TRP:HD1	1.77	0.49
2:B:426:MET:CE	2:B:466:LEU:HD22	2.41	0.49
2:B:518:LEU:HD23	2:B:518:LEU:C	2.32	0.49
1:C:636:LEU:HD12	1:C:640:GLY:HA2	1.95	0.49
1:E:242:TYR:O	1:E:247:GLY:HA3	2.12	0.49
1:E:398:MET:HE1	1:E:488:HIS:HA	1.94	0.49
1:E:634:SER:HB3	1:E:666:SER:CB	2.42	0.49
2:F:400:LEU:CD1	2:F:866:THR:HG21	2.42	0.49
2:H:410:ILE:HA	2:H:444:VAL:O	2.11	0.49
2:H:626:TRP:CE2	2:H:661:PRO:HG3	2.47	0.49
2:B:521:VAL:HG13	2:B:526:ILE:HD13	1.94	0.49
2:D:683:ILE:O	2:D:712:LEU:HD12	2.13	0.49
2:D:830:THR:HA	2:D:848:PRO:HB3	1.94	0.49
1:E:800:ARG:HG3	2:H:790:LEU:CD1	2.42	0.49
1:E:941:ASN:O	1:E:944:GLU:HG3	2.12	0.49
1:E:977:ALA:O	1:E:979:VAL:N	2.44	0.49
2:F:298:CYS:SG	2:F:343:THR:HG22	2.53	0.49
2:F:851:PRO:O	2:F:854:VAL:HG22	2.12	0.49
1:A:251:GLY:CA	1:A:294:ASN:ND2	2.75	0.49
1:A:893:GLU:HA	1:A:893:GLU:OE2	2.12	0.49
2:B:711:VAL:CG2	2:B:910:VAL:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:786:SER:HB3	1:C:823:LEU:HG	1.93	0.49
2:F:253:GLU:O	2:F:256:ARG:HB3	2.13	0.49
2:F:400:LEU:HD12	2:F:866:THR:HG21	1.92	0.49
2:F:522:ASN:HD21	2:F:529:LYS:NZ	2.09	0.49
2:H:201:VAL:HG11	2:H:218:ILE:CD1	2.42	0.49
2:H:268:THR:O	2:H:268:THR:HG23	2.12	0.49
2:H:590:ALA:HA	2:H:620:TYR:O	2.13	0.49
1:A:538:LEU:C	1:A:538:LEU:HD23	2.32	0.49
2:B:587:LEU:HD12	2:B:587:LEU:H	1.75	0.49
2:B:770:THR:CG2	2:B:946:ARG:HD2	2.42	0.49
2:D:381:HIS:CB	2:D:383:ARG:HG3	2.38	0.49
2:D:679:ASP:HB3	2:D:883:GLN:HE22	1.76	0.49
2:D:753:GLY:HA2	2:D:804:PHE:CD2	2.47	0.49
1:E:599:VAL:HG13	1:E:629:ILE:CB	2.30	0.49
2:F:528:ARG:O	2:F:529:LYS:HD2	2.12	0.49
2:F:800:LEU:HD21	2:F:817:ILE:HD11	1.95	0.49
2:B:220:ARG:HD2	2:B:252:TRP:CE2	2.48	0.49
1:C:833:TYR:HA	1:C:837:LEU:HD23	1.94	0.49
2:D:523:GLU:O	2:D:524:ASN:C	2.50	0.49
1:C:746:TYR:CE1	2:D:854:VAL:HG11	2.47	0.49
1:E:253:LYS:C	1:E:255:LEU:N	2.64	0.49
1:E:342:PRO:HG2	1:E:343:TYR:CD1	2.47	0.49
1:E:805:LEU:HD23	1:E:805:LEU:N	2.28	0.49
1:G:309:ASP:OD1	1:G:310:GLY:N	2.46	0.49
2:H:353:THR:CG2	2:H:534:SER:HA	2.43	0.49
1:A:242:TYR:N	1:A:242:TYR:CD1	2.81	0.49
1:A:975:LEU:O	1:A:979:VAL:HG23	2.13	0.49
2:B:327:ILE:HB	2:B:331:GLN:NE2	2.27	0.49
2:B:382:SER:HA	2:B:439:ARG:O	2.12	0.49
2:B:662:GLU:HG3	2:B:695:GLN:NE2	2.28	0.49
2:B:904:SER:O	2:B:906:THR:N	2.44	0.49
1:C:374:ARG:NH2	1:C:494:THR:O	2.45	0.49
1:C:782:THR:HG22	1:C:784:ALA:N	2.28	0.49
2:D:453:ASP:CG	2:D:455:THR:HG23	2.33	0.49
2:D:916:HIS:O	2:D:917:VAL:HG23	2.12	0.49
2:F:281:LEU:HD12	2:F:317:LEU:HD23	1.94	0.49
2:F:256:ARG:NH1	2:F:813:PHE:CE1	2.80	0.49
1:G:746:TYR:CE1	2:H:854:VAL:HG11	2.47	0.49
1:G:765:GLU:HA	1:G:825:ARG:O	2.13	0.49
1:G:974:LYS:CG	1:G:975:LEU:N	2.68	0.49
1:A:508:VAL:HG21	1:A:969:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:626:TRP:CE2	2:B:661:PRO:HG3	2.47	0.49
1:C:242:TYR:O	1:C:247:GLY:HA3	2.13	0.49
2:D:626:TRP:CE2	2:D:661:PRO:HG3	2.48	0.49
2:D:726:TYR:CE1	2:D:730:SER:HB3	2.48	0.49
2:D:946:ARG:HH21	2:D:946:ARG:CG	2.21	0.49
1:E:651:GLU:HG3	1:E:652:ASN:ND2	2.28	0.49
1:A:247:GLY:HA2	1:A:254:TYR:HD2	1.77	0.49
1:C:210:VAL:HG12	1:C:304:VAL:HB	1.95	0.49
1:C:928:CYS:O	1:C:934:VAL:HA	2.12	0.49
2:D:438:LYS:HG2	2:D:440:THR:O	2.13	0.49
1:E:242:TYR:CD1	1:E:242:TYR:N	2.81	0.49
2:F:453:ASP:O	2:F:454:LEU:HB2	2.12	0.49
1:G:375:ILE:HD13	1:G:397:VAL:HG11	1.94	0.49
2:H:381:HIS:CB	2:H:383:ARG:HG3	2.40	0.49
2:H:593:ASN:HA	2:H:684:VAL:O	2.13	0.49
2:H:587:LEU:CD2	2:H:883:GLN:NE2	2.75	0.49
1:A:772:GLY:C	1:A:959:TRP:CZ3	2.86	0.49
2:B:549:ASP:OD2	2:B:552:ARG:HB2	2.12	0.49
1:C:651:GLU:HG3	1:C:652:ASN:ND2	2.27	0.49
1:C:703:ARG:HD2	1:C:703:ARG:C	2.33	0.49
1:C:975:LEU:O	1:C:979:VAL:HG23	2.12	0.49
1:E:398:MET:HG3	1:E:490:GLN:NE2	2.28	0.49
1:E:422:GLU:CG	1:E:564:ARG:HD2	2.41	0.49
1:E:716:MET:O	1:E:924:ALA:HA	2.13	0.49
1:E:746:TYR:CE1	2:F:854:VAL:CG1	2.96	0.49
2:F:798:GLU:O	2:F:801:ALA:HB3	2.13	0.49
1:G:959:TRP:CD1	1:G:959:TRP:N	2.81	0.49
2:H:665:ASP:OD1	2:H:668:MET:HG2	2.13	0.49
1:A:317:LEU:N	1:A:317:LEU:HD12	2.28	0.48
2:B:786:GLU:OE2	2:B:946:ARG:NH2	2.31	0.48
1:C:315:ALA:O	1:C:348:ILE:HD13	2.13	0.48
1:C:947:THR:O	1:C:947:THR:HG23	2.13	0.48
2:D:304:LEU:HD13	2:D:518:LEU:HD12	1.94	0.48
2:D:518:LEU:HD23	2:D:518:LEU:C	2.34	0.48
2:D:608:MET:SD	2:D:608:MET:C	2.91	0.48
2:D:874:LYS:HD2	2:D:917:VAL:HG21	1.95	0.48
1:E:581:LYS:C	1:E:583:ASP:H	2.15	0.48
2:F:322:LEU:O	2:F:324:THR:N	2.42	0.48
2:F:740:TYR:CE1	2:F:851:PRO:HB3	2.48	0.48
1:G:342:PRO:HG2	1:G:343:TYR:CD1	2.48	0.48
1:G:744:VAL:HG12	1:G:745:ASN:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:281:LEU:CD2	2:H:326:ARG:NH2	2.75	0.48
2:H:779:GLN:HA	2:H:953:VAL:HG21	1.94	0.48
2:B:781:SER:HA	2:B:818:LEU:O	2.13	0.48
2:B:956:LYS:NZ	2:B:956:LYS:CA	2.73	0.48
2:D:707:ARG:HE	2:D:897:ASN:CG	2.15	0.48
1:E:943:TRP:HA	1:E:946:GLU:HG3	1.94	0.48
2:F:421:GLU:O	2:F:425:GLN:HB2	2.13	0.48
1:A:864:GLY:CA	2:B:743:VAL:HG22	2.44	0.48
2:B:690:PHE:HA	2:B:712:LEU:HD22	1.94	0.48
1:C:548:VAL:O	1:C:552:ILE:HG12	2.13	0.48
1:C:788:TYR:HB3	1:C:794:ILE:HD11	1.93	0.48
1:E:466:THR:HB	1:E:469:ASP:CG	2.31	0.48
1:E:360:SER:HB3	1:E:545:THR:HG22	1.94	0.48
1:E:583:ASP:O	1:E:583:ASP:OD2	2.31	0.48
1:E:930:ASN:O	1:E:931:GLY:C	2.51	0.48
2:F:327:ILE:CA	2:F:331:GLN:NE2	2.76	0.48
2:F:723:GLY:O	2:F:911:GLY:HA3	2.13	0.48
1:A:466:THR:CG2	1:A:468:ASN:H	2.15	0.48
1:A:398:MET:HG3	1:A:490:GLN:NE2	2.28	0.48
1:A:822:LEU:C	1:A:822:LEU:CD1	2.81	0.48
1:A:964:LYS:H	1:A:964:LYS:CD	2.23	0.48
2:B:499:GLN:HG2	2:B:526:ILE:HD12	1.95	0.48
2:B:648:SER:HA	2:B:865:ARG:HD3	1.94	0.48
2:D:288:ILE:HA	2:D:335:MET:CE	2.43	0.48
2:D:378:ALA:HB2	2:D:385:PHE:CE1	2.48	0.48
2:D:692:SER:O	2:D:693:LEU:C	2.51	0.48
2:F:647:GLN:HE22	2:F:869:THR:CG2	2.27	0.48
1:G:421:PRO:HB3	1:G:456:GLY:O	2.12	0.48
1:A:746:TYR:CE1	2:B:854:VAL:CG1	2.97	0.48
1:C:292:ALA:O	1:C:296:ILE:HG13	2.14	0.48
1:C:410:GLY:HA2	1:C:452:ILE:HD12	1.94	0.48
1:C:773:TYR:N	1:C:959:TRP:CH2	2.80	0.48
1:E:501:TRP:HZ2	1:E:962:TYR:HH	1.59	0.48
1:E:586:GLU:O	1:E:587:LEU:C	2.52	0.48
2:F:321:LEU:O	2:F:325:ASN:O	2.31	0.48
2:F:453:ASP:CG	2:F:455:THR:HG23	2.32	0.48
1:G:942:LEU:C	1:G:944:GLU:H	2.16	0.48
1:A:581:LYS:C	1:A:583:ASP:H	2.17	0.48
1:A:586:GLU:O	1:A:587:LEU:C	2.50	0.48
2:B:608:MET:SD	2:B:608:MET:C	2.92	0.48
1:C:631:ASN:OD1	2:D:752:ARG:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:601:VAL:O	1:E:691:GLY:HA3	2.14	0.48
2:F:658:ARG:HH21	4:F:6:FDP:H62	1.78	0.48
1:G:360:SER:HB3	1:G:545:THR:HG22	1.95	0.48
1:G:772:GLY:HA2	1:G:826:ASN:HD22	1.78	0.48
1:G:822:LEU:C	1:G:822:LEU:CD1	2.80	0.48
1:A:410:GLY:HA2	1:A:452:ILE:HD12	1.96	0.48
1:A:508:VAL:CG2	1:A:969:LEU:HD11	2.44	0.48
1:A:968:ILE:CD1	1:A:973:LEU:HD12	2.44	0.48
2:B:201:VAL:HA	2:B:296:ILE:O	2.14	0.48
2:B:354:THR:CB	2:B:520:ALA:HB1	2.44	0.48
2:B:594:VAL:HB	2:B:689:ALA:HB2	1.95	0.48
1:C:341:ALA:HB3	1:C:342:PRO:HD3	1.96	0.48
2:D:522:ASN:O	2:D:523:GLU:C	2.52	0.48
1:E:250:ARG:HG3	1:E:250:ARG:NH1	2.29	0.48
1:E:319:ARG:NH1	1:E:517:PHE:CE2	2.80	0.48
1:E:548:VAL:O	1:E:552:ILE:HG12	2.14	0.48
1:E:942:LEU:C	1:E:944:GLU:H	2.17	0.48
2:F:418:THR:HA	2:F:421:GLU:CB	2.39	0.48
1:G:740:LEU:HD13	1:G:777:PHE:CE2	2.48	0.48
2:H:220:ARG:HD2	2:H:252:TRP:CE2	2.48	0.48
2:H:662:GLU:H	2:H:695:GLN:NE2	2.12	0.48
1:A:966:GLY:O	1:A:970:SER:CB	2.62	0.48
1:A:804:THR:CG2	1:A:979:VAL:HG21	2.44	0.48
2:B:466:LEU:HD12	2:B:472:LEU:HD11	1.95	0.48
2:D:521:VAL:HG13	2:D:526:ILE:HD13	1.95	0.48
2:D:701:GLU:CD	2:D:701:GLU:O	2.52	0.48
1:E:247:GLY:HA2	1:E:254:TYR:HD2	1.78	0.48
2:F:353:THR:HG21	2:F:534:SER:HA	1.95	0.48
1:A:253:LYS:C	1:A:255:LEU:N	2.66	0.48
1:A:466:THR:CG2	1:A:467:ALA:N	2.77	0.48
1:A:558:ASP:O	1:A:561:ILE:HG22	2.13	0.48
1:A:977:ALA:C	1:A:979:VAL:N	2.67	0.48
2:B:467:VAL:O	2:B:471:GLY:CA	2.58	0.48
2:B:946:ARG:CG	2:B:946:ARG:HH21	2.21	0.48
1:C:947:THR:O	1:C:948:ASN:O	2.32	0.48
2:D:354:THR:HB	2:D:520:ALA:HB1	1.95	0.48
2:F:418:THR:HG21	2:F:422:TRP:HD1	1.78	0.48
1:G:315:ALA:O	1:G:348:ILE:HD13	2.13	0.48
1:A:212:THR:CG2	1:A:275:GLY:O	2.62	0.48
1:A:289:ARG:NH2	1:A:328:GLU:OE2	2.45	0.48
1:A:676:ALA:HB2	1:A:712:PHE:CZ	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LYS:C	1:C:255:LEU:N	2.66	0.48
2:F:709:PRO:HB2	2:F:879:ILE:HD13	1.96	0.48
1:G:790:PRO:HD2	1:G:791:GLU:OE1	2.14	0.48
2:H:626:TRP:NE1	2:H:661:PRO:HG3	2.29	0.48
2:H:874:LYS:CD	2:H:917:VAL:HG21	2.43	0.48
1:A:805:LEU:N	1:A:805:LEU:HD23	2.29	0.47
1:A:755:SER:HB3	1:A:817:ASN:O	2.14	0.47
2:B:853:HIS:C	2:B:855:GLN:N	2.66	0.47
1:C:421:PRO:C	1:C:423:ARG:N	2.67	0.47
2:D:518:LEU:HD23	2:D:518:LEU:O	2.14	0.47
1:E:690:LEU:HD23	1:E:719:ILE:HB	1.96	0.47
2:F:312:SER:O	2:F:315:PRO:HD2	2.14	0.47
2:F:522:ASN:HD21	2:F:529:LYS:HE3	1.79	0.47
2:F:770:THR:OG1	2:F:946:ARG:HD3	2.14	0.47
2:H:390:MET:HB3	3:H:986:F6P:O3	2.13	0.47
2:H:522:ASN:HD21	2:H:529:LYS:HE3	1.78	0.47
2:H:887:ALA:C	2:H:889:ALA:H	2.17	0.47
1:A:289:ARG:N	1:A:325:LEU:HD13	2.29	0.47
2:B:607:SER:OG	2:B:869:THR:CB	2.61	0.47
1:C:423:ARG:CD	1:C:561:ILE:HD12	2.44	0.47
2:D:344:VAL:HG22	2:D:357:THR:HG22	1.96	0.47
2:F:946:ARG:HG3	2:F:946:ARG:NH2	2.25	0.47
1:G:242:TYR:N	1:G:242:TYR:CD1	2.81	0.47
2:H:383:ARG:NH1	2:H:475:ARG:CZ	2.77	0.47
2:H:770:THR:HG23	2:H:946:ARG:HD2	1.96	0.47
2:H:830:THR:HA	2:H:848:PRO:HB3	1.97	0.47
2:H:829:ALA:HB3	2:H:850:TYR:CZ	2.49	0.47
2:B:494:ILE:HD13	2:B:771:TYR:HD2	1.79	0.47
1:C:350:GLY:O	1:C:351:LEU:HD23	2.14	0.47
1:C:746:TYR:CD1	2:D:854:VAL:CG1	2.97	0.47
1:C:766:VAL:CG1	1:C:774:ILE:HG22	2.44	0.47
1:C:825:ARG:NH2	1:C:834:SER:HA	2.30	0.47
2:D:911:GLY:O	2:D:917:VAL:HA	2.13	0.47
1:E:529:LEU:HA	1:E:529:LEU:HD23	1.70	0.47
1:E:216:ASP:OD2	2:F:377:THR:HA	2.14	0.47
2:H:298:CYS:CB	2:H:343:THR:HG22	2.44	0.47
2:H:587:LEU:HD23	2:H:679:ASP:HB3	1.96	0.47
1:A:583:ASP:C	1:A:585:SER:H	2.16	0.47
2:B:295:LEU:O	2:B:340:ILE:HA	2.14	0.47
2:B:684:VAL:HG22	2:B:713:ILE:HB	1.95	0.47
1:C:391:ARG:NH1	1:C:482:LYS:HE3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:GLU:O	1:C:587:LEU:C	2.51	0.47
1:C:804:THR:O	1:C:805:LEU:C	2.53	0.47
1:C:755:SER:HB3	1:C:817:ASN:O	2.13	0.47
2:D:717:LEU:C	2:D:717:LEU:HD12	2.34	0.47
2:F:201:VAL:HG13	2:F:218:ILE:HG21	1.96	0.47
2:F:426:MET:CE	2:F:466:LEU:HD22	2.44	0.47
2:F:662:GLU:H	2:F:695:GLN:NE2	2.13	0.47
2:F:706:PHE:C	2:F:708:ILE:H	2.17	0.47
1:G:808:GLU:O	1:G:809:ASN:C	2.53	0.47
1:A:518:THR:CB	1:A:519:PRO:HD2	2.44	0.47
1:A:958:HIS:ND1	1:A:959:TRP:HD1	2.12	0.47
2:B:285:GLN:OE1	2:B:326:ARG:HD2	2.14	0.47
1:C:317:LEU:N	1:C:317:LEU:HD12	2.29	0.47
1:C:696:PHE:HA	1:C:718:LEU:HD22	1.96	0.47
2:D:347:ILE:HB	2:D:363:ALA:CB	2.45	0.47
2:D:935:ARG:HH12	4:D:4:FDP:P1	2.38	0.47
1:E:685:ASP:O	1:E:714:ILE:HB	2.14	0.47
2:F:202:MET:HE3	2:F:295:LEU:HD21	1.97	0.47
2:H:418:THR:HA	2:H:421:GLU:CB	2.40	0.47
1:A:211:MET:HG3	1:A:244:GLY:HA2	1.96	0.47
1:A:667:VAL:HG11	1:A:697:ARG:HD3	1.97	0.47
2:B:327:ILE:CA	2:B:331:GLN:NE2	2.78	0.47
2:B:940:ILE:HD12	2:B:943:GLN:NE2	2.29	0.47
1:C:322:TRP:O	1:C:326:VAL:HG23	2.15	0.47
2:D:481:HIS:O	2:D:482:VAL:C	2.52	0.47
1:E:732:TYR:CE1	1:E:736:VAL:HB	2.50	0.47
2:F:718:SER:HB3	2:F:762:GLY:HA2	1.97	0.47
2:H:285:GLN:OE1	2:H:326:ARG:HD2	2.15	0.47
2:H:420:SER:O	2:H:423:GLN:HG2	2.15	0.47
2:H:591:ILE:HB	2:H:608:MET:CE	2.44	0.47
2:H:832:LEU:HA	2:H:832:LEU:HD12	1.80	0.47
1:A:252:GLY:O	1:A:253:LYS:HB3	2.14	0.47
1:A:315:ALA:O	1:A:348:ILE:HD13	2.14	0.47
1:A:421:PRO:C	1:A:423:ARG:H	2.16	0.47
1:A:674:THR:O	1:A:677:TYR:HB3	2.15	0.47
2:B:392:ARG:HH21	3:B:980:F6P:C1	2.23	0.47
2:B:416:PRO:HD2	2:B:550:PHE:CD1	2.49	0.47
2:B:475:ARG:HG2	2:B:475:ARG:HH11	1.80	0.47
1:C:328:GLU:O	1:C:332:GLU:CG	2.59	0.47
1:C:822:LEU:CD1	1:C:822:LEU:C	2.83	0.47
2:D:327:ILE:HG13	2:D:327:ILE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:418:THR:OG1	2:D:419:SER:N	2.44	0.47
2:D:418:THR:HG21	2:D:422:TRP:HD1	1.79	0.47
1:E:622:HIS:HD2	1:E:886:GLU:OE1	1.98	0.47
2:F:431:SER:OG	2:F:470:LEU:HD11	2.14	0.47
1:G:433:GLU:O	1:G:437:VAL:HG23	2.14	0.47
1:G:746:TYR:CE1	2:H:854:VAL:HG13	2.49	0.47
2:H:428:ASP:CG	2:H:432:LYS:NZ	2.67	0.47
2:H:740:TYR:CE1	2:H:851:PRO:HB3	2.50	0.47
1:A:514:VAL:HG12	1:A:515:LEU:N	2.29	0.47
1:A:548:VAL:O	1:A:552:ILE:HG12	2.15	0.47
1:C:391:ARG:HG2	1:C:480:ASP:HB3	1.96	0.47
1:C:581:LYS:C	1:C:583:ASP:H	2.18	0.47
1:E:439:GLN:OE1	1:E:439:GLN:HA	2.15	0.47
1:E:586:GLU:CG	1:E:587:LEU:N	2.78	0.47
1:E:746:TYR:CE2	1:E:857:PRO:HG3	2.50	0.47
2:F:657:ASN:OD1	2:F:659:VAL:HG23	2.15	0.47
2:F:365:ASP:HA	2:F:862:PRO:HG2	1.97	0.47
1:G:391:ARG:O	1:G:448:ASN:HA	2.15	0.47
1:G:972:ARG:HH11	1:G:972:ARG:HG3	1.80	0.47
2:H:264:THR:HG22	2:H:266:ILE:N	2.27	0.47
2:H:288:ILE:HA	2:H:335:MET:HE1	1.96	0.47
1:A:336:THR:HG23	1:A:339:GLU:OE1	2.15	0.47
1:A:758:ARG:NH1	2:B:655:GLY:HA3	2.30	0.47
1:C:212:THR:CG2	1:C:274:ILE:HG13	2.44	0.47
2:D:324:THR:O	2:D:325:ASN:HB2	2.15	0.47
2:F:327:ILE:HB	2:F:331:GLN:NE2	2.30	0.47
2:F:593:ASN:HA	2:F:684:VAL:O	2.14	0.47
1:G:812:HIS:CD2	1:G:812:HIS:N	2.82	0.47
2:H:344:VAL:HG22	2:H:357:THR:HG22	1.97	0.47
2:H:647:GLN:HE22	2:H:869:THR:HG22	1.79	0.47
2:B:946:ARG:HG3	2:B:946:ARG:NH2	2.26	0.47
1:C:416:ASP:OD2	1:C:449:ASN:HA	2.15	0.47
2:B:827:LEU:HD21	1:C:837:LEU:HD11	1.96	0.47
2:F:518:LEU:HD23	2:F:518:LEU:O	2.15	0.47
2:F:680:GLY:HA3	2:F:879:ILE:HD12	1.97	0.47
2:F:770:THR:OG1	2:F:946:ARG:CD	2.63	0.47
1:A:418:ILE:HG12	1:A:575:PHE:CE2	2.49	0.47
2:B:706:PHE:C	2:B:708:ILE:H	2.18	0.47
2:D:304:LEU:O	2:D:307:ALA:HB3	2.14	0.47
2:D:421:GLU:O	2:D:425:GLN:HB2	2.15	0.47
2:D:453:ASP:OD2	2:D:455:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:522:ASN:ND2	2:D:529:LYS:HE3	2.30	0.47
2:D:662:GLU:H	2:D:695:GLN:NE2	2.13	0.47
1:E:398:MET:HB3	3:E:988:F6P:O3	2.15	0.47
2:F:416:PRO:HG2	2:F:550:PHE:CZ	2.50	0.47
2:F:631:ARG:O	2:F:632:HIS:ND1	2.48	0.47
1:G:315:ALA:O	1:G:348:ILE:CD1	2.63	0.47
1:G:949:VAL:O	1:G:950:GLU:C	2.52	0.47
2:H:867:ARG:O	2:H:871:MET:HG2	2.15	0.47
2:H:946:ARG:HH21	2:H:946:ARG:CG	2.21	0.47
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.72	0.46
1:A:588:LEU:O	1:A:589:PRO:O	2.32	0.46
1:C:697:ARG:O	1:C:701:GLN:HG3	2.15	0.46
2:D:690:PHE:HA	2:D:712:LEU:HD22	1.97	0.46
1:E:821:LYS:NZ	1:E:821:LYS:HB2	2.17	0.46
1:E:803:ILE:HD13	1:E:845:ALA:CB	2.45	0.46
1:G:630:MET:SD	1:G:643:LYS:HD3	2.55	0.46
1:G:773:TYR:HA	1:G:959:TRP:CE3	2.50	0.46
2:H:623:TYR:HB2	2:H:634:SER:HB2	1.97	0.46
1:A:952:ARG:HH11	1:A:952:ARG:HG3	1.81	0.46
1:A:773:TYR:N	1:A:959:TRP:CH2	2.83	0.46
1:C:216:ASP:HA	1:C:220:MET:SD	2.56	0.46
1:C:514:VAL:O	1:C:517:PHE:HB2	2.15	0.46
2:D:416:PRO:HB2	2:D:452:ALA:HA	1.98	0.46
2:D:701:GLU:HB2	2:D:897:ASN:ND2	2.30	0.46
1:E:676:ALA:HB2	1:E:712:PHE:CZ	2.50	0.46
1:E:754:ALA:HB2	1:E:762:PHE:CE1	2.50	0.46
2:F:632:HIS:O	2:F:633:GLU:C	2.54	0.46
2:F:825:LYS:N	1:G:844:GLU:OE2	2.48	0.46
2:F:935:ARG:O	2:F:936:MET:HB3	2.15	0.46
1:A:832:VAL:HG12	1:A:833:TYR:N	2.30	0.46
1:A:951:LEU:H	1:A:951:LEU:HD23	1.80	0.46
2:B:889:ALA:C	2:B:891:ALA:N	2.64	0.46
1:C:486:LEU:O	1:C:489:VAL:HG22	2.15	0.46
1:C:640:GLY:HA3	1:C:678:TYR:CE2	2.50	0.46
2:D:417:ALA:O	2:D:418:THR:HB	2.14	0.46
2:D:420:SER:O	2:D:423:GLN:HG2	2.16	0.46
2:D:560:GLU:OE1	2:D:870:ARG:NH1	2.48	0.46
2:D:711:VAL:CG2	2:D:910:VAL:HG22	2.44	0.46
1:E:586:GLU:CD	1:E:587:LEU:H	2.17	0.46
1:E:596:ILE:CD1	1:E:885:ILE:HG21	2.46	0.46
1:G:650:VAL:HG23	1:G:653:TRP:CE3	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:293:ASP:HB3	2:H:335:MET:HE3	1.97	0.46
2:H:341:CYS:HB2	2:H:507:VAL:CG1	2.45	0.46
2:H:347:ILE:HB	2:H:363:ALA:CB	2.45	0.46
2:H:587:LEU:HD21	2:H:883:GLN:HG3	1.98	0.46
1:A:294:ASN:O	1:A:297:SER:HB3	2.14	0.46
2:B:587:LEU:N	2:B:617:HIS:HD1	2.09	0.46
2:B:623:TYR:HB2	2:B:634:SER:HB2	1.98	0.46
1:C:716:MET:O	1:C:924:ALA:HA	2.15	0.46
2:D:400:LEU:CD1	2:D:866:THR:HG21	2.45	0.46
1:E:212:THR:CG2	1:E:212:THR:O	2.62	0.46
1:E:856:ILE:O	1:E:857:PRO:C	2.53	0.46
1:E:976:ARG:O	1:E:979:VAL:N	2.47	0.46
2:F:244:PRO:O	2:F:245:GLU:CB	2.60	0.46
2:F:432:LYS:HE2	2:F:577:ASN:ND2	2.30	0.46
1:G:216:ASP:H	2:H:381:HIS:CE1	2.33	0.46
2:H:325:ASN:C	2:H:327:ILE:H	2.17	0.46
2:B:420:SER:C	2:B:423:GLN:HE21	2.19	0.46
1:C:703:ARG:O	1:C:703:ARG:HD2	2.15	0.46
2:D:740:TYR:CE1	2:D:851:PRO:HB3	2.50	0.46
1:E:611:ALA:HB2	1:E:874:ALA:HB1	1.96	0.46
2:F:523:GLU:O	2:F:524:ASN:C	2.53	0.46
1:G:585:SER:O	1:G:586:GLU:O	2.32	0.46
1:G:584:GLY:O	1:G:588:LEU:HB2	2.16	0.46
1:G:766:VAL:HG11	1:G:774:ILE:HG22	1.98	0.46
2:H:662:GLU:HG3	2:H:695:GLN:NE2	2.31	0.46
2:B:420:SER:O	2:B:423:GLN:HG2	2.16	0.46
2:B:591:ILE:HD13	2:B:682:ILE:O	2.16	0.46
2:B:740:TYR:CD1	2:B:851:PRO:HB3	2.51	0.46
2:B:876:VAL:HG12	2:B:880:LYS:HE3	1.97	0.46
1:E:323:PRO:O	1:E:326:VAL:HB	2.16	0.46
1:A:864:GLY:HA3	2:B:743:VAL:HG22	1.96	0.46
2:B:583:LYS:O	2:B:585:LYS:HB2	2.15	0.46
1:C:526:ILE:HD13	1:C:535:ARG:HG2	1.98	0.46
2:F:626:TRP:CE2	2:F:661:PRO:HG3	2.50	0.46
2:F:679:ASP:O	2:F:708:ILE:HB	2.15	0.46
1:A:506:GLN:HG2	1:A:526:ILE:HG22	1.98	0.46
2:B:911:GLY:O	2:B:917:VAL:HA	2.16	0.46
2:D:552:ARG:O	2:D:552:ARG:HD3	2.15	0.46
2:D:704:PRO:CA	2:D:707:ARG:NH1	2.79	0.46
1:E:853:ARG:HG2	1:E:853:ARG:HH11	1.80	0.46
2:F:577:ASN:CA	2:F:579:PRO:HD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:547:SER:O	1:G:550:THR:HB	2.15	0.46
1:G:759:ARG:HA	1:G:810:PHE:CE2	2.50	0.46
2:H:581:LEU:HB2	2:H:615:GLN:NE2	2.31	0.46
2:H:717:LEU:HG	4:H:8:FDP:O3	2.16	0.46
1:A:289:ARG:CA	1:A:325:LEU:HD13	2.46	0.46
1:A:589:PRO:O	1:A:590:VAL:O	2.34	0.46
1:A:650:VAL:HG13	1:A:650:VAL:O	2.16	0.46
2:B:704:PRO:CA	2:B:707:ARG:NH1	2.79	0.46
1:C:514:VAL:HG12	1:C:515:LEU:N	2.31	0.46
1:C:883:LYS:O	1:C:887:GLN:HG3	2.16	0.46
2:D:706:PHE:C	2:D:708:ILE:H	2.19	0.46
1:E:331:ALA:O	1:E:333:GLY:N	2.49	0.46
1:E:613:ARG:HA	1:E:650:VAL:CG2	2.46	0.46
2:F:314:TRP:HB3	2:F:315:PRO:HD3	1.98	0.46
2:F:547:ALA:O	2:F:549:ASP:N	2.49	0.46
2:F:416:PRO:HD2	2:F:550:PHE:CD1	2.50	0.46
1:G:230:THR:OG1	1:G:508:VAL:HG22	2.16	0.46
1:G:601:VAL:O	1:G:691:GLY:HA3	2.16	0.46
1:G:960:ALA:C	1:G:962:TYR:N	2.66	0.46
1:A:717:CYS:HA	1:A:925:ALA:O	2.16	0.46
1:A:765:GLU:HA	1:A:825:ARG:O	2.16	0.46
2:B:200:ALA:HA	2:B:230:PHE:O	2.15	0.46
2:F:947:LEU:HD22	2:F:951:HIS:NE2	2.30	0.46
1:G:366:ILE:HD13	1:G:503:ALA:CB	2.46	0.46
2:H:755:ALA:HA	2:H:815:LYS:O	2.15	0.46
2:H:256:ARG:CZ	2:H:813:PHE:CE1	2.98	0.46
1:A:525:LEU:HD23	1:A:525:LEU:C	2.36	0.45
1:A:526:ILE:HD13	1:A:535:ARG:HG2	1.98	0.45
1:A:655:ASN:O	1:A:865:VAL:HG22	2.16	0.45
2:B:341:CYS:SG	2:B:519:ILE:CD1	3.04	0.45
1:C:207:LYS:HB3	1:C:300:ILE:HG12	1.98	0.45
1:E:773:TYR:HA	1:E:959:TRP:CD2	2.50	0.45
2:F:420:SER:HA	2:F:423:GLN:NE2	2.30	0.45
2:F:832:LEU:HA	2:F:832:LEU:HD12	1.78	0.45
2:H:200:ALA:HB2	2:H:230:PHE:HB2	1.98	0.45
2:H:288:ILE:HG12	2:H:335:MET:HE2	1.98	0.45
2:H:796:ASP:O	2:H:800:LEU:HB2	2.15	0.45
2:H:892:ALA:C	2:H:894:GLU:N	2.70	0.45
2:B:414:GLU:N	2:B:414:GLU:OE2	2.45	0.45
2:B:420:SER:CA	2:B:423:GLN:NE2	2.80	0.45
2:B:615:GLN:HB2	2:B:617:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:701:GLU:O	2:B:701:GLU:OE2	2.34	0.45
1:C:466:THR:CG2	1:C:467:ALA:N	2.79	0.45
1:C:732:TYR:CE1	1:C:736:VAL:HB	2.51	0.45
2:D:511:THR:OG1	2:D:514:THR:HG23	2.15	0.45
2:D:547:ALA:O	2:D:549:ASP:N	2.49	0.45
1:E:315:ALA:O	1:E:348:ILE:CD1	2.64	0.45
1:E:488:HIS:C	1:E:490:GLN:N	2.67	0.45
1:E:696:PHE:HA	1:E:718:LEU:HD22	1.98	0.45
1:E:710:PRO:HA	1:E:713:ASN:ND2	2.31	0.45
2:F:607:SER:OG	2:F:869:THR:CB	2.52	0.45
2:H:420:SER:HA	2:H:423:GLN:NE2	2.30	0.45
2:H:581:LEU:CB	2:H:582:PRO:HD3	2.42	0.45
1:A:255:LEU:C	1:A:255:LEU:HD23	2.36	0.45
1:A:291:ALA:O	1:A:292:ALA:C	2.54	0.45
1:A:356:ASP:OD2	3:A:988:F6P:C1	2.56	0.45
1:A:486:LEU:O	1:A:489:VAL:HG22	2.16	0.45
1:A:613:ARG:NH1	1:A:613:ARG:HG2	2.31	0.45
1:C:496:VAL:O	1:C:500:ARG:HG3	2.16	0.45
1:C:519:PRO:HG2	1:C:520:GLU:H	1.79	0.45
1:C:952:ARG:HH11	1:C:952:ARG:HG3	1.78	0.45
1:C:809:ASN:N	1:C:975:LEU:HD22	2.31	0.45
2:D:587:LEU:N	2:D:617:HIS:HD1	2.07	0.45
1:E:613:ARG:NH1	1:E:613:ARG:HG2	2.30	0.45
1:G:746:TYR:CE2	1:G:857:PRO:HG3	2.51	0.45
2:H:414:GLU:HB3	2:H:554:MET:HE2	1.98	0.45
2:H:883:GLN:O	2:H:887:ALA:CB	2.64	0.45
2:H:348:ASP:CG	3:H:986:F6P:H11	2.36	0.45
1:A:747:THR:O	1:A:751:LYS:HB2	2.17	0.45
2:B:298:CYS:SG	2:B:343:THR:CG2	3.04	0.45
2:B:424:ASP:OD1	2:B:469:ARG:NH2	2.49	0.45
2:B:354:THR:HB	2:B:520:ALA:HB1	1.98	0.45
1:C:759:ARG:HD2	1:C:849:LYS:O	2.17	0.45
2:D:382:SER:HA	2:D:439:ARG:O	2.17	0.45
2:D:693:LEU:CD2	2:D:922:ILE:HB	2.46	0.45
1:E:922:ASP:HA	1:E:938:PRO:HG3	1.97	0.45
2:F:717:LEU:HB2	2:F:733:ALA:CB	2.45	0.45
2:H:633:GLU:O	2:H:633:GLU:HG2	2.16	0.45
1:A:804:THR:O	1:A:805:LEU:C	2.55	0.45
1:A:813:ASP:O	1:A:815:GLY:N	2.46	0.45
2:B:220:ARG:HD2	2:B:252:TRP:CZ2	2.51	0.45
2:B:418:THR:O	2:B:419:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:418:THR:OG1	2:B:419:SER:N	2.49	0.45
2:B:523:GLU:O	2:B:524:ASN:C	2.55	0.45
2:B:770:THR:HG23	2:B:946:ARG:HD2	1.97	0.45
1:C:809:ASN:HB2	1:C:975:LEU:HD21	1.99	0.45
2:D:781:SER:HA	2:D:818:LEU:O	2.16	0.45
1:E:796:LEU:HD21	2:H:835:VAL:HG11	1.98	0.45
2:F:264:THR:HG22	2:F:266:ILE:N	2.29	0.45
2:F:484:ARG:HG3	2:F:484:ARG:NH1	2.31	0.45
2:F:633:GLU:HB2	2:F:672:TYR:OH	2.16	0.45
2:F:684:VAL:HG22	2:F:713:ILE:HB	1.99	0.45
1:G:466:THR:HB	1:G:469:ASP:CG	2.36	0.45
2:H:323:LYS:O	2:H:324:THR:CB	2.63	0.45
2:H:522:ASN:ND2	2:H:529:LYS:HE3	2.32	0.45
2:H:698:ARG:HD2	2:H:698:ARG:O	2.16	0.45
1:A:322:TRP:CZ3	1:A:343:TYR:O	2.70	0.45
1:A:451:ILE:HD12	1:A:451:ILE:N	2.32	0.45
1:A:716:MET:O	1:A:924:ALA:HA	2.17	0.45
1:C:856:ILE:O	1:C:857:PRO:C	2.53	0.45
2:D:578:GLU:C	2:D:580:LYS:N	2.69	0.45
1:E:289:ARG:CA	1:E:325:LEU:HD13	2.46	0.45
1:G:221:ASN:ND2	1:G:270:GLY:O	2.49	0.45
2:H:518:LEU:C	2:H:518:LEU:HD23	2.36	0.45
1:E:832:VAL:CG2	2:H:834:GLU:HB3	2.45	0.45
1:A:766:VAL:CG1	1:A:774:ILE:HG22	2.47	0.45
2:B:347:ILE:HB	2:B:363:ALA:HB2	1.98	0.45
2:B:416:PRO:O	2:B:417:ALA:C	2.54	0.45
1:C:334:ARG:HG3	1:C:335:PHE:CE1	2.51	0.45
1:E:439:GLN:NE2	1:E:477:LEU:HD11	2.32	0.45
1:E:832:VAL:HG12	1:E:833:TYR:N	2.32	0.45
2:F:484:ARG:HG3	2:F:484:ARG:HH11	1.82	0.45
1:G:209:ALA:O	1:G:303:LEU:HD12	2.16	0.45
1:G:435:LYS:HD3	1:G:477:LEU:HB2	1.99	0.45
2:H:499:GLN:HG2	2:H:526:ILE:HD12	1.99	0.45
2:H:761:GLN:HG3	2:H:855:GLN:NE2	2.30	0.45
2:B:422:TRP:CZ3	2:B:465:VAL:HG21	2.51	0.45
2:B:662:GLU:H	2:B:695:GLN:NE2	2.14	0.45
1:C:400:ARG:NH1	1:C:400:ARG:HG2	2.30	0.45
1:C:584:GLY:O	1:C:585:SER:O	2.35	0.45
2:D:426:MET:CE	2:D:466:LEU:HD22	2.46	0.45
2:D:900:ASP:O	2:D:901:LYS:C	2.56	0.45
2:D:946:ARG:HG3	2:D:946:ARG:NH2	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:440:ARG:HH11	1:E:440:ARG:HB2	1.81	0.45
1:E:505:LEU:HB2	1:E:533:ILE:HD11	1.97	0.45
1:E:236:CYS:SG	1:E:515:LEU:HD21	2.57	0.45
2:F:354:THR:CB	2:F:520:ALA:HB1	2.47	0.45
2:F:900:ASP:O	2:F:901:LYS:C	2.54	0.45
2:F:931:GLU:O	2:F:931:GLU:HG3	2.16	0.45
2:F:771:TYR:OH	2:F:945:THR:HG21	2.17	0.45
1:G:586:GLU:CD	1:G:587:LEU:H	2.20	0.45
2:F:791:GLU:HG3	1:G:800:ARG:NH2	2.31	0.45
2:H:281:LEU:HD12	2:H:317:LEU:HD22	1.99	0.45
2:H:462:VAL:O	2:H:466:LEU:HD23	2.17	0.45
2:H:684:VAL:HG22	2:H:713:ILE:HB	1.98	0.45
1:A:557:PHE:O	1:A:560:ALA:HB3	2.17	0.45
1:A:589:PRO:HD2	1:A:622:HIS:HB3	1.99	0.45
1:A:761:VAL:HA	1:A:821:LYS:O	2.16	0.45
2:B:463:HIS:CD2	2:B:474:THR:HG22	2.49	0.45
2:B:518:LEU:HD23	2:B:518:LEU:O	2.16	0.45
2:B:609:ALA:O	2:B:612:CYS:HB2	2.16	0.45
1:C:211:MET:CE	1:C:305:VAL:HG22	2.47	0.45
2:D:900:ASP:O	2:D:903:ILE:HG13	2.17	0.45
1:E:448:ASN:H	1:E:448:ASN:ND2	2.15	0.45
2:F:744:VAL:O	2:F:747:SER:HB3	2.17	0.45
1:G:249:LEU:HD13	1:G:290:GLN:HG2	1.98	0.45
1:G:927:ILE:O	1:G:927:ILE:HG23	2.17	0.45
2:H:511:THR:OG1	2:H:514:THR:HG23	2.16	0.45
2:H:755:ALA:O	2:H:846:ALA:HA	2.16	0.45
1:A:407:LEU:HD11	1:A:572:TYR:HA	1.97	0.45
1:A:942:LEU:C	1:A:944:GLU:H	2.19	0.45
2:B:590:ALA:HA	2:B:620:TYR:O	2.17	0.45
2:B:717:LEU:HB2	2:B:733:ALA:HB2	1.98	0.45
1:C:248:LEU:HG	1:C:291:ALA:HB1	1.98	0.45
1:C:485:ILE:N	1:C:485:ILE:HD12	2.32	0.45
2:D:312:SER:O	2:D:315:PRO:HD2	2.17	0.45
2:D:892:ALA:CB	2:D:894:GLU:HG2	2.43	0.45
1:E:255:LEU:HD23	1:E:256:LYS:N	2.32	0.45
2:F:595:GLY:O	2:F:656:THR:OG1	2.30	0.45
2:F:887:ALA:C	2:F:889:ALA:H	2.21	0.45
1:G:323:PRO:O	1:G:326:VAL:HB	2.17	0.45
2:H:578:GLU:C	2:H:580:LYS:N	2.67	0.45
1:A:960:ALA:O	1:A:961:GLU:C	2.56	0.44
1:C:451:ILE:N	1:C:451:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:514:VAL:HG12	1:G:515:LEU:N	2.33	0.44
1:G:960:ALA:O	1:G:962:TYR:N	2.50	0.44
2:H:679:ASP:HB3	2:H:883:GLN:HE22	1.81	0.44
2:H:726:TYR:CE1	2:H:730:SER:HB3	2.52	0.44
2:H:831:LYS:HA	2:H:831:LYS:HD3	1.60	0.44
1:A:215:GLY:HA2	2:B:381:HIS:HE2	1.82	0.44
1:C:385:THR:HA	2:D:207:ASP:OD2	2.17	0.44
1:E:230:THR:OG1	1:E:508:VAL:HG22	2.16	0.44
2:F:830:THR:HA	2:F:848:PRO:HB3	1.99	0.44
1:E:796:LEU:CD1	2:H:793:LEU:HD13	2.43	0.44
1:A:442:ARG:NH1	1:A:449:ASN:OD1	2.39	0.44
1:A:264:ARG:HD2	1:A:819:ASN:HD22	1.81	0.44
2:B:537:LEU:O	2:B:540:ALA:HB3	2.18	0.44
1:C:594:LEU:CD2	1:C:889:ASN:ND2	2.78	0.44
2:D:196:GLN:CD	2:D:228:ARG:HG2	2.36	0.44
2:D:717:LEU:HB2	2:D:733:ALA:HB2	1.98	0.44
2:F:711:VAL:CG2	2:F:910:VAL:HG22	2.47	0.44
1:G:249:LEU:HD12	1:G:249:LEU:C	2.37	0.44
1:G:421:PRO:C	1:G:423:ARG:N	2.71	0.44
1:G:585:SER:O	1:G:586:GLU:C	2.53	0.44
1:G:780:LEU:C	1:G:780:LEU:HD13	2.37	0.44
1:G:960:ALA:C	1:G:962:TYR:H	2.20	0.44
1:G:963:ASN:N	1:G:963:ASN:HD22	2.12	0.44
1:A:794:ILE:O	1:A:794:ILE:HG22	2.17	0.44
2:B:239:LEU:HD22	2:B:287:LEU:HD22	1.99	0.44
2:D:327:ILE:HB	2:D:331:GLN:HE21	1.83	0.44
2:D:918:VAL:HG12	2:D:919:TYR:H	1.83	0.44
1:E:255:LEU:C	1:E:255:LEU:HD23	2.37	0.44
1:E:650:VAL:O	1:E:650:VAL:HG13	2.16	0.44
1:E:697:ARG:O	1:E:701:GLN:HG3	2.18	0.44
2:F:697:GLU:HA	2:F:700:ARG:HD3	1.99	0.44
1:G:421:PRO:HG2	1:G:422:GLU:OE2	2.17	0.44
1:G:946:GLU:O	1:G:955:PHE:CZ	2.71	0.44
1:G:947:THR:O	1:G:950:GLU:N	2.50	0.44
1:A:746:TYR:CD1	2:B:854:VAL:CG1	3.00	0.44
1:A:746:TYR:CE1	2:B:854:VAL:HG13	2.52	0.44
2:B:591:ILE:HB	2:B:608:MET:CE	2.46	0.44
2:B:867:ARG:O	2:B:871:MET:HG2	2.17	0.44
2:B:886:ILE:O	2:B:890:ARG:CB	2.59	0.44
1:C:554:ASN:O	1:C:556:ASP:N	2.50	0.44
1:C:746:TYR:CE2	1:C:857:PRO:HG3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:648:SER:HA	2:D:865:ARG:HD3	1.98	0.44
2:D:589:ILE:CD1	2:D:879:ILE:HG21	2.46	0.44
1:E:301:ASP:OD1	1:E:301:ASP:N	2.51	0.44
1:E:416:ASP:OD2	1:E:449:ASN:HA	2.16	0.44
1:E:739:CYS:SG	1:E:861:GLN:HB3	2.57	0.44
2:F:522:ASN:ND2	2:F:529:LYS:HE3	2.32	0.44
2:F:690:PHE:HA	2:F:712:LEU:HD22	1.99	0.44
2:H:348:ASP:OD1	2:H:391:GLY:HA2	2.17	0.44
1:A:423:ARG:O	1:A:424:ALA:C	2.56	0.44
2:B:481:HIS:C	2:B:483:GLN:N	2.68	0.44
1:C:291:ALA:HA	1:C:294:ASN:ND2	2.33	0.44
1:C:423:ARG:O	1:C:424:ALA:C	2.56	0.44
1:C:418:ILE:HG12	1:C:575:PHE:CE2	2.53	0.44
2:D:541:VAL:HG22	2:D:556:LEU:HB2	1.99	0.44
1:E:210:VAL:HG23	1:E:210:VAL:O	2.17	0.44
2:F:578:GLU:C	2:F:580:LYS:N	2.70	0.44
2:F:591:ILE:HB	2:F:608:MET:CE	2.48	0.44
2:F:755:ALA:HA	2:F:815:LYS:O	2.16	0.44
1:G:809:ASN:C	1:G:809:ASN:OD1	2.55	0.44
2:H:453:ASP:OD2	2:H:455:THR:HG23	2.18	0.44
2:H:574:ALA:CB	2:H:610:THR:HB	2.47	0.44
2:H:608:MET:C	2:H:608:MET:SD	2.95	0.44
1:A:589:PRO:O	1:A:593:ARG:NH1	2.50	0.44
2:B:416:PRO:HG2	2:B:550:PHE:CZ	2.53	0.44
2:B:935:ARG:O	2:B:936:MET:HB3	2.18	0.44
1:C:572:TYR:CE2	1:C:576:LEU:HD11	2.53	0.44
1:C:690:LEU:HD23	1:C:719:ILE:HB	2.00	0.44
1:C:927:ILE:O	1:C:927:ILE:HG23	2.18	0.44
2:D:501:LEU:HD12	2:D:501:LEU:O	2.18	0.44
1:E:578:THR:HG23	1:E:578:THR:O	2.16	0.44
1:E:785:VAL:O	1:E:785:VAL:CG2	2.65	0.44
2:F:354:THR:HB	2:F:520:ALA:HB1	2.00	0.44
2:F:883:GLN:O	2:F:887:ALA:CB	2.66	0.44
1:G:255:LEU:HD23	1:G:255:LEU:C	2.38	0.44
2:H:771:TYR:OH	2:H:945:THR:HG21	2.17	0.44
1:A:767:GLN:HB3	4:A:1:FDP:O1	2.18	0.44
2:B:344:VAL:HG22	2:B:357:THR:HG22	1.99	0.44
2:B:692:SER:O	2:B:693:LEU:C	2.56	0.44
1:C:249:LEU:C	1:C:249:LEU:HD12	2.37	0.44
1:C:547:SER:O	1:C:550:THR:HB	2.18	0.44
1:C:596:ILE:CD1	1:C:885:ILE:HG21	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:389:VAL:O	2:D:447:GLU:HB3	2.18	0.44
1:E:485:ILE:CD1	1:E:485:ILE:N	2.80	0.44
2:F:349:ASN:OD1	2:F:356:ALA:HA	2.17	0.44
2:F:554:MET:CG	2:F:562:ILE:HG12	2.39	0.44
1:G:212:THR:O	1:G:212:THR:CG2	2.63	0.44
2:H:327:ILE:HB	2:H:331:GLN:NE2	2.33	0.44
2:H:349:ASN:OD1	2:H:356:ALA:HA	2.17	0.44
2:H:717:LEU:HD23	2:H:856:GLN:HG2	1.99	0.44
2:B:561:PHE:CD2	2:B:561:PHE:C	2.91	0.44
1:C:405:LEU:HA	1:C:405:LEU:HD12	1.88	0.44
1:C:823:LEU:HD12	1:C:823:LEU:N	2.33	0.44
2:F:238:GLY:O	2:F:241:ARG:O	2.35	0.44
2:F:740:TYR:CD1	2:F:851:PRO:HB3	2.52	0.44
1:G:366:ILE:HD13	1:G:503:ALA:HB2	1.99	0.44
2:H:414:GLU:N	2:H:414:GLU:OE2	2.51	0.44
1:A:247:GLY:HA2	1:A:254:TYR:CD2	2.53	0.43
1:A:423:ARG:CD	1:A:561:ILE:HD12	2.48	0.43
2:B:298:CYS:CB	2:B:343:THR:HG22	2.48	0.43
2:B:900:ASP:CG	2:B:903:ILE:HG13	2.38	0.43
1:C:211:MET:HE3	1:C:305:VAL:HG22	2.00	0.43
1:C:587:LEU:CB	1:C:622:HIS:CE1	2.99	0.43
1:C:724:SER:OG	4:C:3:FDP:H12	2.18	0.43
2:D:892:ALA:HB3	2:D:894:GLU:CG	2.46	0.43
1:E:339:GLU:C	1:E:341:ALA:H	2.21	0.43
1:E:374:ARG:HG2	1:E:489:VAL:O	2.17	0.43
1:E:837:LEU:HD13	2:H:831:LYS:HG3	1.98	0.43
1:G:426:PRO:O	1:G:428:GLY:N	2.51	0.43
1:G:679:PHE:HE2	1:G:687:LEU:HD22	1.82	0.43
1:G:685:ASP:O	1:G:715:PRO:HD2	2.17	0.43
2:H:416:PRO:HB2	2:H:452:ALA:HA	2.00	0.43
2:B:438:LYS:HG2	2:B:440:THR:O	2.17	0.43
2:B:567:ASN:O	2:B:571:ILE:HG12	2.17	0.43
2:B:711:VAL:HG22	2:B:910:VAL:CG2	2.48	0.43
1:C:330:VAL:HG22	1:C:340:VAL:HG11	1.99	0.43
1:C:382:ILE:O	1:C:385:THR:HG22	2.17	0.43
1:C:961:GLU:O	1:C:962:TYR:C	2.57	0.43
2:D:494:ILE:HD13	2:D:771:TYR:HD2	1.83	0.43
1:E:947:THR:HG22	1:E:953:LYS:O	2.18	0.43
2:F:608:MET:SD	2:F:608:MET:C	2.97	0.43
2:F:692:SER:O	2:F:693:LEU:C	2.56	0.43
4:F:6:FDP:O2P	4:F:6:FDP:O5	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:398:MET:HG3	1:G:490:GLN:NE2	2.34	0.43
2:H:239:LEU:O	2:H:286:HIS:CD2	2.67	0.43
2:H:701:GLU:O	2:H:701:GLU:OE2	2.36	0.43
2:H:704:PRO:CA	2:H:707:ARG:NH1	2.81	0.43
1:E:800:ARG:HH22	2:H:791:GLU:HG3	1.81	0.43
2:H:946:ARG:CG	2:H:946:ARG:NH2	2.80	0.43
1:C:315:ALA:O	1:C:348:ILE:CD1	2.67	0.43
1:C:680:GLN:HB3	1:G:680:GLN:HE22	1.82	0.43
1:C:757:THR:HG23	2:D:597:PRO:HD3	2.01	0.43
2:F:580:LYS:O	2:F:581:LEU:C	2.55	0.43
2:F:661:PRO:HD2	2:F:695:GLN:NE2	2.33	0.43
2:F:894:GLU:O	2:F:896:PHE:N	2.50	0.43
1:G:246:GLU:HA	1:G:279:SER:HB2	2.00	0.43
1:G:591:SER:HA	1:G:593:ARG:HG3	2.00	0.43
1:G:665:ARG:HG2	1:G:665:ARG:HH11	1.83	0.43
1:G:806:LEU:O	1:G:807:LYS:C	2.56	0.43
1:G:813:ASP:O	1:G:815:GLY:N	2.46	0.43
2:H:313:GLU:O	2:H:317:LEU:HG	2.18	0.43
2:H:327:ILE:CA	2:H:331:GLN:NE2	2.81	0.43
2:H:428:ASP:OD2	2:H:432:LYS:NZ	2.51	0.43
1:A:405:LEU:HD12	1:A:405:LEU:HA	1.83	0.43
1:A:606:ALA:O	1:A:866:PRO:HB3	2.19	0.43
1:A:944:GLU:HA	1:A:946:GLU:OE1	2.18	0.43
1:A:731:GLU:HG2	1:A:958:HIS:CD2	2.53	0.43
1:A:979:VAL:O	1:A:980:ALA:HB2	2.18	0.43
2:B:740:TYR:CZ	2:B:851:PRO:HB3	2.53	0.43
2:B:763:GLY:O	2:B:822:ASN:HB2	2.19	0.43
2:B:587:LEU:CD2	2:B:883:GLN:NE2	2.81	0.43
1:C:421:PRO:HG2	1:C:422:GLU:OE2	2.19	0.43
2:D:201:VAL:HA	2:D:296:ILE:O	2.18	0.43
2:D:418:THR:HG23	2:D:451:ALA:HB1	2.00	0.43
2:D:418:THR:O	2:D:419:SER:HB2	2.19	0.43
1:E:246:GLU:O	1:E:249:LEU:HB3	2.18	0.43
1:E:421:PRO:C	1:E:423:ARG:H	2.20	0.43
1:E:433:GLU:O	1:E:437:VAL:HG23	2.18	0.43
1:E:589:PRO:O	1:E:590:VAL:O	2.35	0.43
1:E:703:ARG:HD2	1:E:703:ARG:O	2.18	0.43
2:F:201:VAL:CG1	2:F:218:ILE:HG21	2.48	0.43
2:F:239:LEU:HA	2:F:239:LEU:HD23	1.84	0.43
2:F:792:GLN:HE22	2:F:957:ARG:CB	2.31	0.43
1:G:271:GLY:HA3	2:H:380:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:448:ASN:ND2	1:G:448:ASN:N	2.61	0.43
1:G:407:LEU:HD11	1:G:572:TYR:HA	2.00	0.43
2:H:344:VAL:CG2	2:H:357:THR:HG22	2.49	0.43
2:H:467:VAL:O	2:H:471:GLY:CA	2.61	0.43
2:H:723:GLY:O	2:H:911:GLY:HA3	2.18	0.43
2:H:693:LEU:CD2	2:H:922:ILE:HB	2.49	0.43
1:A:251:GLY:HA3	1:A:294:ASN:ND2	2.33	0.43
1:A:285:ARG:NH1	1:A:325:LEU:HD23	2.33	0.43
1:A:973:LEU:HA	1:A:973:LEU:HD23	1.71	0.43
2:B:236:TYR:O	2:B:239:LEU:N	2.45	0.43
2:B:264:THR:HG22	2:B:266:ILE:HG12	1.98	0.43
2:B:631:ARG:O	2:B:632:HIS:ND1	2.51	0.43
2:B:633:GLU:CG	2:B:672:TYR:CE1	3.02	0.43
2:B:633:GLU:HG3	2:B:672:TYR:CE1	2.54	0.43
2:B:723:GLY:O	2:B:911:GLY:HA3	2.17	0.43
1:C:801:GLU:OE1	1:C:976:ARG:CZ	2.67	0.43
1:C:950:GLU:HG3	1:C:951:LEU:HG	2.00	0.43
2:D:499:GLN:HG2	2:D:526:ILE:HD12	2.01	0.43
2:D:580:LYS:O	2:D:582:PRO:N	2.52	0.43
1:E:322:TRP:HB3	1:E:323:PRO:HD3	2.00	0.43
1:E:592:ASP:C	1:E:592:ASP:OD1	2.57	0.43
2:H:421:GLU:O	2:H:425:GLN:HB2	2.18	0.43
1:A:853:ARG:HG2	1:A:853:ARG:HH11	1.83	0.43
1:A:959:TRP:N	1:A:959:TRP:CD1	2.87	0.43
2:B:744:VAL:O	2:B:747:SER:HB3	2.19	0.43
2:B:947:LEU:HD22	2:B:951:HIS:CE1	2.54	0.43
1:C:625:LYS:HG2	1:C:644:GLU:OE2	2.18	0.43
2:D:295:LEU:O	2:D:340:ILE:HA	2.18	0.43
2:D:420:SER:C	2:D:423:GLN:HE21	2.22	0.43
2:D:883:GLN:O	2:D:887:ALA:CB	2.66	0.43
2:D:707:ARG:NE	2:D:897:ASN:CG	2.72	0.43
1:E:959:TRP:N	1:E:959:TRP:CD1	2.83	0.43
1:G:548:VAL:HG22	1:G:563:LEU:HD13	1.99	0.43
2:H:420:SER:C	2:H:423:GLN:HE21	2.22	0.43
2:H:552:ARG:HD3	2:H:552:ARG:O	2.17	0.43
2:H:647:GLN:HE22	2:H:869:THR:HG21	1.80	0.43
1:A:319:ARG:HB2	1:A:348:ILE:CD1	2.34	0.43
1:A:703:ARG:C	1:A:703:ARG:HD2	2.39	0.43
2:B:273:GLU:H	2:B:273:GLU:CD	2.19	0.43
2:B:580:LYS:O	2:B:581:LEU:C	2.57	0.43
2:B:639:ASN:O	2:B:640:TRP:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:VAL:HG12	1:C:979:VAL:O	2.19	0.43
2:D:341:CYS:HB2	2:D:507:VAL:CG1	2.49	0.43
2:D:519:ILE:HD12	2:D:519:ILE:N	2.33	0.43
2:D:784:PRO:HA	2:D:823:ALA:HA	1.99	0.43
1:E:755:SER:O	1:E:758:ARG:NH2	2.34	0.43
2:F:295:LEU:O	2:F:340:ILE:HA	2.18	0.43
2:F:545:ILE:HD11	2:F:553:ALA:CB	2.49	0.43
1:G:247:GLY:HA2	1:G:254:TYR:CD2	2.49	0.43
1:G:270:GLY:O	1:G:271:GLY:C	2.56	0.43
1:G:357:ASN:HA	1:G:365:THR:CG2	2.49	0.43
2:H:312:SER:O	2:H:315:PRO:HD2	2.19	0.43
2:H:632:HIS:O	2:H:633:GLU:C	2.57	0.43
2:H:918:VAL:HG12	2:H:919:TYR:H	1.83	0.43
2:B:627:SER:HB3	2:B:659:VAL:HG21	2.01	0.43
2:B:494:ILE:HG23	2:B:774:LEU:HD23	1.99	0.43
2:B:894:GLU:O	2:B:896:PHE:N	2.51	0.43
1:C:806:LEU:O	1:C:807:LYS:C	2.57	0.43
1:C:805:LEU:HA	1:C:975:LEU:HB3	2.01	0.43
1:E:585:SER:O	1:E:586:GLU:C	2.57	0.43
1:E:743:LEU:HD23	1:E:743:LEU:HA	1.81	0.43
1:E:765:GLU:HA	1:E:825:ARG:O	2.19	0.43
2:F:581:LEU:HB2	2:F:615:GLN:NE2	2.34	0.43
2:F:633:GLU:O	2:F:633:GLU:HG2	2.19	0.43
1:G:342:PRO:HG2	1:G:343:TYR:CE1	2.54	0.43
1:G:674:THR:O	1:G:677:TYR:HB3	2.18	0.43
1:G:724:SER:OG	1:G:768:GLY:HA2	2.18	0.43
2:H:575:ASP:C	2:H:575:ASP:OD1	2.56	0.43
2:B:239:LEU:HA	2:B:239:LEU:HD23	1.77	0.43
2:B:575:ASP:OD1	2:B:575:ASP:C	2.56	0.43
1:A:756:ALA:HB2	2:B:651:GLY:HA2	2.00	0.43
2:B:715:ALA:CB	2:B:728:LEU:HB2	2.49	0.43
1:A:860:VAL:CG1	2:B:740:TYR:CE1	3.02	0.43
2:B:800:LEU:HD21	2:B:817:ILE:HD11	2.01	0.43
2:B:830:THR:HA	2:B:848:PRO:HB3	2.01	0.43
1:C:611:ALA:HB2	1:C:874:ALA:HB1	2.01	0.43
2:D:231:VAL:HG13	2:D:266:ILE:HG21	1.99	0.43
2:D:202:MET:CE	2:D:295:LEU:HD21	2.49	0.43
2:D:726:TYR:OH	2:D:864:ASP:OD2	2.29	0.43
2:D:647:GLN:HE22	2:D:869:THR:HG22	1.84	0.43
1:E:391:ARG:NH2	3:F:984:F6P:O2P	2.51	0.43
1:G:526:ILE:HD13	1:G:535:ARG:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:523:GLU:O	2:H:524:ASN:C	2.56	0.43
1:A:530:GLU:HA	1:A:932:SER:HB3	2.01	0.43
2:B:238:GLY:O	2:B:241:ARG:O	2.37	0.43
2:B:278:GLU:OE1	2:B:278:GLU:CA	2.67	0.43
2:B:420:SER:CA	2:B:423:GLN:HE21	2.31	0.43
2:B:558:ASP:O	2:B:560:GLU:N	2.51	0.43
1:C:543:LYS:NZ	1:C:543:LYS:HB2	2.34	0.43
1:C:794:ILE:HD11	1:C:829:ALA:HB1	2.00	0.43
2:D:253:GLU:O	2:D:256:ARG:HB3	2.19	0.43
2:D:288:ILE:HD11	2:D:318:ILE:HG22	2.00	0.43
1:E:674:THR:O	1:E:677:TYR:HB3	2.19	0.43
2:H:314:TRP:CD2	2:H:338:LEU:HB2	2.54	0.43
2:H:353:THR:HG21	2:H:534:SER:HA	2.01	0.43
2:H:587:LEU:HB3	2:H:679:ASP:HB2	2.01	0.43
2:H:661:PRO:HD2	2:H:695:GLN:NE2	2.34	0.43
1:A:317:LEU:H	1:A:317:LEU:CD1	2.31	0.42
1:A:703:ARG:NH1	1:A:921:ASP:OD2	2.52	0.42
1:A:744:VAL:HG12	1:A:745:ASN:N	2.33	0.42
1:C:587:LEU:O	1:C:589:PRO:HD3	2.18	0.42
1:E:962:TYR:N	1:E:962:TYR:CD2	2.85	0.42
2:F:765:SER:HB2	2:F:936:MET:CE	2.48	0.42
1:G:229:ARG:HD3	1:G:260:TRP:CZ2	2.53	0.42
1:G:271:GLY:HA3	2:H:380:SER:HG	1.84	0.42
2:H:947:LEU:HD22	2:H:951:HIS:NE2	2.34	0.42
1:A:634:SER:HB3	1:A:666:SER:OG	2.18	0.42
1:A:942:LEU:O	1:A:944:GLU:N	2.45	0.42
1:A:943:TRP:HA	1:A:946:GLU:HG3	2.01	0.42
2:B:580:LYS:CD	2:B:586:ARG:NH2	2.82	0.42
2:B:947:LEU:HD22	2:B:951:HIS:NE2	2.33	0.42
1:C:569:ILE:H	1:C:569:ILE:HD12	1.84	0.42
2:D:880:LYS:HE2	2:D:880:LYS:HB3	1.76	0.42
2:D:679:ASP:HB3	2:D:883:GLN:NE2	2.34	0.42
1:E:270:GLY:O	1:E:271:GLY:O	2.37	0.42
1:E:397:VAL:O	1:E:455:GLU:HG3	2.19	0.42
2:F:665:ASP:OD1	2:F:668:MET:HG2	2.19	0.42
1:A:856:ILE:O	1:A:857:PRO:C	2.58	0.42
1:C:323:PRO:O	1:C:326:VAL:HB	2.19	0.42
1:C:655:ASN:HB3	1:C:871:ARG:NH1	2.34	0.42
2:D:607:SER:OG	2:D:869:THR:CB	2.60	0.42
2:D:892:ALA:HB1	2:D:894:GLU:OE1	2.19	0.42
1:E:246:GLU:OE1	1:E:246:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:418:THR:HA	2:F:421:GLU:HG3	2.01	0.42
1:G:339:GLU:C	1:G:341:ALA:H	2.22	0.42
1:G:663:THR:O	1:G:663:THR:HG23	2.18	0.42
1:G:877:PHE:CZ	1:G:929:VAL:HG22	2.54	0.42
2:H:355:ASP:OD1	2:H:559:THR:HG22	2.19	0.42
2:H:717:LEU:HB2	2:H:733:ALA:HB2	2.00	0.42
1:A:212:THR:O	1:A:212:THR:CG2	2.66	0.42
1:A:421:PRO:C	1:A:423:ARG:N	2.72	0.42
1:A:440:ARG:HH11	1:A:440:ARG:HB2	1.84	0.42
1:A:529:LEU:HD12	1:A:534:ILE:HD13	2.00	0.42
1:A:837:LEU:HD11	2:D:827:LEU:HD21	2.00	0.42
2:B:593:ASN:HA	2:B:684:VAL:O	2.19	0.42
2:B:880:LYS:HE2	2:B:880:LYS:HB3	1.69	0.42
2:B:931:GLU:HG3	2:B:931:GLU:O	2.19	0.42
1:C:223:ALA:O	1:C:227:VAL:HG23	2.19	0.42
1:C:261:GLU:CD	1:C:261:GLU:H	2.23	0.42
1:C:278:ARG:NH1	1:C:278:ARG:HG3	2.33	0.42
2:D:410:ILE:HA	2:D:444:VAL:O	2.20	0.42
1:E:526:ILE:HD13	1:E:535:ARG:HG2	2.02	0.42
1:E:703:ARG:HD2	1:E:703:ARG:C	2.39	0.42
1:E:865:VAL:CG1	1:E:871:ARG:HH21	2.32	0.42
2:F:314:TRP:O	2:F:315:PRO:C	2.56	0.42
1:G:421:PRO:O	1:G:423:ARG:N	2.52	0.42
1:G:534:ILE:HD11	1:G:536:MET:HE2	2.01	0.42
1:G:746:TYR:CD1	2:H:854:VAL:HG11	2.54	0.42
2:B:379:ASN:HA	2:B:440:THR:HG23	2.01	0.42
2:B:665:ASP:OD1	2:B:668:MET:HG2	2.19	0.42
1:E:833:TYR:HA	1:E:837:LEU:HD23	2.02	0.42
2:F:422:TRP:CH2	2:F:465:VAL:HG21	2.53	0.42
2:F:590:ALA:HA	2:F:620:TYR:O	2.19	0.42
2:F:892:ALA:C	2:F:894:GLU:N	2.73	0.42
1:G:212:THR:CG2	1:G:275:GLY:O	2.68	0.42
1:G:211:MET:CE	1:G:305:VAL:HG22	2.48	0.42
1:G:461:GLN:HB2	1:G:463:ASN:ND2	2.35	0.42
1:G:972:ARG:HH11	1:G:972:ARG:CG	2.31	0.42
2:H:706:PHE:C	2:H:708:ILE:H	2.22	0.42
1:A:317:LEU:O	1:A:321:GLU:HB3	2.20	0.42
1:A:711:ILE:O	1:A:714:ILE:HG23	2.19	0.42
2:B:666:LEU:HD12	2:B:666:LEU:HA	1.81	0.42
2:B:796:ASP:O	2:B:800:LEU:HB2	2.20	0.42
2:B:755:ALA:O	2:B:846:ALA:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:936:MET:CB	2:B:937:PRO:HD2	2.36	0.42
1:C:246:GLU:O	1:C:249:LEU:HB3	2.20	0.42
1:E:230:THR:HG22	1:E:511:VAL:HG11	2.01	0.42
2:F:288:ILE:HD11	2:F:318:ILE:HG22	2.01	0.42
1:G:838:LEU:HA	1:G:838:LEU:HD12	1.86	0.42
1:G:964:LYS:HG2	1:G:964:LYS:H	1.57	0.42
1:G:962:TYR:O	1:G:965:ILE:N	2.52	0.42
2:H:701:GLU:O	2:H:701:GLU:CD	2.58	0.42
1:A:613:ARG:HG2	1:A:613:ARG:HH11	1.85	0.42
2:B:831:LYS:HA	2:B:831:LYS:HD3	1.79	0.42
1:C:278:ARG:HG3	1:C:278:ARG:HH11	1.84	0.42
1:C:326:VAL:HG13	1:C:340:VAL:HG22	1.99	0.42
1:C:529:LEU:HB2	1:C:534:ILE:HD13	2.01	0.42
1:C:694:GLU:CD	1:C:952:ARG:HH21	2.23	0.42
2:D:587:LEU:HB3	2:D:679:ASP:OD2	2.19	0.42
2:D:887:ALA:C	2:D:889:ALA:H	2.22	0.42
1:E:317:LEU:HD12	1:E:317:LEU:N	2.34	0.42
1:E:442:ARG:NH1	1:E:449:ASN:OD1	2.43	0.42
1:E:663:THR:HG23	1:E:663:THR:O	2.19	0.42
1:E:944:GLU:C	1:E:945:ASN:HD22	2.22	0.42
2:F:328:SER:N	2:F:331:GLN:NE2	2.66	0.42
1:E:216:ASP:H	2:F:381:HIS:HE1	1.67	0.42
2:F:835:VAL:HG13	1:G:833:TYR:OH	2.19	0.42
1:G:761:VAL:O	1:G:852:VAL:HA	2.19	0.42
2:H:580:LYS:O	2:H:581:LEU:C	2.58	0.42
2:H:687:PHE:CE2	2:H:935:ARG:HA	2.55	0.42
1:A:808:GLU:O	1:A:809:ASN:C	2.57	0.42
2:D:607:SER:CB	2:D:869:THR:HB	2.49	0.42
2:D:946:ARG:NH2	2:D:946:ARG:CG	2.80	0.42
1:E:249:LEU:C	1:E:249:LEU:HD12	2.40	0.42
1:E:291:ALA:O	1:E:294:ASN:N	2.53	0.42
1:E:518:THR:CB	1:E:519:PRO:HD2	2.49	0.42
2:F:715:ALA:HB2	2:F:728:LEU:HB2	2.02	0.42
1:G:569:ILE:H	1:G:569:ILE:HD12	1.84	0.42
1:G:574:ASN:O	1:G:578:THR:HB	2.19	0.42
2:H:578:GLU:O	2:H:580:LYS:CG	2.54	0.42
2:H:591:ILE:HB	2:H:608:MET:HE1	2.02	0.42
2:H:617:HIS:NE2	2:H:880:LYS:NZ	2.62	0.42
1:A:587:LEU:HB3	1:A:622:HIS:CE1	2.55	0.42
1:A:968:ILE:HD13	1:A:968:ILE:HA	1.81	0.42
2:B:717:LEU:HD12	2:B:717:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:679:PHE:CE2	1:C:687:LEU:HD22	2.54	0.42
1:C:808:GLU:OE2	1:C:978:GLU:OE1	2.38	0.42
2:D:202:MET:HE3	2:D:295:LEU:HD21	2.01	0.42
1:E:302:ALA:HA	1:E:347:SER:HB2	2.02	0.42
1:E:586:GLU:HG3	1:E:587:LEU:N	2.34	0.42
1:E:731:GLU:HG2	1:E:958:HIS:CG	2.55	0.42
2:F:623:TYR:HB2	2:F:634:SER:HB2	2.02	0.42
1:G:246:GLU:CA	1:G:279:SER:HB2	2.50	0.42
1:G:930:ASN:O	1:G:931:GLY:C	2.57	0.42
2:H:201:VAL:HA	2:H:296:ILE:O	2.20	0.42
2:H:420:SER:CA	2:H:423:GLN:HE21	2.33	0.42
2:H:433:HIS:ND1	2:H:640:TRP:CZ2	2.88	0.42
1:A:416:ASP:OD2	1:A:449:ASN:HA	2.20	0.42
2:B:578:GLU:O	2:B:580:LYS:CG	2.53	0.42
2:D:219:VAL:O	2:D:223:ILE:HG13	2.20	0.42
2:D:666:LEU:HA	2:D:666:LEU:HD12	1.90	0.42
2:D:876:VAL:HG12	2:D:880:LYS:HE3	2.01	0.42
2:D:900:ASP:CG	2:D:903:ILE:HG13	2.40	0.42
2:D:392:ARG:NH2	3:D:982:F6P:H12	2.33	0.42
1:E:322:TRP:O	1:E:326:VAL:HG23	2.20	0.42
2:F:428:ASP:CG	2:F:432:LYS:HZ3	2.23	0.42
2:F:911:GLY:O	2:F:917:VAL:HA	2.19	0.42
1:G:578:THR:O	1:G:578:THR:HG23	2.20	0.42
2:H:522:ASN:O	2:H:523:GLU:C	2.58	0.42
2:H:545:ILE:HD11	2:H:553:ALA:CB	2.49	0.42
2:H:400:LEU:CD1	2:H:866:THR:HG21	2.48	0.42
2:H:935:ARG:O	2:H:936:MET:HB3	2.18	0.42
2:B:231:VAL:HG13	2:B:266:ILE:HG21	2.02	0.41
2:B:419:SER:O	2:B:423:GLN:NE2	2.52	0.41
2:B:416:PRO:HB2	2:B:452:ALA:HA	2.03	0.41
1:A:862:GLN:NE2	2:B:747:SER:OG	2.53	0.41
2:B:892:ALA:C	2:B:894:GLU:N	2.71	0.41
2:B:882:ASN:ND2	2:B:906:THR:HG22	2.17	0.41
1:C:440:ARG:HB2	1:C:440:ARG:HH11	1.86	0.41
1:C:756:ALA:HB2	2:D:651:GLY:HA2	2.01	0.41
2:D:662:GLU:HG3	2:D:695:GLN:NE2	2.34	0.41
2:F:594:VAL:O	2:F:685:GLY:HA3	2.19	0.41
1:G:317:LEU:CD1	1:G:317:LEU:N	2.81	0.41
1:G:728:PRO:HG3	1:G:954:GLY:CA	2.50	0.41
1:G:974:LYS:CD	1:G:975:LEU:HD13	2.50	0.41
2:H:258:TRP:CH2	2:H:265:ASN:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:886:ILE:O	2:H:890:ARG:N	2.52	0.41
2:H:918:VAL:HG12	2:H:919:TYR:N	2.35	0.41
1:A:282:PHE:HZ	1:A:318:PHE:CD1	2.38	0.41
1:A:424:ALA:HA	1:A:458:LEU:O	2.20	0.41
1:A:801:GLU:O	1:A:805:LEU:HG	2.20	0.41
1:A:233:HIS:NE2	1:A:968:ILE:HD12	2.35	0.41
2:B:239:LEU:O	2:B:286:HIS:CD2	2.72	0.41
2:B:288:ILE:HG12	2:B:335:MET:HE2	2.01	0.41
1:C:229:ARG:NH1	1:C:969:LEU:O	2.52	0.41
2:D:575:ASP:C	2:D:575:ASP:OD1	2.57	0.41
1:E:211:MET:HG3	1:E:244:GLY:HA2	2.02	0.41
1:E:471:LYS:HG3	1:E:481:THR:HG22	2.02	0.41
2:F:418:THR:CG2	2:F:422:TRP:HD1	2.31	0.41
2:F:573:SER:O	2:F:574:ALA:O	2.39	0.41
1:G:346:LEU:HD13	1:G:348:ILE:HD11	2.02	0.41
1:G:877:PHE:HZ	1:G:929:VAL:HG22	1.85	0.41
1:G:972:ARG:NH1	1:G:972:ARG:CG	2.83	0.41
2:B:327:ILE:O	2:B:327:ILE:HG13	2.20	0.41
2:B:341:CYS:HB2	2:B:507:VAL:CG1	2.48	0.41
1:C:242:TYR:N	1:C:242:TYR:CD1	2.88	0.41
2:D:298:CYS:CB	2:D:343:THR:HG22	2.50	0.41
2:D:587:LEU:HB3	2:D:679:ASP:HB2	2.02	0.41
1:E:355:ILE:HB	1:E:371:ALA:HB2	2.02	0.41
1:E:787:VAL:HA	1:E:824:VAL:O	2.20	0.41
1:E:963:ASN:HD22	1:E:963:ASN:N	2.17	0.41
2:F:236:TYR:O	2:F:239:LEU:HB2	2.21	0.41
2:F:415:LYS:N	2:F:416:PRO:HD3	2.35	0.41
2:F:516:SER:O	2:F:531:LEU:HB2	2.20	0.41
2:F:626:TRP:NE1	2:F:661:PRO:HG3	2.35	0.41
1:G:724:SER:CB	1:G:768:GLY:HA2	2.50	0.41
2:H:886:ILE:O	2:H:890:ARG:HB2	2.20	0.41
2:H:887:ALA:C	2:H:889:ALA:N	2.74	0.41
1:A:927:ILE:O	1:A:927:ILE:HG23	2.19	0.41
2:B:647:GLN:HE22	2:B:869:THR:HG21	1.83	0.41
2:B:894:GLU:C	2:B:896:PHE:N	2.74	0.41
2:B:904:SER:C	2:B:906:THR:H	2.23	0.41
1:C:474:LEU:HD22	1:C:479:LEU:HD12	2.03	0.41
1:C:488:HIS:C	1:C:490:GLN:N	2.71	0.41
1:C:506:GLN:HG2	1:C:526:ILE:HG22	2.03	0.41
2:D:420:SER:CA	2:D:423:GLN:NE2	2.83	0.41
2:D:587:LEU:HD23	2:D:679:ASP:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:800:LEU:HD21	2:D:817:ILE:HD11	2.02	0.41
1:E:209:ALA:HA	1:E:239:PHE:O	2.21	0.41
2:F:417:ALA:O	2:F:418:THR:CB	2.69	0.41
2:F:694:HIS:HA	2:F:922:ILE:HG12	2.01	0.41
1:G:289:ARG:HA	1:G:325:LEU:HD13	2.02	0.41
1:G:586:GLU:CG	1:G:587:LEU:N	2.83	0.41
1:G:651:GLU:HG3	1:G:652:ASN:ND2	2.35	0.41
1:G:728:PRO:HG3	1:G:954:GLY:HA2	2.02	0.41
1:G:780:LEU:O	1:G:780:LEU:HD13	2.20	0.41
2:H:717:LEU:HD11	2:H:761:GLN:HE21	1.86	0.41
2:H:792:GLN:NE2	2:H:957:ARG:HB3	2.29	0.41
1:A:823:LEU:N	1:A:823:LEU:CD1	2.83	0.41
2:B:343:THR:HG22	2:B:343:THR:O	2.21	0.41
2:B:475:ARG:HG2	2:B:475:ARG:NH1	2.36	0.41
1:A:746:TYR:CE1	2:B:854:VAL:HG11	2.55	0.41
1:C:787:VAL:HA	1:C:824:VAL:O	2.21	0.41
2:D:573:SER:O	2:D:574:ALA:C	2.59	0.41
2:D:591:ILE:HB	2:D:608:MET:HE3	2.02	0.41
2:D:672:TYR:O	2:D:676:TYR:HD1	2.03	0.41
1:E:606:ALA:O	1:E:866:PRO:HB3	2.20	0.41
1:E:788:TYR:HE1	1:E:823:LEU:HD23	1.85	0.41
2:F:293:ASP:HB3	2:F:335:MET:HE3	2.01	0.41
2:F:413:PRO:HB3	2:F:448:GLY:O	2.20	0.41
2:F:755:ALA:O	2:F:846:ALA:HA	2.20	0.41
2:F:797:ILE:HD13	2:F:836:ILE:HA	2.03	0.41
2:F:796:ASP:O	2:F:800:LEU:HB2	2.19	0.41
2:F:916:HIS:O	2:F:917:VAL:HB	2.21	0.41
1:G:962:TYR:O	1:G:964:LYS:N	2.54	0.41
2:H:298:CYS:HB2	2:H:343:THR:CG2	2.50	0.41
2:H:288:ILE:HD11	2:H:318:ILE:HG22	2.02	0.41
2:H:295:LEU:O	2:H:340:ILE:HA	2.20	0.41
2:H:428:ASP:O	2:H:432:LYS:HG3	2.20	0.41
2:H:711:VAL:CG1	2:H:711:VAL:O	2.67	0.41
1:A:947:THR:O	1:A:950:GLU:O	2.37	0.41
1:A:950:GLU:O	1:A:952:ARG:N	2.47	0.41
2:B:418:THR:CG2	2:B:422:TRP:HD1	2.33	0.41
2:B:453:ASP:O	2:B:454:LEU:HB2	2.20	0.41
2:B:622:ILE:HG23	2:B:629:LEU:HD13	2.02	0.41
2:B:946:ARG:CG	2:B:946:ARG:NH2	2.80	0.41
1:C:759:ARG:HG2	1:C:810:PHE:CD2	2.56	0.41
2:D:467:VAL:O	2:D:471:GLY:CA	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:747:SER:O	2:D:750:SER:HB2	2.20	0.41
1:E:246:GLU:CA	1:E:279:SER:HB2	2.50	0.41
1:E:421:PRO:HG2	1:E:422:GLU:OE2	2.20	0.41
1:E:782:THR:HG22	1:E:784:ALA:N	2.36	0.41
1:E:734:LEU:HD21	1:E:873:THR:HG22	2.02	0.41
2:F:365:ASP:OD2	2:F:369:LYS:NZ	2.46	0.41
2:F:414:GLU:C	2:F:416:PRO:HD3	2.41	0.41
1:G:246:GLU:OE1	1:G:246:GLU:HA	2.20	0.41
1:G:450:THR:C	1:G:451:ILE:HD12	2.40	0.41
2:H:347:ILE:CG2	2:H:363:ALA:HB2	2.50	0.41
2:H:429:ILE:HG13	2:H:433:HIS:CD2	2.55	0.41
2:H:462:VAL:HG12	2:H:466:LEU:HD23	2.02	0.41
2:H:365:ASP:HA	2:H:862:PRO:HG2	2.02	0.41
2:H:930:THR:HG22	2:H:932:VAL:H	1.83	0.41
1:A:697:ARG:NH1	1:A:943:TRP:HH2	2.19	0.41
2:B:418:THR:OG1	2:B:422:TRP:N	2.35	0.41
2:B:524:ASN:HB2	2:B:914:GLY:HA2	2.02	0.41
1:C:805:LEU:HD23	1:C:805:LEU:N	2.35	0.41
1:C:922:ASP:HA	1:C:938:PRO:HG3	2.02	0.41
2:D:207:ASP:HA	2:D:211:MET:SD	2.61	0.41
2:D:574:ALA:CB	2:D:610:THR:O	2.68	0.41
2:D:831:LYS:HA	2:D:831:LYS:HD3	1.82	0.41
1:E:341:ALA:CB	1:E:342:PRO:CD	2.98	0.41
1:E:968:ILE:CG1	1:E:973:LEU:HD12	2.51	0.41
2:F:236:TYR:O	2:F:239:LEU:N	2.52	0.41
2:F:407:ALA:HB1	2:F:442:ILE:O	2.21	0.41
2:F:717:LEU:HD12	2:F:718:SER:N	2.36	0.41
2:F:761:GLN:HB3	4:F:6:FDP:O1	2.21	0.41
1:E:746:TYR:CE1	2:F:854:VAL:HG13	2.55	0.41
2:F:694:HIS:CA	2:F:922:ILE:HG12	2.51	0.41
2:H:390:MET:HG3	2:H:483:GLN:HE22	1.82	0.41
2:H:690:PHE:HA	2:H:712:LEU:HD22	2.03	0.41
2:H:888:GLU:OE1	2:H:889:ALA:HB2	2.20	0.41
1:A:357:ASN:OD1	1:A:364:SER:HA	2.21	0.41
1:A:758:ARG:NH2	1:A:817:ASN:HA	2.36	0.41
2:B:577:ASN:CA	2:B:579:PRO:HD2	2.51	0.41
2:B:900:ASP:O	2:B:901:LYS:C	2.59	0.41
1:C:216:ASP:H	2:D:381:HIS:CE1	2.33	0.41
1:C:266:TRP:CD2	1:C:273:LEU:HD12	2.55	0.41
1:C:317:LEU:CD1	1:C:317:LEU:H	2.34	0.41
1:C:697:ARG:NH1	1:C:943:TRP:HH2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:930:THR:HG22	2:D:931:GLU:N	2.35	0.41
1:E:591:SER:HA	1:E:593:ARG:HG3	2.02	0.41
1:E:819:ASN:O	1:E:821:LYS:HE3	2.20	0.41
2:F:438:LYS:HG2	2:F:440:THR:O	2.21	0.41
2:F:522:ASN:O	2:F:523:GLU:C	2.59	0.41
2:F:765:SER:HB2	2:F:936:MET:HE3	2.03	0.41
1:G:317:LEU:O	1:G:321:GLU:HB3	2.21	0.41
2:H:612:CYS:HB3	2:H:617:HIS:HB2	2.03	0.41
2:H:648:SER:HA	2:H:865:ARG:HD3	2.03	0.41
1:A:421:PRO:O	1:A:423:ARG:N	2.54	0.41
2:B:219:VAL:O	2:B:223:ILE:HG13	2.21	0.41
2:B:341:CYS:CB	2:B:507:VAL:HG13	2.47	0.41
2:B:611:TYR:CG	2:B:873:ILE:HG12	2.56	0.41
1:A:660:GLU:C	2:B:752:ARG:HH22	2.24	0.41
2:B:903:ILE:HG13	2:B:903:ILE:H	1.68	0.41
1:C:424:ALA:HB1	1:C:459:ASP:O	2.21	0.41
1:C:774:ILE:HD13	1:C:774:ILE:HA	1.98	0.41
1:C:765:GLU:HA	1:C:825:ARG:O	2.20	0.41
2:D:314:TRP:O	2:D:315:PRO:C	2.59	0.41
2:D:494:ILE:HG23	2:D:774:LEU:HD23	2.03	0.41
2:D:723:GLY:O	2:D:911:GLY:HA3	2.21	0.41
1:E:289:ARG:N	1:E:325:LEU:HD13	2.35	0.41
1:E:431:GLN:N	1:E:431:GLN:NE2	2.50	0.41
1:E:554:ASN:O	1:E:555:LYS:C	2.59	0.41
2:H:314:TRP:O	2:H:315:PRO:C	2.55	0.41
2:H:325:ASN:O	2:H:326:ARG:HB2	2.20	0.41
1:A:788:TYR:HE1	1:A:823:LEU:HD23	1.85	0.41
2:B:410:ILE:HA	2:B:444:VAL:O	2.21	0.41
1:C:606:ALA:O	1:C:866:PRO:HB3	2.21	0.41
1:C:613:ARG:HG2	1:C:613:ARG:NH1	2.36	0.41
2:D:239:LEU:HA	2:D:239:LEU:HD23	1.87	0.41
2:D:379:ASN:HA	2:D:440:THR:HG23	2.02	0.41
2:D:673:PHE:HZ	2:D:681:LEU:HD22	1.86	0.41
2:D:752:ARG:CZ	2:D:811:GLY:HA2	2.50	0.41
1:E:247:GLY:HA2	1:E:254:TYR:CD2	2.55	0.41
1:E:249:LEU:HD13	1:E:290:GLN:HG2	2.01	0.41
1:E:399:GLY:O	1:E:400:ARG:HB3	2.21	0.41
2:F:349:ASN:HA	2:F:357:THR:OG1	2.21	0.41
2:F:662:GLU:HG3	2:F:695:GLN:NE2	2.36	0.41
1:G:590:VAL:CG2	1:G:591:SER:H	2.22	0.41
2:H:381:HIS:CD2	2:H:383:ARG:HH21	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:ARG:NH2	1:A:834:SER:HA	2.36	0.41
1:A:930:ASN:O	1:A:931:GLY:C	2.58	0.41
2:B:726:TYR:CE1	2:B:730:SER:HB3	2.55	0.41
2:B:755:ALA:HA	2:B:815:LYS:O	2.21	0.41
1:C:317:LEU:O	1:C:321:GLU:HB3	2.21	0.41
1:C:788:TYR:OH	1:C:802:ASP:OD2	2.37	0.41
2:D:523:GLU:OE1	2:D:915:SER:HB3	2.21	0.41
2:D:879:ILE:HD13	2:D:879:ILE:HA	1.92	0.41
1:E:710:PRO:HA	1:E:713:ASN:HD22	1.86	0.41
2:F:591:ILE:HG12	2:F:682:ILE:CG2	2.51	0.41
1:G:589:PRO:O	1:G:593:ARG:NH1	2.54	0.41
1:A:433:GLU:O	1:A:437:VAL:HG23	2.20	0.40
1:A:638:GLN:HG3	1:A:638:GLN:O	2.20	0.40
1:A:837:LEU:HD11	1:A:841:ILE:HD11	2.02	0.40
1:A:498:HIS:HD2	1:A:869:LYS:NZ	2.19	0.40
2:B:390:MET:HG3	2:B:483:GLN:HE22	1.82	0.40
1:C:518:THR:OG1	1:C:521:THR:CG2	2.53	0.40
1:C:711:ILE:O	1:C:714:ILE:HG23	2.20	0.40
2:D:365:ASP:HA	2:D:862:PRO:HG2	2.03	0.40
2:D:590:ALA:HA	2:D:620:TYR:O	2.21	0.40
2:D:853:HIS:C	2:D:855:GLN:N	2.74	0.40
1:E:211:MET:CE	1:E:305:VAL:HG22	2.49	0.40
1:E:539:VAL:O	1:E:542:VAL:CG2	2.68	0.40
2:F:347:ILE:CG2	2:F:363:ALA:HB2	2.51	0.40
2:F:587:LEU:N	2:F:617:HIS:HD1	2.16	0.40
1:G:530:GLU:HA	1:G:932:SER:HB3	2.02	0.40
1:G:558:ASP:O	1:G:561:ILE:HG22	2.20	0.40
1:G:625:LYS:HG2	1:G:644:GLU:OE2	2.21	0.40
1:G:750:ILE:HG13	1:G:751:LYS:N	2.35	0.40
1:G:754:ALA:HB2	1:G:762:PHE:HE1	1.86	0.40
2:H:239:LEU:HD22	2:H:287:LEU:HD22	2.02	0.40
2:H:322:LEU:HD23	2:H:322:LEU:HA	1.86	0.40
2:H:541:VAL:HG22	2:H:556:LEU:HB2	2.03	0.40
2:H:587:LEU:N	2:H:587:LEU:CD1	2.84	0.40
2:H:726:TYR:O	2:H:726:TYR:CD2	2.74	0.40
1:A:554:ASN:O	1:A:556:ASP:N	2.55	0.40
3:A:988:F6P:O2P	2:B:383:ARG:NH2	2.48	0.40
2:B:752:ARG:CZ	2:B:811:GLY:HA2	2.51	0.40
1:C:247:GLY:HA2	1:C:254:TYR:HD2	1.85	0.40
1:C:864:GLY:HA3	2:D:743:VAL:HG22	2.04	0.40
2:D:344:VAL:CG2	2:D:357:THR:HG22	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:466:THR:CG2	1:E:467:ALA:N	2.84	0.40
1:E:975:LEU:O	1:E:978:GLU:HB2	2.21	0.40
2:F:341:CYS:SG	2:F:519:ILE:CD1	3.09	0.40
2:F:916:HIS:O	2:F:917:VAL:CB	2.69	0.40
2:F:930:THR:HG22	2:F:931:GLU:N	2.36	0.40
1:G:231:GLY:O	1:G:232:ILE:C	2.59	0.40
1:G:832:VAL:HG12	1:G:833:TYR:N	2.36	0.40
2:H:341:CYS:CB	2:H:507:VAL:HG13	2.49	0.40
2:H:563:GLU:OE2	2:H:870:ARG:NE	2.34	0.40
1:A:625:LYS:HG2	1:A:644:GLU:OE2	2.20	0.40
1:A:743:LEU:HD23	1:A:743:LEU:HA	1.93	0.40
1:A:947:THR:HG21	1:A:951:LEU:CB	2.43	0.40
1:C:483:VAL:HG12	1:C:485:ILE:CD1	2.51	0.40
1:C:700:LYS:NZ	1:C:704:ASP:OD2	2.54	0.40
2:D:244:PRO:O	2:D:245:GLU:CB	2.68	0.40
2:D:408:ASP:OD1	2:D:441:THR:HA	2.22	0.40
2:D:545:ILE:HD11	2:D:553:ALA:CB	2.51	0.40
2:D:580:LYS:O	2:D:581:LEU:C	2.59	0.40
2:D:711:VAL:HG22	2:D:910:VAL:CG2	2.51	0.40
2:D:884:ALA:O	2:D:887:ALA:HB3	2.20	0.40
1:E:584:GLY:O	1:E:588:LEU:HB2	2.20	0.40
2:F:288:ILE:HG12	2:F:335:MET:HE2	2.03	0.40
2:F:366:ARG:NH2	2:F:487:THR:O	2.53	0.40
2:F:679:ASP:HB3	2:F:883:GLN:HE22	1.86	0.40
1:G:975:LEU:HD22	1:G:975:LEU:N	2.20	0.40
2:H:239:LEU:HD23	2:H:239:LEU:HA	1.87	0.40
2:H:666:LEU:O	2:H:669:ILE:HB	2.21	0.40
2:H:800:LEU:HD21	2:H:817:ILE:HD11	2.03	0.40
2:H:900:ASP:O	2:H:901:LYS:C	2.60	0.40
1:A:770:HIS:CG	1:A:951:LEU:HA	2.55	0.40
2:B:519:ILE:HD12	2:B:519:ILE:N	2.37	0.40
1:C:404:TRP:HE3	1:C:405:LEU:HD13	1.86	0.40
1:C:584:GLY:O	1:C:588:LEU:HB2	2.21	0.40
1:C:720:PRO:HG2	1:C:730:THR:HG21	2.04	0.40
2:D:201:VAL:HG13	2:D:218:ILE:HG21	2.03	0.40
2:D:419:SER:O	2:D:423:GLN:NE2	2.55	0.40
2:D:701:GLU:O	2:D:701:GLU:OE2	2.39	0.40
1:E:448:ASN:HD22	1:E:448:ASN:H	1.67	0.40
1:E:514:VAL:HG12	1:E:515:LEU:N	2.36	0.40
1:E:648:ILE:HD13	1:E:648:ILE:O	2.22	0.40
1:E:780:LEU:HD13	1:E:780:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:837:LEU:HD22	2:H:831:LYS:CD	2.51	0.40
2:F:888:GLU:OE1	2:F:889:ALA:HB2	2.20	0.40
2:F:936:MET:CB	2:F:937:PRO:HD2	2.37	0.40
1:G:225:ARG:HA	1:G:263:VAL:HG11	2.03	0.40
1:G:754:ALA:HB2	1:G:762:PHE:CD1	2.56	0.40
2:H:325:ASN:C	2:H:327:ILE:N	2.74	0.40
2:H:420:SER:CA	2:H:423:GLN:NE2	2.85	0.40
2:H:946:ARG:HG3	2:H:946:ARG:NH2	2.27	0.40
1:A:255:LEU:HD23	1:A:256:LYS:N	2.37	0.40
1:A:382:ILE:O	1:A:385:THR:HG22	2.22	0.40
1:A:803:ILE:HD13	1:A:845:ALA:CB	2.52	0.40
1:A:760:ARG:NH1	4:B:2:FDP:O6P	2.53	0.40
2:B:832:LEU:HD12	2:B:832:LEU:HA	1.77	0.40
2:B:949:ALA:O	2:B:953:VAL:HG12	2.21	0.40
1:C:518:THR:HG23	1:C:521:THR:HG21	2.03	0.40
1:C:589:PRO:HD2	1:C:622:HIS:HB3	2.03	0.40
2:D:475:ARG:HG2	2:D:475:ARG:HH11	1.87	0.40
2:D:587:LEU:HB3	2:D:679:ASP:CB	2.52	0.40
1:A:837:LEU:HD11	2:D:827:LEU:CD2	2.51	0.40
1:E:484:THR:C	1:E:485:ILE:HD12	2.41	0.40
1:E:669:SER:HB3	1:E:701:GLN:CD	2.42	0.40
2:F:647:GLN:HE22	2:F:869:THR:HG22	1.86	0.40
1:E:746:TYR:CE1	2:F:854:VAL:HG11	2.57	0.40
1:G:278:ARG:HG3	1:G:278:ARG:NH1	2.36	0.40
1:G:432:ASP:O	1:G:436:GLU:HB2	2.21	0.40
1:G:761:VAL:HA	1:G:821:LYS:O	2.21	0.40
2:H:740:TYR:CD1	2:H:851:PRO:HB3	2.56	0.40
2:H:945:THR:HA	2:H:948:ILE:HG12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:333:GLU:OE2	2:H:578:GLU:OE1[4_446]	2.14	0.06

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	746/787 (95%)	630 (84%)	87 (12%)	29 (4%)	3	12
1	C	746/787 (95%)	634 (85%)	85 (11%)	27 (4%)	3	14
1	E	748/787 (95%)	643 (86%)	74 (10%)	31 (4%)	3	11
1	G	742/787 (94%)	632 (85%)	79 (11%)	31 (4%)	3	10
2	B	761/766 (99%)	675 (89%)	61 (8%)	25 (3%)	4	15
2	D	761/766 (99%)	672 (88%)	59 (8%)	30 (4%)	3	12
2	F	760/766 (99%)	674 (89%)	58 (8%)	28 (4%)	3	13
2	H	761/766 (99%)	680 (89%)	53 (7%)	28 (4%)	3	13
All	All	6025/6212 (97%)	5240 (87%)	556 (9%)	229 (4%)	3	13

All (229) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	GLY
1	A	321	GLU
1	A	331	ALA
1	A	585	SER
1	A	587	LEU
1	A	589	PRO
1	A	590	VAL
1	A	817	ASN
1	A	948	ASN
2	B	324	THR
2	B	418	THR
2	B	548	LYS
2	B	559	THR
2	B	574	ALA
2	B	579	PRO
2	B	580	LYS
2	B	584	ASP

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Mol	Chain	Res	Type
2	B	884	ALA
2	B	885	ALA
2	B	891	ALA
2	B	905	ASP
2	B	917	VAL
1	C	252	GLY
1	C	321	GLU
1	C	331	ALA
1	C	555	LYS
1	C	585	SER
1	C	586	GLU
1	C	587	LEU
1	C	590	VAL
1	C	671	ASP
1	C	817	ASN
1	C	948	ASN
1	C	949	VAL
2	D	324	THR
2	D	418	THR
2	D	548	LYS
2	D	574	ALA
2	D	579	PRO
2	D	580	LYS
2	D	584	ASP
2	D	884	ALA
2	D	885	ALA
2	D	891	ALA
1	E	252	GLY
1	E	271	GLY
1	E	321	GLU
1	E	331	ALA
1	E	555	LYS
1	E	585	SER
1	E	590	VAL
1	E	817	ASN
1	E	950	GLU
1	E	976	ARG
2	F	324	THR
2	F	418	THR
2	F	548	LYS
2	F	574	ALA
2	F	579	PRO

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Mol	Chain	Res	Type
2	F	580	LYS
2	F	584	ASP
2	F	884	ALA
2	F	885	ALA
2	F	891	ALA
1	G	252	GLY
1	G	271	GLY
1	G	321	GLU
1	G	331	ALA
1	G	427	HIS
1	G	555	LYS
1	G	585	SER
1	G	586	GLU
1	G	590	VAL
1	G	817	ASN
1	G	948	ASN
1	G	950	GLU
2	H	324	THR
2	H	418	THR
2	H	548	LYS
2	H	574	ALA
2	H	579	PRO
2	H	580	LYS
2	H	584	ASP
2	H	885	ALA
2	H	891	ALA
1	A	271	GLY
1	A	275	GLY
1	A	332	GLU
1	A	334	ARG
1	A	555	LYS
1	A	586	GLU
1	A	671	ASP
1	A	848	GLY
1	A	951	LEU
1	A	961	GLU
2	B	417	ALA
2	B	625	GLY
2	B	700	ARG
2	B	702	SER
2	B	711	VAL
2	B	890	ARG

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Mol	Chain	Res	Type
2	B	893	GLU
2	B	895	ASN
2	B	932	VAL
1	C	271	GLY
1	C	332	GLU
1	C	333	GLY
1	C	334	ARG
1	C	422	GLU
1	C	427	HIS
1	C	589	PRO
1	C	848	GLY
2	D	323	LYS
2	D	417	ALA
2	D	559	THR
2	D	702	SER
2	D	711	VAL
2	D	810	ARG
2	D	890	ARG
2	D	893	GLU
2	D	895	ASN
2	D	905	ASP
2	D	917	VAL
2	D	932	VAL
1	E	332	GLU
1	E	334	ARG
1	E	586	GLU
1	E	587	LEU
1	E	589	PRO
1	E	671	ASP
1	E	848	GLY
1	E	949	VAL
2	F	417	ALA
2	F	702	SER
2	F	711	VAL
2	F	890	ARG
2	F	893	GLU
2	F	895	ASN
2	F	905	ASP
2	F	917	VAL
1	G	332	GLU
1	G	334	ARG
1	G	587	LEU

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Mol	Chain	Res	Type
1	G	848	GLY
1	G	972	ARG
2	H	417	ALA
2	H	559	THR
2	H	700	ARG
2	H	702	SER
2	H	711	VAL
2	H	890	ARG
2	H	893	GLU
2	H	895	ASN
2	H	917	VAL
1	A	427	HIS
1	A	944	GLU
2	B	323	LYS
1	C	806	LEU
1	C	952	ARG
2	D	625	GLY
2	D	700	ARG
1	E	333	GLY
1	E	427	HIS
1	E	632	GLY
1	E	806	LEU
1	E	948	ASN
1	E	951	LEU
1	E	978	GLU
2	F	559	THR
2	F	700	ARG
1	G	251	GLY
1	G	333	GLY
1	G	589	PRO
1	G	671	ASP
1	G	963	ASN
2	H	323	LYS
2	H	665	ASP
2	H	884	ALA
2	H	905	ASP
1	A	806	LEU
1	A	963	ASN
1	C	632	GLY
1	C	944	GLU
2	D	557	ARG
2	D	956	LYS

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Mol	Chain	Res	Type
2	F	665	ASP
2	F	752	ARG
1	G	422	GLU
1	G	426	PRO
1	G	806	LEU
1	G	944	GLU
1	G	949	VAL
1	G	974	LYS
2	H	752	ARG
1	A	251	GLY
1	A	758	ARG
1	C	426	PRO
2	D	581	LEU
2	D	752	ARG
1	E	275	GLY
1	E	426	PRO
1	E	974	LYS
2	F	325	ASN
2	F	932	VAL
1	G	758	ARG
2	H	956	LYS
1	A	949	VAL
2	B	581	LEU
2	B	914	GLY
1	C	950	GLU
2	D	665	ASP
1	E	758	ARG
2	F	581	LEU
1	G	759	ARG
2	H	325	ASN
2	H	914	GLY
1	A	340	VAL
2	F	886	ILE
2	H	581	LEU
1	E	251	GLY
2	F	914	GLY
1	A	333	GLY
1	A	426	PRO
2	D	243	GLY
1	E	340	VAL
1	G	968	ILE
1	C	275	GLY

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Mol	Chain	Res	Type
2	F	243	GLY
2	H	886	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	614/645 (95%)	567 (92%)	47 (8%)	13	35
1	C	614/645 (95%)	567 (92%)	47 (8%)	13	35
1	E	616/645 (96%)	565 (92%)	51 (8%)	11	32
1	G	612/645 (95%)	561 (92%)	51 (8%)	11	32
2	B	612/615 (100%)	552 (90%)	60 (10%)	8	24
2	D	612/615 (100%)	552 (90%)	60 (10%)	8	24
2	F	611/615 (99%)	554 (91%)	57 (9%)	9	27
2	H	612/615 (100%)	553 (90%)	59 (10%)	8	25
All	All	4903/5040 (97%)	4471 (91%)	432 (9%)	10	30

All (432) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	LYS
1	A	237	ASP
1	A	249	LEU
1	A	264	ARG
1	A	309	ASP
1	A	322	TRP
1	A	328	GLU
1	A	332	GLU
1	A	334	ARG
1	A	340	VAL
1	A	346	LEU
1	A	359	MET
1	A	405	LEU

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Mol	Chain	Res	Type
1	A	423	ARG
1	A	427	HIS
1	A	431	GLN
1	A	436	GLU
1	A	458	LEU
1	A	502	LEU
1	A	514	VAL
1	A	517	PHE
1	A	524	PRO
1	A	539	VAL
1	A	555	LYS
1	A	578	THR
1	A	588	LEU
1	A	589	PRO
1	A	599	VAL
1	A	605	SER
1	A	622	HIS
1	A	648	ILE
1	A	650	VAL
1	A	656	LEU
1	A	703	ARG
1	A	758	ARG
1	A	782	THR
1	A	785	VAL
1	A	814	LYS
1	A	819	ASN
1	A	821	LYS
1	A	822	LEU
1	A	891	LYS
1	A	934	VAL
1	A	946	GLU
1	A	952	ARG
1	A	959	TRP
1	A	964	LYS
2	B	201	VAL
2	B	253	GLU
2	B	256	ARG
2	B	259	SER
2	B	273	GLU
2	B	281	LEU
2	B	287	LEU
2	B	297	VAL

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Mol	Chain	Res	Type
2	B	301	ASP
2	B	322	LEU
2	B	336	LYS
2	B	343	THR
2	B	366	ARG
2	B	389	VAL
2	B	423	GLN
2	B	436	ARG
2	B	469	ARG
2	B	472	LEU
2	B	487	THR
2	B	510	SER
2	B	518	LEU
2	B	521	VAL
2	B	525	LYS
2	B	531	LEU
2	B	551	LYS
2	B	552	ARG
2	B	565	LEU
2	B	575	ASP
2	B	579	PRO
2	B	583	LYS
2	B	584	ASP
2	B	586	ARG
2	B	587	LEU
2	B	591	ILE
2	B	608	MET
2	B	619	PRO
2	B	673	PHE
2	B	688	GLU
2	B	698	ARG
2	B	700	ARG
2	B	701	GLU
2	B	702	SER
2	B	707	ARG
2	B	711	VAL
2	B	716	THR
2	B	793	LEU
2	B	794	SER
2	B	800	LEU
2	B	808	GLU
2	B	810	ARG

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Mol	Chain	Res	Type
2	B	867	ARG
2	B	869	THR
2	B	888	GLU
2	B	893	GLU
2	B	902	THR
2	B	916	HIS
2	B	925	LEU
2	B	945	THR
2	B	947	LEU
2	B	956	LYS
1	C	205	LYS
1	C	210	VAL
1	C	249	LEU
1	C	309	ASP
1	C	319	ARG
1	C	322	TRP
1	C	328	GLU
1	C	332	GLU
1	C	340	VAL
1	C	346	LEU
1	C	359	MET
1	C	405	LEU
1	C	423	ARG
1	C	427	HIS
1	C	431	GLN
1	C	436	GLU
1	C	458	LEU
1	C	502	LEU
1	C	514	VAL
1	C	517	PHE
1	C	539	VAL
1	C	555	LYS
1	C	564	ARG
1	C	578	THR
1	C	588	LEU
1	C	589	PRO
1	C	599	VAL
1	C	605	SER
1	C	648	ILE
1	C	650	VAL
1	C	656	LEU
1	C	722	THR

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Mol	Chain	Res	Type
1	C	758	ARG
1	C	782	THR
1	C	785	VAL
1	C	814	LYS
1	C	819	ASN
1	C	821	LYS
1	C	822	LEU
1	C	832	VAL
1	C	891	LYS
1	C	929	VAL
1	C	934	VAL
1	C	946	GLU
1	C	955	PHE
1	C	959	TRP
1	C	967	ASP
2	D	201	VAL
2	D	250	PHE
2	D	253	GLU
2	D	256	ARG
2	D	259	SER
2	D	273	GLU
2	D	281	LEU
2	D	287	LEU
2	D	297	VAL
2	D	301	ASP
2	D	322	LEU
2	D	336	LYS
2	D	343	THR
2	D	344	VAL
2	D	366	ARG
2	D	389	VAL
2	D	423	GLN
2	D	436	ARG
2	D	469	ARG
2	D	472	LEU
2	D	487	THR
2	D	510	SER
2	D	517	PRO
2	D	518	LEU
2	D	521	VAL
2	D	525	LYS
2	D	531	LEU

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Mol	Chain	Res	Type
2	D	551	LYS
2	D	552	ARG
2	D	565	LEU
2	D	575	ASP
2	D	579	PRO
2	D	584	ASP
2	D	586	ARG
2	D	587	LEU
2	D	591	ILE
2	D	608	MET
2	D	673	PHE
2	D	688	GLU
2	D	698	ARG
2	D	700	ARG
2	D	701	GLU
2	D	702	SER
2	D	707	ARG
2	D	711	VAL
2	D	716	THR
2	D	793	LEU
2	D	794	SER
2	D	800	LEU
2	D	808	GLU
2	D	810	ARG
2	D	867	ARG
2	D	869	THR
2	D	888	GLU
2	D	916	HIS
2	D	932	VAL
2	D	945	THR
2	D	947	LEU
2	D	956	LYS
2	D	957	ARG
1	E	203	GLN
1	E	207	LYS
1	E	237	ASP
1	E	249	LEU
1	E	264	ARG
1	E	306	CYS
1	E	309	ASP
1	E	322	TRP
1	E	328	GLU

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Mol	Chain	Res	Type
1	E	332	GLU
1	E	334	ARG
1	E	340	VAL
1	E	346	LEU
1	E	359	MET
1	E	405	LEU
1	E	423	ARG
1	E	427	HIS
1	E	431	GLN
1	E	436	GLU
1	E	448	ASN
1	E	458	LEU
1	E	502	LEU
1	E	514	VAL
1	E	517	PHE
1	E	539	VAL
1	E	555	LYS
1	E	564	ARG
1	E	578	THR
1	E	588	LEU
1	E	589	PRO
1	E	599	VAL
1	E	605	SER
1	E	622	HIS
1	E	648	ILE
1	E	650	VAL
1	E	656	LEU
1	E	758	ARG
1	E	766	VAL
1	E	782	THR
1	E	785	VAL
1	E	814	LYS
1	E	819	ASN
1	E	821	LYS
1	E	822	LEU
1	E	891	LYS
1	E	929	VAL
1	E	934	VAL
1	E	944	GLU
1	E	946	GLU
1	E	959	TRP
1	E	976	ARG

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Mol	Chain	Res	Type
2	F	201	VAL
2	F	253	GLU
2	F	256	ARG
2	F	259	SER
2	F	273	GLU
2	F	277	ARG
2	F	281	LEU
2	F	287	LEU
2	F	301	ASP
2	F	322	LEU
2	F	336	LYS
2	F	343	THR
2	F	344	VAL
2	F	366	ARG
2	F	389	VAL
2	F	423	GLN
2	F	469	ARG
2	F	472	LEU
2	F	487	THR
2	F	510	SER
2	F	518	LEU
2	F	521	VAL
2	F	525	LYS
2	F	531	LEU
2	F	551	LYS
2	F	552	ARG
2	F	565	LEU
2	F	575	ASP
2	F	579	PRO
2	F	583	LYS
2	F	586	ARG
2	F	587	LEU
2	F	591	ILE
2	F	608	MET
2	F	636	ARG
2	F	673	PHE
2	F	688	GLU
2	F	700	ARG
2	F	701	GLU
2	F	702	SER
2	F	707	ARG
2	F	711	VAL

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Mol	Chain	Res	Type
2	F	716	THR
2	F	793	LEU
2	F	794	SER
2	F	800	LEU
2	F	808	GLU
2	F	810	ARG
2	F	867	ARG
2	F	869	THR
2	F	888	GLU
2	F	893	GLU
2	F	916	HIS
2	F	925	LEU
2	F	945	THR
2	F	947	LEU
2	F	956	LYS
1	G	205	LYS
1	G	237	ASP
1	G	249	LEU
1	G	309	ASP
1	G	322	TRP
1	G	324	SER
1	G	328	GLU
1	G	332	GLU
1	G	340	VAL
1	G	346	LEU
1	G	359	MET
1	G	374	ARG
1	G	405	LEU
1	G	423	ARG
1	G	427	HIS
1	G	431	GLN
1	G	436	GLU
1	G	448	ASN
1	G	458	LEU
1	G	489	VAL
1	G	502	LEU
1	G	514	VAL
1	G	517	PHE
1	G	539	VAL
1	G	555	LYS
1	G	578	THR
1	G	588	LEU

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Mol	Chain	Res	Type
1	G	589	PRO
1	G	599	VAL
1	G	605	SER
1	G	648	ILE
1	G	650	VAL
1	G	656	LEU
1	G	766	VAL
1	G	782	THR
1	G	785	VAL
1	G	814	LYS
1	G	821	LYS
1	G	822	LEU
1	G	832	VAL
1	G	891	LYS
1	G	929	VAL
1	G	934	VAL
1	G	944	GLU
1	G	946	GLU
1	G	948	ASN
1	G	950	GLU
1	G	959	TRP
1	G	963	ASN
1	G	972	ARG
1	G	975	LEU
2	H	201	VAL
2	H	253	GLU
2	H	256	ARG
2	H	259	SER
2	H	273	GLU
2	H	281	LEU
2	H	287	LEU
2	H	297	VAL
2	H	301	ASP
2	H	322	LEU
2	H	336	LYS
2	H	343	THR
2	H	366	ARG
2	H	423	GLN
2	H	436	ARG
2	H	469	ARG
2	H	472	LEU
2	H	487	THR

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Mol	Chain	Res	Type
2	H	510	SER
2	H	517	PRO
2	H	518	LEU
2	H	521	VAL
2	H	525	LYS
2	H	529	LYS
2	H	531	LEU
2	H	551	LYS
2	H	552	ARG
2	H	565	LEU
2	H	575	ASP
2	H	579	PRO
2	H	586	ARG
2	H	587	LEU
2	H	591	ILE
2	H	656	THR
2	H	673	PHE
2	H	688	GLU
2	H	700	ARG
2	H	701	GLU
2	H	702	SER
2	H	707	ARG
2	H	711	VAL
2	H	716	THR
2	H	793	LEU
2	H	794	SER
2	H	800	LEU
2	H	808	GLU
2	H	810	ARG
2	H	867	ARG
2	H	869	THR
2	H	888	GLU
2	H	900	ASP
2	H	902	THR
2	H	904	SER
2	H	916	HIS
2	H	925	LEU
2	H	932	VAL
2	H	945	THR
2	H	947	LEU
2	H	956	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (144) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN
1	A	431	GLN
1	A	448	ASN
1	A	498	HIS
1	A	506	GLN
1	A	600	HIS
1	A	652	ASN
1	A	701	GLN
1	A	767	GLN
1	A	770	HIS
1	A	812	HIS
1	A	819	ASN
1	A	828	GLN
1	A	836	GLN
1	A	862	GLN
1	A	889	ASN
1	A	930	ASN
1	A	945	ASN
2	B	196	GLN
2	B	214	ASN
2	B	286	HIS
2	B	331	GLN
2	B	381	HIS
2	B	423	GLN
2	B	463	HIS
2	B	572	ASN
2	B	577	ASN
2	B	674	GLN
2	B	695	GLN
2	B	761	GLN
2	B	882	ASN
2	B	943	GLN
1	C	431	GLN
1	C	448	ASN
1	C	463	ASN
1	C	498	HIS
1	C	506	GLN
1	C	574	ASN
1	C	600	HIS
1	C	622	HIS
1	C	652	ASN
1	C	701	GLN

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Mol	Chain	Res	Type
1	C	708	GLN
1	C	709	HIS
1	C	767	GLN
1	C	812	HIS
1	C	819	ASN
1	C	828	GLN
1	C	836	GLN
1	C	862	GLN
1	C	889	ASN
2	D	196	GLN
2	D	214	ASN
2	D	286	HIS
2	D	331	GLN
2	D	381	HIS
2	D	423	GLN
2	D	463	HIS
2	D	522	ASN
2	D	572	ASN
2	D	577	ASN
2	D	674	GLN
2	D	695	GLN
2	D	746	GLN
2	D	761	GLN
2	D	792	GLN
2	D	882	ASN
2	D	897	ASN
2	D	941	HIS
2	D	943	GLN
1	E	294	ASN
1	E	431	GLN
1	E	448	ASN
1	E	463	ASN
1	E	498	HIS
1	E	506	GLN
1	E	600	HIS
1	E	622	HIS
1	E	652	ASN
1	E	701	GLN
1	E	767	GLN
1	E	770	HIS
1	E	812	HIS
1	E	828	GLN

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Mol	Chain	Res	Type
1	E	836	GLN
1	E	862	GLN
1	E	889	ASN
1	E	930	ASN
1	E	945	ASN
1	E	958	HIS
1	E	963	ASN
2	F	196	GLN
2	F	214	ASN
2	F	286	HIS
2	F	331	GLN
2	F	381	HIS
2	F	423	GLN
2	F	463	HIS
2	F	522	ASN
2	F	572	ASN
2	F	577	ASN
2	F	695	GLN
2	F	746	GLN
2	F	792	GLN
2	F	882	ASN
2	F	897	ASN
2	F	943	GLN
1	G	431	GLN
1	G	448	ASN
1	G	463	ASN
1	G	498	HIS
1	G	506	GLN
1	G	600	HIS
1	G	652	ASN
1	G	680	GLN
1	G	701	GLN
1	G	709	HIS
1	G	767	GLN
1	G	812	HIS
1	G	819	ASN
1	G	828	GLN
1	G	836	GLN
1	G	862	GLN
1	G	889	ASN
1	G	930	ASN
1	G	945	ASN

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Mol	Chain	Res	Type
1	G	963	ASN
2	H	196	GLN
2	H	214	ASN
2	H	286	HIS
2	H	331	GLN
2	H	381	HIS
2	H	423	GLN
2	H	463	HIS
2	H	522	ASN
2	H	572	ASN
2	H	577	ASN
2	H	674	GLN
2	H	695	GLN
2	H	761	GLN
2	H	792	GLN
2	H	882	ASN
2	H	897	ASN
2	H	943	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	F6P	B	980	-	15,16,16	1.02	1 (6%)	17,25,25	1.26	2 (11%)
4	FDP	A	1	-	19,20,20	0.90	0	30,32,32	0.74	0
4	FDP	E	5	-	19,20,20	0.91	0	30,32,32	0.87	1 (3%)
3	F6P	D	982	-	15,16,16	0.88	0	17,25,25	1.05	1 (5%)
3	F6P	E	988	-	15,16,16	0.83	0	17,25,25	1.10	1 (5%)
3	F6P	H	986	-	15,16,16	0.82	0	17,25,25	1.00	1 (5%)
3	F6P	G	988	-	15,16,16	1.07	1 (6%)	17,25,25	3.64	6 (35%)
4	FDP	G	7	-	19,20,20	0.90	0	30,32,32	0.79	1 (3%)
3	F6P	A	988	-	15,16,16	0.91	0	17,25,25	3.74	6 (35%)
3	F6P	C	988	-	15,16,16	0.89	0	17,25,25	1.17	1 (5%)
4	FDP	F	6	-	19,20,20	0.91	0	30,32,32	0.89	2 (6%)
4	FDP	C	3	-	19,20,20	0.93	0	30,32,32	0.79	0
3	F6P	F	984	-	15,16,16	0.88	0	17,25,25	1.16	1 (5%)
4	FDP	B	2	-	19,20,20	0.89	0	30,32,32	0.83	0
4	FDP	D	4	-	19,20,20	0.90	0	30,32,32	0.83	1 (3%)
4	FDP	H	8	-	19,20,20	0.91	0	30,32,32	0.91	1 (3%)

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
3	F6P	B	980	-	-	1/9/28/28	0/1/1/1
4	FDP	A	1	-	-	3/12/34/34	0/1/1/1
4	FDP	E	5	-	-	3/12/34/34	0/1/1/1
3	F6P	D	982	-	-	1/9/28/28	0/1/1/1
3	F6P	E	988	-	-	1/9/28/28	0/1/1/1
3	F6P	H	986	-	-	1/9/28/28	0/1/1/1
3	F6P	G	988	-	-	3/9/28/28	0/1/1/1
4	FDP	G	7	-	-	1/12/34/34	0/1/1/1
3	F6P	A	988	-	-	3/9/28/28	0/1/1/1
3	F6P	C	988	-	-	1/9/28/28	0/1/1/1
4	FDP	F	6	-	-	6/12/34/34	0/1/1/1
4	FDP	C	3	-	-	0/12/34/34	0/1/1/1
3	F6P	F	984	-	-	1/9/28/28	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FDP	B	2	-	-	0/12/34/34	0/1/1/1
4	FDP	D	4	-	-	2/12/34/34	0/1/1/1
4	FDP	H	8	-	-	1/12/34/34	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	988	F6P	O5-C2	-2.27	1.39	1.43
3	B	980	F6P	P-O3P	2.16	1.63	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	988	F6P	O3P-P-O6	-8.80	83.32	106.73
3	G	988	F6P	O3P-P-O6	-8.72	83.52	106.73
3	A	988	F6P	O3P-P-O1P	-6.79	84.12	110.68
3	A	988	F6P	O6-P-O1P	6.60	124.98	106.47
3	G	988	F6P	O6-P-O1P	6.53	124.80	106.47
3	A	988	F6P	O3P-P-O2P	-6.39	83.21	107.64
3	G	988	F6P	O3P-P-O1P	-6.37	85.74	110.68
3	G	988	F6P	O3P-P-O2P	-5.97	84.83	107.64
3	A	988	F6P	P-O6-C6	-3.77	107.90	118.30
3	A	988	F6P	O2P-P-O6	3.39	115.76	106.73
3	G	988	F6P	P-O6-C6	-3.39	108.96	118.30
3	C	988	F6P	P-O6-C6	-3.31	109.19	118.30
3	F	984	F6P	P-O6-C6	-3.23	109.39	118.30
3	E	988	F6P	P-O6-C6	-3.18	109.53	118.30
3	B	980	F6P	P-O6-C6	-3.05	109.90	118.30
3	D	982	F6P	P-O6-C6	-2.98	110.08	118.30
3	G	988	F6P	O2P-P-O6	2.93	114.54	106.73
3	H	986	F6P	P-O6-C6	-2.69	110.89	118.30
4	F	6	FDP	O6-P2-O4P	2.42	113.26	106.47
4	E	5	FDP	O6-P2-O4P	2.37	113.13	106.47
3	B	980	F6P	O5-C5-C6	-2.33	104.31	109.45
4	D	4	FDP	O6-P2-O4P	2.19	112.61	106.47
4	F	6	FDP	C2-O5-C5	-2.16	102.27	108.28
4	G	7	FDP	O6-P2-O4P	2.06	112.25	106.47
4	H	8	FDP	O5-C5-C6	2.00	113.86	109.45

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	5	FDP	C6-O6-P2-O4P
4	E	5	FDP	C6-O6-P2-O5P
4	E	5	FDP	C6-O6-P2-O6P
4	A	1	FDP	C6-O6-P2-O4P
4	A	1	FDP	C6-O6-P2-O5P
4	F	6	FDP	C6-O6-P2-O4P
4	F	6	FDP	C6-O6-P2-O6P
3	G	988	F6P	C6-O6-P-O1P
3	G	988	F6P	C6-O6-P-O3P
3	A	988	F6P	C6-O6-P-O3P
4	D	4	FDP	C6-O6-P2-O4P
4	D	4	FDP	C6-O6-P2-O6P
4	F	6	FDP	O5-C5-C6-O6
4	F	6	FDP	C5-C6-O6-P2
4	F	6	FDP	C2-O2-P1-O1P
4	F	6	FDP	C6-O6-P2-O5P
4	G	7	FDP	C6-O6-P2-O5P
3	A	988	F6P	C6-O6-P-O1P
3	B	980	F6P	O1-C1-C2-C3
3	D	982	F6P	O1-C1-C2-C3
3	E	988	F6P	O1-C1-C2-C3
3	H	986	F6P	O1-C1-C2-C3
3	G	988	F6P	O1-C1-C2-C3
3	A	988	F6P	O1-C1-C2-C3
3	C	988	F6P	O1-C1-C2-C3
3	F	984	F6P	O1-C1-C2-C3
4	A	1	FDP	O5-C5-C6-O6
4	H	8	FDP	O1-C1-C2-C3

There are no ring outliers.

14 monomers are involved in 42 short contacts:

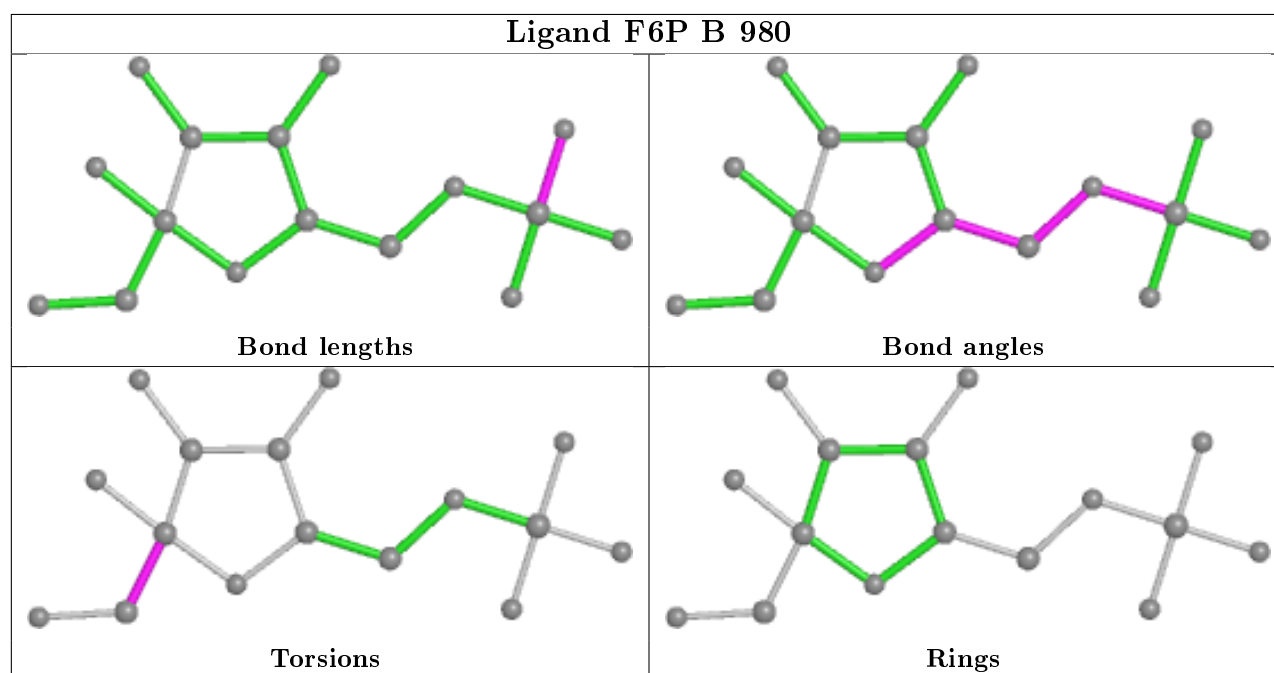
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	980	F6P	4	0
4	A	1	FDP	6	0
3	D	982	F6P	3	0
3	E	988	F6P	2	0
3	H	986	F6P	5	0
3	G	988	F6P	2	0
3	A	988	F6P	4	0
3	C	988	F6P	1	0
4	F	6	FDP	3	0
4	C	3	FDP	1	0

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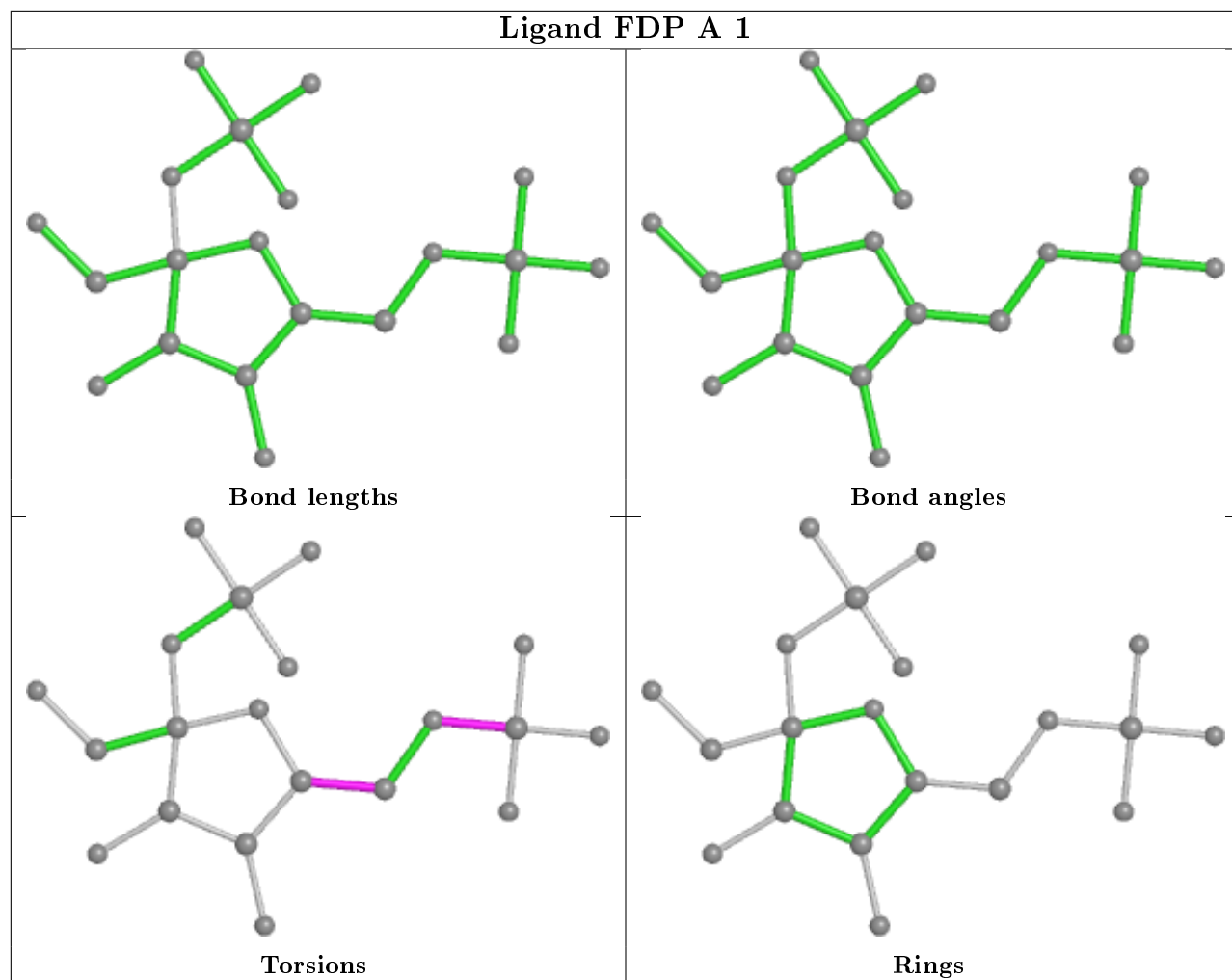
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	984	F6P	4	0
4	B	2	FDP	3	0
4	D	4	FDP	2	0
4	H	8	FDP	2	0

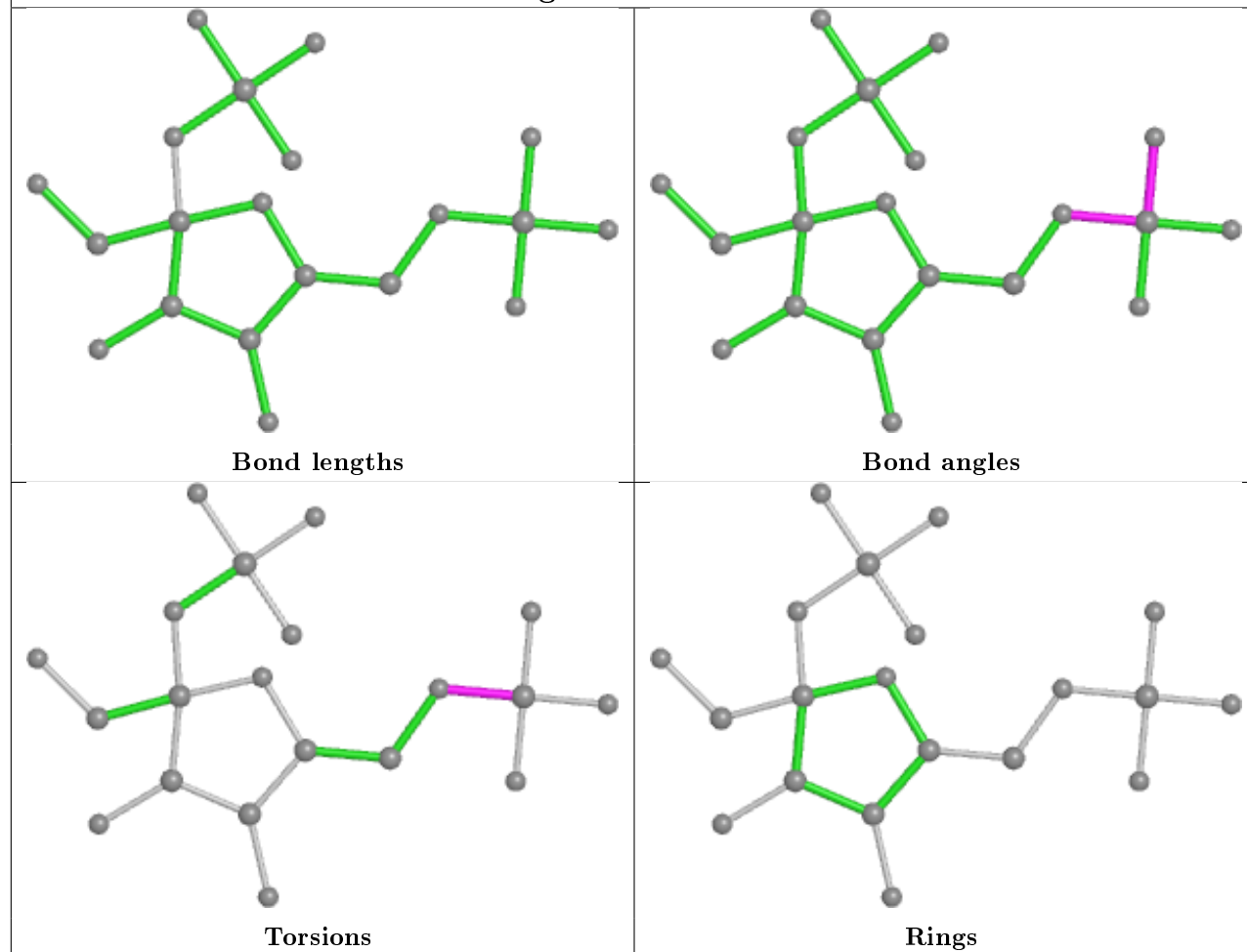
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



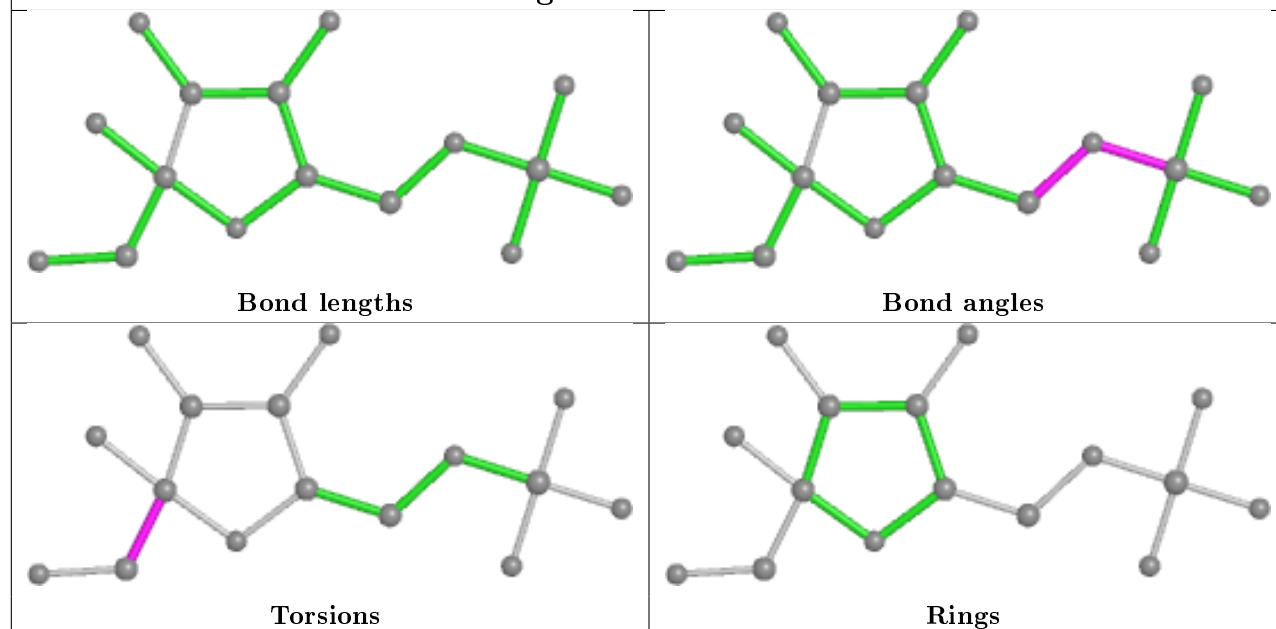
Ligand FDP A 1



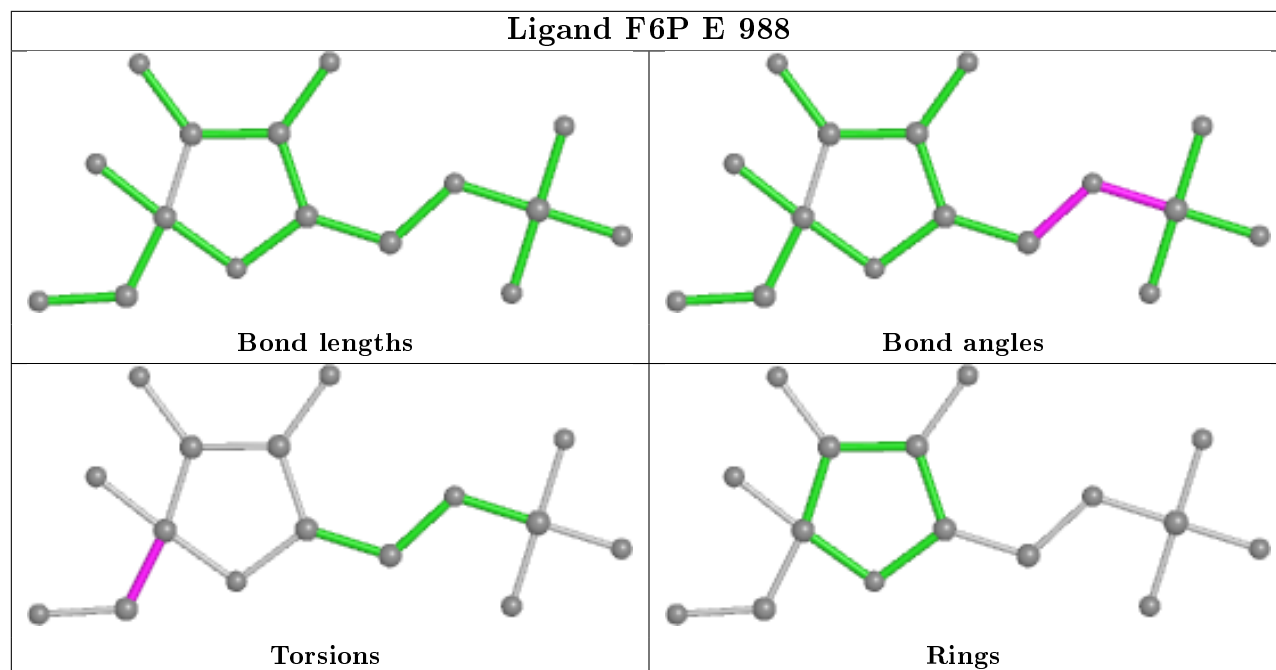
Ligand FDP E 5



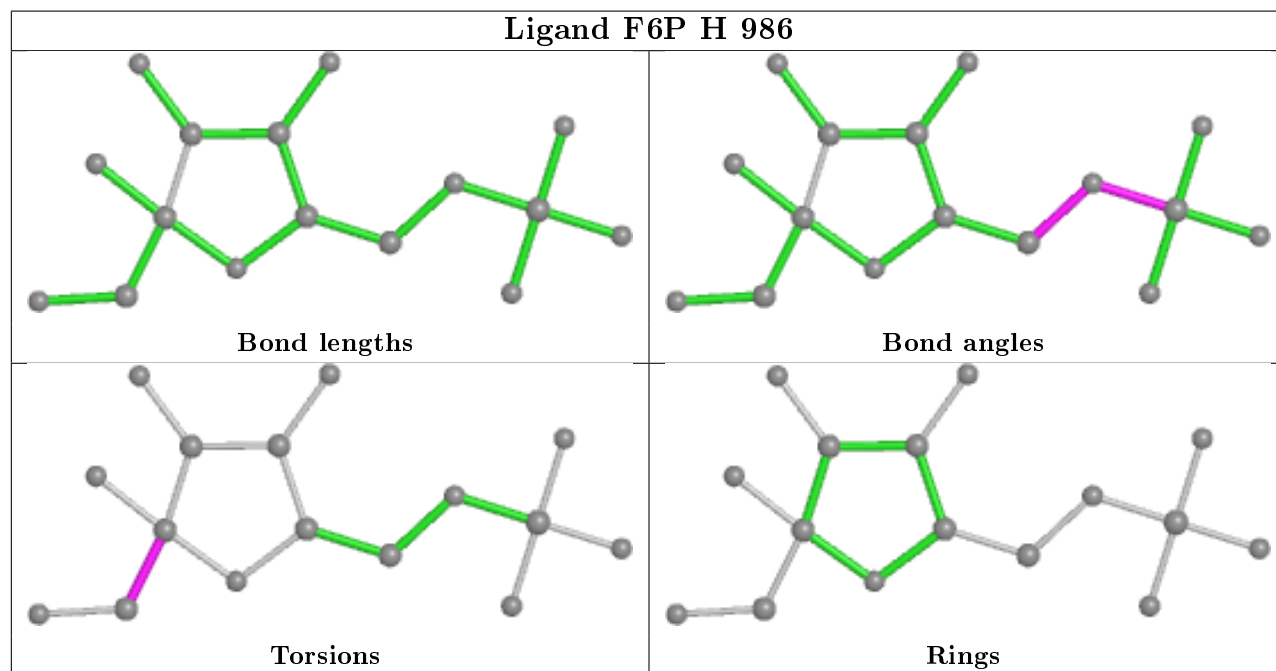
Ligand F6P D 982



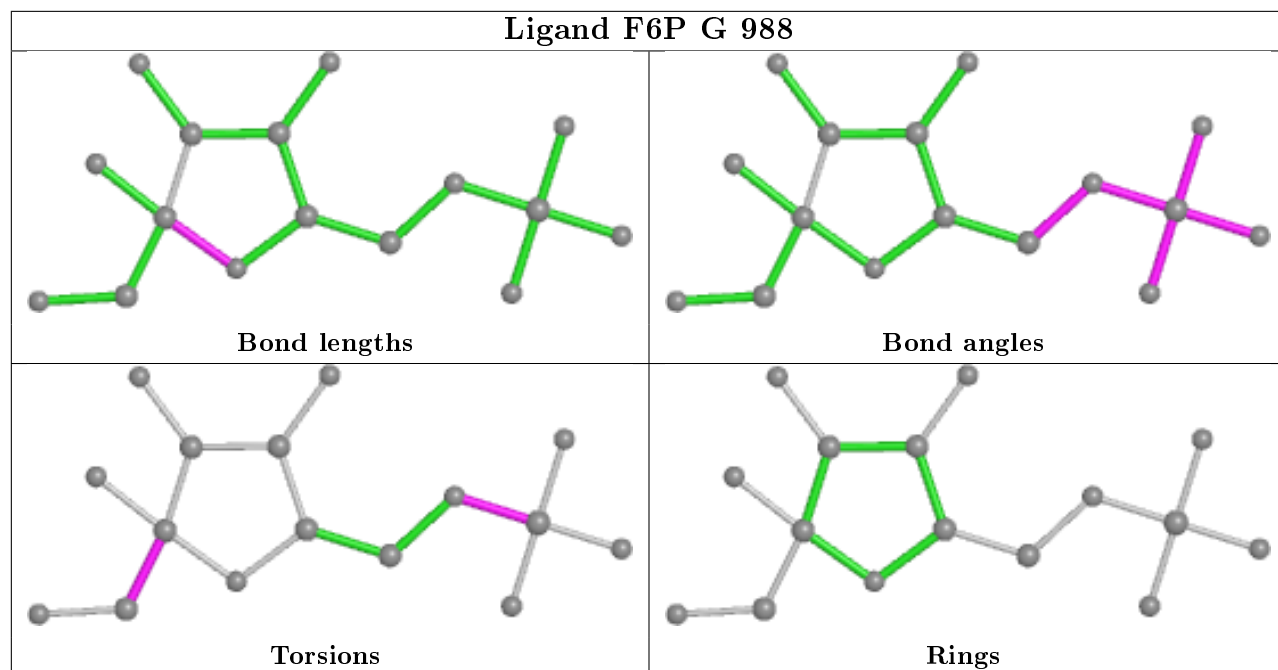
Ligand F6P E 988



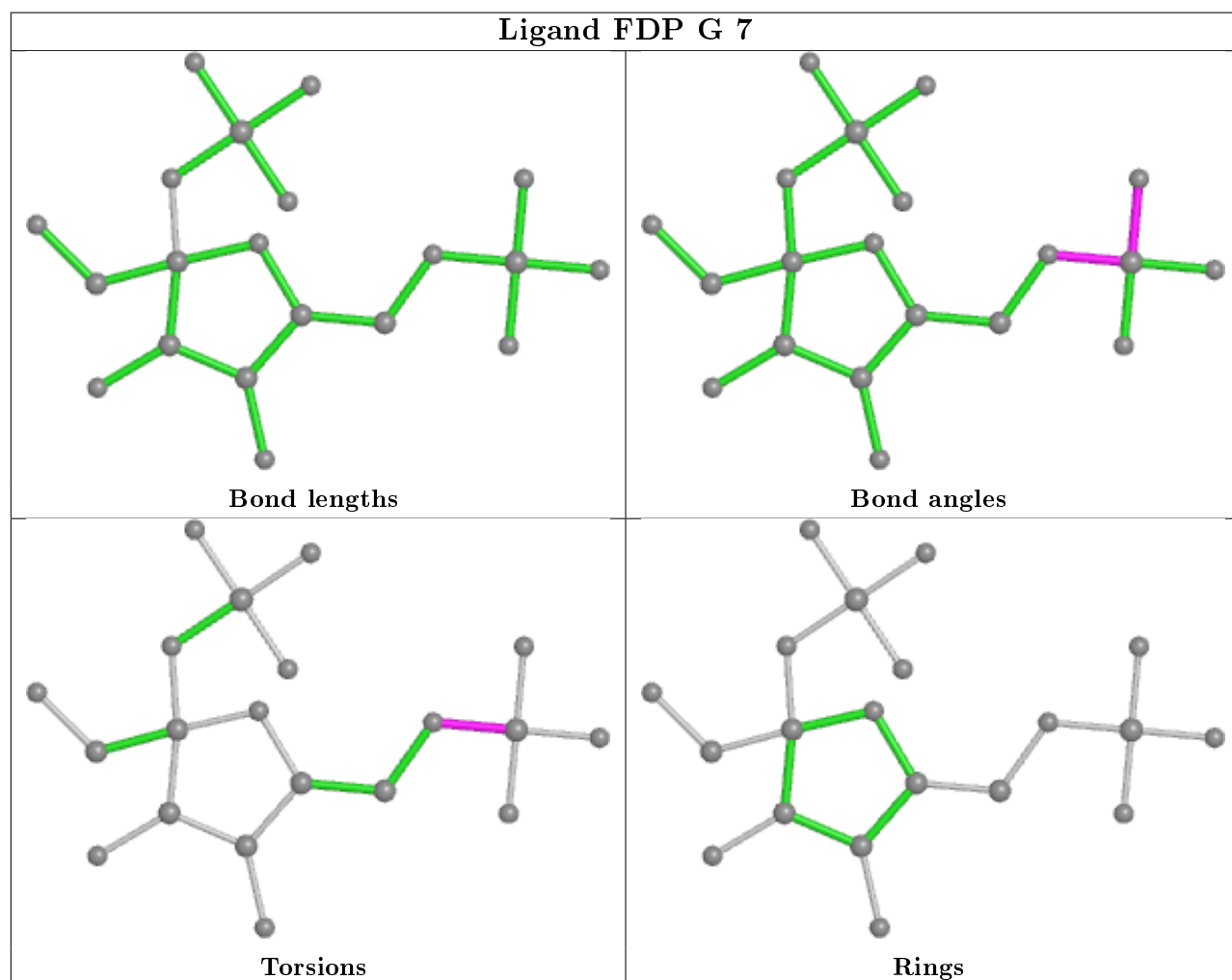
Ligand F6P H 986



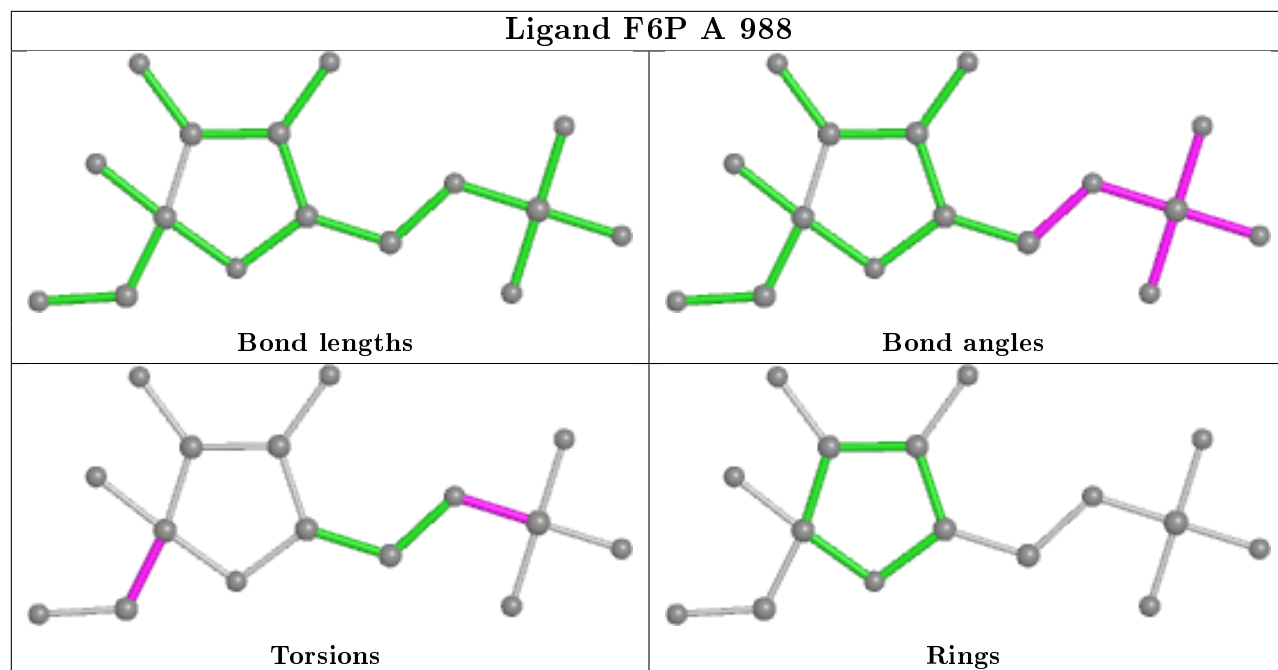
Ligand F6P G 988



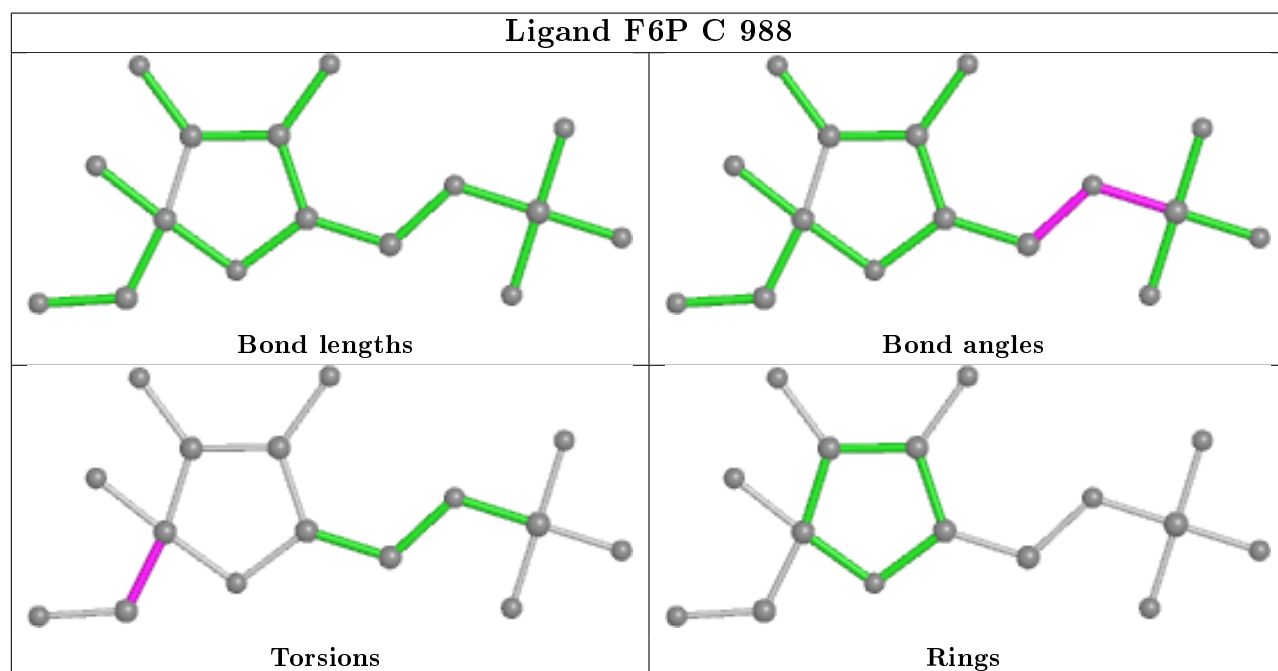
Ligand FDP G 7



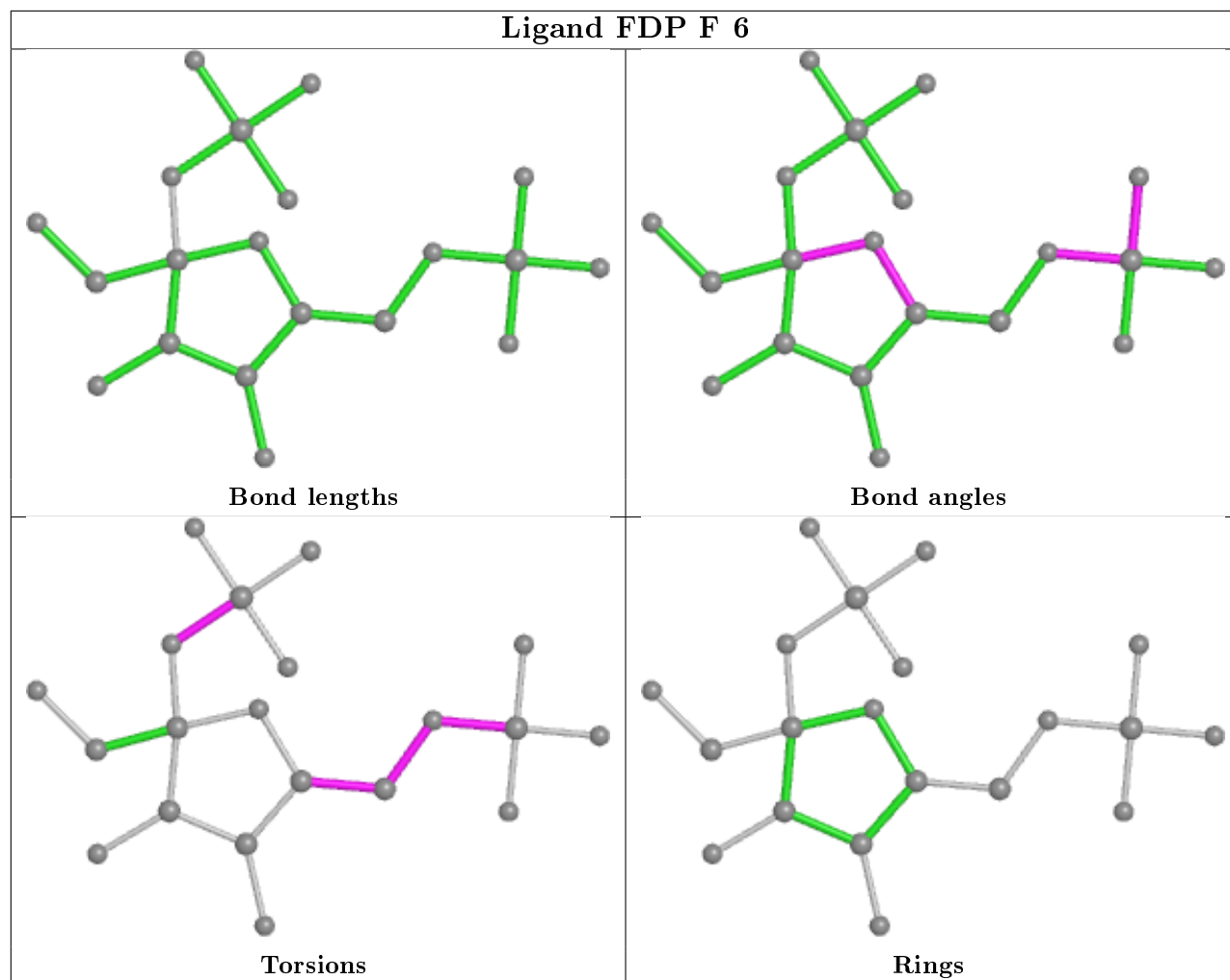
Ligand F6P A 988



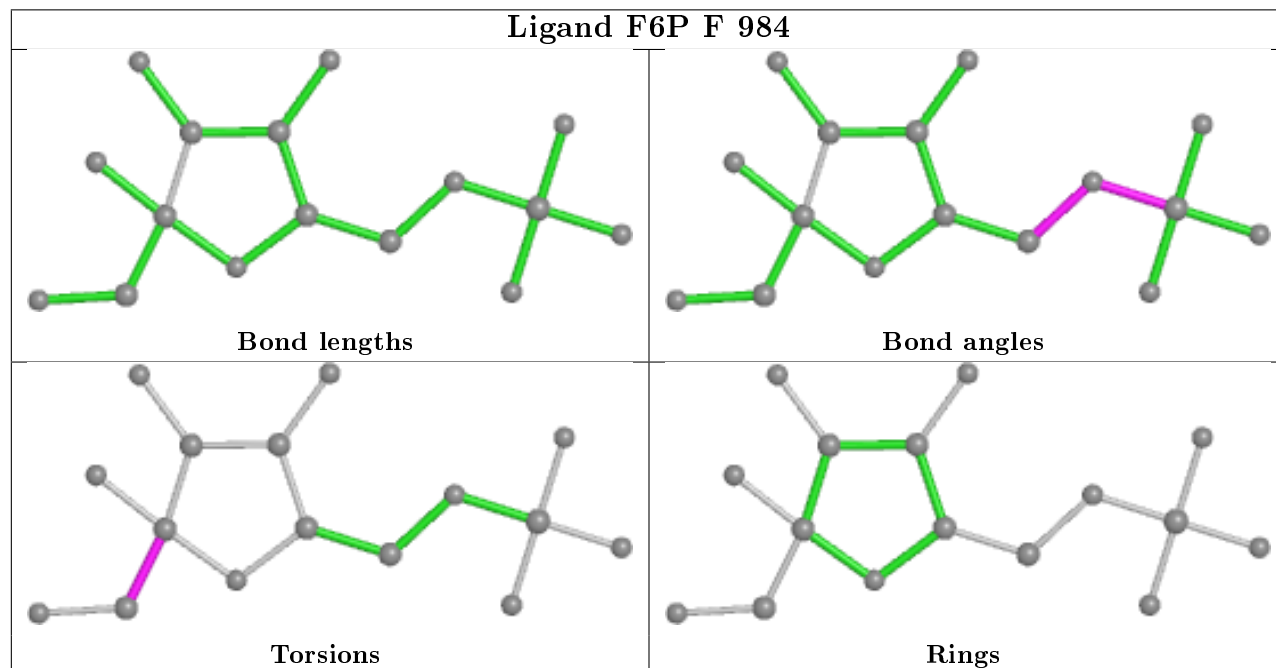
Ligand F6P C 988

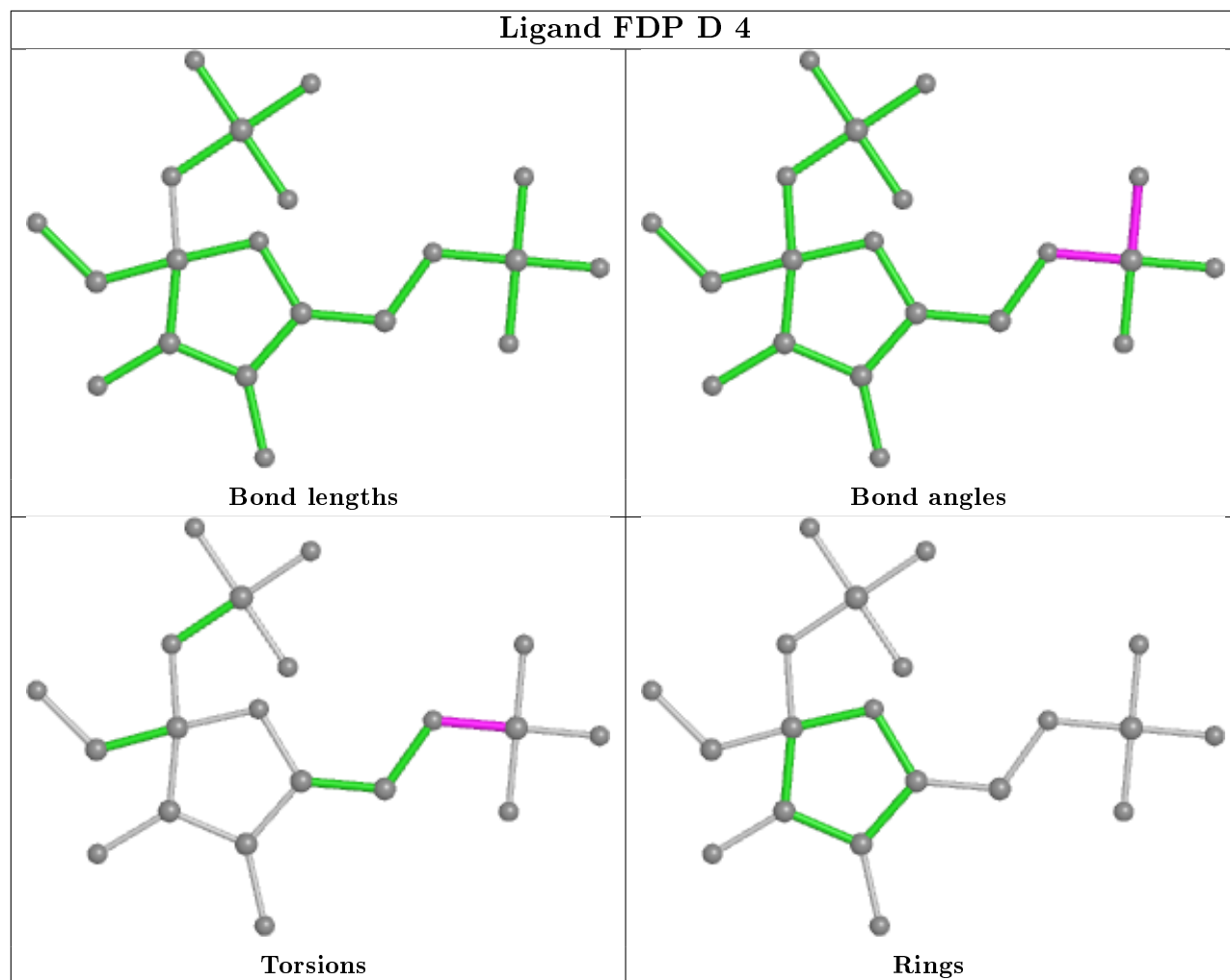


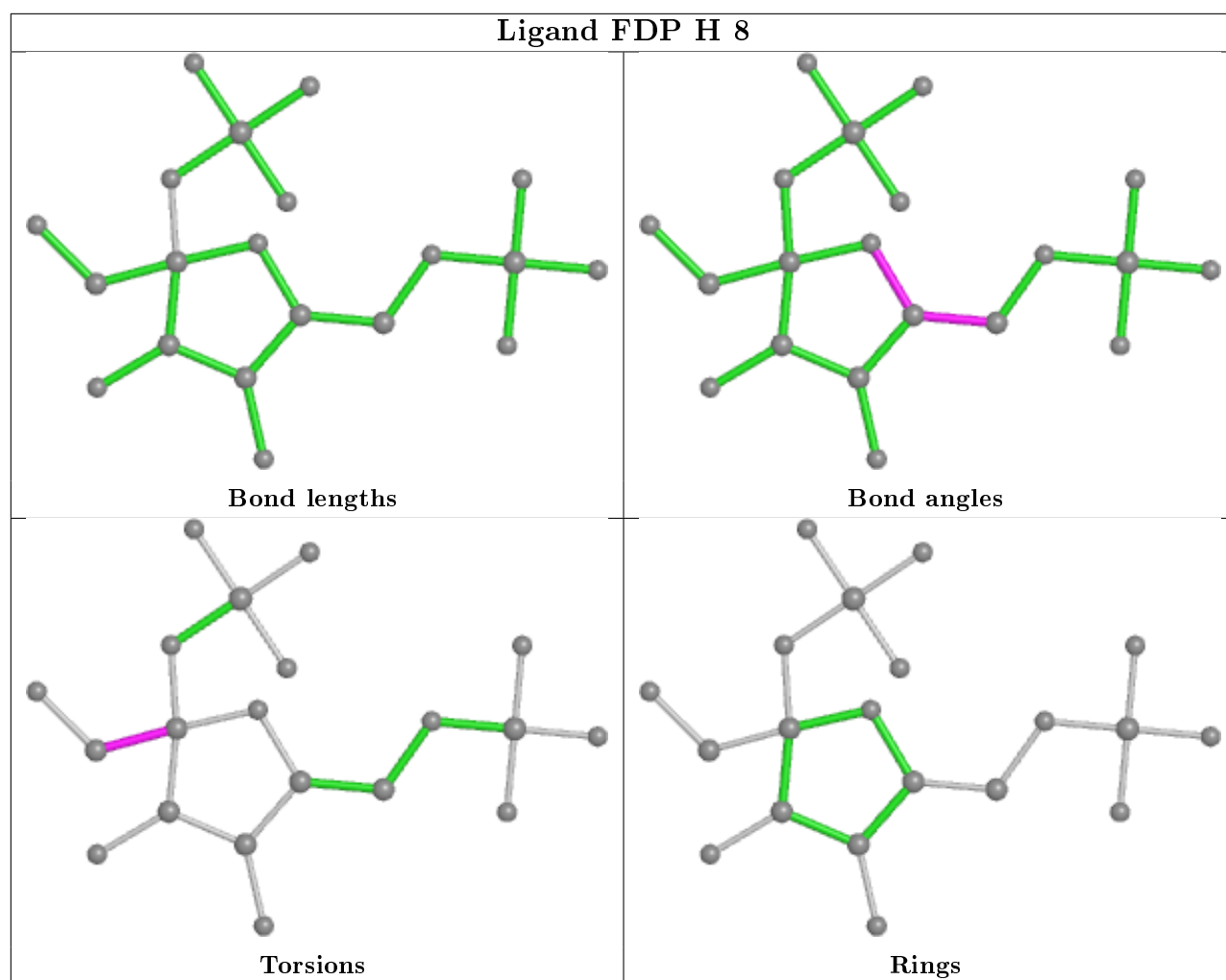
Ligand FDP F 6



Ligand F6P F 984







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	750/787 (95%)	0.00	26 (3%)	44	38	22, 61, 81, 81	67 (8%)
1	C	750/787 (95%)	0.04	35 (4%)	31	28	16, 56, 81, 81	49 (6%)
1	E	752/787 (95%)	-0.07	21 (2%)	53	49	22, 53, 81, 81	58 (7%)
1	G	744/787 (94%)	-0.12	27 (3%)	42	37	19, 52, 81, 81	60 (8%)
2	B	763/766 (99%)	0.04	25 (3%)	46	41	27, 70, 81, 81	88 (11%)
2	D	761/766 (99%)	-0.15	15 (1%)	65	63	20, 60, 81, 81	54 (7%)
2	F	762/766 (99%)	-0.08	22 (2%)	51	47	25, 61, 81, 81	61 (8%)
2	H	763/766 (99%)	-0.31	6 (0%)	86	86	21, 47, 79, 81	37 (4%)
All	All	6045/6212 (97%)	-0.08	177 (2%)	51	47	16, 57, 81, 81	474 (7%)

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	812	HIS	7.0
1	C	815	GLY	7.0
1	G	327	ASP	6.4
1	G	326	VAL	6.1
1	C	949	VAL	5.9
1	C	813	ASP	5.7
2	F	895	ASN	5.6
1	G	342	PRO	5.1
1	G	338	GLU	4.9
1	G	325	LEU	4.9
2	F	896	PHE	4.6
2	D	941	HIS	4.6
2	F	893	GLU	4.6
1	C	805	LEU	4.5
1	C	587	LEU	4.5
1	A	949	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	812	HIS	4.3
1	E	325	LEU	4.1
2	F	271	CYS	4.0
1	C	955	PHE	4.0
1	G	341	ALA	4.0
2	F	582	PRO	4.0
2	D	895	ASN	3.9
1	C	954	GLY	3.8
1	C	829	ALA	3.8
2	F	581	LEU	3.8
1	E	811	ARG	3.6
1	A	340	VAL	3.6
1	G	322	TRP	3.6
2	F	553	ALA	3.5
2	F	892	ALA	3.5
1	C	556	ASP	3.5
2	F	545	ILE	3.5
2	D	417	ALA	3.4
2	B	472	LEU	3.4
2	D	666	LEU	3.4
1	G	323	PRO	3.4
1	C	845	ALA	3.4
1	C	552	ILE	3.4
2	B	417	ALA	3.4
2	F	325	ASN	3.4
1	E	326	VAL	3.3
1	A	587	LEU	3.3
1	E	552	ILE	3.3
1	E	980	ALA	3.3
1	A	813	ASP	3.2
1	G	320	HIS	3.2
1	A	279	SER	3.2
1	G	330	VAL	3.1
1	A	467	ALA	3.1
2	B	896	PHE	3.1
1	C	814	LYS	3.1
1	C	554	ASN	3.1
2	H	891	ALA	3.1
1	A	334	ARG	3.1
1	E	544	LEU	3.0
1	C	589	PRO	3.0
1	G	339	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	277	ALA	3.0
1	C	948	ASN	3.0
1	A	335	PHE	3.0
1	E	819	ASN	3.0
1	A	978	GLU	2.9
1	G	754	ALA	2.9
1	A	517	PHE	2.9
1	C	560	ALA	2.9
1	G	788	TYR	2.8
1	C	788	TYR	2.8
2	D	926	TYR	2.8
1	E	948	ASN	2.8
1	C	797	ALA	2.8
1	G	757	THR	2.8
2	F	899	ASP	2.8
1	A	470	VAL	2.8
1	A	333	GLY	2.7
1	G	347	SER	2.7
2	D	897	ASN	2.7
2	B	466	LEU	2.7
2	F	938	LYS	2.7
1	G	302	ALA	2.7
1	C	846	SER	2.6
2	B	538	THR	2.6
2	F	542	ALA	2.6
1	G	824	VAL	2.6
1	E	250	ARG	2.6
2	D	603	SER	2.6
1	E	345	ASN	2.6
2	B	666	LEU	2.6
1	G	948	ASN	2.6
2	H	933	SER	2.5
2	D	665	ASP	2.5
1	G	321	GLU	2.5
1	E	548	VAL	2.5
1	G	324	SER	2.5
2	B	887	ALA	2.5
2	D	892	ALA	2.5
1	A	979	VAL	2.5
1	C	282	PHE	2.5
2	B	811	GLY	2.4
1	A	521	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	339	GLU	2.4
2	B	545	ILE	2.4
2	F	702	SER	2.4
1	E	560	ALA	2.4
1	C	557	PHE	2.4
2	H	892	ALA	2.4
1	A	815	GLY	2.4
2	B	273	GLU	2.4
1	C	541	SER	2.4
1	A	479	LEU	2.4
1	C	298	GLN	2.3
2	D	807	ALA	2.3
2	B	541	VAL	2.3
1	E	808	GLU	2.3
2	D	545	ILE	2.3
1	E	821	LYS	2.3
1	C	830	SER	2.3
1	G	848	GLY	2.3
1	E	327	ASP	2.3
1	G	343	TYR	2.3
2	B	455	THR	2.3
1	C	606	ALA	2.3
1	A	288	ARG	2.3
2	H	896	PHE	2.3
1	A	947	THR	2.3
2	B	895	ASN	2.3
1	C	951	LEU	2.3
1	G	286	GLU	2.3
2	F	933	SER	2.2
1	A	287	GLY	2.2
1	C	329	LEU	2.2
1	G	340	VAL	2.2
2	F	703	TYR	2.2
2	B	956	LYS	2.2
2	F	329	ASN	2.2
2	B	886	ILE	2.2
2	D	664	ALA	2.2
2	B	279	GLY	2.2
1	E	733	SER	2.2
2	D	452	ALA	2.2
2	H	931	GLU	2.2
1	A	955	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	803	ILE	2.2
2	B	582	PRO	2.2
2	B	703	TYR	2.2
2	B	888	GLU	2.2
2	F	808	GLU	2.2
1	A	325	LEU	2.2
1	C	943	TRP	2.2
1	G	552	ILE	2.2
1	E	333	GLY	2.1
1	C	945	ASN	2.1
1	A	332	GLU	2.1
1	C	893	GLU	2.1
2	F	664	ALA	2.1
2	B	356	ALA	2.1
2	F	243	GLY	2.1
2	F	931	GLU	2.1
1	G	279	SER	2.1
1	C	950	GLU	2.1
2	B	702	SER	2.1
1	C	553	GLU	2.1
1	C	254	TYR	2.1
2	D	418	THR	2.1
2	B	911	GLY	2.1
2	B	576	HIS	2.1
2	D	537	LEU	2.1
2	F	541	VAL	2.1
2	B	915	SER	2.0
1	E	722	THR	2.0
1	G	465	VAL	2.0
1	C	563	LEU	2.0
1	A	948	ASN	2.0
2	H	890	ARG	2.0
1	E	807	LYS	2.0
1	E	949	VAL	2.0
2	B	957	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

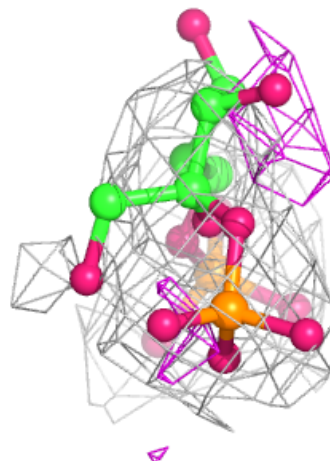
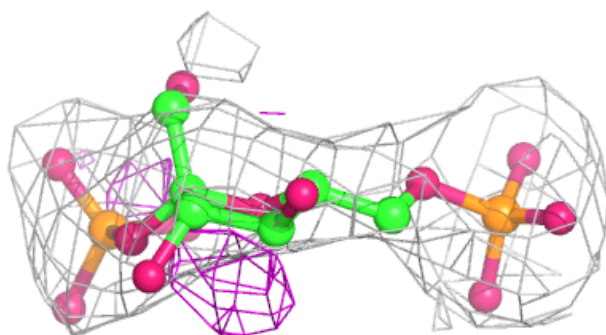
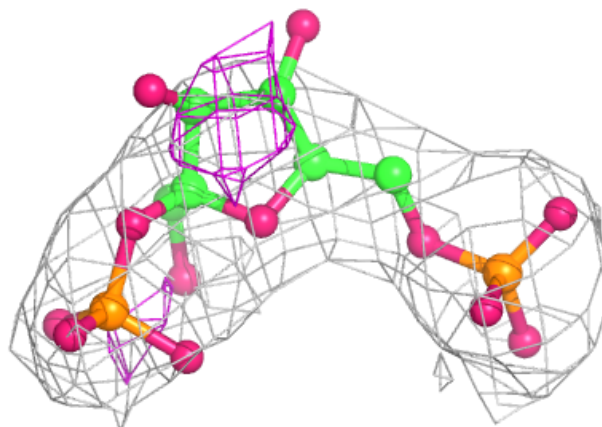
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FDP	C	3	20/20	0.85	0.35	79,82,82,82	0
4	FDP	H	8	20/20	0.85	0.33	81,82,82,82	0
4	FDP	F	6	20/20	0.89	0.27	81,82,82,82	0
3	F6P	A	988	16/16	0.91	0.17	79,82,82,82	0
4	FDP	A	1	20/20	0.91	0.21	77,82,82,82	0
4	FDP	G	7	20/20	0.91	0.18	80,82,82,82	0
3	F6P	C	988	16/16	0.92	0.19	75,78,80,80	0
3	F6P	B	980	16/16	0.93	0.16	77,80,82,82	0
3	F6P	E	988	16/16	0.94	0.19	62,66,66,68	0
3	F6P	D	982	16/16	0.94	0.22	65,67,70,71	0
4	FDP	E	5	20/20	0.95	0.15	66,70,74,74	0
3	F6P	F	984	16/16	0.95	0.18	56,57,63,64	0
4	FDP	B	2	20/20	0.95	0.17	65,68,70,71	0
4	FDP	D	4	20/20	0.96	0.14	52,54,56,57	0
3	F6P	G	988	16/16	0.96	0.20	61,62,64,68	0
3	F6P	H	986	16/16	0.97	0.16	41,47,47,49	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.

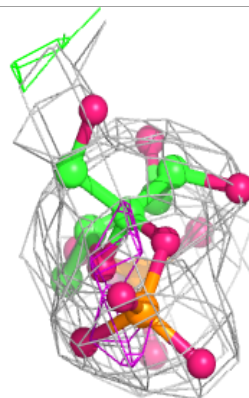
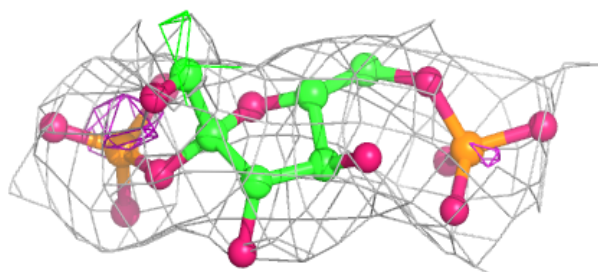
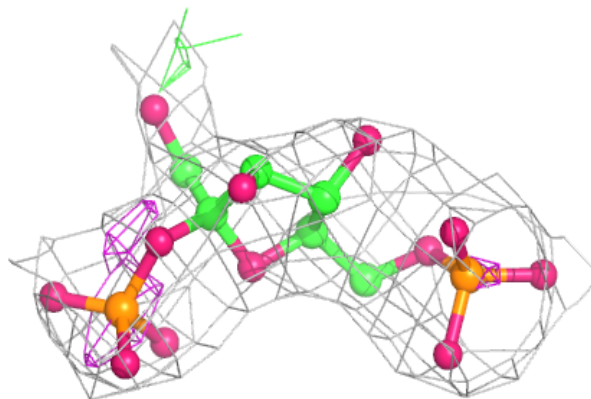
Electron density around FDP H 8:

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

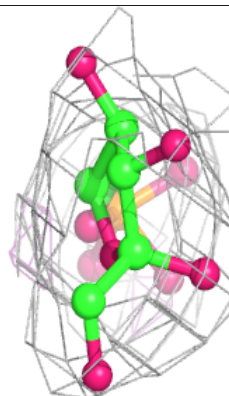
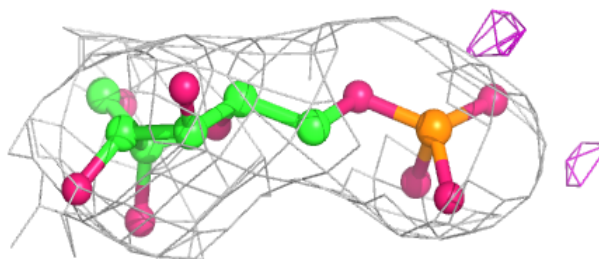
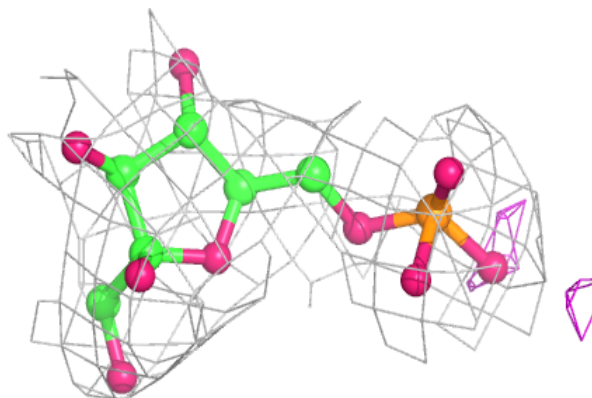


Electron density around FDP F 6:

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

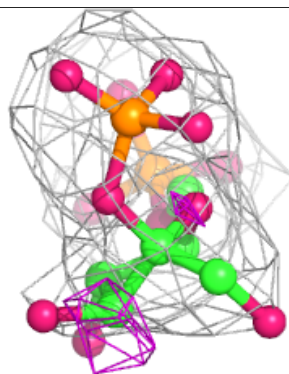
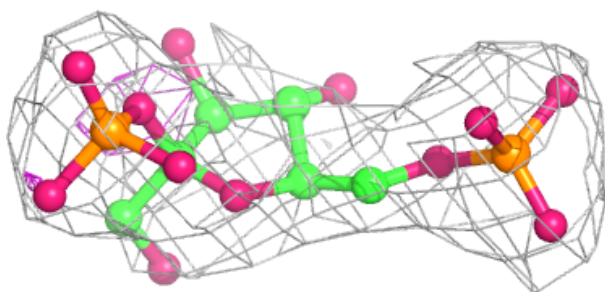
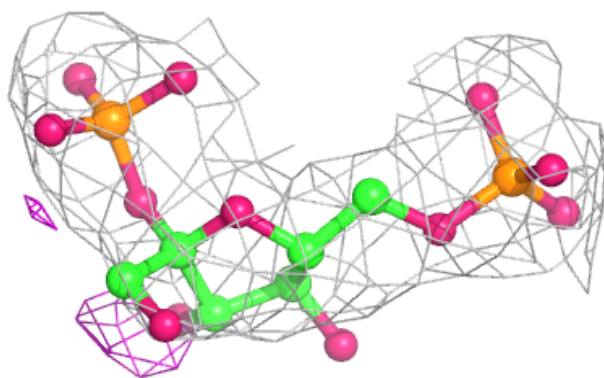
**Electron density around F6P A 988:**

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



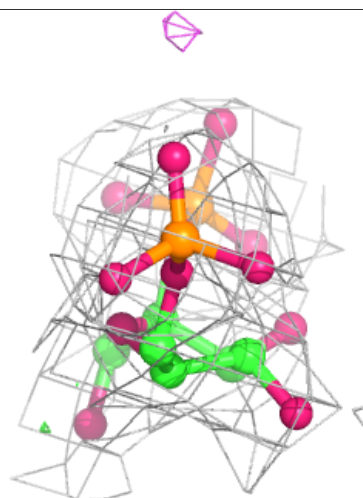
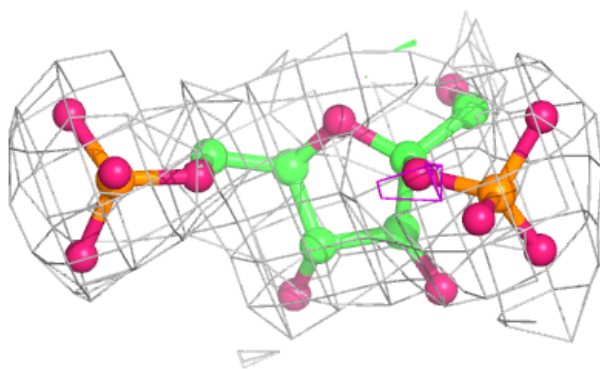
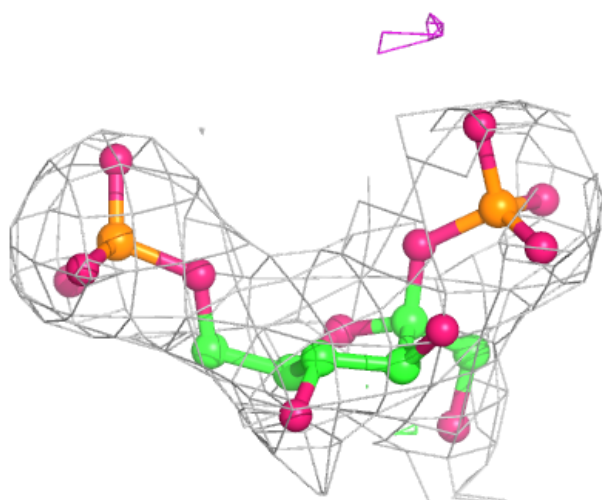
Electron density around FDP A 1:

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



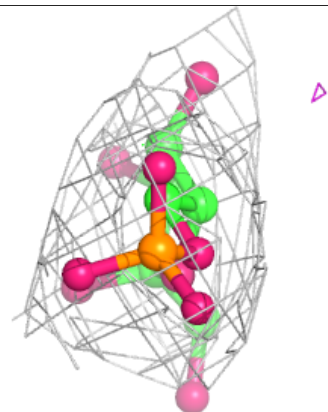
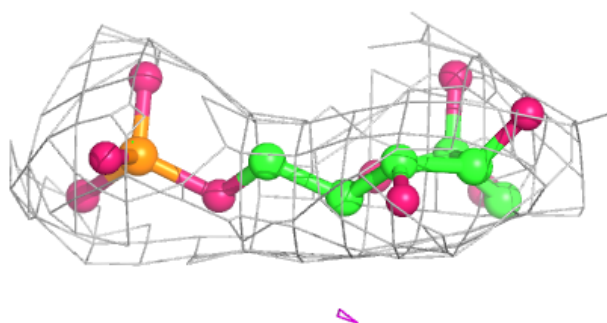
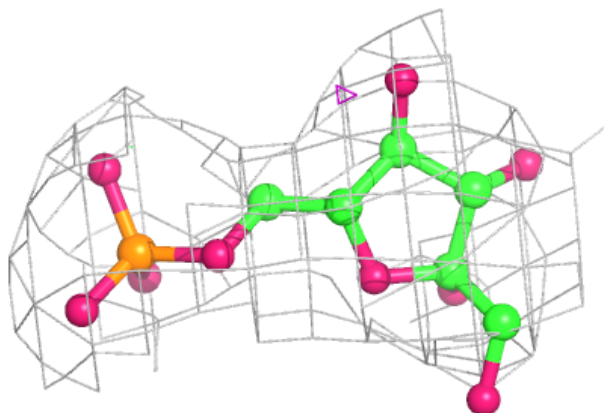
Electron density around FDP G 7:

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

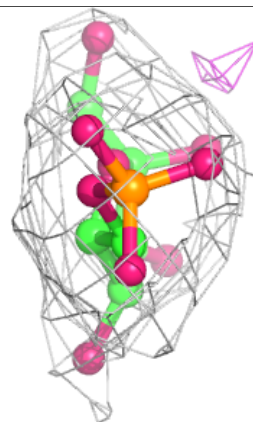
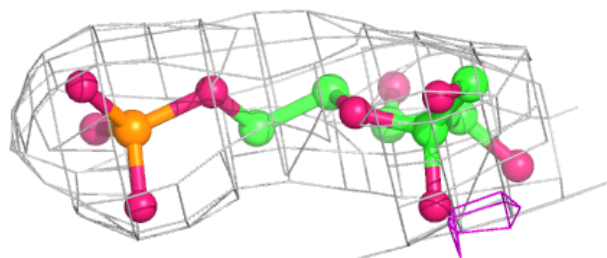
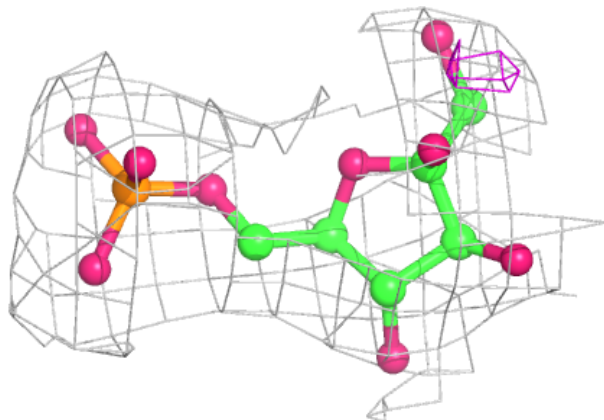


Electron density around F6P C 988:

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

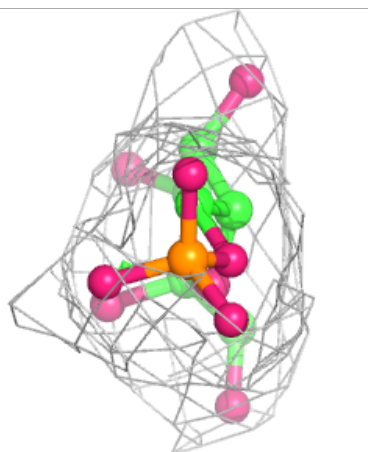
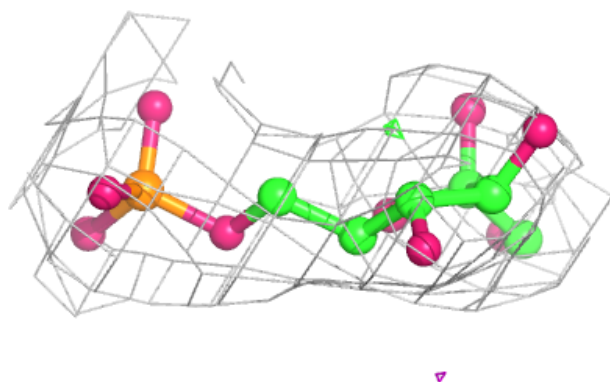
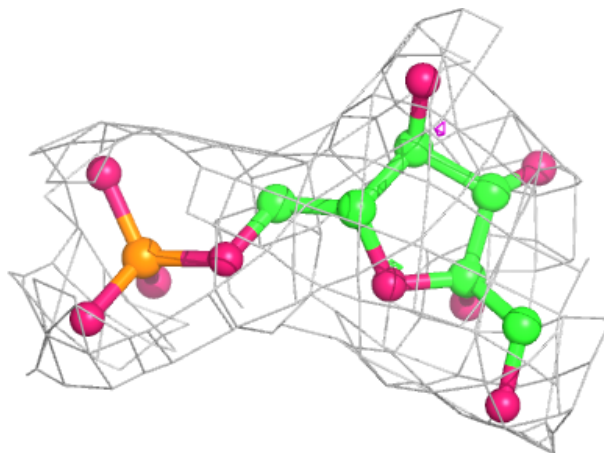
**Electron density around F6P B 980:**

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



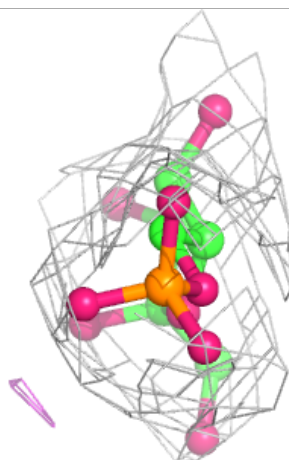
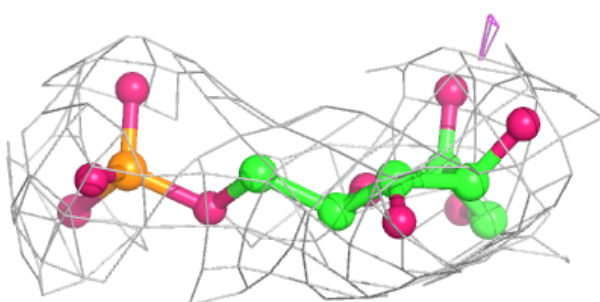
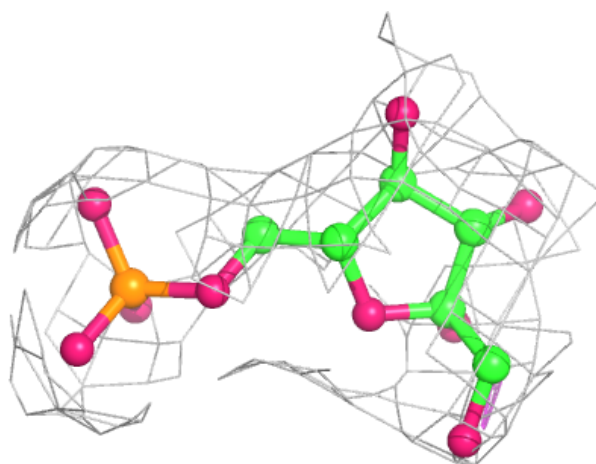
Electron density around F6P E 988:

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



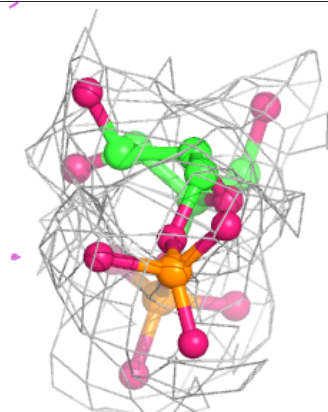
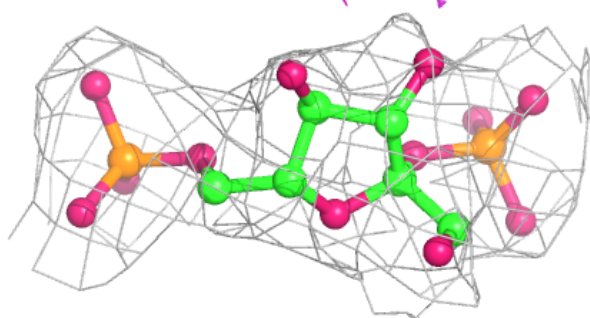
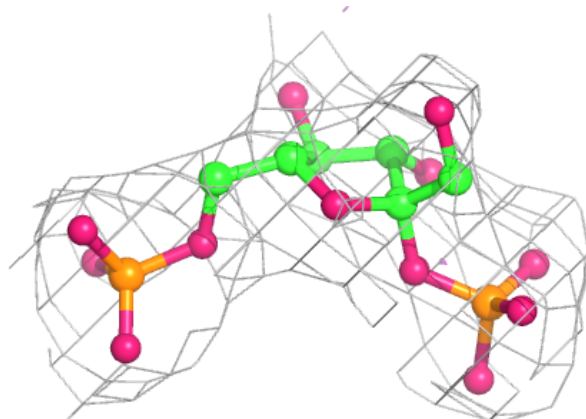
Electron density around F6P D 982:

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



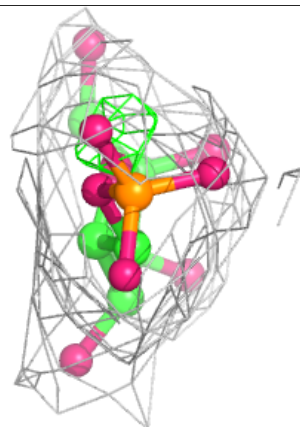
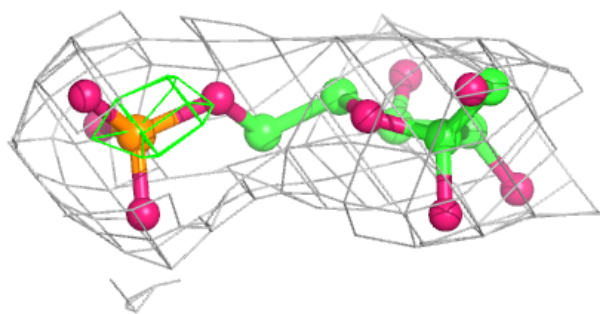
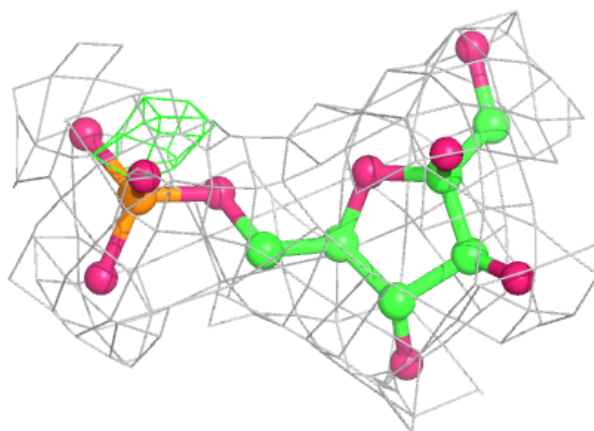
Electron density around FDP E 5:

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



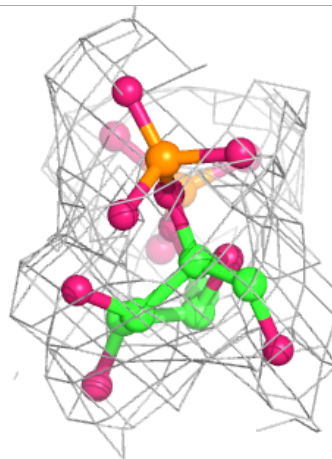
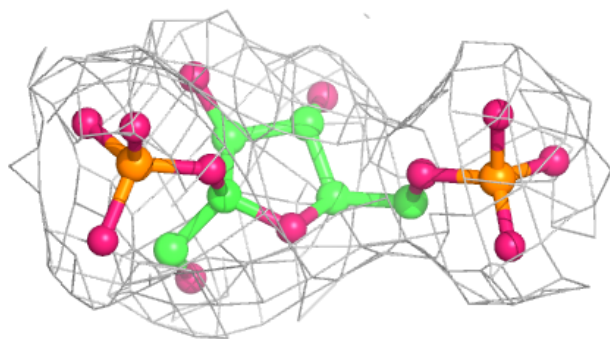
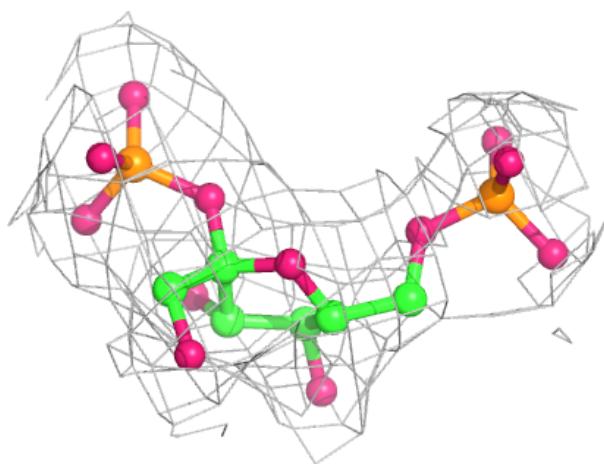
Electron density around F6P F 984:

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



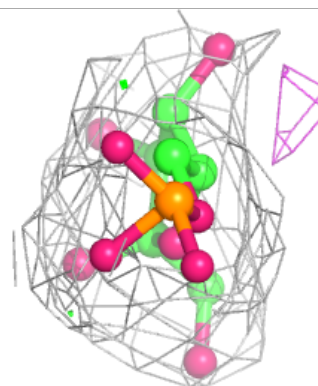
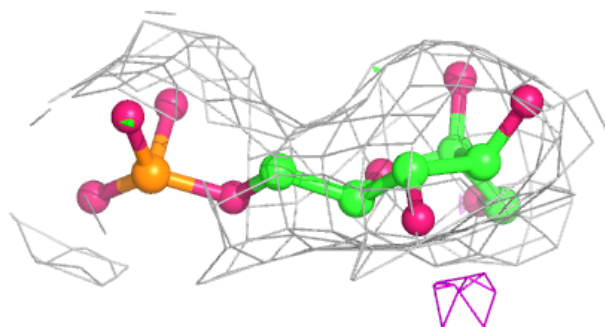
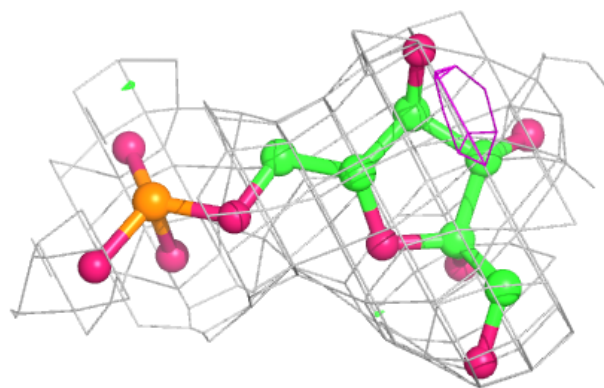
Electron density around FDP D 4:

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



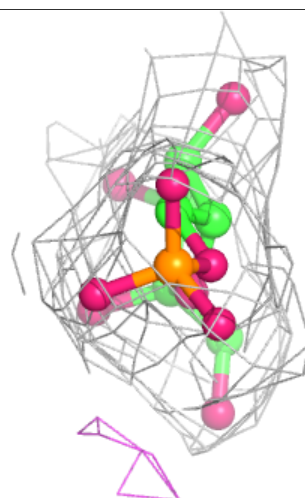
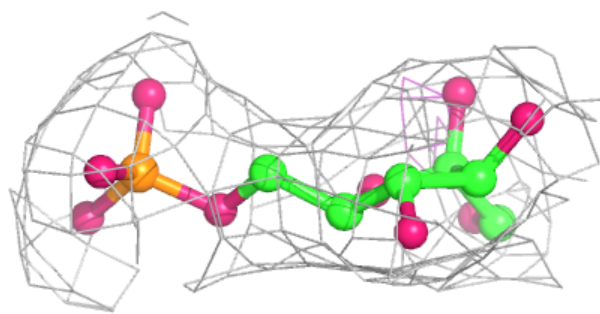
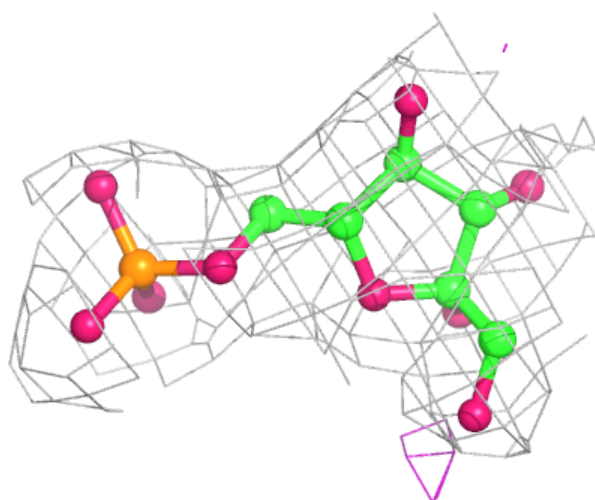
Electron density around F6P G 988:

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



Electron density around F6P H 986:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.