



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:06 PM UTC

PDB ID : 3O8O / pdb_00003o8o
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 types of validation reports are described at

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

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

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

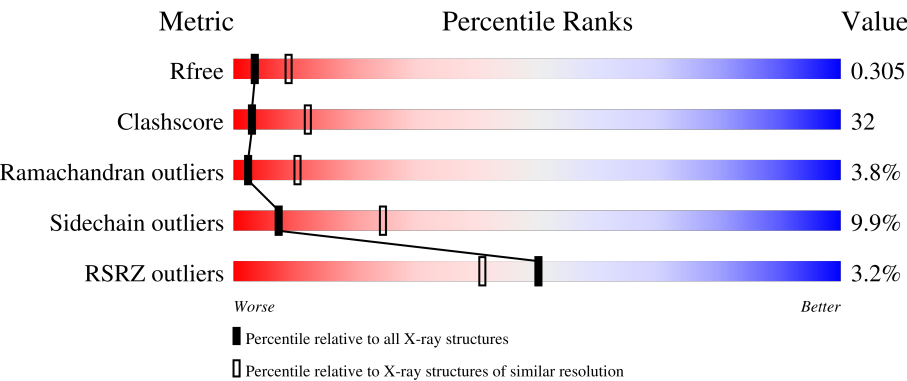
1 Overall quality at a glance i

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	787	4% 48%37%8%• 5%
1	C	787	4% 47%39%8%• 5%
1	E	787	2% 49%37%9%• •
1	G	787	5% 49%35%8%• 5%
2	B	766	5% 51%39%8%•

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Mol	Chain	Length	Quality of chain
2	D	766	2% 51% 40% 8%
2	F	766	% 51% 39% 8%
2	H	766	2% 51% 40% 8%

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.

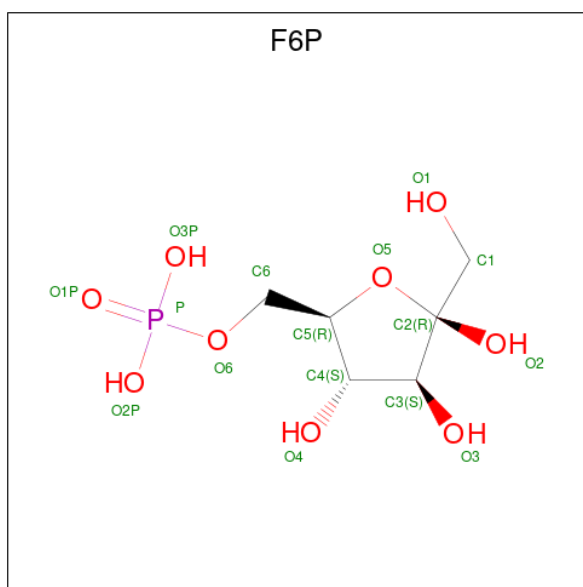
- Molecule 1 is a protein called 6-phosphofructokinase subunit alpha.

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.

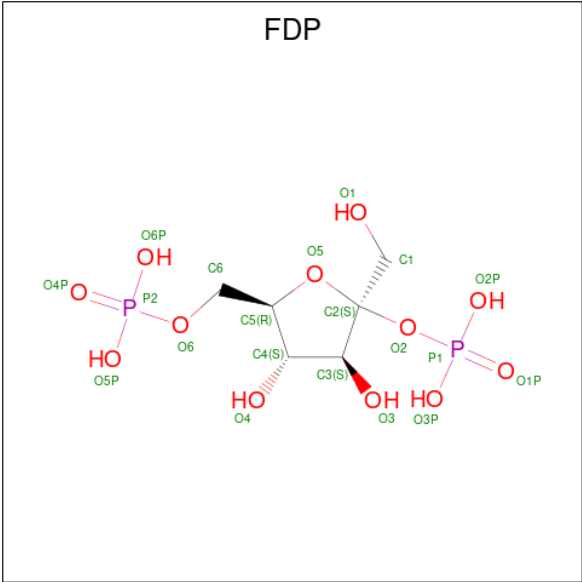
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	763	Total	C	N	O	S	364	0	0
			5834	3652	1034	1118	30			
2	D	763	Total	C	N	O	S	266	0	0
			5834	3652	1034	1118	30			
2	F	762	Total	C	N	O	S	279	0	0
			5827	3647	1033	1117	30			
2	H	763	Total	C	N	O	S	173	0	0
			5834	3652	1034	1118	30			

- Molecule 3 is 6-O-phosphono-beta-D-fructofuranose (CCD ID: 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 (CCD ID: FDP) (formula: $C_6H_{14}O_{12}P_2$).

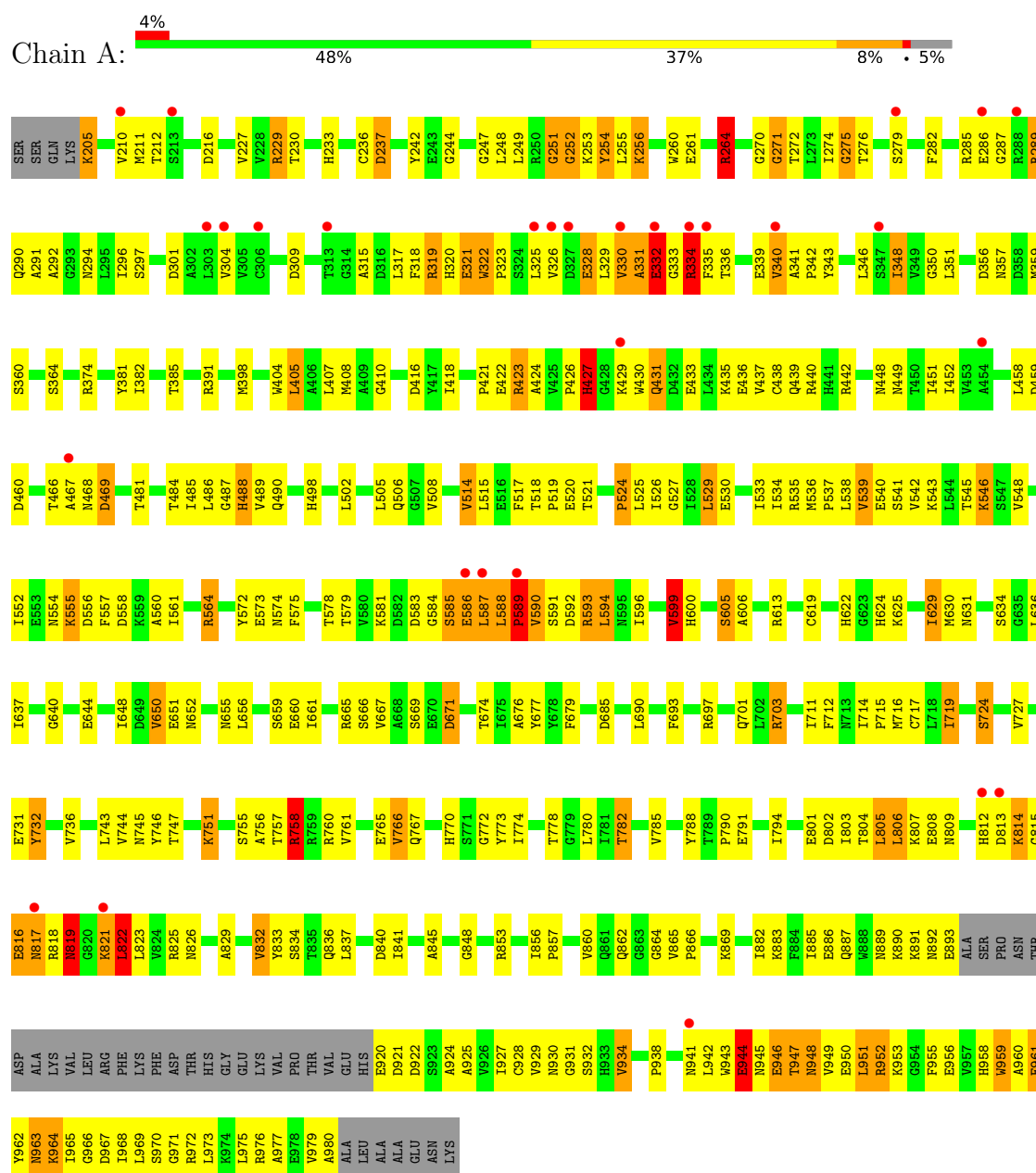


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		
4	E	1	Total	C	O	P	0	0
			20	6	12	2		
4	F	1	Total	C	O	P	0	0
			20	6	12	2		
4	G	1	Total	C	O	P	0	0
			20	6	12	2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

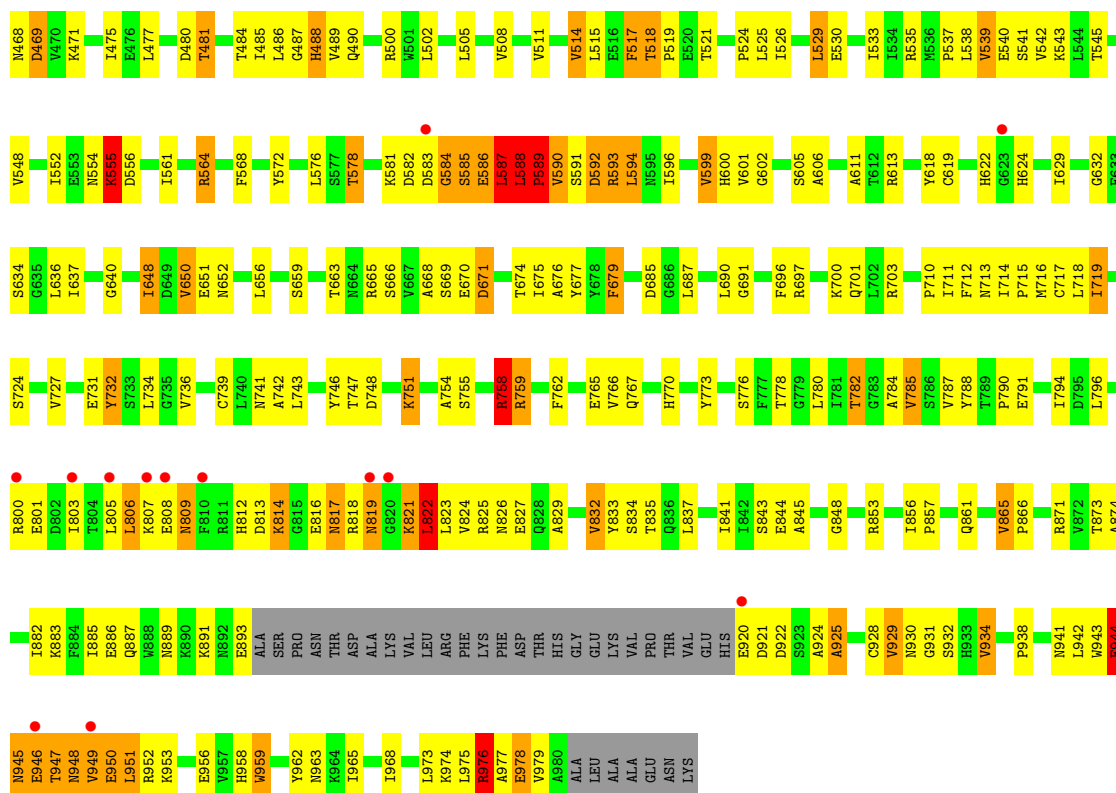
3 Residue-property plots

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.

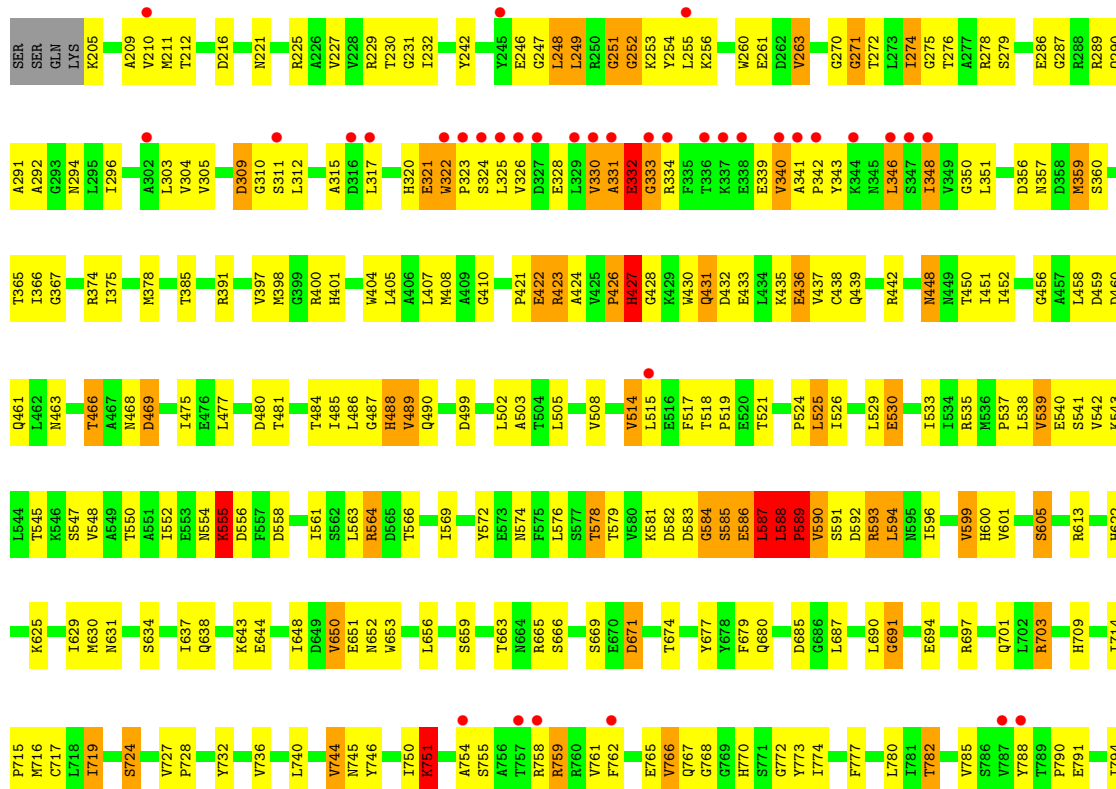
- Molecule 1: 6-phosphofructokinase subunit alpha

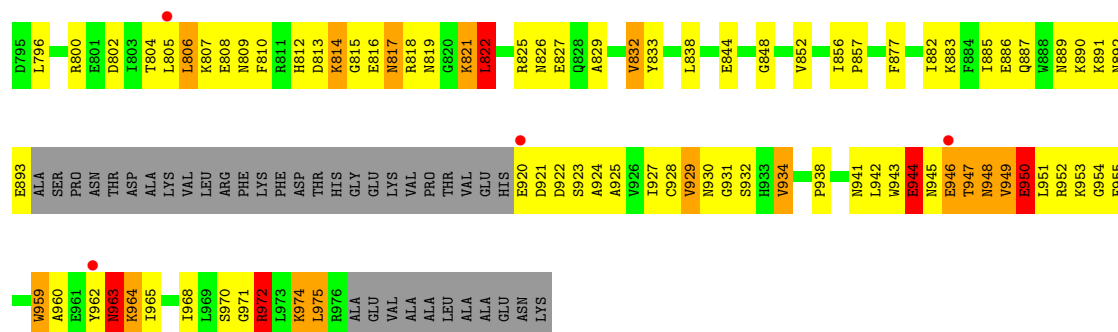


- Molecule 1: 6-phosphofructokinase subunit alpha

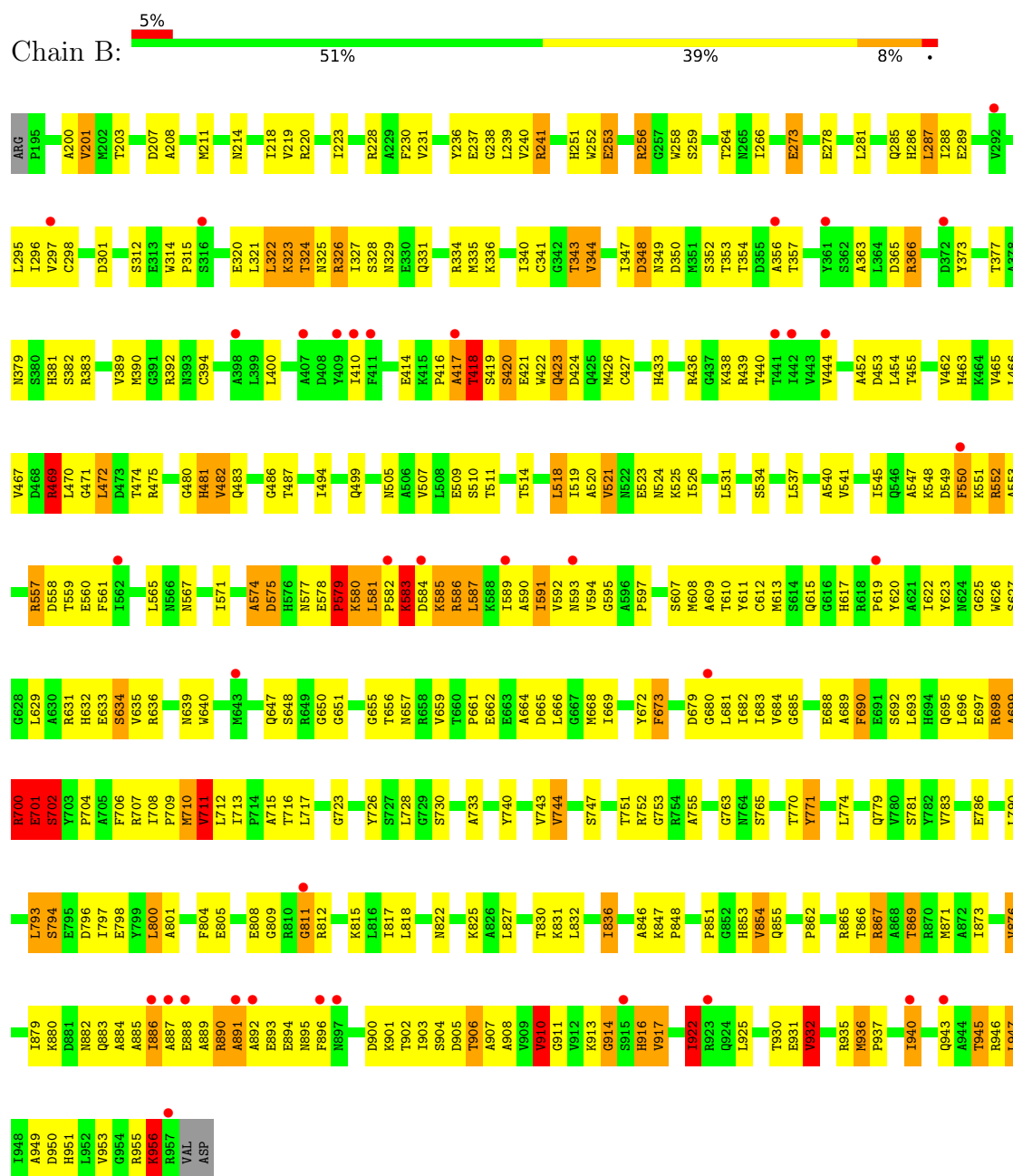


• Molecule 1: 6-phosphofructokinase subunit alpha

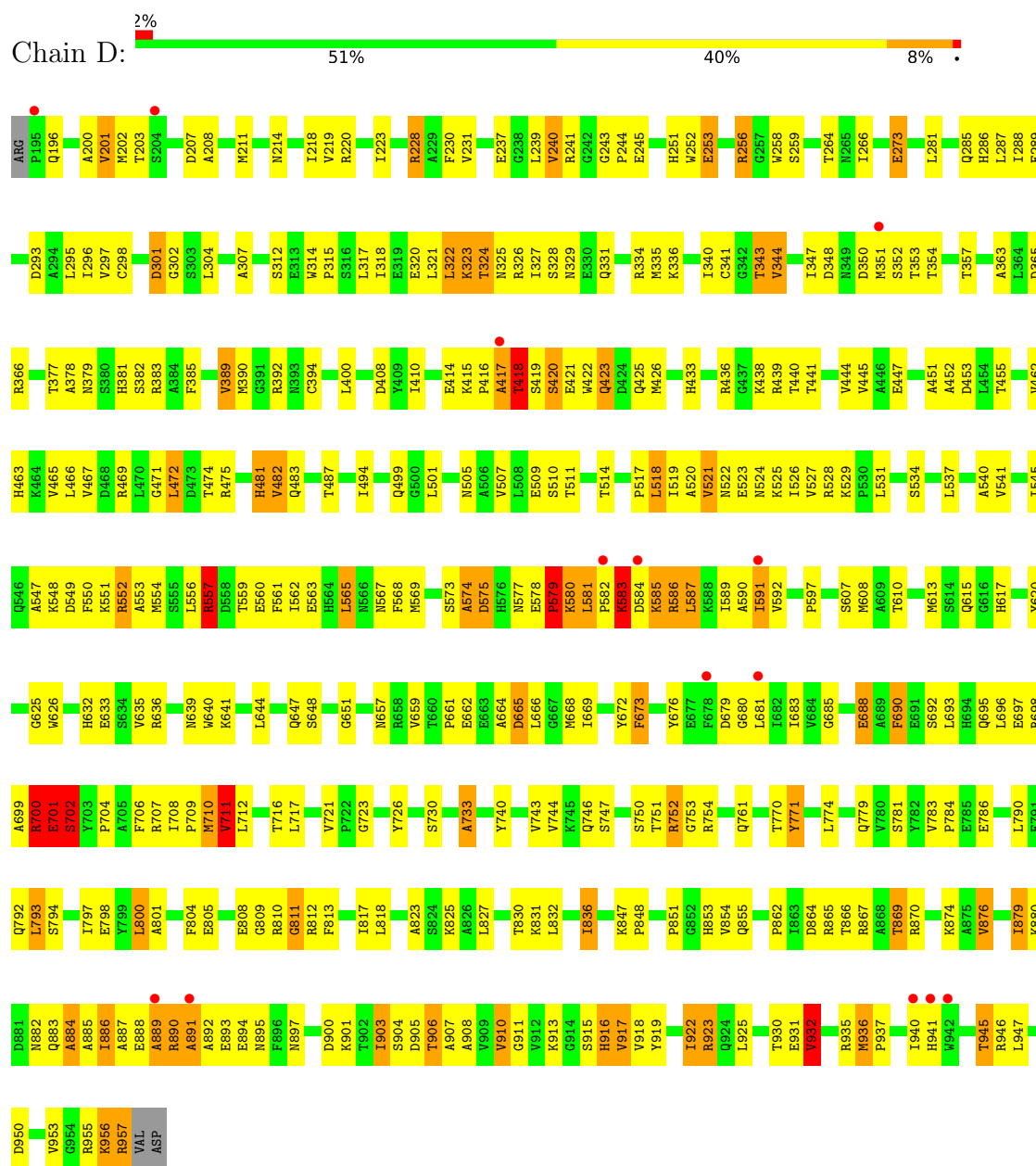




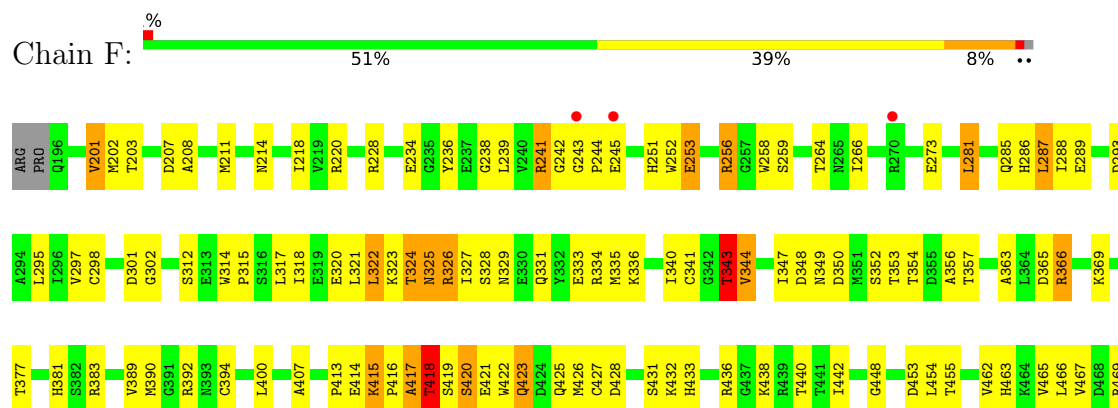
• Molecule 2: 6-phosphofructokinase subunit beta

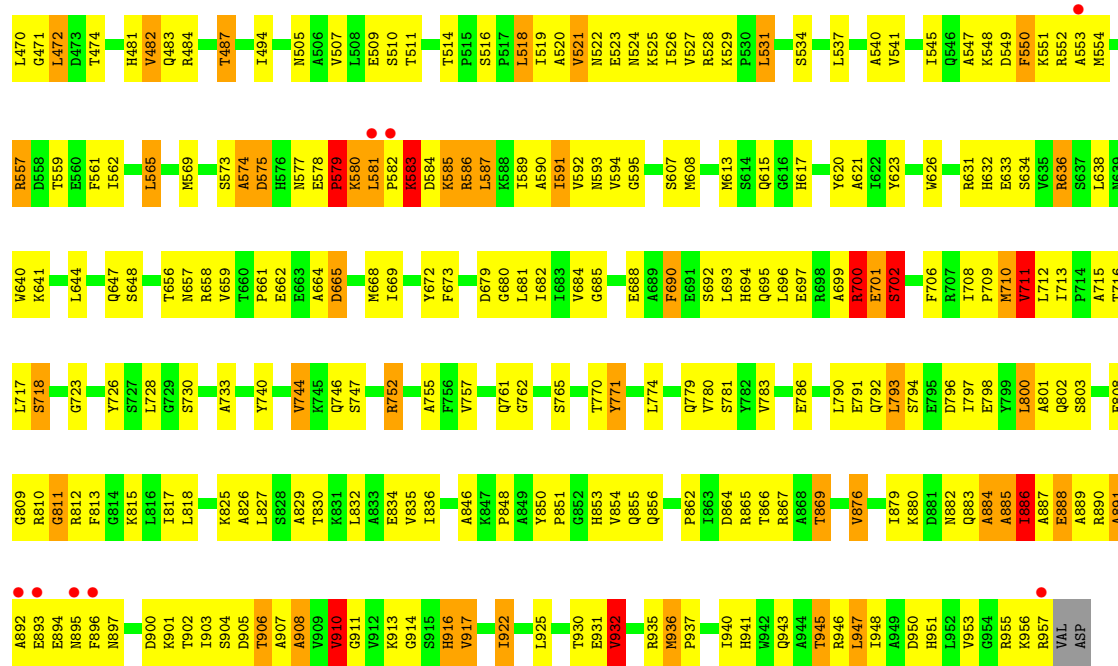


• Molecule 2: 6-phosphofructokinase subunit beta

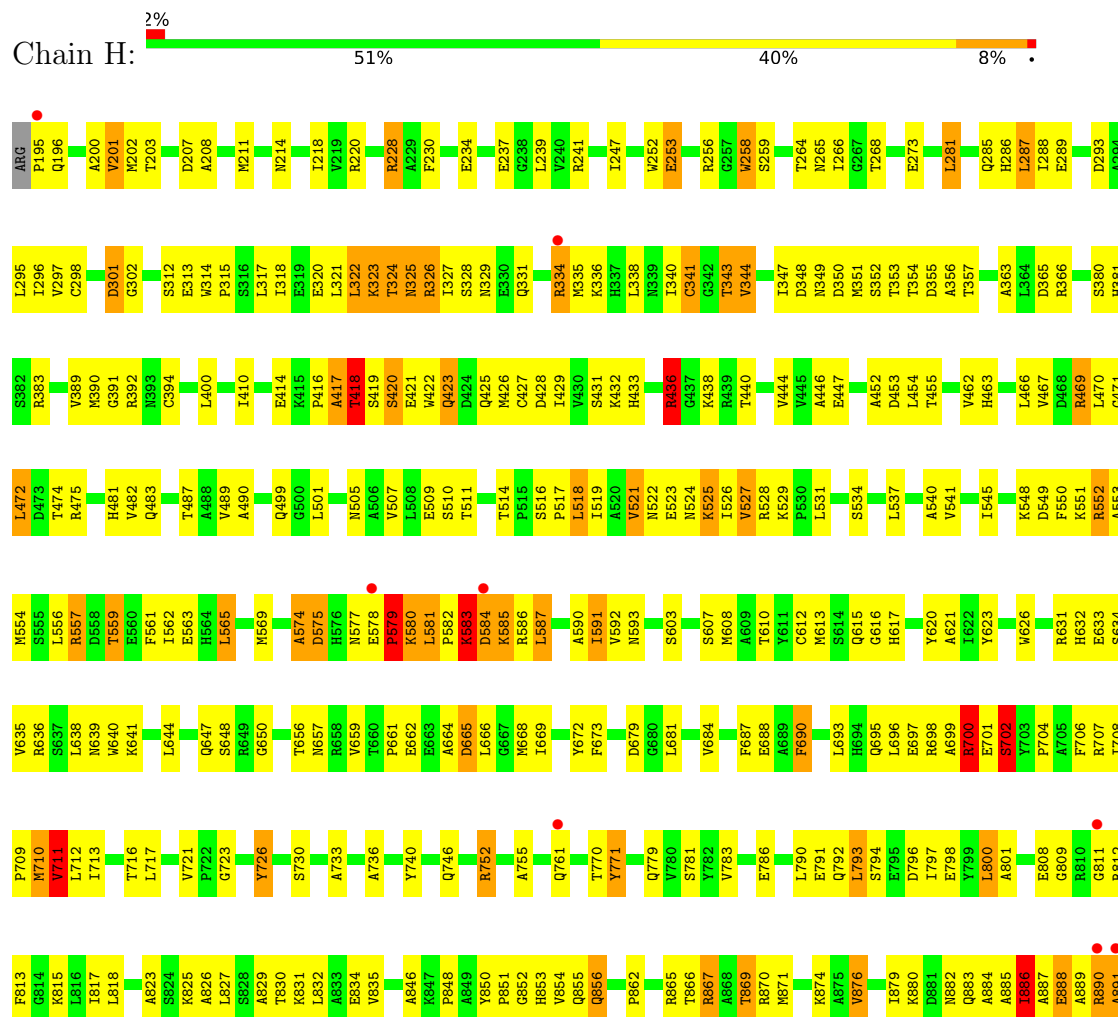


• Molecule 2: 6-phosphofructokinase subunit beta





● 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 35.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.90) 98.3 (35.00-2.90)	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 0.257 , 0.305	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)	0.29 , 56.0	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: F6P, FDP

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	0.67	2/5860 (0.0%)	1.11	41/7925 (0.5%)
1	C	0.72	1/5860 (0.0%)	1.12	38/7925 (0.5%)
1	E	0.73	0/5878	1.14	47/7948 (0.6%)
1	G	0.75	0/5834	1.13	37/7889 (0.5%)
2	B	0.65	2/5940 (0.0%)	1.11	32/8038 (0.4%)
2	D	0.70	3/5940 (0.1%)	1.13	40/8038 (0.5%)
2	F	0.64	1/5932 (0.0%)	1.11	36/8027 (0.4%)
2	H	0.75	1/5940 (0.0%)	1.16	45/8038 (0.6%)
All	All	0.70	10/47184 (0.0%)	1.13	316/63828 (0.5%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	836	ILE	CA-CB	6.96	1.62	1.54
1	A	719	ILE	CA-CB	6.09	1.60	1.53
2	D	733	ALA	CA-CB	5.88	1.62	1.53
2	H	736	ALA	CA-CB	-5.83	1.44	1.53
2	B	783	VAL	CA-CB	-5.58	1.50	1.55
2	F	757	VAL	CA-CB	-5.49	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	710	MET	SD-CE	5.37	1.93	1.79
2	D	836	ILE	CA-CB	5.07	1.60	1.54
1	C	742	ALA	CA-CB	-5.03	1.45	1.53
1	A	629	ILE	CA-CB	5.01	1.58	1.53

All (316) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	592	ASP	N-CA-C	-13.36	94.65	110.41
2	H	811	GLY	N-CA-C	11.95	128.62	114.16
2	B	811	GLY	N-CA-C	11.75	128.38	114.16
2	H	352	SER	N-CA-C	11.53	125.28	111.33
2	D	811	GLY	N-CA-C	11.10	128.42	114.66
2	F	352	SER	N-CA-C	11.05	124.69	111.33
2	D	585	LYS	N-CA-C	-11.02	97.32	112.30
2	B	585	LYS	N-CA-C	-10.96	96.68	113.02
2	F	811	GLY	N-CA-C	10.95	127.41	114.16
2	D	352	SER	N-CA-C	10.48	124.02	111.33
1	C	584	GLY	N-CA-C	-10.47	100.63	114.25
1	E	584	GLY	N-CA-C	-10.35	100.79	114.25
1	C	945	ASN	N-CA-C	-10.20	99.06	114.16
1	A	945	ASN	N-CA-C	-10.15	99.14	114.16
1	A	584	GLY	N-CA-C	-10.15	101.06	114.25
1	G	945	ASN	N-CA-C	-10.05	96.92	113.50
1	G	530	GLU	N-CA-C	-10.03	98.40	110.44
1	E	719	ILE	N-CA-C	-10.01	96.89	107.60
1	E	530	GLU	N-CA-C	-9.98	98.46	110.44
2	B	352	SER	N-CA-C	9.85	124.36	111.75
2	F	585	LYS	N-CA-C	-9.79	98.44	113.02
1	E	945	ASN	N-CA-C	-9.58	97.70	113.50
1	G	719	ILE	N-CA-C	-9.57	97.36	107.60
1	G	584	GLY	N-CA-C	-9.38	101.44	114.67
2	D	936	MET	N-CA-C	9.09	116.31	108.13
2	H	585	LYS	N-CA-C	-8.92	99.07	112.54
1	G	330	VAL	N-CA-C	-8.79	101.98	110.42
2	D	241	ARG	N-CA-C	-8.74	99.66	110.41
1	A	719	ILE	N-CA-C	-8.61	98.39	107.60
1	C	592	ASP	N-CA-C	-8.58	92.53	110.80
1	C	469	ASP	N-CA-C	-8.56	101.91	111.07
1	G	593	ARG	N-CA-C	-8.48	97.96	110.52
2	H	936	MET	N-CA-C	8.39	115.68	108.13
1	C	530	GLU	N-CA-C	-8.23	99.53	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	593	ARG	N-CA-C	-8.18	97.32	110.32
2	B	936	MET	N-CA-C	8.17	115.48	108.13
2	D	583	LYS	N-CA-C	-8.14	99.56	110.55
2	F	241	ARG	N-CA-C	-8.11	99.82	110.53
1	E	488	HIS	N-CA-C	8.11	122.60	112.87
1	E	592	ASP	N-CA-C	-8.00	93.76	110.80
1	G	592	ASP	N-CA-C	-7.87	94.04	110.80
2	H	420	SER	N-CA-C	-7.73	104.74	114.56
1	A	469	ASP	N-CA-C	-7.60	102.94	111.07
2	B	241	ARG	N-CA-C	-7.52	100.60	110.53
1	G	727	VAL	CA-C-N	7.52	127.57	119.90
1	G	727	VAL	C-N-CA	7.52	127.57	119.90
1	G	469	ASP	N-CA-C	-7.47	103.08	111.07
2	B	481	HIS	N-CA-C	7.38	121.72	112.87
1	E	469	ASP	N-CA-C	-7.33	103.23	111.07
1	G	588	LEU	N-CA-C	-7.33	96.97	110.02
2	D	481	HIS	N-CA-C	7.29	121.76	113.01
1	E	588	LEU	N-CA-C	-7.26	97.09	110.02
2	H	690	PHE	N-CA-C	-7.16	103.08	111.03
2	B	690	PHE	N-CA-C	-7.14	103.10	111.03
1	C	593	ARG	N-CA-C	-6.98	99.22	110.32
1	G	430	TRP	N-CA-C	6.98	119.73	111.71
2	H	910	VAL	CB-CA-C	-6.98	103.74	111.35
1	C	256	LYS	N-CA-C	6.97	120.92	109.06
2	H	241	ARG	N-CA-C	-6.97	101.33	110.53
1	A	430	TRP	N-CA-C	6.95	119.70	111.71
2	F	690	PHE	N-CA-C	-6.94	103.32	111.03
2	F	583	LYS	N-CA-C	-6.93	100.22	110.48
1	E	330	VAL	N-CA-C	-6.88	103.81	110.42
2	H	516	SER	CA-C-N	6.88	127.34	120.52
2	H	516	SER	C-N-CA	6.88	127.34	120.52
1	A	594	LEU	N-CA-C	6.87	119.85	109.41
2	F	906	THR	N-CA-C	-6.85	104.12	113.30
2	F	876	VAL	N-CA-C	-6.85	103.64	110.62
1	C	599	VAL	CB-CA-C	-6.83	99.76	110.69
1	E	594	LEU	N-CA-C	6.83	119.79	109.41
1	G	882	ILE	N-CA-C	-6.83	103.82	110.72
1	E	529	LEU	N-CA-C	6.77	122.18	113.18
2	H	941	HIS	N-CA-C	6.77	120.44	112.72
2	H	710	MET	N-CA-C	6.75	121.16	112.12
1	A	256	LYS	N-CA-C	6.75	120.53	109.06
1	G	488	HIS	N-CA-C	6.72	121.19	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	691	GLY	N-CA-C	6.70	119.60	110.69
1	E	481	THR	N-CA-C	6.68	119.79	108.90
1	C	283	ARG	NE-CZ-NH2	6.66	125.19	119.20
2	B	876	VAL	N-CA-C	-6.64	104.05	110.42
2	F	420	SER	N-CA-C	-6.64	106.13	114.56
2	B	699	ALA	N-CA-C	-6.63	104.42	113.30
2	F	783	VAL	N-CA-C	6.60	115.16	107.84
1	C	594	LEU	N-CA-C	6.57	119.70	109.52
1	E	204	LYS	N-CA-C	6.57	120.04	109.86
1	C	956	GLU	N-CA-C	6.55	118.99	110.53
1	E	205	LYS	N-CA-C	6.54	124.73	110.80
2	B	420	SER	N-CA-C	-6.53	105.89	114.31
2	H	783	VAL	N-CA-C	6.52	115.07	107.84
2	D	783	VAL	N-CA-C	6.51	115.07	107.84
1	E	724	SER	N-CA-C	6.50	120.31	112.38
1	A	488	HIS	N-CA-C	6.50	120.92	113.19
1	G	348	ILE	N-CA-C	6.49	117.37	107.77
2	B	854	VAL	N-CA-C	-6.49	104.57	113.00
1	A	724	SER	N-CA-C	6.47	120.44	112.54
2	D	699	ALA	N-CA-C	-6.46	104.64	113.30
1	E	582	ASP	N-CA-C	-6.45	105.79	113.21
1	A	330	VAL	N-CA-C	-6.45	104.23	110.42
1	E	732	TYR	N-CA-C	6.43	117.97	107.23
2	F	482	VAL	N-CA-C	-6.42	103.03	111.05
2	F	241	ARG	CA-C-N	-6.41	115.18	122.42
2	F	241	ARG	C-N-CA	-6.41	115.18	122.42
2	F	810	ARG	N-CA-C	6.40	118.56	110.24
1	E	430	TRP	N-CA-C	6.36	119.02	111.71
1	E	759	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	A	286	GLU	N-CA-C	-6.32	104.31	111.07
1	A	727	VAL	CA-C-N	6.32	126.34	119.90
1	A	727	VAL	C-N-CA	6.32	126.34	119.90
1	A	289	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	A	593	ARG	N-CA-C	-6.27	100.34	110.32
2	D	701	GLU	N-CA-C	-6.27	100.37	109.59
2	D	906	THR	N-CA-C	-6.27	104.90	113.30
1	E	256	LYS	N-CA-C	6.26	119.71	109.06
2	D	876	VAL	N-CA-C	-6.26	104.23	110.62
2	D	420	SER	N-CA-C	-6.25	106.25	114.31
1	A	819	ASN	N-CA-C	6.24	120.53	112.41
1	A	947	THR	N-CA-C	-6.22	102.41	111.30
1	G	529	LEU	N-CA-C	6.20	121.43	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	823	ALA	N-CA-C	-6.18	105.59	113.01
1	E	759	ARG	NE-CZ-NH1	-6.18	115.32	121.50
2	B	783	VAL	N-CA-C	6.18	114.70	107.84
1	C	430	TRP	N-CA-C	6.18	118.81	111.71
1	G	822	LEU	N-CA-C	6.17	118.80	109.23
1	E	751	LYS	N-CA-C	-6.17	104.47	111.07
1	G	724	SER	N-CA-C	6.14	120.03	112.54
1	C	529	LEU	N-CA-C	6.11	121.31	113.18
1	E	882	ILE	N-CA-C	-6.11	104.55	110.42
2	D	690	PHE	N-CA-C	-6.10	104.26	111.03
1	G	582	ASP	N-CA-C	-6.07	106.23	113.21
2	H	436	ARG	NE-CZ-NH1	-6.06	115.44	121.50
2	F	910	VAL	CB-CA-C	-6.05	104.69	111.23
2	D	258	TRP	N-CA-C	6.05	118.65	111.33
1	A	289	ARG	NE-CZ-NH1	-6.03	115.47	121.50
1	G	256	LYS	N-CA-C	6.03	119.31	109.06
2	F	710	MET	N-CA-C	6.02	120.19	112.12
1	C	283	ARG	NE-CZ-NH1	-6.02	115.48	121.50
2	B	583	LYS	N-CA-C	-6.00	101.59	110.48
1	E	959	TRP	N-CA-C	6.00	119.65	112.93
2	B	348	ASP	N-CA-C	5.96	118.73	111.82
2	H	583	LYS	N-CA-C	-5.95	102.52	110.55
1	C	348	ILE	N-CA-C	5.95	116.64	107.78
1	E	348	ILE	N-CA-C	5.94	116.67	108.12
1	C	947	THR	N-CA-C	-5.93	102.81	111.30
2	B	910	VAL	CB-CA-C	-5.93	104.89	111.35
1	A	481	THR	N-CA-C	5.93	119.06	109.40
2	D	237	GLU	N-CA-C	-5.89	104.20	111.33
1	A	822	LEU	N-CA-C	5.87	118.33	109.23
2	H	329	ASN	N-CA-C	-5.87	104.97	111.36
1	E	727	VAL	CA-C-N	5.87	127.17	119.84
1	E	727	VAL	C-N-CA	5.87	127.17	119.84
2	B	710	MET	N-CA-C	5.86	119.97	112.12
1	C	344	LYS	N-CA-C	5.82	117.43	111.14
2	D	710	MET	N-CA-C	5.82	119.92	112.12
1	G	691	GLY	N-CA-C	5.79	118.38	110.69
1	A	732	TYR	N-CA-C	5.78	118.59	107.44
2	F	418	THR	N-CA-C	5.76	123.06	110.80
2	F	636	ARG	NE-CZ-NH2	5.74	124.36	119.20
2	B	329	ASN	N-CA-C	-5.73	105.11	111.36
1	E	429	LYS	N-CA-C	5.73	120.43	113.38
1	A	971	GLY	N-CA-C	-5.73	107.36	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	944	GLU	CA-C-N	5.73	128.99	120.17
1	E	944	GLU	C-N-CA	5.73	128.99	120.17
1	G	631	ASN	N-CA-C	5.72	119.32	111.54
2	H	418	THR	N-CA-C	5.71	122.96	110.80
2	D	334	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	C	429	LYS	N-CA-C	5.69	120.22	113.28
1	A	529	LEU	N-CA-C	5.68	120.74	113.18
1	A	631	ASN	N-CA-C	5.68	119.23	111.39
2	H	234	GLU	N-CA-C	5.68	119.26	111.54
2	F	746	GLN	N-CA-C	-5.67	105.11	111.28
2	B	906	THR	N-CA-C	-5.66	105.71	113.30
1	G	605	SER	N-CA-C	-5.65	101.55	109.69
2	H	746	GLN	N-CA-C	-5.65	105.12	111.28
1	A	264	ARG	NE-CZ-NH2	5.64	124.28	119.20
2	F	415	LYS	CA-C-N	5.64	125.49	119.28
2	F	415	LYS	C-N-CA	5.64	125.49	119.28
2	D	334	ARG	NE-CZ-NH1	-5.63	115.87	121.50
2	F	941	HIS	N-CA-C	5.63	119.14	112.72
1	E	500	ARG	N-CA-C	-5.61	105.07	111.07
2	D	688	GLU	N-CA-C	-5.60	105.17	112.23
2	B	258	TRP	N-CA-C	5.60	118.15	111.71
1	E	925	ALA	N-CA-C	5.59	118.00	109.95
1	A	348	ILE	N-CA-C	5.58	116.15	108.12
2	H	650	GLY	N-CA-C	-5.57	102.74	112.55
1	A	599	VAL	CB-CA-C	-5.57	102.08	110.55
1	A	605	SER	N-CA-C	-5.57	101.67	109.69
1	C	925	ALA	N-CA-C	5.57	117.71	109.69
1	G	274	ILE	N-CA-C	-5.56	105.99	111.88
1	A	546	LYS	N-CA-C	-5.55	105.33	111.71
1	G	944	GLU	CA-C-N	5.53	128.69	120.17
1	G	944	GLU	C-N-CA	5.53	128.69	120.17
2	H	906	THR	N-CA-C	-5.52	105.90	113.30
1	C	605	SER	N-CA-C	-5.52	101.74	109.69
1	E	822	LEU	N-CA-C	5.51	117.64	108.99
1	E	675	ILE	N-CA-C	-5.51	104.96	110.30
2	H	631	ARG	NE-CZ-NH2	5.50	124.15	119.20
2	H	699	ALA	N-CA-C	-5.50	105.78	112.88
1	A	229	ARG	N-CA-C	5.49	117.26	111.28
1	A	679	PHE	N-CA-C	-5.48	105.31	111.28
1	C	818	ARG	NE-CZ-NH2	5.48	124.13	119.20
2	H	711	VAL	N-CA-C	5.48	120.73	109.34
1	C	724	SER	N-CA-C	5.47	118.17	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	258	TRP	N-CA-C	5.46	117.99	111.71
2	D	240	VAL	N-CA-C	-5.45	105.29	110.42
2	F	936	MET	CA-C-N	5.45	125.45	119.89
2	F	936	MET	C-N-CA	5.45	125.45	119.89
2	D	923	ARG	NE-CZ-NH2	5.45	124.11	119.20
1	C	822	LEU	N-CA-C	5.44	117.66	109.23
2	H	916	HIS	N-CA-C	5.43	121.10	110.56
2	H	436	ARG	NE-CZ-NH2	5.42	124.07	119.20
2	B	698	ARG	NE-CZ-NH2	5.42	124.07	119.20
1	G	970	SER	N-CA-C	-5.41	105.07	110.97
1	E	229	ARG	N-CA-C	5.40	117.92	111.71
2	B	956	LYS	N-CA-C	5.39	122.29	110.80
1	C	751	LYS	N-CA-C	-5.39	105.40	111.28
2	B	922	ILE	N-CA-C	-5.36	104.35	111.05
2	H	228	ARG	N-CA-C	-5.36	100.97	109.76
2	D	418	THR	N-CA-C	5.36	122.21	110.80
1	G	466	THR	N-CA-C	5.36	118.84	110.32
2	H	631	ARG	NE-CZ-NH1	-5.34	116.16	121.50
2	D	711	VAL	N-CA-C	5.33	120.44	109.34
2	F	550	PHE	N-CA-C	5.33	117.17	111.36
2	H	876	VAL	N-CA-C	-5.32	105.19	110.62
1	C	568	PHE	N-CA-C	5.32	117.51	111.02
2	H	341	CYS	CA-C-N	-5.31	117.45	122.66
2	H	341	CYS	C-N-CA	-5.31	117.45	122.66
1	G	263	VAL	CB-CA-C	-5.31	105.17	111.65
2	F	908	ALA	N-CA-C	5.31	116.72	109.18
2	B	469	ARG	N-CA-C	5.30	116.74	111.07
2	D	326	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	E	843	SER	N-CA-C	-5.28	105.22	110.97
2	F	258	TRP	N-CA-C	5.28	117.78	111.71
1	E	602	GLY	N-CA-C	5.27	117.69	111.63
1	A	816	GLU	CB-CA-C	-5.27	110.48	116.54
2	F	329	ASN	N-CA-C	-5.26	105.62	111.36
2	H	935	ARG	N-CA-C	5.26	118.64	111.39
1	C	818	ARG	NE-CZ-NH1	-5.25	116.25	121.50
2	B	650	GLY	N-CA-C	-5.24	104.55	112.41
1	G	286	GLU	N-CA-C	-5.24	105.46	111.07
2	D	482	VAL	N-CA-C	-5.24	104.51	111.05
2	D	941	HIS	N-CA-C	5.23	118.68	112.72
1	A	254	TYR	N-CA-C	-5.22	106.16	113.37
2	D	746	GLN	N-CA-C	-5.22	105.48	111.07
2	F	228	ARG	N-CA-C	-5.22	101.19	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	343	THR	N-CA-C	-5.22	99.15	108.13
2	H	469	ARG	N-CA-C	5.22	116.66	111.07
2	D	721	VAL	CA-C-N	5.22	125.15	119.78
2	D	721	VAL	C-N-CA	5.22	125.15	119.78
2	D	329	ASN	N-CA-C	-5.21	105.68	111.36
1	E	947	THR	N-CA-C	-5.19	99.74	110.80
1	G	248	LEU	N-CA-C	-5.19	105.70	111.36
2	H	247	ILE	N-CA-C	-5.19	98.54	109.34
2	D	910	VAL	CB-CA-C	-5.19	104.38	111.33
2	F	234	GLU	N-CA-C	5.19	118.60	111.54
1	G	751	LYS	N-CA-C	-5.18	105.63	111.28
2	D	889	ALA	N-CA-C	-5.18	107.62	114.04
1	A	944	GLU	CA-C-N	5.17	129.13	120.70
1	A	944	GLU	C-N-CA	5.17	129.13	120.70
2	B	701	GLU	N-CA-C	-5.17	101.99	109.59
2	H	856	GLN	N-CA-C	-5.16	106.98	113.28
1	C	307	GLY	N-CA-C	5.16	117.55	110.69
2	B	482	VAL	N-CA-C	-5.16	104.47	111.89
1	G	579	THR	N-CA-C	5.16	120.04	113.18
1	E	568	PHE	N-CA-C	5.15	117.31	111.02
1	A	319	ARG	NE-CZ-NH2	5.15	123.83	119.20
2	F	242	GLY	N-CA-C	5.14	121.23	110.69
2	H	726	TYR	N-CA-C	5.14	115.82	107.23
1	E	665	ARG	N-CA-C	5.13	118.81	112.54
2	H	946	ARG	N-CA-C	-5.13	105.12	111.33
2	F	636	ARG	NE-CZ-NH1	-5.13	116.37	121.50
2	H	527	VAL	N-CA-C	5.12	117.40	108.90
2	D	685	GLY	N-CA-C	5.12	117.50	110.69
1	E	475	ILE	N-CA-C	-5.12	105.55	110.72
2	B	685	GLY	N-CA-C	5.12	117.75	110.74
1	A	579	THR	N-CA-C	5.12	119.99	113.18
1	C	286	GLU	N-CA-C	-5.11	105.60	111.07
1	E	254	TYR	N-CA-C	-5.11	106.32	113.37
1	C	732	TYR	N-CA-C	5.11	116.50	107.61
1	A	429	LYS	N-CA-C	5.11	119.66	113.38
2	F	856	GLN	N-CA-C	-5.11	106.83	113.16
2	H	721	VAL	CA-C-N	5.10	125.04	119.78
2	H	721	VAL	C-N-CA	5.10	125.04	119.78
1	C	481	THR	N-CA-C	5.10	117.72	109.40
2	H	481	HIS	N-CA-C	5.10	121.65	110.80
1	G	481	THR	N-CA-C	5.09	117.70	109.40
2	F	711	VAL	N-CA-C	5.09	119.93	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	679	PHE	N-CA-C	-5.08	105.74	111.28
1	G	947	THR	N-CA-C	-5.08	99.97	110.80
2	H	616	GLY	N-CA-C	-5.07	108.00	114.85
2	B	936	MET	CB-CG-SD	-5.07	97.48	112.70
1	C	330	VAL	N-CA-C	-5.07	105.60	110.72
1	E	929	VAL	CB-CA-C	-5.06	103.14	110.63
1	C	582	ASP	N-CA-C	-5.06	107.39	113.21
2	D	326	ARG	NE-CZ-NH1	-5.06	116.44	121.50
2	H	237	GLU	N-CA-C	-5.06	105.21	111.33
1	G	475	ILE	N-CA-C	-5.06	105.46	110.62
2	D	228	ARG	N-CA-C	-5.05	101.47	109.76
2	B	418	THR	N-CA-C	5.04	121.54	110.80
2	B	634	SER	N-CA-C	5.04	118.32	112.97
2	D	415	LYS	CA-C-N	5.04	124.83	119.28
2	D	415	LYS	C-N-CA	5.04	124.83	119.28
1	A	279	SER	N-CA-C	5.04	116.84	108.02
1	C	631	ASN	N-CA-C	5.04	118.35	111.39
1	C	841	ILE	N-CA-C	-5.04	105.48	110.62
2	D	923	ARG	NE-CZ-NH1	-5.04	116.46	121.50
1	E	416	ASP	N-CA-C	-5.04	106.98	113.23
2	D	445	VAL	N-CA-C	5.03	115.28	107.28
2	B	550	PHE	N-CA-C	5.03	116.84	111.36
2	F	699	ALA	N-CA-C	-5.03	106.56	113.30
1	A	630	MET	N-CA-C	5.02	117.51	110.23
1	G	594	LEU	N-CA-C	5.02	117.05	109.41
1	C	819	ASN	N-CA-C	5.02	119.12	112.30
1	E	758	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	B	228	ARG	N-CA-C	-5.00	101.55	109.76
1	C	944	GLU	CA-C-N	5.00	128.85	120.70
1	C	944	GLU	C-N-CA	5.00	128.85	120.70

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
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	355	0
1	C	5759	0	5758	349	0
1	E	5777	0	5779	343	0
1	G	5733	0	5733	330	0
2	B	5834	0	5799	385	0
2	D	5834	0	5799	373	0
2	F	5827	0	5791	349	1
2	H	5834	0	5799	392	1
3	A	16	0	11	5	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	2783	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 32.

All (2783) 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
2:F:418:THR:HG1	2:F:422:TRP:CD1	1.72	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:418:THR:HG1	2:D:422:TRP:CD1	1.77	1.02
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: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:577:ASN:C	2:F:579:PRO:HD2	1.93	0.93
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
1:E:821:LYS:HB2	1:E:821:LYS:HZ2	1.34	0.93
2:H:418:THR:HG1	2:H:422:TRP:CD1	1.86	0.93
2:B:701:GLU:O	2:B:702:SER:HB2	1.69	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:418:THR:HG23	2:H:419:SER:H	1.32	0.93
2:B:577:ASN:C	2:B:579:PRO:HD2	1.93	0.93
1:A:466:THR:HG22	1:A:468:ASN:H	1.32	0.93
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:H	1:E:431:GLN:NE2	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:NE2	1:C:431:GLN:H	1.68	0.90
2:F:607:SER:OG	2:F:869:THR:HB	1.69	0.90
2:H:577:ASN:C	2:H:579:PRO:HD2	1.96	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
2:D:577:ASN:C	2:D:579:PRO:HD2	1.96	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
1:E:212:THR:HG21	1:E:272:THR:OG1	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:418:THR:HG1	2:B:422:TRP:CD1	1.92	0.86
2:H:348:ASP:OD2	3:H:986:F6P:H11	1.74	0.86
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
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:HD22	1:G:975:LEU:H	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:B:956:LYS:HZ3	2:B:956:LYS:HA	1.43	0.83
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:E:813:ASP:CG	1:E:814:LYS:H	1.84	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:HD12	1:E:822:LEU:O	1.80	0.81
1:A:212:THR:HG21	1:A:272:THR:OG1	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:813:ASP:CG	1:A:814:LYS:H	1.89	0.80
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
1:C:378:MET:HE3	2:D:482:VAL:HG11	1.62	0.79
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:H:591:ILE:HB	2:H:608:MET:HE3	1.64	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
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
2:D:591:ILE:HB	2:D:608:MET:HE3	1.64	0.78
2:H:889:ALA:C	2:H:891:ALA:H	1.92	0.78
1:C:505:LEU:HB3	1:C:533:ILE:CD1	2.14	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:587:LEU:HD12	2:D:587:LEU:N	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
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
2:F:889:ALA:C	2:F:891:ALA:H	1.92	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:HH21	2:F:946:ARG:HG3	1.49	0.77
1:C:947:THR:HG22	1:C:953:LYS:H	1.50	0.77
1:A:431:GLN:H	1:A:431:GLN:HE21	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
2:H:418:THR:HG1	2:H:422:TRP:HD1	1.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:591:ILE:HB	2:F:608:MET:HE3	1.67	0.76
2:B:418:THR:HG23	2:B:419:SER:N	2.00	0.76
2:B:591:ILE:HB	2:B:608:MET:HE3	1.66	0.76
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
1:A:336:THR:HG23	1:A:339:GLU:CD	2.10	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
1:G:814:LYS:HZ2	1:G:814:LYS:HA	1.52	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:H	1:G:431:GLN:HE21	1.35	0.75
1:A:336:THR:HG1	1:A:339:GLU:HG3	1.50	0.74
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
1:E:822:LEU:HD12	1:E:822:LEU:C	2.12	0.74
2:H:946:ARG:HG3	2:H:946:ARG:HH21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH21	2:B:946:ARG:HG3	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
2:B:889:ALA:C	2:B:891:ALA:H	1.95	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
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
2:D:889:ALA:C	2:D:891:ALA:H	1.97	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
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:703:ARG:HD3	1:E:921:ASP:OD1	1.87	0.72
1:E:832:VAL:O	2:H:831:LYS:NZ	2.20	0.72
2:H:579:PRO:O	2:H:580:LYS:C	2.31	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: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:HA	2:B:956:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:936:MET:HB2	2:D:937:PRO:HD2	1.72	0.72
1:E:947:THR:O	1:E:948:ASN:C	2.32	0.72
1:E:587:LEU:C	1:E:589:PRO:HD3	2.14	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
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:H:323:LYS:O	2:H:324:THR:HB	1.88	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:HD12	2:B:587:LEU:N	2.05	0.71
1:E:385:THR:HA	2:F:207:ASP:OD2	1.90	0.71
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:H:894:GLU:C	2:H:896:PHE:H	1.98	0.71
2:F:288:ILE:HA	2:F:335:MET:HE2	1.71	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
2:F:579:PRO:O	2:F:580:LYS:C	2.33	0.71
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
1:G:427:HIS:CB	1:G:460:ASP:HB2	2.16	0.70
1:A:216:ASP:OD2	2:B:377:THR:HA	1.90	0.70
1:A:822:LEU:O	1:A:822:LEU:HD12	1.91	0.70
1:C:541:SER:O	1:C:545:THR:HG23	1.91	0.70
1:E:832:VAL:HG22	2:H:834:GLU:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:844:GLU:OE2	2:H:825:LYS:N	2.24	0.70
1:E:253:LYS:C	1:E:255:LEU:H	1.98	0.70
1:A:703:ARG:HD3	1:A:921:ASP:OD1	1.91	0.70
2:B:288:ILE:HA	2:B:335:MET:HE2	1.73	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:B:579:PRO:O	2:B:580:LYS:C	2.34	0.70
1:C:587:LEU:C	1:C:589:PRO:HD3	2.15	0.70
2:D:552:ARG:C	2:D:552:ARG:HD3	2.16	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:587:LEU:C	1:A:589:PRO:HD3	2.17	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
1:C:253:LYS:C	1:C:255:LEU:H	2.00	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:O	1:E:947:THR:HG23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:212:THR:HG23	1:C:212:THR:O	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
2:B:453:ASP:CG	2:B:455:THR:HG23	2.17	0.68
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:G:587:LEU:C	1:G:589:PRO:HD3	2.17	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
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
1:A:253:LYS:C	1:A:255:LEU:H	2.00	0.68
1:A:947:THR:O	1:A:948:ASN:C	2.36	0.68
2:B:201:VAL:HG11	2:B:218:ILE:HD13	1.74	0.68
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:D:589:ILE:HD13	2:D:879:ILE:HG21	1.74	0.68
1:A:703:ARG:HH11	1:A:921:ASP:CG	2.01	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
2:H:436:ARG:HH12	2:H:575:ASP:CG	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:814:LYS:HA	1:G:814:LYS:NZ	2.08	0.67
2:H:525:LYS:HB2	2:H:525:LYS:NZ	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
2:H:591:ILE:HD13	2:H:592:VAL:H	1.60	0.67
2:B:577:ASN:C	2:B:579:PRO:CD	2.67	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:776:SER:HB3	1:E:963:ASN:HD21	1.59	0.67
1:E:825:ARG:NH1	1:E:829:ALA:HB3	2.09	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
2:D:418:THR:HG1	2:D:422:TRP:CG	2.13	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
2:H:552:ARG:HD3	2:H:552:ARG:C	2.19	0.67
2:H:577:ASN:C	2:H:579:PRO:CD	2.68	0.67
1:C:249:LEU:CD1	1:C:290:GLN:HG2	2.24	0.67
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
1:G:947:THR:O	1:G:947:THR:HG23	1.94	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
1:A:822:LEU:HD12	1:A:822:LEU:C	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:587:LEU:HD12	2:D:587:LEU:H	1.60	0.66
1:E:505:LEU:HB3	1:E:533:ILE:HD11	1.77	0.66
1:G:822:LEU:HD12	1:G:822:LEU:C	2.19	0.66
1:E:755:SER:HB3	1:E:817:ASN:O	1.96	0.66
1:E:959:TRP:H	1:E:959:TRP:CD1	2.13	0.66
2:F:256:ARG:HD2	2:F:812:ARG:O	1.95	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:HG2	1:G:400:ARG:HH11	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
2:H:892:ALA:C	2:H:894:GLU:H	2.03	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
2:F:244:PRO:O	2:F:245:GLU:HB3	1.95	0.65
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
1:C:427:HIS:HA	1:C:459:ASP:HB2	1.77	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
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
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:822:LEU:C	1:C:822:LEU:HD12	2.22	0.65
2:D:201:VAL:CG1	2:D:218:ILE:HD13	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:792:GLN:HE22	2:D:957:ARG:C	2.04	0.65
2:H:522:ASN:ND2	2:H:527:VAL:HG21	2.11	0.65
1:A:959:TRP:O	1:A:960:ALA:C	2.39	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
1:E:813:ASP:CG	1:E:814:LYS:N	2.55	0.65
2:F:579:PRO:O	2:F:581:LEU:N	2.30	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
1:A:946:GLU:CD	1:A:946:GLU:C	2.65	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:202:MET:HE3	2:D:295:LEU:HD21	1.79	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
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
1:C:427:HIS:ND1	1:C:427:HIS:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:351:MET:HE3	2:D:354:THR:HG22	1.80	0.64
1:E:378:MET:HE3	2:F:482:VAL:HG11	1.79	0.64
2:F:577:ASN:C	2:F:579:PRO:CD	2.68	0.64
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:O	1:A:947:THR:HG23	1.98	0.63
2:B:418:THR:HG1	2:B:422:TRP:HD1	1.44	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:C:216:ASP:OD2	2:D:377:THR:HA	1.99	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
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
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:F:418:THR:HG1	2:F:422:TRP:CG	2.14	0.63
2:B:436:ARG:HG3	2:B:436:ARG:O	1.97	0.63
1:C:336:THR:HG23	1:C:339:GLU:CD	2.24	0.63
1:C:422:GLU:CG	1:C:564:ARG:HD2	2.28	0.63
2:D:579:PRO:O	2:D:580:LYS:C	2.41	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:757:THR:HG23	2:B:597:PRO:HD3	1.81	0.63
2:B:201:VAL:HG11	2:B:218:ILE:CD1	2.28	0.63
1:C:805:LEU:HD21	1:C:976:ARG:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:703:ARG:HH11	1:E:921:ASP:CG	2.06	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:HG23	1:G:276:THR:O	1.98	0.63
1:G:746:TYR:CE1	2:H:854:VAL:CG1	2.82	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
1:C:424:ALA:HB1	1:C:459:ASP:C	2.24	0.62
1:C:703:ARG:HH11	1:C:921:ASP:CG	2.06	0.62
2:D:641:LYS:O	2:D:644:LEU:HD12	1.99	0.62
1:E:946:GLU:C	1:E:946:GLU:CD	2.66	0.62
2:F:494:ILE:HG23	2:F:774:LEU:HD23	1.80	0.62
2:F:701:GLU:HB3	2:F:897:ASN:HD22	1.62	0.62
1:G:253:LYS:C	1:G:255:LEU:H	2.06	0.62
1:G:583:ASP:C	1:G:585:SER:H	2.07	0.62
1:C:348:ILE:O	1:C:524:PRO:HD2	2.00	0.62
2:D:577:ASN:C	2:D:579:PRO:CD	2.70	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:N	1:E:485:ILE:HD12	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
1:C:216:ASP:H	2:D:381:HIS:HE1	1.48	0.62
1:C:251:GLY:O	1:C:252:GLY:O	2.17	0.62
2:D:632:HIS:O	2:D:633:GLU:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:427:HIS:C	1:G:427:HIS:ND1	2.57	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:N	1:G:451:ILE:HD12	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
2:D:892:ALA:C	2:D:894:GLU:H	2.08	0.62
1:E:276:THR:HG23	1:E:276:THR:O	2.00	0.62
1:E:427:HIS:C	1:E:427:HIS:ND1	2.58	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
2:B:892:ALA:C	2:B:894:GLU:H	2.06	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:392:ARG:HH21	3:D:982:F6P:H12	1.65	0.61
2:D:665:ASP:O	2:D:669:ILE:HG12	2.00	0.61
1:G:427:HIS:HA	1:G:459:ASP:HB2	1.81	0.61
1:A:424:ALA:HB1	1:A:459:ASP:C	2.25	0.61
2:B:894:GLU:C	2:B:896:PHE:H	2.07	0.61
1:C:461:GLN:HB2	1:C:463:ASN:ND2	2.14	0.61
2:H:239:LEU:O	2:H:286:HIS:HD2	1.82	0.61
2:H:256:ARG:HD2	2:H:812:ARG:O	1.99	0.61
2:H:341:CYS:HB2	2:H:507:VAL:HG13	1.82	0.61
2:H:578:GLU:C	2:H:580:LYS:H	2.09	0.61
1:A:596:ILE:HD12	1:A:885:ILE:HG21	1.82	0.61
1:E:977:ALA:C	1:E:979:VAL:H	2.07	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
1:C:421:PRO:C	1:C:423:ARG:H	2.08	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
1:G:703:ARG:HH11	1:G:921:ASP:CG	2.08	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:704:PRO:HA	2:B:707:ARG:HH11	1.64	0.61
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:894:GLU:C	2:F:896:PHE:H	2.08	0.61
2:H:288:ILE:HA	2:H:335:MET:HE2	1.81	0.61
2:H:940:ILE:HD12	2:H:943:GLN:NE2	2.15	0.61
1:C:822:LEU:HD12	1:C:822:LEU:O	2.00	0.61
2:D:298:CYS:HA	2:D:343:THR:O	2.00	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
1:C:331:ALA:O	1:C:332:GLU:C	2.43	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
2:F:892:ALA:C	2:F:894:GLU:H	2.09	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:F:202:MET:HE3	2:F:295:LEU:HD21	1.82	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:E:583:ASP:C	1:E:585:SER:H	2.08	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:949:VAL:O	1:E:950:GLU:C	2.41	0.60
1:G:331:ALA:O	1:G:332:GLU:C	2.43	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: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:G:599:VAL:CG1	1:G:629:ILE:HB	2.25	0.60
1:A:398:MET:HE3	1:A:487:GLY:C	2.26	0.60
2:F:521:VAL:HG13	2:F:526:ILE:HD13	1.82	0.60
1:G:424:ALA:HB1	1:G:459:ASP:C	2.27	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
1:E:822:LEU:C	1:E:822:LEU:CD1	2.74	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:C:583:ASP:C	1:C:585:SER:H	2.09	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
1:A:813:ASP:CG	1:A:814:LYS:N	2.60	0.59
4:A:1:FDP:O4P	2:B:847:LYS:NZ	2.34	0.59
2:B:632:HIS:O	2:B:633:GLU:C	2.45	0.59
2:B:701:GLU:O	2:B:701:GLU:CD	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:GLU:O	1:A:946:GLU:CD	2.45	0.59
2:B:288:ILE:HA	2:B:335:MET:CE	2.32	0.59
2:B:578:GLU:C	2:B:580:LYS:H	2.10	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
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:F:889:ALA:C	2:F:891:ALA:N	2.61	0.59
1:A:841:ILE:CG2	2:D:790:LEU:HD11	2.32	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
1:E:594:LEU:N	1:E:624:HIS:ND1	2.48	0.59
1:G:581:LYS:C	1:G:583:ASP:H	2.10	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:578:GLU:C	2:D:580:LYS:H	2.09	0.59
2:D:704:PRO:HA	2:D:707:ARG:NH1	2.18	0.59
2:F:416:PRO:O	2:F:417:ALA:C	2.45	0.59
2:F:554:MET:HG2	2:F:562:ILE:CG1	2.29	0.59
1:G:586:GLU:O	1:G:587:LEU:C	2.46	0.59
1:G:679:PHE:CE2	1:G:687:LEU:HD22	2.38	0.59
2:H:587:LEU:N	2:H:587:LEU:HD12	2.18	0.59
1:A:613:ARG:HA	1:A:650:VAL:CG2	2.33	0.59
1:E:424:ALA:HB1	1:E:459:ASP:C	2.28	0.59
2:F:328:SER:H	2:F:331:GLN:NE2	2.00	0.59
2:F:518:LEU:HD23	2:F:518:LEU:C	2.28	0.59
2:F:575:ASP:OD1	2:F:575:ASP:C	2.45	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
1:E:806:LEU:O	1:E:807:LYS:C	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:439:GLN:OE1	1:A:439:GLN:HA	2.02	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
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:439:GLN:OE1	1:C:439:GLN:HA	2.04	0.58
1:C:766:VAL:HG11	1:C:774:ILE:HG22	1.84	0.58
1:E:539:VAL:O	1:E:542:VAL:HG22	2.03	0.58
1:E:809:ASN:C	1:E:809:ASN:OD1	2.46	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:947:THR:HG22	1:C:953:LYS:N	2.17	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:A:216:ASP:H	2:B:381:HIS:HE1	1.52	0.58
1:A:651:GLU:HG3	1:A:652:ASN:ND2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:E:525:LEU:HD23	1:E:525:LEU:C	2.28	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: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:360:SER:H	1:A:545:THR:HG22	1.67	0.57
1:A:485:ILE:HD12	1:A:485:ILE:N	2.18	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
2:F:792:GLN:HE22	2:F:957:ARG:HB3	1.68	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:N	2:F:414:GLU:OE2	2.35	0.57
2:H:418:THR:OG1	2:H:419:SER:N	2.35	0.57
2:H:717:LEU:C	2:H:717:LEU:HD12	2.29	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:288:ILE:HA	2:D:335:MET:HE2	1.85	0.57
1:E:350:GLY:O	1:E:351:LEU:HD23	2.05	0.57
1:E:590:VAL:HG23	1:E:591:SER:N	2.17	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
2:B:890:ARG:O	2:B:890:ARG:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:958:HIS:C	1:C:959:TRP:CD1	2.82	0.57
2:F:790:LEU:HD22	1:G:796:LEU:HD22	1.87	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: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
1:C:341:ALA:HB3	1:C:342:PRO:CD	2.34	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:HD12	2:H:501:LEU:O	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:F:701:GLU:O	2:F:701:GLU:CD	2.48	0.57
2:H:752:ARG:HD2	2:H:809:GLY:O	2.05	0.57
1:A:205:LYS:HE3	1:A:237:ASP:CG	2.29	0.56
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
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: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: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
1:C:832:VAL:HG12	1:C:833:TYR:N	2.19	0.56
1:E:977:ALA:C	1:E:979:VAL:N	2.62	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:385:THR:HA	2:B:207:ASP:OD2	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
2:B:704:PRO:HA	2:B:707:ARG:NH1	2.21	0.56
1:E:946:GLU:CD	1:E:946:GLU:O	2.49	0.56
2:F:281:LEU:HD12	2:F:317:LEU:CD2	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:347:ILE:HB	2:F:363:ALA:HB2	1.87	0.56
2:F:578:GLU:C	2:F:580:LYS:H	2.13	0.56
2:H:554:MET:HG2	2:H:562:ILE:CG1	2.34	0.56
2:H:633:GLU:HB2	2:H:672:TYR:CZ	2.40	0.56
1:E:451:ILE:N	1:E:451:ILE:HD12	2.20	0.56
1:E:928:CYS:O	1:E:934:VAL:HA	2.05	0.56
2:F:717:LEU:C	2:F:717:LEU:HD12	2.30	0.56
1:G:249:LEU:CD1	1:G:290:GLN:HG2	2.35	0.56
1:G:525:LEU:HD23	1:G:525:LEU:C	2.30	0.56
1:A:778:THR:O	1:A:782:THR:HB	2.05	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:D:889:ALA:C	2:D:891:ALA:N	2.64	0.56
2:H:521:VAL:HG13	2:H:526:ILE:HD13	1.87	0.56
2:H:522:ASN:HD22	2:H:527:VAL:HG21	1.70	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:385:THR:HA	2:H:207:ASP:OD2	2.06	0.56
2:H:202:MET:HE3	2:H:295:LEU:HD21	1.88	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
2:F:752:ARG:HD2	2:F:809:GLY:O	2.05	0.56
1:G:421:PRO:C	1:G:423:ARG:H	2.12	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:A:398:MET:HE3	1:A:487:GLY:O	2.06	0.55
2:B:886:ILE:HD12	2:B:887:ALA:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:TRP:CZ2	1:C:408:MET:HE2	2.41	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
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:CD2	1:C:812:HIS:N	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:538:LEU:HD23	1:E:538:LEU:C	2.31	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
1:C:538:LEU:C	1:C:538:LEU:HD23	2.31	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
1:A:427:HIS:C	1:A:427:HIS:ND1	2.65	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:C:893:GLU:OE2	2.07	0.55
1:E:398:MET:HE3	1:E:487:GLY:C	2.32	0.55
1:C:525:LEU:C	1:C:525:LEU:HD23	2.31	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
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
2:B:587:LEU:HD21	2:B:883:GLN:HG3	1.88	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:HA	1:E:893:GLU:OE2	2.06	0.55
2:F:662:GLU:H	2:F:695:GLN:HE22	1.53	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
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
2:H:453:ASP:CG	2:H:455:THR:HG23	2.32	0.55
1:A:519:PRO:HG2	1:A:520:GLU:H	1.72	0.54
1:C:942:LEU:C	1:C:944:GLU:H	2.16	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
2:H:416:PRO:O	2:H:417:ALA:C	2.49	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
1:C:660:GLU:C	2:D:752:ARG:HH22	2.14	0.54
1:E:837:LEU:HD22	2:H:831:LYS:HD2	1.88	0.54
1:G:423:ARG:CD	1:G:561:ILE:HD12	2.37	0.54
1:G:816:GLU:O	1:G:818:ARG:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:220:ARG:HD2	2:H:252:TRP:CZ2	2.42	0.54
1:A:339:GLU:C	1:A:341:ALA:H	2.15	0.54
1:A:398:MET:HB3	3:A:988:F6P:O3	2.07	0.54
1:A:438:CYS:O	1:A:442:ARG:HG3	2.06	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
2:D:416:PRO:O	2:D:417:ALA:C	2.50	0.54
1:E:466:THR:HB	1:E:469:ASP:CG	2.31	0.54
2:F:780:VAL:HG12	2:F:781:SER:N	2.23	0.54
2:B:278:GLU:OE1	2:B:278:GLU:HA	2.07	0.54
2:B:518:LEU:HD23	2:B:518:LEU:C	2.32	0.54
2:D:680:GLY:HA3	2:D:879:ILE:HD12	1.88	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
1:A:360:SER:HB3	1:A:545:THR:HG22	1.90	0.54
1:A:822:LEU:C	1:A:822:LEU:CD1	2.81	0.54
2:B:325:ASN:O	2:B:327:ILE:N	2.31	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:538:LEU:HD23	1:A:538:LEU:C	2.32	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:813:ASP:OD1	1:E:814:LYS:N	2.17	0.54
2:F:946:ARG:HH21	2:F:946:ARG:CG	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
2:D:523:GLU:O	2:D:524:ASN:C	2.50	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:351:MET:HE3	2:H:354:THR:HG22	1.89	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:709:PRO:HB2	2:B:879:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:740:TYR:CE1	2:B:851:PRO:HB3	2.43	0.54
1:C:801:GLU:O	1:C:805:LEU:HG	2.08	0.54
2:D:453:ASP:CG	2:D:455:THR:HG23	2.33	0.54
2:D:522:ASN:HD21	2:D:529:LYS:CE	2.21	0.54
1:E:253:LYS:C	1:E:255:LEU:N	2.64	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
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:596:ILE:HD12	1:E:885:ILE:HG21	1.90	0.54
1:E:685:ASP:O	1:E:715:PRO:HD2	2.07	0.54
1:E:791:GLU:CD	1:E:959:TRP:HH2	2.15	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
1:A:772:GLY:C	1:A:959:TRP:CZ3	2.86	0.53
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: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: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
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:253:LYS:C	1:C:255:LEU:N	2.66	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:H	1:E:958:HIS:CD2	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:696:LEU:CB	2:B:710:MET:HE1	2.38	0.53
2:D:518:LEU:C	2:D:518:LEU:HD23	2.34	0.53
2:D:608:MET:SD	2:D:608:MET:C	2.91	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
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
1:E:581:LYS:C	1:E:583:ASP:H	2.15	0.53
1:E:930:ASN:O	1:E:931:GLY:C	2.51	0.53
2:F:341:CYS:CB	2:F:507:VAL:HG13	2.38	0.53
1:G:216:ASP:H	2:H:381:HIS:HE1	1.54	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
2:H:428:ASP:CG	2:H:432:LYS:NZ	2.67	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:D:701:GLU:O	2:D:701:GLU:CD	2.52	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
1:C:703:ARG:HD2	1:C:703:ARG:C	2.33	0.53
2:D:541:VAL:O	2:D:545:ILE:HG12	2.08	0.53
2:D:692:SER:O	2:D:693:LEU:C	2.51	0.53
2:D:707:ARG:HE	2:D:897:ASN:CG	2.15	0.53
1:G:942:LEU:C	1:G:944:GLU:H	2.16	0.53
2:H:324:THR:O	2:H:325:ASN:HB2	2.08	0.53
2:H:641:LYS:O	2:H:644:LEU:HD12	2.08	0.53
1:A:212:THR:HG23	1:A:275:GLY:O	2.08	0.53
1:A:248:LEU:HG	1:A:291:ALA:HB1	1.91	0.53
1:A:421:PRO:C	1:A:423:ARG:H	2.16	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
1:E:586:GLU:O	1:E:587:LEU:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:LYS:C	1:A:583:ASP:H	2.17	0.53
1:A:586:GLU:O	1:A:587:LEU:C	2.50	0.53
2:B:208:ALA:O	2:B:211:MET:HG3	2.09	0.53
2:B:608:MET:SD	2:B:608:MET:C	2.92	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:599:VAL:CG1	1:E:629:ILE:HB	2.29	0.53
2:F:453:ASP:CG	2:F:455:THR:HG23	2.32	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:887:ALA:C	2:H:889:ALA:H	2.17	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:D:522:ASN:O	2:D:523:GLU:C	2.52	0.53
1:E:211:MET:HE3	1:E:305:VAL:HG22	1.91	0.53
1:E:942:LEU:C	1:E:944:GLU:H	2.17	0.53
1:G:822:LEU:C	1:G:822:LEU:CD1	2.80	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:350:ASP:HB3	2:D:394:CYS:HB2	1.90	0.53
2:D:353:THR:CG2	2:D:534:SER:HA	2.39	0.53
2:D:353:THR:HG21	2:D:534:SER:HA	1.91	0.53
2:D:522:ASN:HD22	2:D:527:VAL:HG21	1.74	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
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
1:A:583:ASP:C	1:A:585:SER:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:236:CYS:SG	1:A:515:LEU:HD21	2.49	0.52
1:A:301:ASP:OD1	1:A:301:ASP:N	2.43	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:417:ALA:O	2:H:418:THR:HB	2.08	0.52
2:H:664:ALA:O	2:H:665:ASP:CB	2.57	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: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
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:N	1:G:951:LEU:HD22	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
1:C:804:THR:O	1:C:805:LEU:C	2.53	0.52
2:D:537:LEU:O	2:D:540:ALA:HB3	2.08	0.52
2:D:717:LEU:C	2:D:717:LEU:HD12	2.34	0.52
2:F:706:PHE:C	2:F:708:ILE:H	2.17	0.52
1:G:808:GLU:O	1:G:809:ASN:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:586:GLU:O	1:C:587:LEU:C	2.51	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:822:LEU:C	1:C:822:LEU:CD1	2.83	0.52
1:C:947:THR:HG23	1:C:952:ARG:N	2.25	0.52
2:D:343:THR:O	2:D:343:THR:HG22	2.09	0.52
2:D:481:HIS:O	2:D:482:VAL:C	2.52	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: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
1:C:581:LYS:C	1:C:583:ASP:H	2.18	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
2:F:696:LEU:CB	2:F:710:MET:HE1	2.40	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:C:782:THR:HG22	1:C:784:ALA:H	1.75	0.51
1:C:809:ASN:HB2	1:C:975:LEU:HD11	1.91	0.51
1:C:825:ARG:HH11	1:C:829:ALA:HB3	1.75	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
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:591:ILE:HB	2:D:608:MET:CE	2.39	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:OE1	1:G:439:GLN:HA	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
2:B:706:PHE:C	2:B:708:ILE:H	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:THR:O	1:C:276:THR:CG2	2.57	0.51
1:C:746:TYR:CE1	2:D:854:VAL:HG13	2.45	0.51
1:C:805:LEU:HD13	1:C:972:ARG:HA	1.91	0.51
2:D:416:PRO:HD2	2:D:550:PHE:CD1	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:572:TYR:CE2	1:G:576:LEU:HD11	2.45	0.51
1:G:949:VAL:O	1:G:950:GLU:C	2.52	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:894:GLU:C	2:H:896:PHE:N	2.65	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
1:E:776:SER:CB	1:E:963:ASN:HD21	2.23	0.51
2:F:632:HIS:O	2:F:633:GLU:C	2.54	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:525:LEU:HD23	1:A:525:LEU:C	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:ARG:HG2	1:E:400:ARG:HH11	1.76	0.51
1:E:431:GLN:HE21	1:E:431:GLN:N	1.98	0.51
1:E:488:HIS:C	1:E:490:GLN:N	2.67	0.51
1:E:586:GLU:CD	1:E:587:LEU:H	2.17	0.51
1:E:856:ILE:O	1:E:857:PRO:C	2.53	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:325:ASN:C	2:H:327:ILE:H	2.17	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:293:ASP:HB3	2:D:335:MET:HE3	1.93	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:523:GLU:O	2:F:524:ASN:C	2.53	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:758:ARG:NH1	2:B:655:GLY:CA	2.73	0.51
1:A:812:HIS:CD2	1:A:812:HIS:N	2.77	0.51
2:B:201:VAL:HG13	2:B:218:ILE:HG21	1.93	0.51
2:B:889:ALA:C	2:B:891:ALA:N	2.64	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
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:G:312:LEU:CD1	1:G:359:MET:HE3	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:SER:C	2:B:423:GLN:HE21	2.19	0.50
1:C:249:LEU:HD13	1:C:290:GLN:HG2	1.93	0.50
2:D:633:GLU:HB2	2:D:672:TYR:OH	2.12	0.50
2:D:706:PHE:C	2:D:708:ILE:H	2.19	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
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:G:960:ALA:C	1:G:962:TYR:N	2.66	0.50
1:A:942:LEU:C	1:A:944:GLU:H	2.19	0.50
1:A:977:ALA:C	1:A:979:VAL:N	2.67	0.50
1:C:276:THR:CG2	2:D:381:HIS:CE1	2.95	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:962:TYR:O	1:A:965:ILE:N	2.44	0.50
1:C:233:HIS:CE1	1:C:968:ILE:HD13	2.47	0.50
1:C:860:VAL:HG11	2:D:740:TYR:CD1	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:GLY:O	1:C:253:LYS:HB3	2.10	0.50
1:C:431:GLN:NE2	1:C:431:GLN:N	2.50	0.50
2:D:744:VAL:O	2:D:747:SER:HB3	2.12	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:253:LYS:C	1:A:255:LEU:N	2.66	0.50
1:A:255:LEU:HD23	1:A:255:LEU:C	2.36	0.50
1:A:291:ALA:O	1:A:292:ALA:C	2.54	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
1:G:378:MET:HE3	2:H:482:VAL:HG11	1.94	0.50
2:H:253:GLU:O	2:H:256:ARG:HB3	2.12	0.50
2:H:348:ASP:CG	3:H:986:F6P:H11	2.36	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:B:853:HIS:C	2:B:855:GLN:N	2.66	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
1:G:466:THR:HB	1:G:469:ASP:CG	2.36	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:A:804:THR:O	1:A:805:LEU:C	2.55	0.50
2:B:481:HIS:C	2:B:483:GLN:N	2.68	0.50
2:B:523:GLU:O	2:B:524:ASN:C	2.55	0.50
1:C:667:VAL:HG11	1:C:697:ARG:HD3	1.93	0.50
2:D:422:TRP:CH2	2:D:465:VAL:HG21	2.46	0.50
1:G:485:ILE:N	1:G:485:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:GLU:O	2:B:256:ARG:HB3	2.12	0.50
2:B:416:PRO:O	2:B:417:ALA:C	2.54	0.50
1:C:856:ILE:O	1:C:857:PRO:C	2.53	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
2:D:578:GLU:C	2:D:580:LYS:N	2.69	0.50
2:D:662:GLU:H	2:D:695:GLN:HE22	1.59	0.50
2:D:883:GLN:O	2:D:887:ALA:HB2	2.11	0.50
2:D:935:ARG:NH1	4:D:4:FDP:O3P	2.45	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:518:LEU:HD23	2:H:518:LEU:C	2.36	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:696:LEU:HB3	2:B:710:MET:HE1	1.93	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
1:G:291:ALA:HA	1:G:294:ASN:ND2	2.27	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
1:C:636:LEU:HD12	1:C:640:GLY:HA2	1.95	0.49
2:D:900:ASP:O	2:D:901:LYS:C	2.56	0.49
1:E:242:TYR:O	1:E:247:GLY:HA3	2.12	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:F:900:ASP:O	2:F:901:LYS:C	2.54	0.49
1:G:586:GLU:CD	1:G:587:LEU:H	2.20	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:196:GLN:CD	2:D:228:ARG:HG2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OE2	1:A:893:GLU:HA	2.12	0.49
2:B:711:VAL:CG2	2:B:910:VAL:HG22	2.42	0.49
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:F:887:ALA:C	2:F:889:ALA:H	2.21	0.49
2:H:201:VAL:HG11	2:H:218:ILE:CD1	2.42	0.49
2:H:268:THR:HG23	2:H:268:THR:O	2.12	0.49
2:H:578:GLU:C	2:H:580:LYS:N	2.67	0.49
2:H:590:ALA:HA	2:H:620:TYR:O	2.13	0.49
1:A:960:ALA:O	1:A:961:GLU:C	2.56	0.49
2:B:587:LEU:H	2:B:587:LEU:HD12	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:255:LEU:C	1:E:255:LEU:HD23	2.37	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:746:TYR:CE1	2:D:854:VAL:HG11	2.47	0.49
1:C:833:TYR:HA	1:C:837:LEU:HD23	1.94	0.49
1:E:342:PRO:HG2	1:E:343:TYR:CD1	2.47	0.49
1:E:805:LEU:N	1:E:805:LEU:HD23	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:916:HIS:O	2:D:917:VAL:HG23	2.12	0.49
2:F:256:ARG:NH1	2:F:813:PHE:CE1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:281:LEU:HD12	2:F:317:LEU:HD23	1.94	0.49
1:G:249:LEU:C	1:G:249:LEU:HD12	2.37	0.49
1:G:421:PRO:C	1:G:423:ARG:N	2.71	0.49
1:G:585:SER:O	1:G:586:GLU:C	2.53	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:780:LEU:HD13	1:G:780:LEU:C	2.37	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
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
2:B:426:MET:HE3	2:B:466:LEU:HD22	1.94	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:418:THR:OG1	2:F:419:SER:N	2.41	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:587:LEU:CD2	2:H:883:GLN:NE2	2.75	0.49
2:H:593:ASN:HA	2:H:684:VAL:O	2.13	0.49
1:A:423:ARG:O	1:A:424:ALA:C	2.56	0.49
2:B:549:ASP:OD2	2:B:552:ARG:HB2	2.12	0.49
1:C:423:ARG:O	1:C:424:ALA:C	2.56	0.49
1:C:651:GLU:HG3	1:C:652:ASN:ND2	2.27	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:578:GLU:C	2:F:580:LYS:N	2.70	0.49
2:F:798:GLU:O	2:F:801:ALA:HB3	2.13	0.49
1:G:809:ASN:C	1:G:809:ASN:OD1	2.55	0.49
1:G:959:TRP:CD1	1:G:959:TRP:N	2.81	0.49
2:H:608:MET:C	2:H:608:MET:SD	2.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:665:ASP:OD1	2:H:668:MET:HG2	2.13	0.49
1:A:317:LEU:HD12	1:A:317:LEU:N	2.28	0.48
2:B:692:SER:O	2:B:693:LEU:C	2.56	0.48
2:B:786:GLU:OE2	2:B:946:ARG:NH2	2.31	0.48
2:B:892:ALA:C	2:B:894:GLU:N	2.71	0.48
1:C:315:ALA:O	1:C:348:ILE:HD13	2.13	0.48
1:C:947:THR:HG23	1:C:947:THR:O	2.13	0.48
2:D:304:LEU:HD13	2:D:518:LEU:HD12	1.94	0.48
2:D:874:LYS:HD2	2:D:917:VAL:HG21	1.95	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:255:LEU:HD23	1:G:255:LEU:C	2.38	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
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
1:A:404:TRP:CZ2	1:A:408:MET:HE2	2.48	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
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:561:PHE:C	2:B:561:PHE:CD2	2.91	0.48
2:B:690:PHE:HA	2:B:712:LEU:HD22	1.94	0.48
1:C:249:LEU:C	1:C:249:LEU:HD12	2.37	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: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
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:G:960:ALA:C	1:G:962:TYR:H	2.20	0.48
1:A:398:MET:HG3	1:A:490:GLN:NE2	2.28	0.48
1:A:466:THR:CG2	1:A:468:ASN:H	2.15	0.48
1:A:964:LYS:H	1:A:964:LYS:CD	2.23	0.48
2:B:273:GLU:CD	2:B:273:GLU:H	2.19	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:B:900:ASP:CG	2:B:903:ILE:HG13	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:GLU:C	1:E:341:ALA:H	2.21	0.48
2:F:647:GLN:HE22	2:F:869:THR:CG2	2.27	0.48
2:F:692:SER:O	2:F:693:LEU:C	2.56	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
2:B:635:VAL:C	2:B:636:ARG:HD2	2.37	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:C:961:GLU:O	1:C:962:TYR:C	2.57	0.48
2:F:321:LEU:O	2:F:325:ASN:O	2.31	0.48
2:F:608:MET:SD	2:F:608:MET:C	2.97	0.48
1:C:631:ASN:OD1	2:D:752:ARG:HG3	2.13	0.48
1:E:601:VAL:O	1:E:691:GLY:HA3	2.14	0.48
2:F:580:LYS:O	2:F:581:LEU:C	2.55	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:806:LEU:O	1:G:807:LYS:C	2.56	0.48
2:H:892:ALA:C	2:H:894:GLU:N	2.70	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:351:MET:HE3	2:D:354:THR:CG2	2.44	0.48
2:D:668:MET:HE3	2:D:672:TYR:CE2	2.47	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
2:F:418:THR:HA	2:F:421:GLU:CB	2.39	0.48
1:G:404:TRP:CZ2	1:G:408:MET:HE2	2.48	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:804:THR:CG2	1:A:979:VAL:HG21	2.44	0.48
1:A:966:GLY:O	1:A:970:SER:CB	2.62	0.48
2:B:466:LEU:HD12	2:B:472:LEU:HD11	1.95	0.48
2:B:765:SER:HB2	2:B:936:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:521:VAL:HG13	2:D:526:ILE:HD13	1.95	0.48
1:E:247:GLY:HA2	1:E:254:TYR:HD2	1.78	0.48
1:E:421:PRO:C	1:E:423:ARG:H	2.20	0.48
2:F:353:THR:HG21	2:F:534:SER:HA	1.95	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
2:B:467:VAL:O	2:B:471:GLY:CA	2.58	0.48
2:B:946:ARG:HH21	2:B:946:ARG:CG	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
1:A:703:ARG:HD2	1:A:703:ARG:C	2.39	0.48
2:B:580:LYS:O	2:B:581:LEU:C	2.57	0.48
2:D:420:SER:C	2:D:423:GLN:HE21	2.22	0.48
2:D:707:ARG:NE	2:D:897:ASN:CG	2.72	0.48
2:F:709:PRO:HB2	2:F:879:ILE:HD13	1.96	0.48
1:G:270:GLY:O	1:G:271:GLY:C	2.56	0.48
1:G:790:PRO:HD2	1:G:791:GLU:OE1	2.14	0.48
2:H:420:SER:C	2:H:423:GLN:HE21	2.22	0.48
2:H:575:ASP:C	2:H:575:ASP:OD1	2.56	0.48
2:H:626:TRP:NE1	2:H:661:PRO:HG3	2.29	0.48
2:H:632:HIS:O	2:H:633:GLU:C	2.57	0.48
2:H:874:LYS:CD	2:H:917:VAL:HG21	2.43	0.48
1:A:755:SER:HB3	1:A:817:ASN:O	2.14	0.47
1:A:805:LEU:N	1:A:805:LEU:HD23	2.29	0.47
1:C:806:LEU:O	1:C:807:LYS:C	2.57	0.47
2:D:518:LEU:HD23	2:D:518:LEU:O	2.14	0.47
1:E:585:SER:O	1:E:586:GLU:C	2.57	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
1:A:289:ARG:N	1:A:325:LEU:HD13	2.29	0.47
1:A:421:PRO:C	1:A:423:ARG:N	2.72	0.47
2:B:575:ASP:OD1	2:B:575:ASP:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:765:SER:HB2	2:F:936:MET:HE1	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:523:GLU:O	2:H:524:ASN:C	2.56	0.47
2:H:770:THR:HG23	2:H:946:ARG:HD2	1.96	0.47
2:H:829:ALA:HB3	2:H:850:TYR:CZ	2.49	0.47
2:H:830:THR:HA	2:H:848:PRO:HB3	1.97	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:216:ASP:OD2	2:F:377:THR:HA	2.14	0.47
1:E:529:LEU:HD23	1:E:529:LEU:HA	1.70	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
2:H:668:MET:HE3	2:H:672:TYR:CE2	2.50	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
1:C:755:SER:HB3	1:C:817:ASN:O	2.13	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:H:889:ALA:C	2:H:891:ALA:N	2.61	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
2:B:639:ASN:O	2:B:640:TRP:C	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:VAL:HG11	1:A:697:ARG:HD3	1.97	0.47
1:A:856:ILE:O	1:A:857:PRO:C	2.58	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
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:832:LEU:HD12	2:H:832:LEU:HA	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: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: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:391:ARG:HG2	1:C:480:ASP:HB3	1.96	0.47
2:D:327:ILE:O	2:D:327:ILE:HG13	2.14	0.47
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: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:622:HIS:HD2	1:E:886:GLU:OE1	1.98	0.47
1:E:746:TYR:CE2	1:E:857:PRO:HG3	2.50	0.47
2:F:365:ASP:HA	2:F:862:PRO:HG2	1.97	0.47
2:F:431:SER:OG	2:F:470:LEU:HD11	2.14	0.47
2:F:657:ASN:OD1	2:F:659:VAL:HG23	2.15	0.47
1:G:339:GLU:C	1:G:341:ALA:H	2.22	0.47
1:G:391:ARG:O	1:G:448:ASN:HA	2.15	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
1:G:972:ARG:HG3	1:G:972:ARG:HH11	1.80	0.47
2:H:264:THR:HG22	2:H:266:ILE:N	2.27	0.47
2:H:740:TYR:CE1	2:H:851:PRO:HB3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:314:TRP:O	2:F:315:PRO:C	2.56	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
2:F:892:ALA:C	2:F:894:GLU:N	2.73	0.47
1:G:812:HIS:N	1:G:812:HIS:CD2	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:H:701:GLU:O	2:H:701:GLU:CD	2.58	0.47
2:B:827:LEU:HD21	1:C:837:LEU:HD11	1.96	0.47
2:B:946:ARG:HG3	2:B:946:ARG:NH2	2.26	0.47
1:C:261:GLU:H	1:C:261:GLU:CD	2.23	0.47
1:C:416:ASP:OD2	1:C:449:ASN:HA	2.15	0.47
1:C:694:GLU:CD	1:C:952:ARG:HH21	2.23	0.47
2:D:887:ALA:C	2:D:889:ALA:H	2.22	0.47
1:E:703:ARG:HD2	1:E:703:ARG:C	2.39	0.47
1:E:944:GLU:C	1:E:945:ASN:HD22	2.22	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
2:H:580:LYS:O	2:H:581:LEU:C	2.58	0.47
2:H:668:MET:HE3	2:H:672:TYR:HE2	1.79	0.47
2:H:706:PHE:C	2:H:708:ILE:H	2.22	0.47
1:A:418:ILE:HG12	1:A:575:PHE:CE2	2.49	0.47
1:A:808:GLU:O	1:A:809:ASN:C	2.57	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
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:249:LEU:HD12	1:E:249:LEU:C	2.40	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
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:HA	1:A:529:LEU:HD23	1.72	0.46
1:A:588:LEU:O	1:A:589:PRO:O	2.32	0.46
2:B:717:LEU:C	2:B:717:LEU:HD12	2.40	0.46
1:C:697:ARG:O	1:C:701:GLN:HG3	2.15	0.46
2:D:668:MET:HE3	2:D:672:TYR:HE2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:690:PHE:HA	2:D:712:LEU:HD22	1.97	0.46
1:E:803:ILE:HD13	1:E:845:ALA:CB	2.45	0.46
1:E:821:LYS:HB2	1:E:821:LYS:NZ	2.17	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
1:G:930:ASN:O	1:G:931:GLY:C	2.57	0.46
2:H:623:TYR:HB2	2:H:634:SER:HB2	1.97	0.46
1:A:773:TYR:N	1:A:959:TRP:CH2	2.83	0.46
1:A:952:ARG:HH11	1:A:952:ARG:HG3	1.81	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
2:D:900:ASP:CG	2:D:903:ILE:HG13	2.40	0.46
1:E:592:ASP:C	1:E:592:ASP:OD1	2.57	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: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
2:H:522:ASN:O	2:H:523:GLU:C	2.58	0.46
1:A:832:VAL:HG12	1:A:833:TYR:N	2.30	0.46
1:A:951:LEU:HD23	1:A:951:LEU:H	1.80	0.46
2:B:390:MET:HE3	2:B:480:GLY:C	2.40	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:596:ILE:CD1	1:E:885:ILE:HG21	2.46	0.46
1:G:312:LEU:HD12	1:G:359:MET:HE3	1.98	0.46
1:G:650:VAL:HG23	1:G:653:TRP:CE3	2.49	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
2:D:575:ASP:OD1	2:D:575:ASP:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:THR:O	1:E:212:THR:CG2	2.62	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
1:C:703:ARG:HD2	1:C:703:ARG:O	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
1:G:584:GLY:O	1:G:588:LEU:HB2	2.16	0.46
1:G:585:SER:O	1:G:586:GLU:O	2.32	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
2:B:894:GLU:C	2:B:896:PHE:N	2.74	0.46
2:B:904:SER:C	2:B:906:THR:H	2.23	0.46
1:C:488:HIS:C	1:C:490:GLN:N	2.71	0.46
1:E:323:PRO:O	1:E:326:VAL:HB	2.16	0.46
2:F:668:MET:HE3	2:F:672:TYR:CE2	2.51	0.46
1:G:450:THR:C	1:G:451:ILE:HD12	2.40	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:D:573:SER:O	2:D:574:ALA:C	2.59	0.46
2:F:428:ASP:CG	2:F:432:LYS:HZ3	2.24	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
2:H:696:LEU:CB	2:H:710:MET:HE1	2.45	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:HD3	2:D:552:ARG:O	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:VAL:O	1:A:650:VAL:HG13	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
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:416:PRO:HD2	2:F:550:PHE:CD1	2.50	0.46
2:F:547:ALA:O	2:F:549:ASP:N	2.49	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
2:H:288:ILE:HG12	2:H:335:MET:HE2	1.98	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:B:900:ASP:O	2:B:901:LYS:C	2.59	0.46
2:D:314:TRP:O	2:D:315:PRO:C	2.59	0.46
1:E:554:ASN:O	1:E:555:LYS:C	2.59	0.46
2:F:522:ASN:O	2:F:523:GLU:C	2.59	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
1:G:398:MET:HE3	1:G:487:GLY:C	2.41	0.46
2:H:256:ARG:CZ	2:H:813:PHE:CE1	2.98	0.46
2:H:755:ALA:HA	2:H:815:LYS:O	2.15	0.46
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
1:A:660:GLU:C	2:B:752:ARG:HH22	2.24	0.45
2:B:341:CYS:SG	2:B:519:ILE:CD1	3.04	0.45
2:B:668:MET:HE3	2:B:672:TYR:CE2	2.51	0.45
1:C:207:LYS:HB3	1:C:300:ILE:HG12	1.98	0.45
2:D:892:ALA:C	2:D:894:GLU:N	2.73	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:HD12	2:F:832:LEU:HA	1.78	0.45
2:H:200:ALA:HB2	2:H:230:PHE:HB2	1.98	0.45
2:H:796:ASP:O	2:H:800:LEU:HB2	2.15	0.45
2:B:414:GLU:OE2	2:B:414:GLU:N	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
2:B:701:GLU:O	2:B:701:GLU:OE2	2.34	0.45
1:C:732:TYR:CE1	1:C:736:VAL:HB	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:414:GLU:C	2:F:416:PRO:HD3	2.41	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: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:A:930:ASN:O	1:A:931:GLY:C	2.58	0.45
2:B:288:ILE:HG12	2:B:335:MET:HE2	1.99	0.45
1:C:378:MET:HE3	2:D:482:VAL:CG1	2.42	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:809:ASN:N	1:C:975:LEU:HD22	2.31	0.45
1:C:952:ARG:HH11	1:C:952:ARG:HG3	1.78	0.45
2:D:587:LEU:N	2:D:617:HIS:HD1	2.07	0.45
1:E:613:ARG:HG2	1:E:613:ARG:NH1	2.30	0.45
1:G:211:MET:HE3	1:G:305:VAL:HG22	1.97	0.45
1:G:746:TYR:CE2	1:G:857:PRO:HG3	2.51	0.45
2:H:314:TRP:O	2:H:315:PRO:C	2.55	0.45
2:H:883:GLN:O	2:H:887:ALA:CB	2.64	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:354:THR:HB	2:B:520:ALA:HB1	1.98	0.45
2:B:424:ASP:OD1	2:B:469:ARG:NH2	2.49	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:F:894:GLU:C	2:F:896:PHE:N	2.75	0.45
2:H:633:GLU:O	2:H:633:GLU:HG2	2.16	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
2:B:418:THR:OG1	2:B:419:SER:N	2.49	0.45
2:B:770:THR:HG23	2:B:946:ARG:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:853:HIS:C	2:D:855:GLN:N	2.74	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:231:GLY:O	1:G:232:ILE:C	2.59	0.45
1:G:253:LYS:C	1:G:255:LEU:N	2.73	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:O	2:H:698:ARG:HD2	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:E:289:ARG:CA	1:E:325:LEU:HD13	2.46	0.45
1:E:832:VAL:CG2	2:H:834:GLU:HB3	2.45	0.45
1:G:221:ASN:ND2	1:G:270:GLY:O	2.49	0.45
2:H:900:ASP:O	2:H:901:LYS:C	2.60	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
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:780:LEU:HD13	1:E:780:LEU:C	2.42	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:325:ASN:C	2:H:327:ILE:N	2.74	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:HG2	1:C:400:ARG:NH1	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:580:LYS:O	2:D:581:LEU:C	2.59	0.45
2:D:946:ARG:HG3	2:D:946:ARG:NH2	2.27	0.45
1:E:236:CYS:SG	1:E:515:LEU:HD21	2.57	0.45
1:E:440:ARG:HB2	1:E:440:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:505:LEU:HB2	1:E:533:ILE:HD11	1.97	0.45
2:F:354:THR:CB	2:F:520:ALA:HB1	2.47	0.45
2:F:771:TYR:OH	2:F:945:THR:HG21	2.17	0.45
2:F:791:GLU:HG3	1:G:800:ARG:NH2	2.31	0.45
2:F:931:GLU:HG3	2:F:931:GLU:O	2.16	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
2:H:887:ALA:C	2:H:889:ALA:N	2.74	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
1:E:669:SER:HB3	1:E:701:GLN:CD	2.42	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:669:SER:HB3	1:G:701:GLN:CD	2.41	0.45
1:G:927:ILE:HG23	1:G:927:ILE:O	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
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:HD12	1:C:485:ILE:N	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
2:D:936:MET:HB2	2:D:936:MET:HE3	1.91	0.45
1:E:255:LEU:HD23	1:E:256:LYS:N	2.32	0.45
1:E:943:TRP:C	1:E:946:GLU:HG3	2.42	0.45
2:F:595:GLY:O	2:F:656:THR:OG1	2.30	0.45
1:G:323:PRO:O	1:G:326:VAL:HB	2.17	0.45
1:A:251:GLY:HA3	1:A:294:ASN:CG	2.43	0.44
2:B:668:MET:HE3	2:B:672:TYR:HE2	1.82	0.44
1:C:451:ILE:HD12	1:C:451:ILE:N	2.32	0.44
1:C:944:GLU:C	1:C:945:ASN:HD22	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:THR:C	1:E:485:ILE:HD12	2.41	0.44
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:585:SER:O	1:A:586:GLU:C	2.59	0.44
2:B:236:TYR:O	2:B:237:GLU:C	2.60	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
1:E:488:HIS:C	1:E:490:GLN:H	2.25	0.44
1:E:796:LEU:CD1	2:H:793:LEU:HD13	2.43	0.44
2:F:830:THR:HA	2:F:848:PRO:HB3	1.99	0.44
1:A:264:ARG:HD2	1:A:819:ASN:HD22	1.81	0.44
1:A:442:ARG:NH1	1:A:449:ASN:OD1	2.39	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
1:C:808:GLU:O	1:C:809:ASN:C	2.59	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:963:ASN:N	1:G:963:ASN:HD22	2.12	0.44
2:B:239:LEU:HD22	2:B:287:LEU:HD22	1.99	0.44
1:C:466:THR:CG2	1:C:467:ALA:N	2.79	0.44
2:D:327:ILE:HB	2:D:331:GLN:HE21	1.83	0.44
2:D:561:PHE:C	2:D:561:PHE:CD2	2.96	0.44
2:D:918:VAL:HG12	2:D:919:TYR:H	1.83	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: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
2:D:589:ILE:CD1	2:D:879:ILE:HG21	2.46	0.44
2:D:648:SER:HA	2:D:865:ARG:HD3	1.98	0.44
1:E:301:ASP:N	1:E:301:ASP:OD1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:251:HIS:O	2:F:252:TRP:C	2.60	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:C:291:ALA:HA	1:C:294:ASN:ND2	2.33	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:755:ALA:HA	2:F:815:LYS:O	2.16	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
1:A:588:LEU:O	1:A:589:PRO:C	2.59	0.44
1:A:589:PRO:O	1:A:593:ARG:NH1	2.50	0.44
1:A:794:ILE:O	1:A:794:ILE:HG22	2.17	0.44
2:B:325:ASN:C	2:B:327:ILE:H	2.23	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:HG23	1:C:927:ILE:O	2.18	0.44
2:D:251:HIS:O	2:D:252:TRP:C	2.58	0.44
2:D:501:LEU:O	2:D:501:LEU:HD12	2.18	0.44
1:E:578:THR:O	1:E:578:THR:HG23	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
2:H:489:VAL:O	2:H:490:ALA:C	2.58	0.44
2:H:701:GLU:OE2	2:H:701:GLU:C	2.61	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
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
2:D:389:VAL:O	2:D:447:GLU:HB3	2.18	0.44
1:E:485:ILE:N	1:E:485:ILE:CD1	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
1:G:291:ALA:O	1:G:292:ALA:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:772:GLY:C	1:G:959:TRP:CZ3	2.96	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:554:MET:HE3	2:H:554:MET:HB2	1.92	0.44
2:H:717:LEU:HD23	2:H:856:GLN:HG2	1.99	0.44
1:C:405:LEU:HD12	1:C:405:LEU:HA	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
1:G:694:GLU:CD	1:G:952:ARG:HH21	2.26	0.44
2:H:414:GLU:OE2	2:H:414:GLU:N	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
1:C:255:LEU:HD23	1:C:255:LEU:C	2.43	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: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
2:F:696:LEU:HB3	2:F:710:MET:HE1	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
1:G:791:GLU:H	1:G:791:GLU:CD	2.23	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
2:D:494:ILE:HD13	2:D:771:TYR:HD2	1.83	0.43
1:E:800:ARG:HH22	2:H:791:GLU:HG3	1.81	0.43
1:E:947:THR:HG22	1:E:953:LYS:O	2.18	0.43
4:F:6:FDP:O5	4:F:6:FDP:O2P	2.35	0.43
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
2:H:946:ARG:NH2	2:H:946:ARG:CG	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:270:GLY:O	1:E:271:GLY:C	2.60	0.43
1:E:618:TYR:O	1:E:619:CYS:C	2.61	0.43
2:F:293:ASP:HB3	2:F:335:MET:HE3	2.00	0.43
2:F:573:SER:O	2:F:574:ALA:C	2.61	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:423:ARG:O	1:G:424:ALA:C	2.62	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: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:731:GLU:HG2	1:A:958:HIS:CD2	2.53	0.43
1:A:944:GLU:HA	1:A:946:GLU:OE1	2.18	0.43
1:A:979:VAL:O	1:A:980:ALA:HB2	2.18	0.43
2:B:587:LEU:CD2	2:B:883:GLN:NE2	2.81	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
1:C:367:GLY:H	1:C:499:ASP:CG	2.26	0.43
1:C:421:PRO:HG2	1:C:422:GLU:OE2	2.19	0.43
1:C:466:THR:HB	1:C:469:ASP:CG	2.43	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: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:HD23	2:F:239:LEU:HA	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
1:G:407:LEU:HD11	1:G:572:TYR:HA	2.00	0.43
1:G:448:ASN:ND2	1:G:448:ASN:N	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:344:VAL:CG2	2:H:357:THR:HG22	2.49	0.43
2:H:351:MET:HE3	2:H:354:THR:CG2	2.47	0.43
2:H:467:VAL:O	2:H:471:GLY:CA	2.61	0.43
2:H:693:LEU:CD2	2:H:922:ILE:HB	2.49	0.43
2:H:723:GLY:O	2:H:911:GLY:HA3	2.18	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:791:GLU:H	1:A:791:GLU:CD	2.25	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
2:B:853:HIS:C	2:B:855:GLN:H	2.26	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:481:HIS:C	2:D:483:GLN:N	2.71	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:G:211:MET:CE	1:G:305:VAL:HG22	2.48	0.43
2:H:421:GLU:O	2:H:425:GLN:HB2	2.18	0.43
1:A:822:LEU:C	1:A:823:LEU:HD12	2.43	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:887:ALA:C	2:B:889:ALA:H	2.26	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:696:LEU:CB	2:D:710:MET:HE1	2.48	0.43
2:D:883:GLN:O	2:D:887:ALA:CB	2.66	0.43
1:E:959:TRP:CD1	1:E:959:TRP:N	2.83	0.43
1:G:548:VAL:HG22	1:G:563:LEU:HD13	1.99	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:806:LEU:O	1:A:807:LYS:C	2.61	0.43
1:C:809:ASN:C	1:C:809:ASN:OD1	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:979:VAL:O	1:C:979:VAL:HG12	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: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:918:VAL:HG12	2:H:919:TYR:H	1.83	0.43
1:A:890:LYS:C	1:A:892:ASN:H	2.26	0.43
2:B:494:ILE:HG23	2:B:774:LEU:HD23	1.99	0.43
2:B:627:SER:HB3	2:B:659:VAL:HG21	2.01	0.43
2:B:894:GLU:O	2:B:896:PHE:N	2.51	0.43
1:C:805:LEU:HA	1:C:975:LEU:HB3	2.01	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:HG2	2:F:633:GLU:O	2.19	0.43
1:G:310:GLY:O	1:G:311:SER:C	2.62	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
1:G:890:LYS:C	1:G:892:ASN:H	2.26	0.43
2:H:853:HIS:C	2:H:855:GLN:N	2.75	0.43
1:A:756:ALA:HB2	2:B:651:GLY:HA2	2.00	0.43
1:A:860:VAL:CG1	2:B:740:TYR:CE1	3.02	0.43
2:B:239:LEU:HD23	2:B:239:LEU:HA	1.77	0.43
2:B:715:ALA:CB	2:B:728:LEU:HB2	2.49	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:647:GLN:HE22	2:D:869:THR:HG22	1.84	0.43
2:D:726:TYR:OH	2:D:864:ASP:OD2	2.29	0.43
1:E:391:ARG:NH2	3:F:984:F6P:O2P	2.51	0.43
1:G:484:THR:C	1:G:485:ILE:HD12	2.43	0.43
1:G:526:ILE:HD13	1:G:535:ARG:HG2	2.00	0.43
1:G:971:GLY:O	1:G:972:ARG:C	2.62	0.43
1:A:530:GLU:HA	1:A:932:SER:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:398:MET:HE3	1:C:487:GLY:C	2.43	0.43
1:C:543:LYS:HB2	1:C:543:LYS:NZ	2.34	0.43
1:C:791:GLU:H	1:C:791:GLU:CD	2.22	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
1:G:356:ASP:O	1:G:357:ASN:C	2.62	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:639:ASN:O	2:H:640:TRP:C	2.62	0.43
2:H:661:PRO:HD2	2:H:695:GLN:NE2	2.34	0.43
1:A:317:LEU:CD1	1:A:317:LEU:H	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
2:B:701:GLU:CD	2:B:701:GLU:C	2.86	0.42
1:C:587:LEU:O	1:C:589:PRO:HD3	2.18	0.42
1:E:758:ARG:O	1:E:759:ARG:C	2.62	0.42
1:E:791:GLU:CD	1:E:959:TRP:CH2	2.97	0.42
1:E:962:TYR:CD2	1:E:962:TYR:N	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:921:ASP:C	1:G:923:SER:N	2.76	0.42
2:H:301:ASP:O	2:H:302:GLY:C	2.60	0.42
2:H:947:LEU:HD22	2:H:951:HIS:NE2	2.34	0.42
1:A:484:THR:C	1:A:485:ILE:HD12	2.44	0.42
1:A:488:HIS:C	1:A:490:GLN:N	2.74	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
1:C:890:LYS:C	1:C:892:ASN:H	2.27	0.42
2:D:679:ASP:HB3	2:D:883:GLN:NE2	2.34	0.42
2:D:880:LYS:HB3	2:D:880:LYS:HE2	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:418:THR:OG1	2:B:422:TRP:CD1	2.66	0.42
2:B:697:GLU:C	2:B:699:ALA:H	2.27	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
2:F:418:THR:HA	2:F:421:GLU:HG3	2.01	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:707:ARG:HE	2:H:897:ASN:CG	2.27	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:356:ASP:CG	3:A:988:F6P:H11	2.42	0.42
1:A:440:ARG:HB2	1:A:440:ARG:HH11	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:O	2:B:931:GLU:HG3	2.19	0.42
1:C:223:ALA:O	1:C:227:VAL:HG23	2.19	0.42
1:C:278:ARG:HG3	1:C:278:ARG:NH1	2.33	0.42
1:C:828:GLN:O	1:C:829:ALA:C	2.61	0.42
1:C:836:GLN:HE21	1:C:840:ASP:CG	2.28	0.42
2:D:410:ILE:HA	2:D:444:VAL:O	2.20	0.42
1:E:211:MET:CE	1:E:305:VAL:HG22	2.49	0.42
1:E:526:ILE:HD13	1:E:535:ARG:HG2	2.02	0.42
1:E:865:VAL:CG1	1:E:871:ARG:HH21	2.32	0.42
2:F:577:ASN:CA	2:F:579:PRO:HD2	2.46	0.42
1:G:421:PRO:O	1:G:423:ARG:N	2.52	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
2:D:887:ALA:C	2:D:889:ALA:N	2.78	0.42
1:E:404:TRP:CZ2	1:E:408:MET:HE2	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:590:ALA:HA	2:F:620:TYR:O	2.19	0.42
1:G:212:THR:CG2	1:G:275:GLY:O	2.68	0.42
1:G:367:GLY:H	1:G:499:ASP:CG	2.27	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
1:A:317:LEU:O	1:A:321:GLU:HB3	2.20	0.42
1:A:527:GLY:HA3	1:A:536:MET:HE3	2.01	0.42
1:A:711:ILE:O	1:A:714:ILE:HG23	2.19	0.42
2:B:325:ASN:C	2:B:327:ILE:N	2.78	0.42
2:B:666:LEU:HD12	2:B:666:LEU:HA	1.81	0.42
2:B:755:ALA:O	2:B:846:ALA:HA	2.20	0.42
2:B:796:ASP:O	2:B:800:LEU:HB2	2.20	0.42
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
1:E:291:ALA:O	1:E:292:ALA:C	2.62	0.42
1:E:421:PRO:C	1:E:423:ARG:N	2.78	0.42
2:F:288:ILE:HD11	2:F:318:ILE:HG22	2.01	0.42
2:F:420:SER:C	2:F:423:GLN:HE21	2.27	0.42
1:G:838:LEU:HD12	1:G:838:LEU:HA	1.86	0.42
1:G:962:TYR:O	1:G:965:ILE:N	2.52	0.42
1:G:964:LYS:H	1:G:964:LYS:HG2	1.57	0.42
1:A:270:GLY:O	1:A:271:GLY:C	2.62	0.42
1:A:613:ARG:HG2	1:A:613:ARG:HH11	1.85	0.42
2:B:251:HIS:O	2:B:252:TRP:C	2.62	0.42
2:B:831:LYS:HD3	2:B:831:LYS:HA	1.79	0.42
1:C:211:MET:HE3	1:C:305:VAL:HG22	2.02	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
2:D:587:LEU:HB3	2:D:679:ASP:OD2	2.19	0.42
1:E:216:ASP:H	2:F:381:HIS:HE1	1.67	0.42
1:E:317:LEU:N	1:E:317:LEU:HD12	2.34	0.42
1:E:442:ARG:NH1	1:E:449:ASN:OD1	2.43	0.42
1:E:663:THR:O	1:E:663:THR:HG23	2.19	0.42
2:F:328:SER:N	2:F:331:GLN:NE2	2.66	0.42
2:F:665:ASP:OD2	2:F:665:ASP:C	2.61	0.42
2:F:802:GLN:O	2:F:803:SER:C	2.62	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:293:ASP:HB3	2:H:335:MET:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:687:PHE:CE2	2:H:935:ARG:HA	2.55	0.42
1:C:958:HIS:C	1:C:959:TRP:HD1	2.26	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: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
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
1:C:484:THR:C	1:C:485:ILE:HD12	2.45	0.42
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:381:HIS:O	2:D:382:SER:C	2.62	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
2:F:884:ALA:O	2:F:885:ALA:C	2.62	0.42
1:G:246:GLU:CA	1:G:279:SER:HB2	2.50	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
2:H:561:PHE:CD2	2:H:561:PHE:C	2.98	0.42
1:A:416:ASP:OD2	1:A:449:ASN:HA	2.20	0.42
1:A:809:ASN:C	1:A:809:ASN:OD1	2.63	0.42
2:B:578:GLU:O	2:B:580:LYS:CG	2.53	0.42
1:C:270:GLY:O	1:C:271:GLY:C	2.63	0.42
2:D:219:VAL:O	2:D:223:ILE:HG13	2.20	0.42
2:D:392:ARG:NH2	3:D:982:F6P:H12	2.33	0.42
2:D:666:LEU:HD12	2:D:666:LEU:HA	1.90	0.42
2:D:876:VAL:HG12	2:D:880:LYS:HE3	2.01	0.42
1:E:322:TRP:O	1:E:326:VAL:HG23	2.20	0.42
2:F:325:ASN:C	2:F:327:ILE:N	2.77	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
1:G:804:THR:O	1:G:805:LEU:C	2.63	0.42
1:G:856:ILE:O	1:G:857:PRO:C	2.63	0.42
2:H:400:LEU:CD1	2:H:866:THR:HG21	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:545:ILE:HD11	2:H:553:ALA:CB	2.49	0.42
2:H:935:ARG:O	2:H:936:MET:HB3	2.18	0.42
1:A:862:GLN:NE2	2:B:747:SER:OG	2.53	0.41
2:B:231:VAL:HG13	2:B:266:ILE:HG21	2.02	0.41
2:B:285:GLN:C	2:B:289:GLU:HG3	2.45	0.41
2:B:416:PRO:HB2	2:B:452:ALA:HA	2.03	0.41
2:B:419:SER:O	2:B:423:GLN:NE2	2.52	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
2:F:668:MET:HE3	2:F:672:TYR:HE2	1.85	0.41
2:F:853:HIS:C	2:F:855:GLN:N	2.77	0.41
1:G:317:LEU:N	1:G:317:LEU:CD1	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
2:H:886:ILE:O	2:H:890:ARG:N	2.52	0.41
2:H:900:ASP:CG	2:H:903:ILE:HG13	2.45	0.41
2:H:918:VAL:HG12	2:H:919:TYR:N	2.35	0.41
1:A:233:HIS:NE2	1:A:968:ILE:HD12	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
2:B:239:LEU:O	2:B:286:HIS:CD2	2.72	0.41
1:C:229:ARG:NH1	1:C:969:LEU:O	2.52	0.41
2:D:554:MET:HE3	2:D:554:MET:HB2	1.89	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:CG	1:G:972:ARG:NH1	2.83	0.41
2:H:355:ASP:CG	2:H:559:THR:HG22	2.44	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
2:B:751:THR:C	2:B:752:ARG:HG2	2.45	0.41
1:C:242:TYR:CD1	1:C:242:TYR:N	2.88	0.41
1:C:466:THR:O	1:C:467:ALA:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:696:LEU:HB3	2:D:710:MET:HE1	2.03	0.41
1:E:355:ILE:HB	1:E:371:ALA:HB2	2.02	0.41
1:E:668:ALA:C	1:E:670:GLU:H	2.28	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
1:E:976:ARG:O	1:E:977:ALA:C	2.62	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
2:F:900:ASP:CG	2:F:903:ILE:HG13	2.45	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
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
1:C:245:TYR:O	1:C:246:GLU:C	2.61	0.41
1:C:474:LEU:HD22	1:C:479:LEU:HD12	2.03	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
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:481:HIS:C	2:F:483:GLN:N	2.77	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:488:HIS:C	1:G:490:GLN:N	2.74	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:HD13	1:G:780:LEU:O	2.20	0.41
2:H:707:ARG:NE	2:H:897:ASN:CG	2.78	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:746:TYR:CE1	2:B:854:VAL:HG11	2.55	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:C:787:VAL:HA	1:C:824:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:791:GLU:N	1:C:791:GLU:CD	2.79	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
1:E:834:SER:O	1:E:835:THR:C	2.61	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:796:ASP:O	2:F:800:LEU:HB2	2.19	0.41
2:F:797:ILE:HD13	2:F:836:ILE:HA	2.03	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: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:298:CYS:HB2	2:H:343:THR:CG2	2.50	0.41
2:H:428:ASP:O	2:H:432:LYS:HG3	2.20	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:NH2	2:B:946:ARG:CG	2.80	0.41
1:C:759:ARG:HG2	1:C:810:PHE:CD2	2.56	0.41
1:C:807:LYS:O	1:C:808:GLU:C	2.64	0.41
2:D:467:VAL:O	2:D:471:GLY:CA	2.61	0.41
2:D:567:ASN:O	2:D:568:PHE:C	2.64	0.41
2:D:747:SER:O	2:D:750:SER:HB2	2.20	0.41
2:D:751:THR:C	2:D:752:ARG:HG2	2.45	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:734:LEU:HD21	1:E:873:THR:HG22	2.02	0.41
1:E:782:THR:HG22	1:E:784:ALA:N	2.36	0.41
1:E:808:GLU:O	1:E:809:ASN:C	2.64	0.41
1:E:821:LYS:HZ2	1:E:821:LYS:CB	2.12	0.41
2:F:365:ASP:OD2	2:F:369:LYS:NZ	2.46	0.41
1:G:246:GLU:HA	1:G:246:GLU:OE1	2.20	0.41
2:H:347:ILE:CG2	2:H:363:ALA:HB2	2.50	0.41
2:H:365:ASP:HA	2:H:862:PRO:HG2	2.02	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:583:LYS:O	2:H:584:ASP:C	2.61	0.41
2:H:665:ASP:OD2	2:H:665:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:C:805:LEU:HD23	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:700:LYS:O	1:E:701:GLN:C	2.64	0.41
1:E:746:TYR:CE1	2:F:854:VAL:HG13	2.55	0.41
1:E:826:ASN:OD1	1:E:826:ASN:C	2.63	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:694:HIS:CA	2:F:922:ILE:HG12	2.51	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
2:H:390:MET:HG3	2:H:483:GLN:HE22	1.82	0.41
2:H:446:ALA:O	2:H:447:GLU:C	2.59	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
1:A:780:LEU:C	1:A:780:LEU:HD13	2.46	0.41
2:B:577:ASN:CA	2:B:579:PRO:HD2	2.51	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:H	1:C:317:LEU:CD1	2.34	0.41
1:C:697:ARG:NH1	1:C:943:TRP:HH2	2.18	0.41
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:426:MET:HE3	2:F:466:LEU:HD22	2.02	0.41
2:F:438:LYS:HG2	2:F:440:THR:O	2.21	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
1:A:788:TYR:HE1	1:A:823:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:410:ILE:HA	2:B:444:VAL:O	2.21	0.41
2:B:611:TYR:CG	2:B:873:ILE:HG12	2.56	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: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
1:C:765:GLU:HA	1:C:825:ARG:O	2.20	0.41
1:C:774:ILE:HD13	1:C:774:ILE:HA	1.98	0.41
2:D:239:LEU:HD23	2:D:239:LEU:HA	1.87	0.41
2:D:273:GLU:CD	2:D:273:GLU:H	2.26	0.41
2:D:301:ASP:O	2:D:302:GLY:C	2.61	0.41
2:D:379:ASN:HA	2:D:440:THR:HG23	2.02	0.41
2:D:494:ILE:HG23	2:D:774:LEU:HD23	2.03	0.41
2:D:673:PHE:HZ	2:D:681:LEU:HD22	1.86	0.41
2:D:723:GLY:O	2:D:911:GLY:HA3	2.21	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:289:ARG:N	1:E:325:LEU:HD13	2.35	0.41
1:E:399:GLY:O	1:E:400:ARG:HB3	2.21	0.41
1:E:427:HIS:C	1:E:427:HIS:HD1	2.29	0.41
1:E:431:GLN:NE2	1:E:431:GLN:N	2.50	0.41
1:E:747:THR:O	1:E:748:ASP:C	2.64	0.41
2:F:288:ILE:HG12	2:F:335:MET:HE2	2.03	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:554:ASN:O	1:G:555:LYS:C	2.64	0.41
1:G:590:VAL:CG2	1:G:591:SER:H	2.22	0.41
1:G:962:TYR:C	1:G:964:LYS:N	2.78	0.41
2:H:325:ASN:O	2:H:326:ARG:HB2	2.20	0.41
2:H:381:HIS:CD2	2:H:383:ARG:HH21	2.39	0.41
1:A:665:ARG:O	1:A:666:SER:C	2.63	0.41
1:A:825:ARG:NH2	1:A:834:SER:HA	2.36	0.41
1:A:942:LEU:C	1:A:944:GLU:N	2.79	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
2:D:523:GLU:OE1	2:D:915:SER:HB3	2.21	0.41
2:D:701:GLU:CD	2:D:701:GLU:C	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:741:ASN:O	1:E:742:ALA:C	2.59	0.41
2:F:561:PHE:CD2	2:F:561:PHE:C	2.99	0.41
2:F:591:ILE:HG12	2:F:682:ILE:CG2	2.51	0.41
2:F:936:MET:HB2	2:F:936:MET:HE3	1.96	0.41
1:G:589:PRO:O	1:G:593:ARG:NH1	2.54	0.41
2:H:426:MET:HE3	2:H:466:LEU:HD22	2.02	0.41
2:H:888:GLU:OE1	2:H:888:GLU:C	2.64	0.41
1:A:433:GLU:O	1:A:437:VAL:HG23	2.20	0.40
1:A:498:HIS:HD2	1:A:869:LYS:NZ	2.19	0.40
1:A:837:LEU:HD11	1:A:841:ILE:HD11	2.02	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
1:C:879:VAL:O	1:C:880:LYS:C	2.63	0.40
1:C:930:ASN:O	1:C:931:GLY:C	2.62	0.40
1:C:959:TRP:C	1:C:961:GLU:N	2.79	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:697:GLU:C	2:D:697:GLU:OE2	2.64	0.40
1:E:539:VAL:O	1:E:542:VAL:CG2	2.68	0.40
1:E:539:VAL:C	1:E:542:VAL:HG22	2.45	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:538:LEU:HD23	1:G:538:LEU:C	2.46	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:HA	2:H:322:LEU:HD23	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
1:A:826:ASN:OD1	1:A:826:ASN:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:832:VAL:HG12	1:G:833:TYR:N	2.36	0.40
1:G:921:ASP:C	1:G:923:SER:H	2.28	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:331:ALA:O	1:A:332:GLU:C	2.63	0.40
1:A:431:GLN:H	1:A:431:GLN:CD	2.18	0.40
1:A:573:GLU:O	1:A:574:ASN:C	2.63	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
1:C:942:LEU:C	1:C:944:GLU:N	2.78	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: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:301:ASP:O	2:F:302:GLY:C	2.64	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
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:639:ASN:O	2:D:640:TRP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:701:GLU:O	2:D:701:GLU:OE2	2.39	0.40
1:E:448:ASN:H	1:E:448:ASN:HD22	1.67	0.40
1:E:514:VAL:HG12	1:E:515:LEU:N	2.36	0.40
1:E:648:ILE:O	1:E:648:ILE:HD13	2.22	0.40
1:E:668:ALA:C	1:E:670:GLU:N	2.79	0.40
1:E:837:LEU:HD22	2:H:831:LYS:CD	2.51	0.40
2:F:285:GLN:C	2:F:289:GLU:HG3	2.46	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: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:760:ARG:NH1	4:B:2:FDP:O6P	2.53	0.40
1:A:803:ILE:HD13	1:A:845:ALA:CB	2.52	0.40
1:A:836:GLN:HE21	1:A:840:ASP:CG	2.30	0.40
1:A:837:LEU:HD11	2:D:827:LEU:CD2	2.51	0.40
2:B:832:LEU:HA	2:B:832:LEU:HD12	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:HH11	2:D:475:ARG:HG2	1.87	0.40
2:D:587:LEU:HB3	2:D:679:ASP:CB	2.52	0.40
1:E:746:TYR:CE1	2:F:854:VAL:HG11	2.57	0.40
2:F:647:GLN:HE22	2:F:869:THR:HG22	1.86	0.40
2:F:887:ALA:C	2:F:889:ALA:N	2.78	0.40
1:G:278:ARG:NH1	1:G:278:ARG:HG3	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%)	2	10
1	C	746/787 (95%)	634 (85%)	85 (11%)	27 (4%)	2	11
1	E	748/787 (95%)	643 (86%)	74 (10%)	31 (4%)	2	9
1	G	742/787 (94%)	632 (85%)	79 (11%)	31 (4%)	2	9
2	B	761/766 (99%)	675 (89%)	61 (8%)	25 (3%)	3	13
2	D	761/766 (99%)	672 (88%)	59 (8%)	30 (4%)	2	10
2	F	760/766 (99%)	674 (89%)	58 (8%)	28 (4%)	2	11
2	H	761/766 (99%)	680 (89%)	53 (7%)	28 (4%)	2	11
All	All	6025/6212 (97%)	5240 (87%)	556 (9%)	229 (4%)	2	10

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%)	559 (91%)	55 (9%)	9	28
1	C	614/645 (95%)	556 (91%)	58 (9%)	8	26
1	E	616/645 (96%)	558 (91%)	58 (9%)	8	26
1	G	612/645 (95%)	551 (90%)	61 (10%)	7	24
2	B	612/615 (100%)	547 (89%)	65 (11%)	6	22
2	D	612/615 (100%)	547 (89%)	65 (11%)	6	22
2	F	611/615 (99%)	549 (90%)	62 (10%)	7	24
2	H	612/615 (100%)	552 (90%)	60 (10%)	7	25
All	All	4903/5040 (97%)	4419 (90%)	484 (10%)	7	24

All (484) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	LYS
1	A	237	ASP
1	A	249	LEU
1	A	261	GLU
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

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Mol	Chain	Res	Type
1	A	405	LEU
1	A	423	ARG
1	A	427	HIS
1	A	431	GLN
1	A	436	GLU
1	A	502	LEU
1	A	514	VAL
1	A	517	PHE
1	A	524	PRO
1	A	539	VAL
1	A	543	LYS
1	A	555	LYS
1	A	564	ARG
1	A	578	THR
1	A	588	LEU
1	A	589	PRO
1	A	599	VAL
1	A	605	SER
1	A	648	ILE
1	A	650	VAL
1	A	656	LEU
1	A	703	ARG
1	A	751	LYS
1	A	758	ARG
1	A	766	VAL
1	A	782	THR
1	A	785	VAL
1	A	805	LEU
1	A	814	LYS
1	A	819	ASN
1	A	821	LYS
1	A	822	LEU
1	A	832	VAL
1	A	891	LYS
1	A	920	GLU
1	A	929	VAL
1	A	934	VAL
1	A	946	GLU
1	A	952	ARG
1	A	956	GLU
1	A	959	TRP
1	A	964	LYS

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Mol	Chain	Res	Type
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
2	B	301	ASP
2	B	322	LEU
2	B	326	ARG
2	B	334	ARG
2	B	336	LYS
2	B	343	THR
2	B	344	VAL
2	B	366	ARG
2	B	389	VAL
2	B	423	GLN
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	557	ARG
2	B	565	LEU
2	B	575	ASP
2	B	579	PRO
2	B	583	LYS
2	B	586	ARG
2	B	587	LEU
2	B	591	ILE
2	B	619	PRO
2	B	673	PHE
2	B	688	GLU
2	B	698	ARG
2	B	700	ARG
2	B	701	GLU

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Mol	Chain	Res	Type
2	B	702	SER
2	B	711	VAL
2	B	716	THR
2	B	744	VAL
2	B	793	LEU
2	B	794	SER
2	B	800	LEU
2	B	808	GLU
2	B	825	LYS
2	B	867	ARG
2	B	869	THR
2	B	886	ILE
2	B	888	GLU
2	B	902	THR
2	B	910	VAL
2	B	916	HIS
2	B	922	ILE
2	B	925	LEU
2	B	932	VAL
2	B	940	ILE
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	261	GLU
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

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Mol	Chain	Res	Type
1	C	514	VAL
1	C	517	PHE
1	C	525	LEU
1	C	530	GLU
1	C	539	VAL
1	C	543	LYS
1	C	555	LYS
1	C	564	ARG
1	C	578	THR
1	C	587	LEU
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
1	C	751	LYS
1	C	758	ARG
1	C	766	VAL
1	C	782	THR
1	C	785	VAL
1	C	805	LEU
1	C	812	HIS
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	920	GLU
1	C	929	VAL
1	C	934	VAL
1	C	946	GLU
1	C	955	PHE
1	C	959	TRP
1	C	964	LYS
1	C	967	ASP
2	D	201	VAL
2	D	253	GLU
2	D	256	ARG

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Mol	Chain	Res	Type
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	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
2	D	551	LYS
2	D	552	ARG
2	D	557	ARG
2	D	565	LEU
2	D	575	ASP
2	D	579	PRO
2	D	583	LYS
2	D	586	ARG
2	D	587	LEU
2	D	591	ILE
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	711	VAL
2	D	716	THR
2	D	793	LEU
2	D	794	SER

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Mol	Chain	Res	Type
2	D	800	LEU
2	D	808	GLU
2	D	825	LYS
2	D	867	ARG
2	D	869	THR
2	D	879	ILE
2	D	886	ILE
2	D	888	GLU
2	D	890	ARG
2	D	903	ILE
2	D	916	HIS
2	D	922	ILE
2	D	923	ARG
2	D	925	LEU
2	D	932	VAL
2	D	940	ILE
2	D	945	THR
2	D	947	LEU
2	D	956	LYS
2	D	957	ARG
1	E	203	GLN
1	E	204	LYS
1	E	249	LEU
1	E	261	GLU
1	E	264	ARG
1	E	306	CYS
1	E	309	ASP
1	E	322	TRP
1	E	328	GLU
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	451	ILE
1	E	458	LEU
1	E	502	LEU

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Mol	Chain	Res	Type
1	E	514	VAL
1	E	517	PHE
1	E	518	THR
1	E	539	VAL
1	E	543	LYS
1	E	555	LYS
1	E	564	ARG
1	E	578	THR
1	E	587	LEU
1	E	588	LEU
1	E	589	PRO
1	E	599	VAL
1	E	605	SER
1	E	648	ILE
1	E	650	VAL
1	E	656	LEU
1	E	751	LYS
1	E	758	ARG
1	E	766	VAL
1	E	782	THR
1	E	785	VAL
1	E	809	ASN
1	E	814	LYS
1	E	819	ASN
1	E	821	LYS
1	E	822	LEU
1	E	832	VAL
1	E	865	VAL
1	E	891	LYS
1	E	920	GLU
1	E	929	VAL
1	E	934	VAL
1	E	944	GLU
1	E	946	GLU
1	E	956	GLU
1	E	976	ARG
2	F	201	VAL
2	F	253	GLU
2	F	256	ARG
2	F	259	SER
2	F	273	GLU
2	F	281	LEU

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Mol	Chain	Res	Type
2	F	287	LEU
2	F	297	VAL
2	F	322	LEU
2	F	326	ARG
2	F	334	ARG
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	557	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	636	ARG
2	F	673	PHE
2	F	688	GLU
2	F	700	ARG
2	F	701	GLU
2	F	702	SER
2	F	711	VAL
2	F	716	THR
2	F	718	SER
2	F	744	VAL
2	F	793	LEU
2	F	794	SER
2	F	800	LEU

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Mol	Chain	Res	Type
2	F	808	GLU
2	F	867	ARG
2	F	869	THR
2	F	886	ILE
2	F	888	GLU
2	F	902	THR
2	F	910	VAL
2	F	916	HIS
2	F	922	ILE
2	F	925	LEU
2	F	932	VAL
2	F	945	THR
2	F	947	LEU
2	F	956	LYS
1	G	205	LYS
1	G	249	LEU
1	G	261	GLU
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	525	LEU
1	G	539	VAL
1	G	543	LYS
1	G	555	LYS
1	G	564	ARG

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Mol	Chain	Res	Type
1	G	566	THR
1	G	578	THR
1	G	587	LEU
1	G	588	LEU
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	703	ARG
1	G	744	VAL
1	G	751	LYS
1	G	766	VAL
1	G	782	THR
1	G	785	VAL
1	G	814	LYS
1	G	819	ASN
1	G	821	LYS
1	G	822	LEU
1	G	832	VAL
1	G	891	LYS
1	G	920	GLU
1	G	929	VAL
1	G	934	VAL
1	G	946	GLU
1	G	948	ASN
1	G	950	GLU
1	G	959	TRP
1	G	963	ASN
1	G	964	LYS
1	G	972	ARG
1	G	975	LEU
2	H	201	VAL
2	H	253	GLU
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

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Mol	Chain	Res	Type
2	H	326	ARG
2	H	334	ARG
2	H	336	LYS
2	H	343	THR
2	H	344	VAL
2	H	366	ARG
2	H	389	VAL
2	H	423	GLN
2	H	436	ARG
2	H	469	ARG
2	H	472	LEU
2	H	487	THR
2	H	510	SER
2	H	517	PRO
2	H	518	LEU
2	H	521	VAL
2	H	525	LYS
2	H	531	LEU
2	H	551	LYS
2	H	552	ARG
2	H	557	ARG
2	H	565	LEU
2	H	575	ASP
2	H	579	PRO
2	H	583	LYS
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	702	SER
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	867	ARG
2	H	869	THR
2	H	886	ILE

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Mol	Chain	Res	Type
2	H	888	GLU
2	H	902	THR
2	H	910	VAL
2	H	916	HIS
2	H	925	LEU
2	H	932	VAL
2	H	945	THR
2	H	947	LEU
2	H	956	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	ASN
1	A	431	GLN
1	A	448	ASN
1	A	468	ASN
1	A	498	HIS
1	A	506	GLN
1	A	574	ASN
1	A	600	HIS
1	A	631	ASN
1	A	652	ASN
1	A	654	HIS
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	887	GLN
1	A	889	ASN
1	A	930	ASN
1	A	933	HIS
1	A	945	ASN
2	B	196	GLN
2	B	214	ASN
2	B	286	HIS
2	B	331	GLN
2	B	381	HIS

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Mol	Chain	Res	Type
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	792	GLN
2	B	882	ASN
2	B	943	GLN
1	C	233	HIS
1	C	294	ASN
1	C	298	GLN
1	C	431	GLN
1	C	448	ASN
1	C	463	ASN
1	C	468	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
1	C	708	GLN
1	C	709	HIS
1	C	713	ASN
1	C	767	GLN
1	C	770	HIS
1	C	812	HIS
1	C	819	ASN
1	C	828	GLN
1	C	836	GLN
1	C	862	GLN
1	C	887	GLN
1	C	889	ASN
1	C	930	ASN
1	C	933	HIS
1	C	945	ASN
2	D	196	GLN
2	D	214	ASN
2	D	286	HIS

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Mol	Chain	Res	Type
2	D	331	GLN
2	D	381	HIS
2	D	423	GLN
2	D	463	HIS
2	D	522	ASN
2	D	564	HIS
2	D	572	ASN
2	D	577	ASN
2	D	674	GLN
2	D	695	GLN
2	D	761	GLN
2	D	792	GLN
2	D	855	GLN
2	D	882	ASN
2	D	897	ASN
2	D	941	HIS
2	D	943	GLN
1	E	233	HIS
1	E	294	ASN
1	E	431	GLN
1	E	448	ASN
1	E	498	HIS
1	E	506	GLN
1	E	600	HIS
1	E	622	HIS
1	E	631	ASN
1	E	652	ASN
1	E	701	GLN
1	E	713	ASN
1	E	767	GLN
1	E	770	HIS
1	E	812	HIS
1	E	828	GLN
1	E	862	GLN
1	E	887	GLN
1	E	889	ASN
1	E	930	ASN
1	E	933	HIS
1	E	945	ASN
1	E	958	HIS
1	E	963	ASN
2	F	196	GLN

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Mol	Chain	Res	Type
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	694	HIS
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	294	ASN
1	G	431	GLN
1	G	448	ASN
1	G	498	HIS
1	G	506	GLN
1	G	574	ASN
1	G	600	HIS
1	G	652	ASN
1	G	680	GLN
1	G	701	GLN
1	G	709	HIS
1	G	713	ASN
1	G	767	GLN
1	G	812	HIS
1	G	817	ASN
1	G	819	ASN
1	G	828	GLN
1	G	836	GLN
1	G	862	GLN
1	G	887	GLN
1	G	889	ASN
1	G	930	ASN
1	G	933	HIS
1	G	945	ASN
1	G	963	ASN
2	H	196	GLN

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Mol	Chain	Res	Type
2	H	214	ASN
2	H	286	HIS
2	H	331	GLN
2	H	337	HIS
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	746	GLN
2	H	761	GLN
2	H	792	GLN
2	H	853	HIS
2	H	882	ASN
2	H	897	ASN
2	H	941	HIS
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 oligosaccharides 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
4	FDP	F	6	-	19,20,20	0.94	0	29,32,32	0.91	2 (6%)
4	FDP	A	1	-	19,20,20	0.93	0	29,32,32	0.77	0
4	FDP	B	2	-	19,20,20	0.92	0	29,32,32	0.85	1 (3%)
4	FDP	G	7	-	19,20,20	0.93	0	29,32,32	0.81	1 (3%)
4	FDP	E	5	-	19,20,20	0.95	0	29,32,32	0.89	1 (3%)
3	F6P	E	988	-	15,16,16	0.84	0	16,25,25	0.81	0
4	FDP	C	3	-	19,20,20	0.96	0	29,32,32	0.80	0
4	FDP	H	8	-	19,20,20	0.94	0	29,32,32	0.93	1 (3%)
3	F6P	H	986	-	15,16,16	0.83	0	16,25,25	0.79	1 (6%)
3	F6P	D	982	-	15,16,16	0.90	0	16,25,25	0.78	0
3	F6P	A	988	-	15,16,16	0.92	0	16,25,25	3.82	5 (31%)
4	FDP	D	4	-	19,20,20	0.93	0	29,32,32	0.85	1 (3%)
3	F6P	F	984	-	15,16,16	0.89	0	16,25,25	0.89	0
3	F6P	B	980	-	15,16,16	1.04	1 (6%)	16,25,25	1.03	1 (6%)
3	F6P	C	988	-	15,16,16	0.90	0	16,25,25	0.88	0
3	F6P	G	988	-	15,16,16	1.09	1 (6%)	16,25,25	3.74	5 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FDP	F	6	-	-	6/12/34/34	0/1/1/1
4	FDP	A	1	-	-	2/12/34/34	0/1/1/1
4	FDP	B	2	-	-	0/12/34/34	0/1/1/1
4	FDP	G	7	-	-	1/12/34/34	0/1/1/1
4	FDP	E	5	-	-	3/12/34/34	0/1/1/1
3	F6P	E	988	-	-	1/9/28/28	0/1/1/1
4	FDP	C	3	-	-	0/12/34/34	0/1/1/1
4	FDP	H	8	-	-	1/12/34/34	0/1/1/1
3	F6P	H	986	-	-	1/9/28/28	0/1/1/1
3	F6P	D	982	-	-	1/9/28/28	0/1/1/1
3	F6P	A	988	-	-	3/9/28/28	0/1/1/1
4	FDP	D	4	-	-	2/12/34/34	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	F6P	F	984	-	-	1/9/28/28	0/1/1/1
3	F6P	B	980	-	-	1/9/28/28	0/1/1/1
3	F6P	C	988	-	-	1/9/28/28	0/1/1/1
3	F6P	G	988	-	-	3/9/28/28	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	-2.35	1.39	1.43
3	B	980	F6P	P-O3P	2.25	1.63	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	988	F6P	O3P-P-O6	-8.96	83.32	106.67
3	G	988	F6P	O3P-P-O6	-8.88	83.52	106.67
3	A	988	F6P	O6-P-O1P	6.86	124.98	106.44
3	A	988	F6P	O3P-P-O1P	-6.86	84.12	110.83
3	G	988	F6P	O6-P-O1P	6.79	124.80	106.44
3	A	988	F6P	O3P-P-O2P	-6.56	83.21	107.80
3	G	988	F6P	O3P-P-O1P	-6.44	85.74	110.83
3	G	988	F6P	O3P-P-O2P	-6.13	84.83	107.80
3	A	988	F6P	O2P-P-O6	3.49	115.76	106.67
3	G	988	F6P	O2P-P-O6	3.02	114.54	106.67
4	F	6	FDP	O6-P2-O4P	2.52	113.26	106.44
4	E	5	FDP	O6-P2-O4P	2.47	113.13	106.44
4	D	4	FDP	O6-P2-O4P	2.28	112.61	106.44
3	B	980	F6P	O5-C5-C6	-2.21	104.31	109.50
4	G	7	FDP	O6-P2-O4P	2.15	112.25	106.44
4	F	6	FDP	C2-O5-C5	-2.13	102.27	108.14
3	H	986	F6P	O3P-P-O6	2.02	111.93	106.67
4	H	8	FDP	O6-P2-O4P	2.01	111.88	106.44
4	B	2	FDP	O6-P2-O4P	2.01	111.87	106.44

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	988	F6P	C6-O6-P-O3P
3	G	988	F6P	C6-O6-P-O1P
3	G	988	F6P	C6-O6-P-O3P

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

There are no ring outliers.

14 monomers are involved in 43 short contacts:

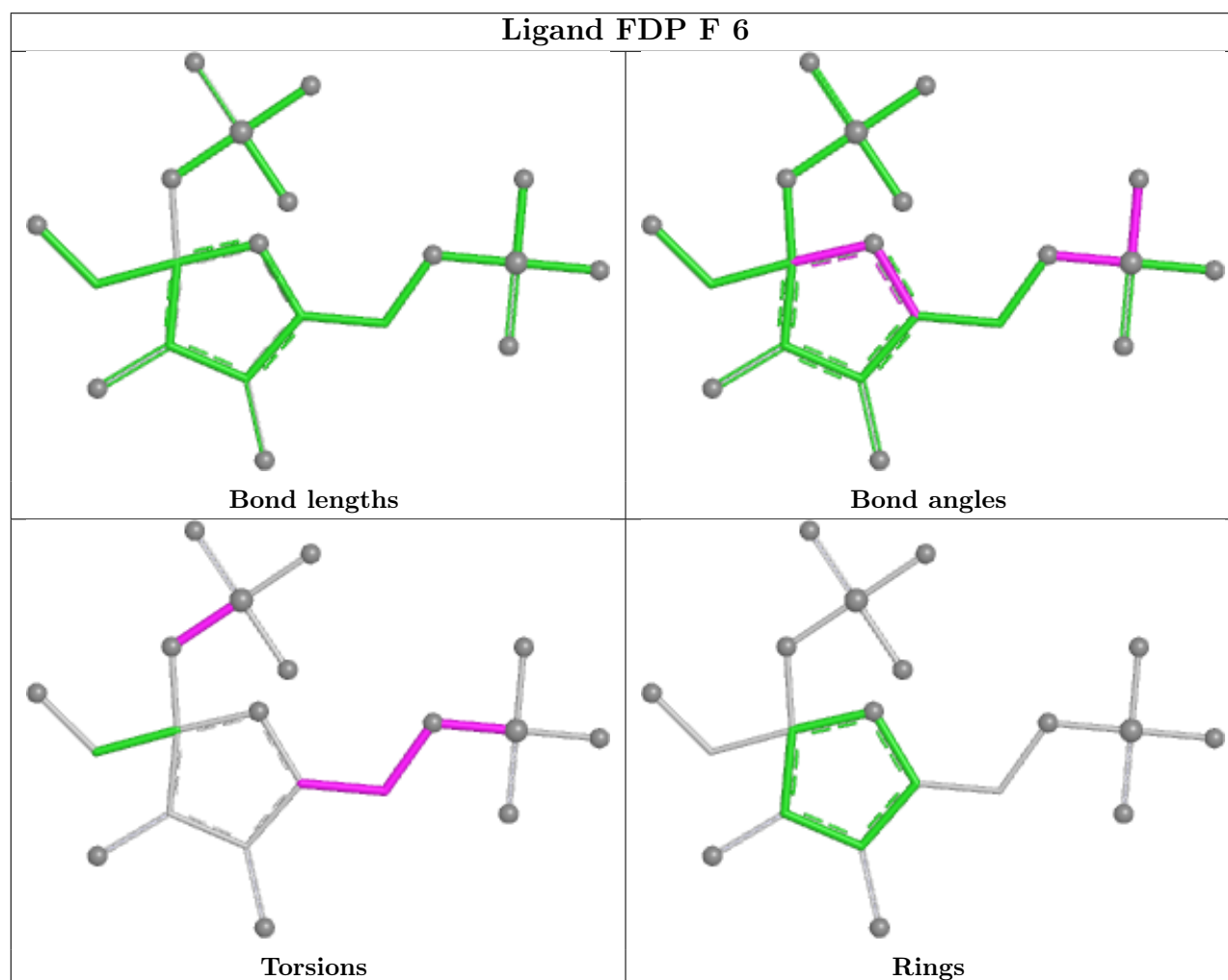
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	6	FDP	3	0
4	A	1	FDP	6	0
4	B	2	FDP	3	0
3	E	988	F6P	2	0
4	C	3	FDP	1	0
4	H	8	FDP	2	0
3	H	986	F6P	5	0
3	D	982	F6P	3	0
3	A	988	F6P	5	0
4	D	4	FDP	2	0
3	F	984	F6P	4	0
3	B	980	F6P	4	0
3	C	988	F6P	1	0

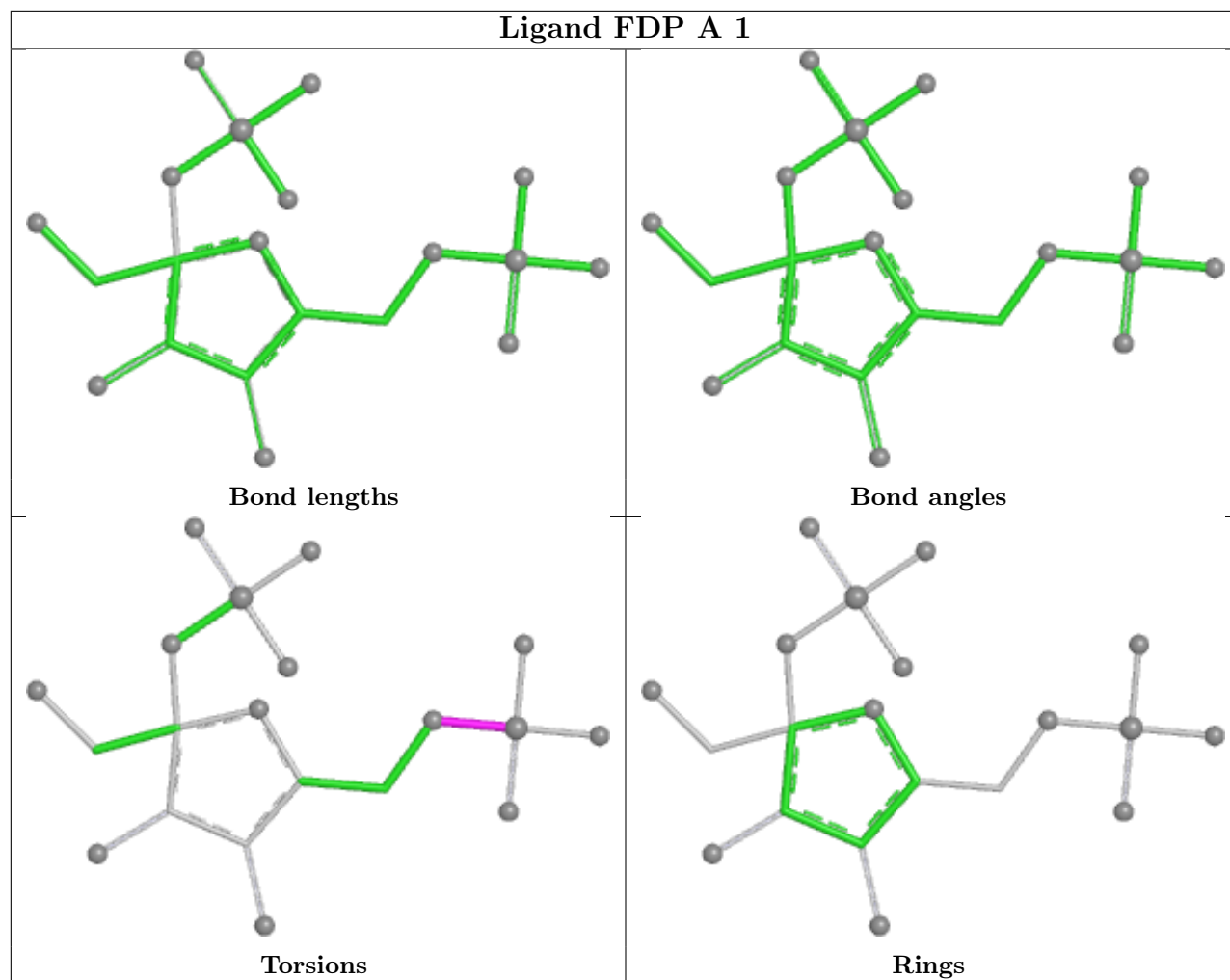
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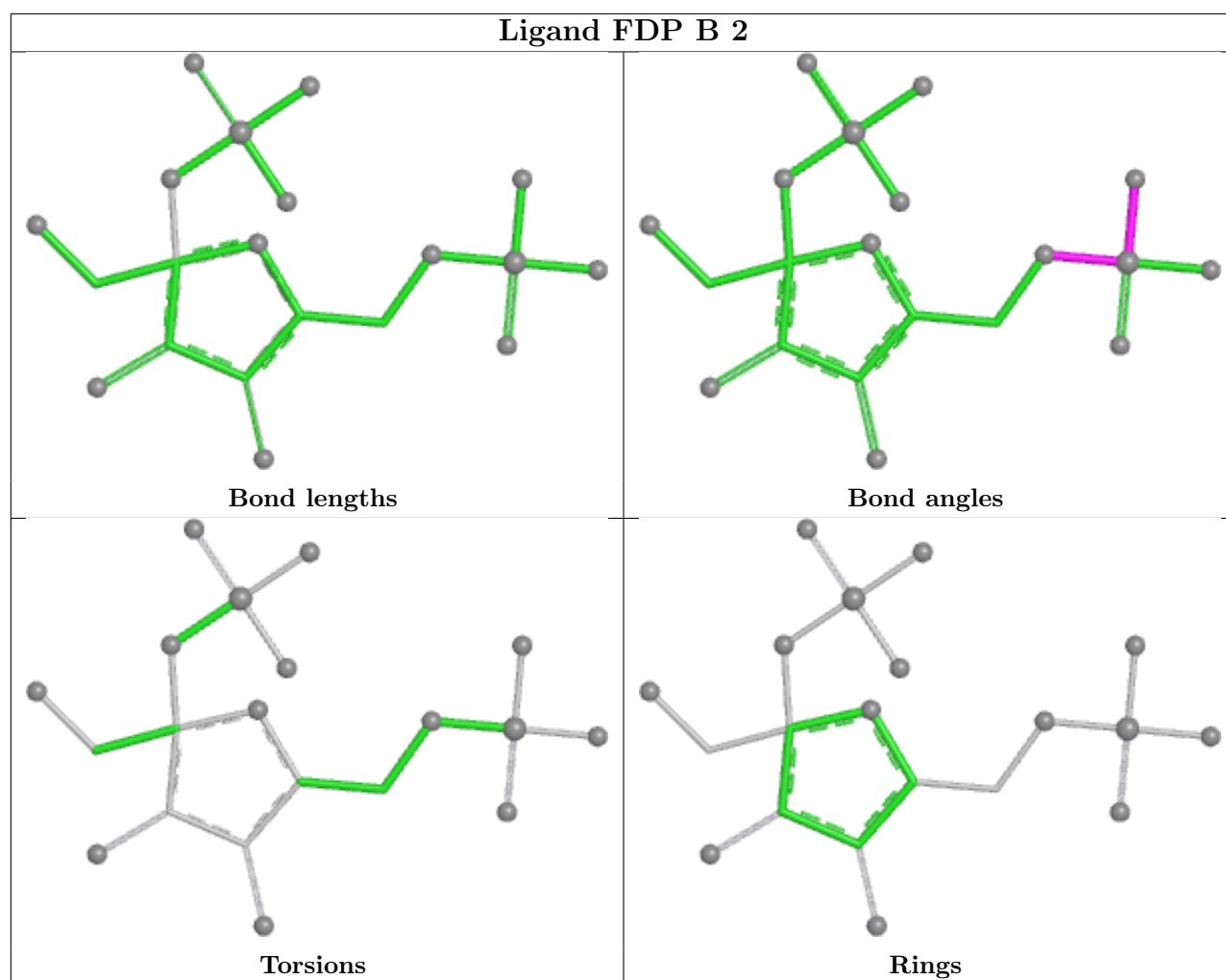
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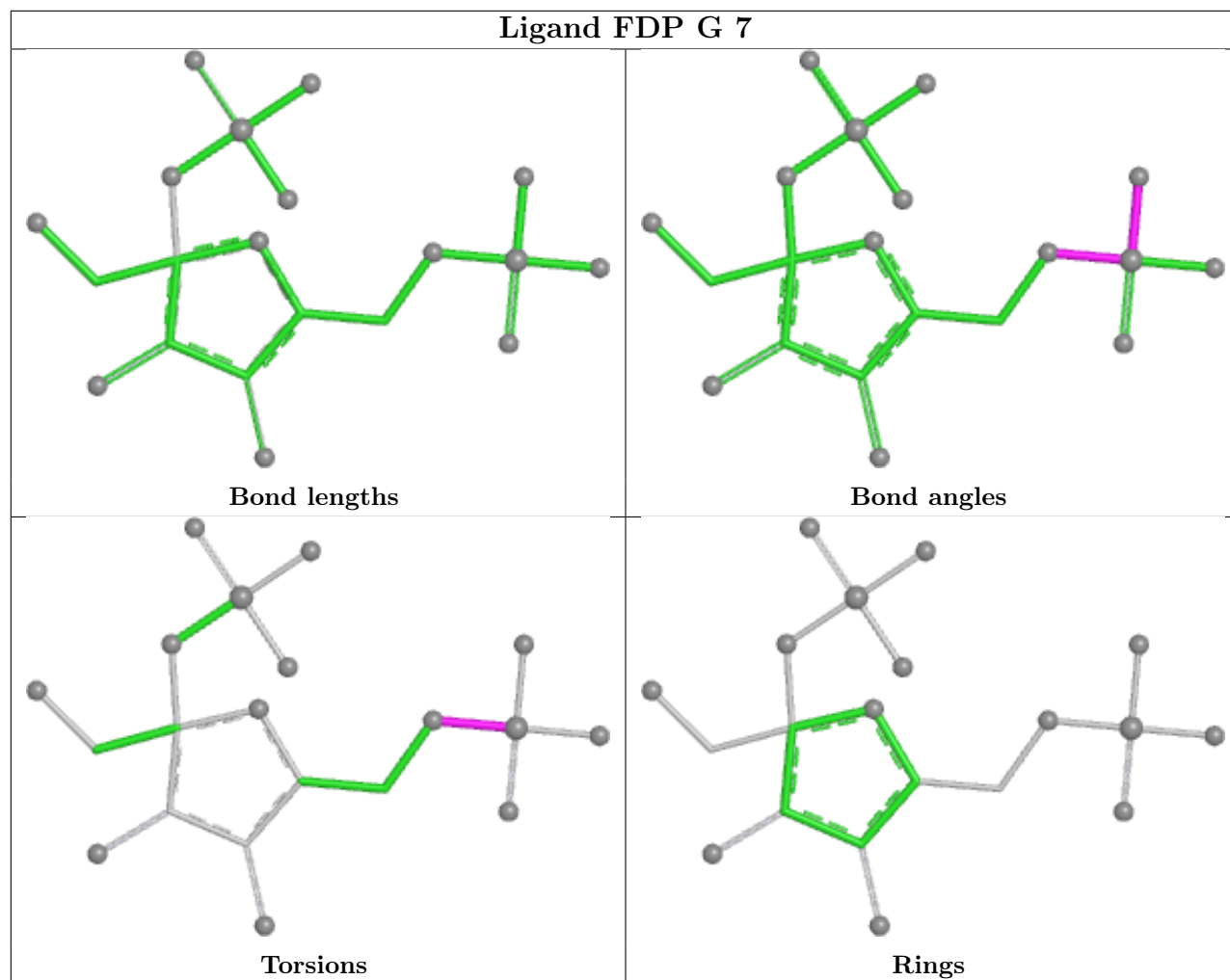
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	988	F6P	2	0

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.

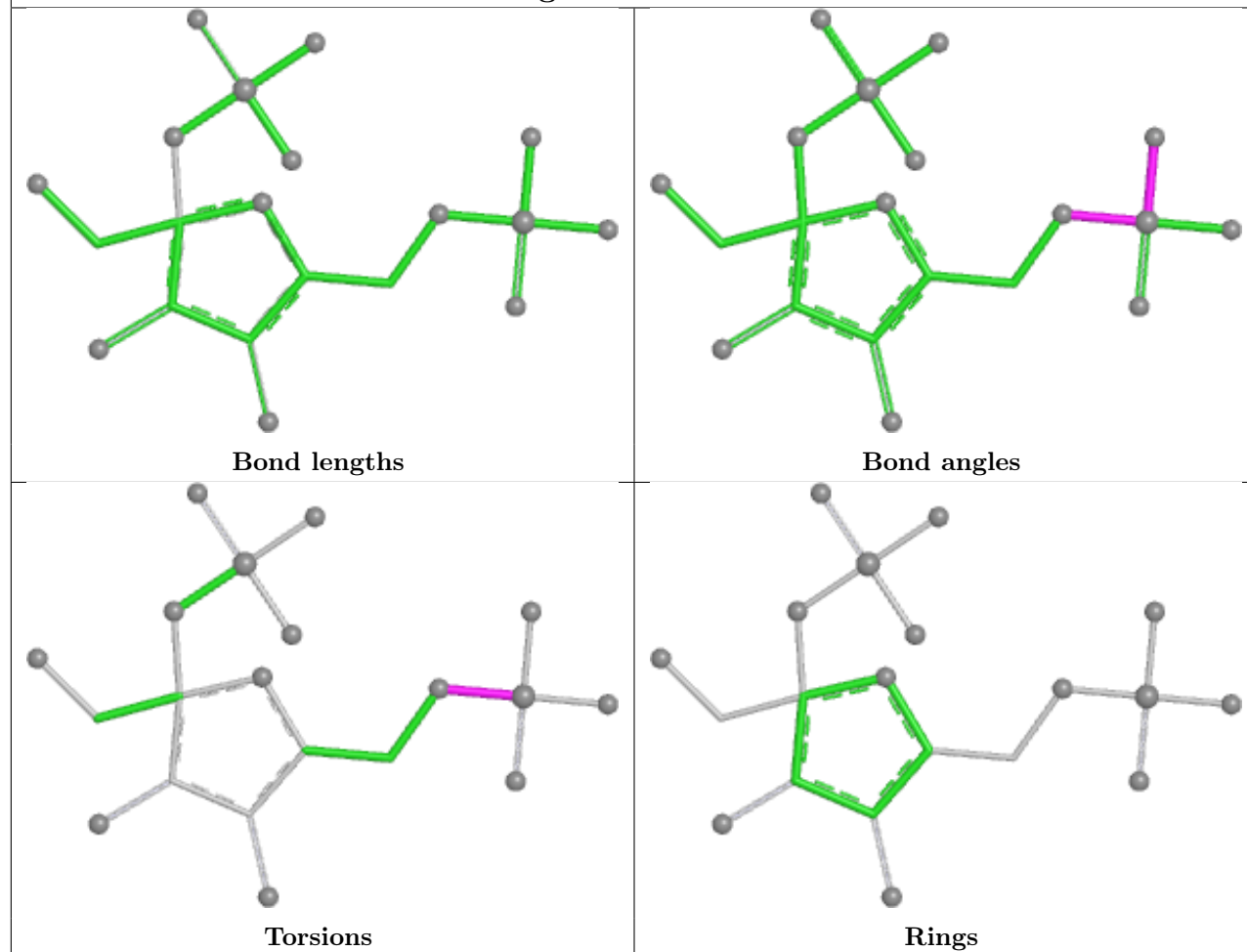




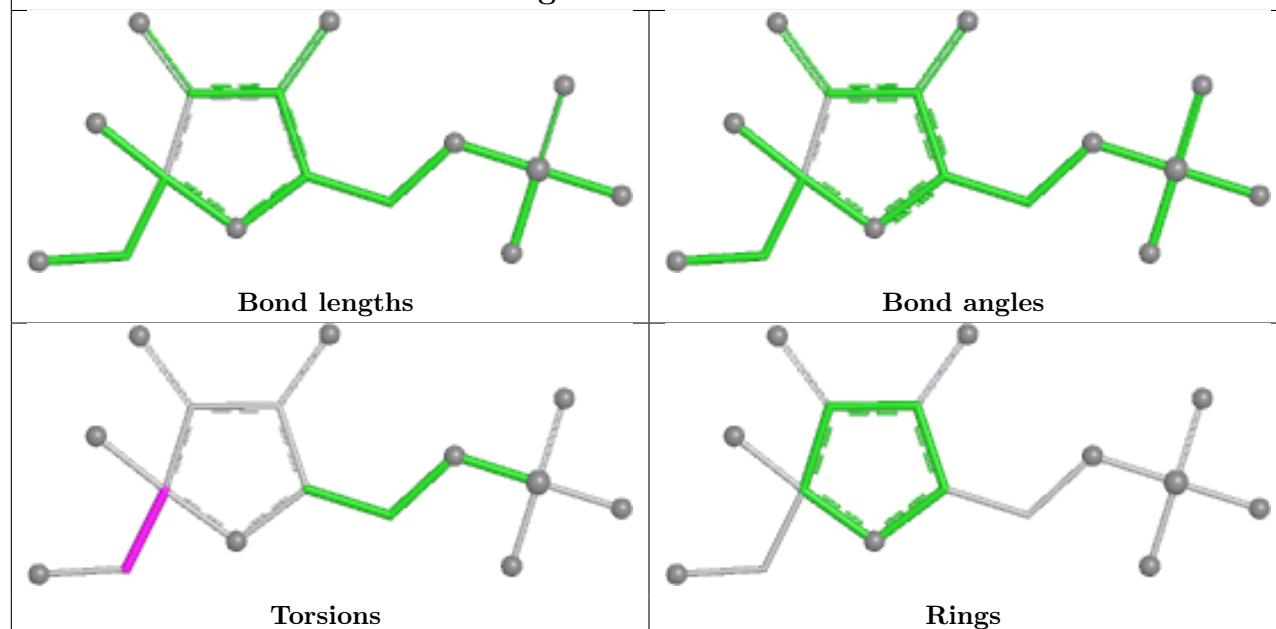




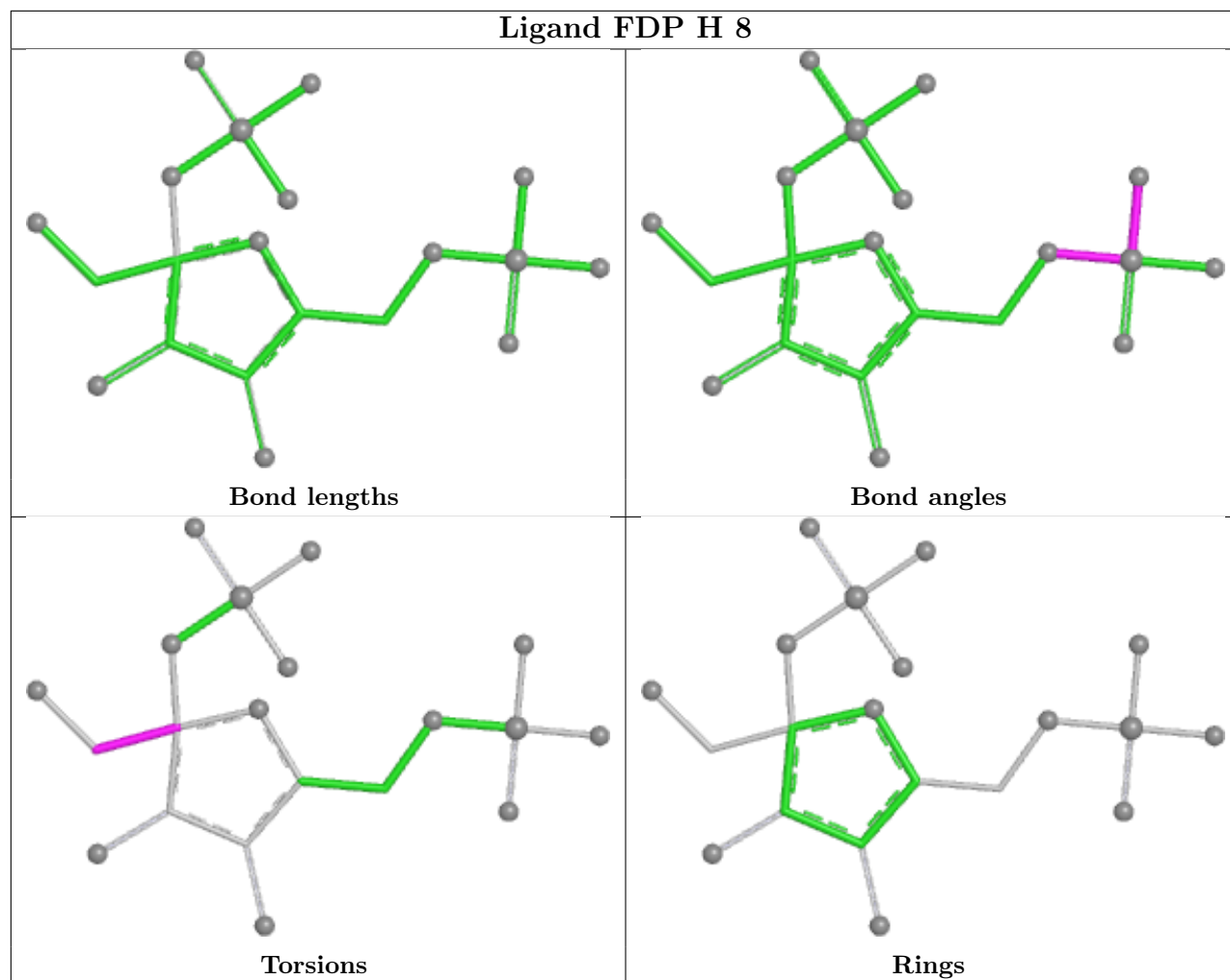
Ligand FDP E 5



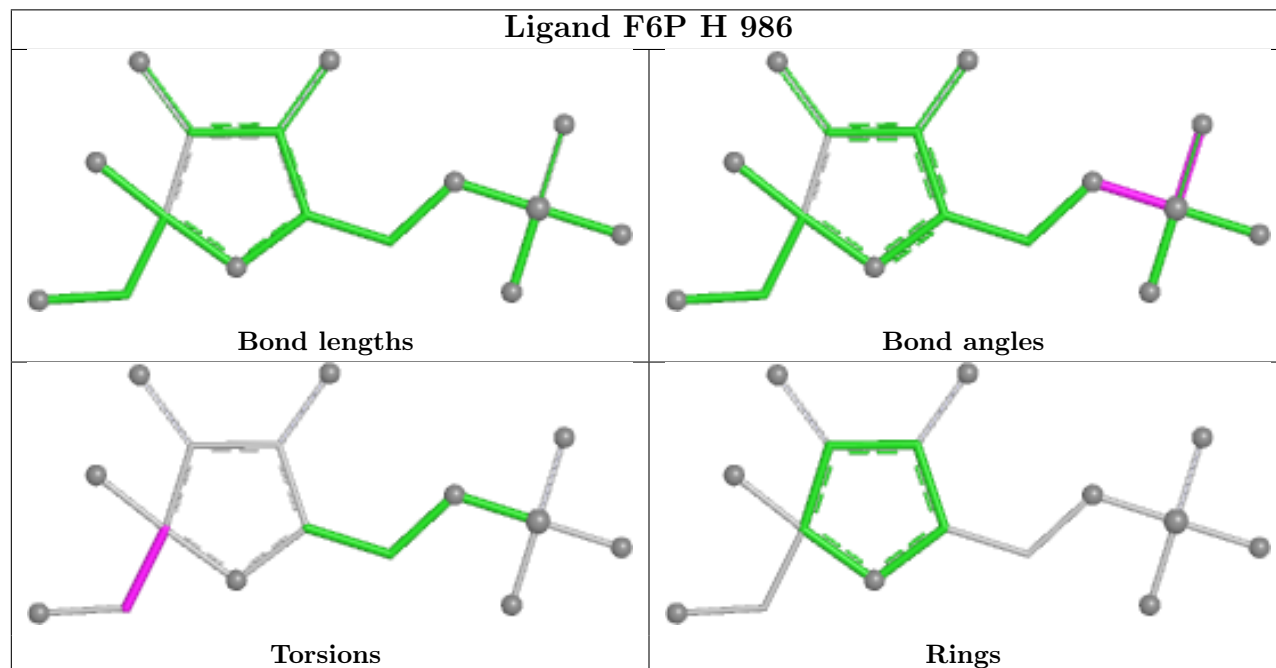
Ligand F6P E 988



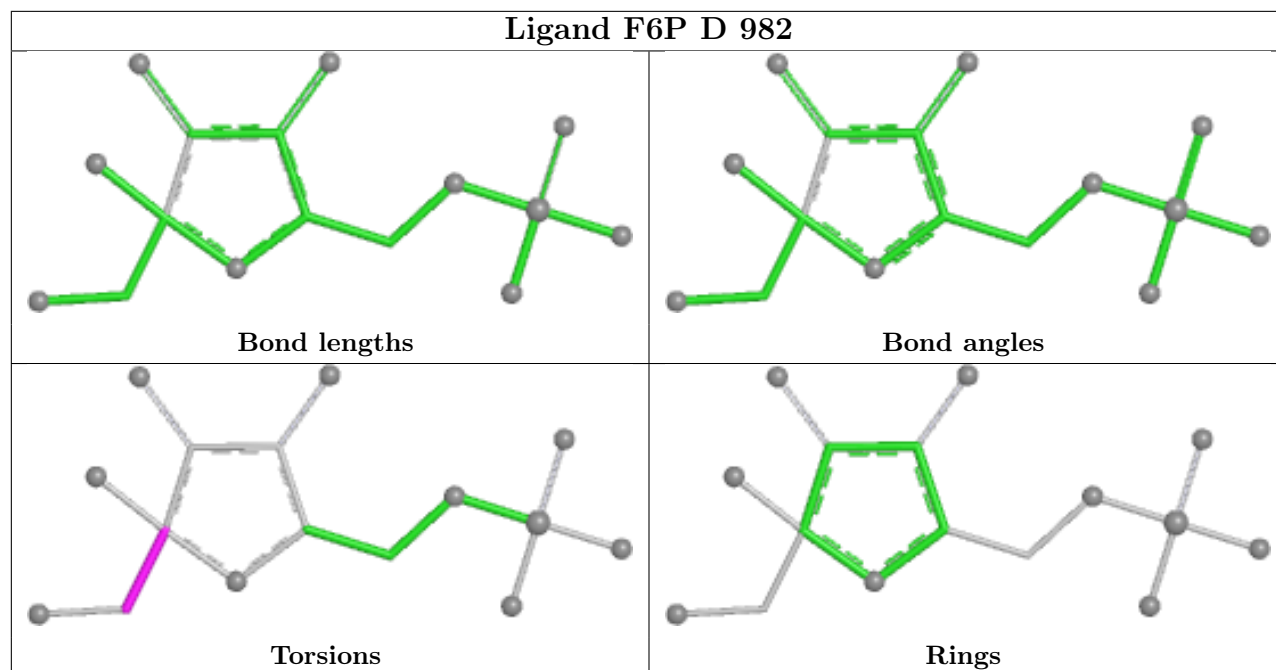
Ligand FDP H 8



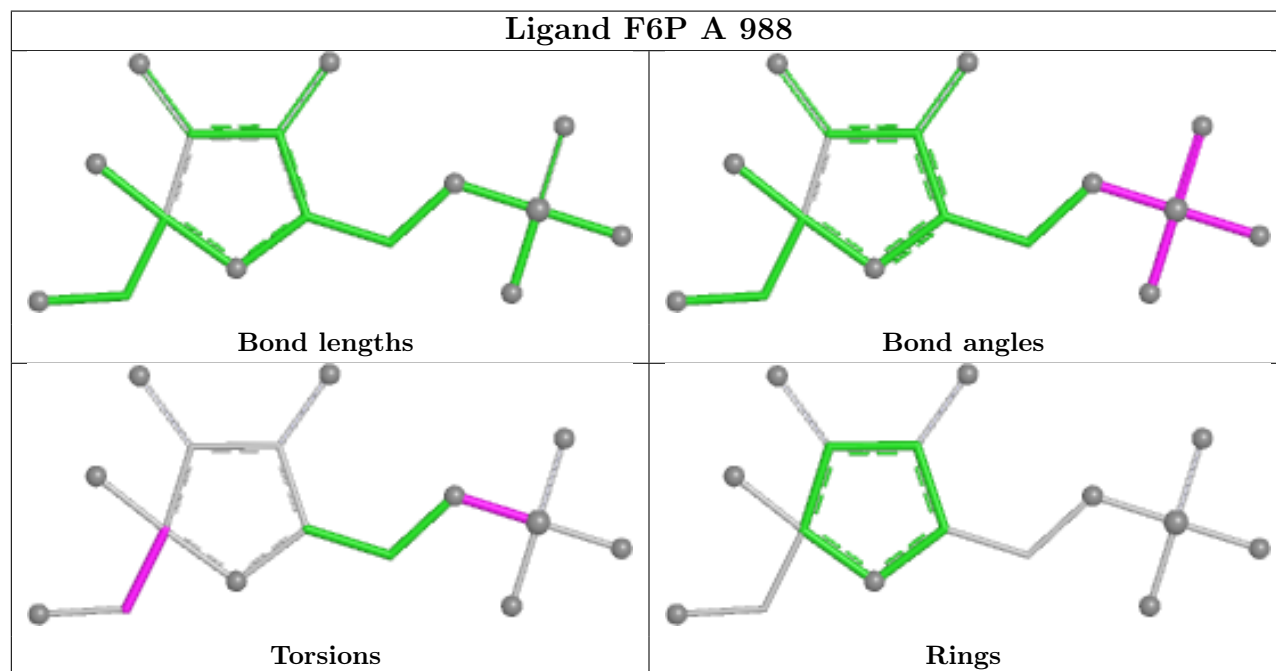
Ligand F6P H 986



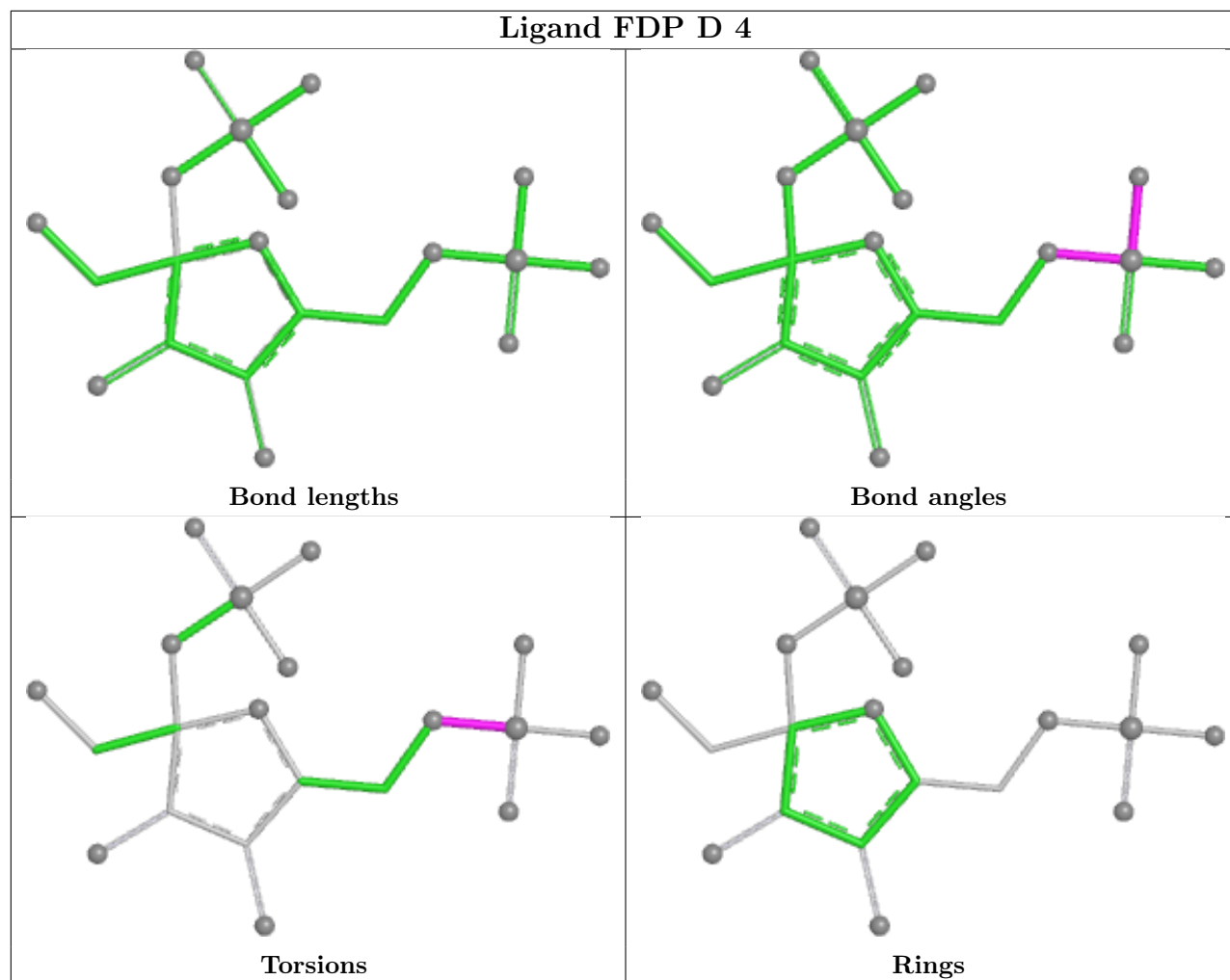
Ligand F6P D 982



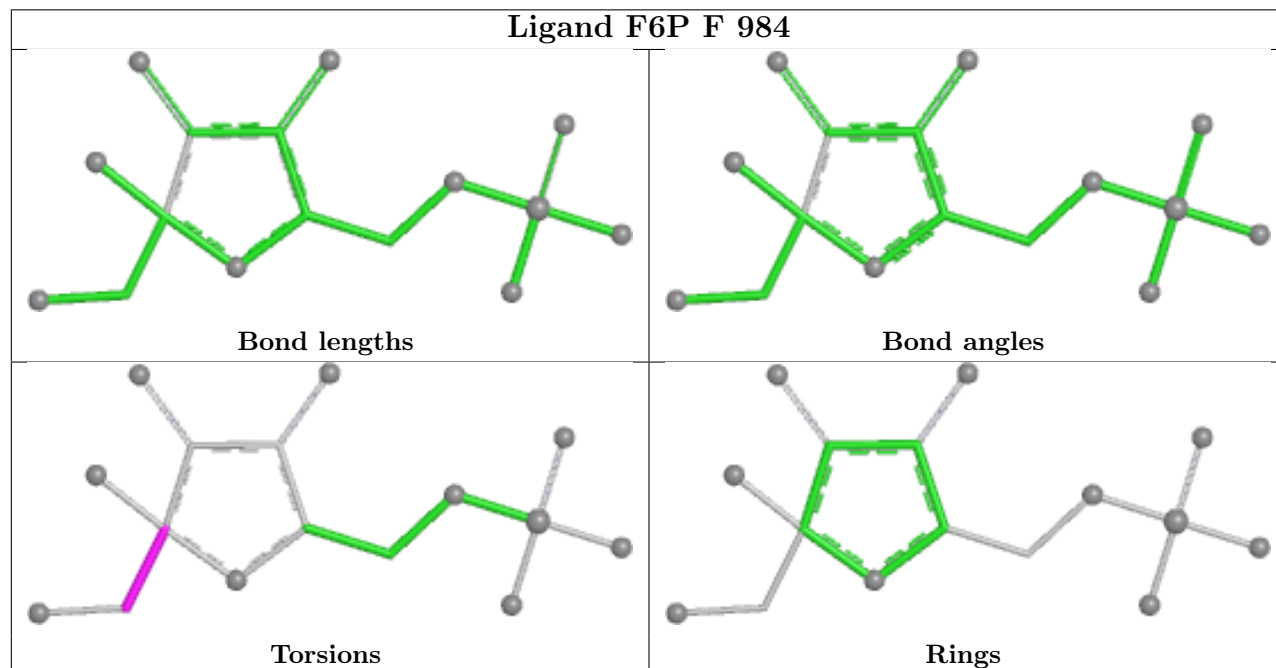
Ligand F6P A 988



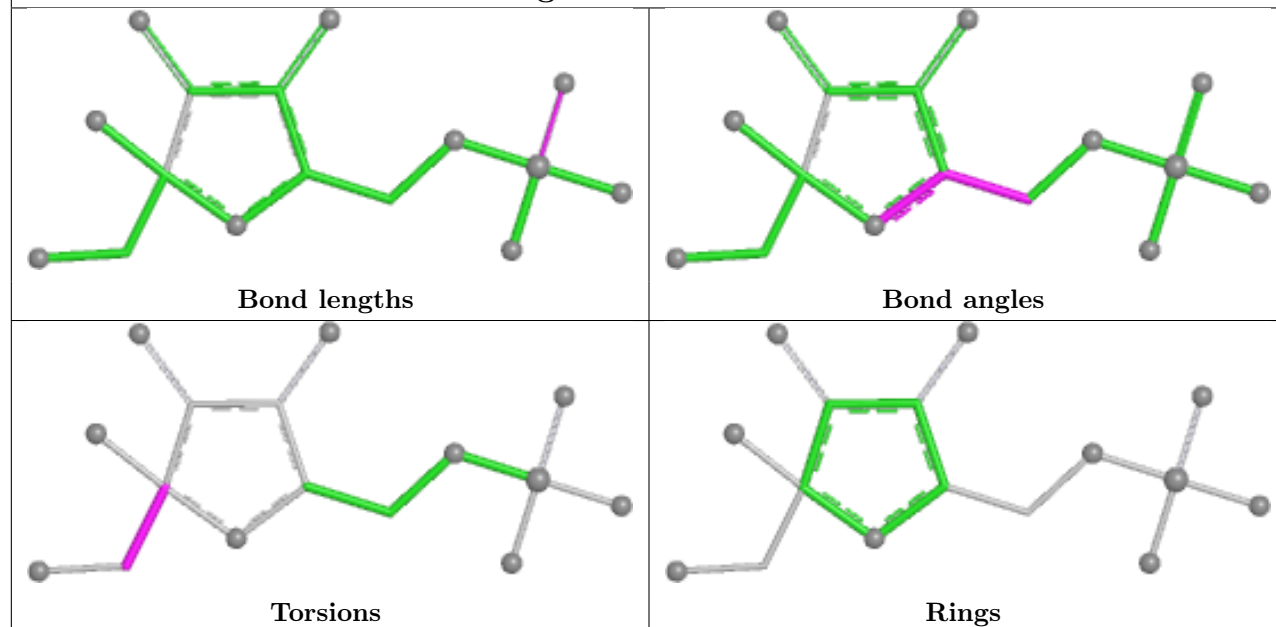
Ligand FDP D 4



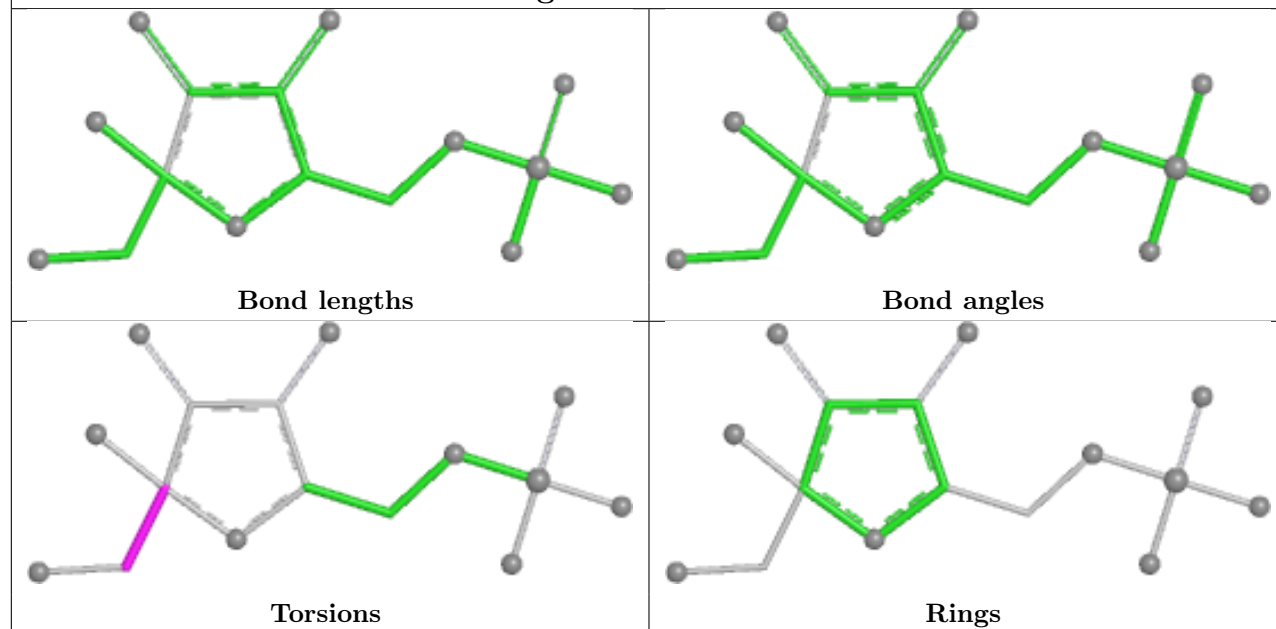
Ligand F6P F 984

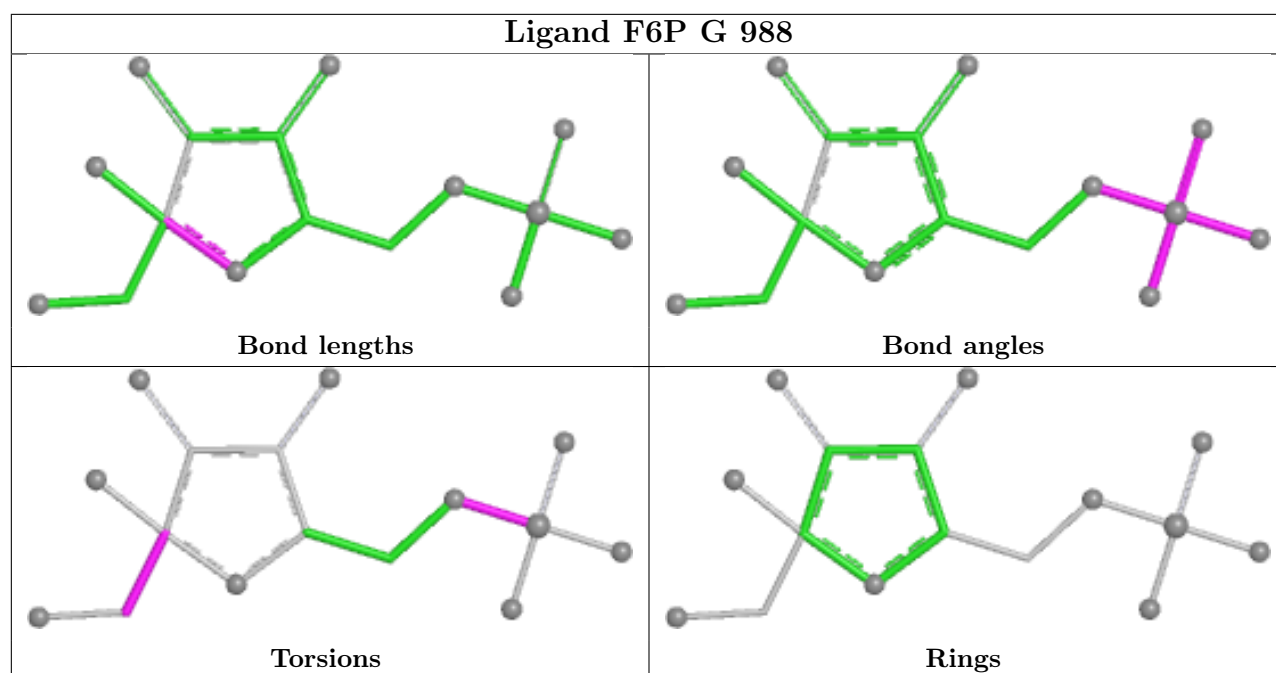


Ligand F6P B 980



Ligand F6P C 988





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%)	0.27	29 (3%)	43	35	17, 56, 81, 81	67 (8%)
1	C	750/787 (95%)	0.34	35 (4%)	36	28	16, 53, 81, 81	49 (6%)
1	E	752/787 (95%)	0.15	18 (2%)	59	50	12, 50, 81, 81	58 (7%)
1	G	744/787 (94%)	0.19	39 (5%)	33	26	19, 49, 81, 81	60 (8%)
2	B	763/766 (99%)	0.43	37 (4%)	35	28	17, 65, 81, 81	88 (11%)
2	D	761/766 (99%)	0.15	14 (1%)	67	59	20, 57, 81, 81	54 (7%)
2	F	762/766 (99%)	0.12	11 (1%)	73	65	24, 58, 81, 81	61 (8%)
2	H	763/766 (99%)	-0.14	12 (1%)	70	62	17, 45, 77, 81	37 (4%)
All	All	6045/6212 (97%)	0.19	195 (3%)	50	41	12, 54, 81, 81	474 (7%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	805	LEU	7.1
1	C	788	TYR	7.0
1	G	326	VAL	6.9
2	B	896	PHE	6.6
1	G	327	ASP	6.0
1	C	815	GLY	5.7
1	G	330	VAL	5.3
1	G	302	ALA	4.8
1	G	325	LEU	4.8
2	B	417	ALA	4.7
1	G	245	TYR	4.7
1	C	587	LEU	4.6
1	C	812	HIS	4.5
1	C	949	VAL	4.5
1	C	813	ASP	4.5
1	C	845	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	G	338	GLU	4.3
2	D	941	HIS	4.2
1	E	805	LEU	4.1
2	B	589	ILE	4.0
2	H	896	PHE	3.9
1	G	322	TRP	3.9
1	G	323	PRO	3.9
1	E	332	GLU	3.8
1	A	340	VAL	3.8
1	G	324	SER	3.8
1	E	807	LYS	3.7
1	C	846	SER	3.5
1	C	797	ALA	3.5
1	C	796	LEU	3.4
2	F	581	LEU	3.4
2	D	940	ILE	3.4
1	A	335	PHE	3.4
2	H	578	GLU	3.4
2	H	891	ALA	3.4
2	B	411	PHE	3.4
1	A	325	LEU	3.3
1	A	813	ASP	3.3
2	D	417	ALA	3.3
2	D	891	ALA	3.3
2	F	895	ASN	3.2
2	B	407	ALA	3.2
2	F	553	ALA	3.2
1	G	340	VAL	3.2
1	A	334	ARG	3.2
2	H	195	PRO	3.2
1	A	587	LEU	3.2
2	B	887	ALA	3.1
1	G	348	ILE	3.1
1	E	800	ARG	3.1
1	A	303	LEU	3.0
1	G	331	ALA	3.0
1	G	333	GLY	3.0
2	B	562	ILE	3.0
1	C	800	ARG	3.0
2	F	582	PRO	3.0
1	G	329	LEU	2.9
2	D	204	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	814	LYS	2.9
1	A	941	ASN	2.9
1	A	326	VAL	2.9
1	A	821	LYS	2.9
1	G	342	PRO	2.9
1	G	344	LYS	2.9
2	F	957	ARG	2.9
2	B	940	ILE	2.8
1	C	820	GLY	2.8
2	B	292	VAL	2.8
2	B	886	ILE	2.8
1	G	788	TYR	2.8
2	B	680	GLY	2.8
1	A	586	GLU	2.7
1	A	304	VAL	2.7
2	H	584	ASP	2.7
2	D	942	TRP	2.7
2	B	957	ARG	2.7
1	E	946	GLU	2.7
2	F	893	GLU	2.7
2	D	678	PHE	2.7
2	B	593	ASN	2.7
1	C	329	LEU	2.7
2	F	243	GLY	2.6
1	C	552	ILE	2.6
1	A	213	SER	2.6
1	A	347	SER	2.6
2	B	923	ARG	2.6
1	A	589	PRO	2.6
2	H	811	GLY	2.6
2	B	410	ILE	2.6
2	B	943	GLN	2.6
2	D	591	ILE	2.6
1	E	583	ASP	2.6
2	D	584	ASP	2.6
1	G	346	LEU	2.6
1	G	754	ALA	2.6
1	A	817	ASN	2.6
2	F	892	ALA	2.6
1	G	311	SER	2.5
2	B	409	TYR	2.5
1	G	758	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	589	PRO	2.5
1	A	210	VAL	2.5
1	E	808	GLU	2.5
1	E	803	ILE	2.5
1	E	920	GLU	2.5
1	G	757	THR	2.5
1	A	306	CYS	2.5
1	G	316	ASP	2.4
1	E	820	GLY	2.4
1	E	949	VAL	2.4
2	H	890	ARG	2.4
1	A	279	SER	2.4
1	A	288	ARG	2.4
1	G	337	LYS	2.4
1	G	336	THR	2.4
1	C	605	SER	2.4
2	D	889	ALA	2.4
2	D	195	PRO	2.4
1	A	429	LYS	2.4
1	G	334	ARG	2.4
2	B	550	PHE	2.4
1	C	798	SER	2.4
2	B	442	ILE	2.4
1	G	787	VAL	2.3
1	E	312	LEU	2.3
1	C	817	ASN	2.3
2	B	892	ALA	2.3
1	E	333	GLY	2.3
1	E	819	ASN	2.3
2	B	897	ASN	2.3
1	G	946	GLU	2.3
1	C	322	TRP	2.3
1	E	810	PHE	2.3
1	A	286	GLU	2.3
1	G	341	ALA	2.3
2	B	888	GLU	2.3
1	E	303	LEU	2.3
1	E	322	TRP	2.3
2	D	351	MET	2.2
1	A	467	ALA	2.2
1	C	816	GLU	2.2
1	A	327	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	282	PHE	2.2
1	A	332	GLU	2.2
1	C	809	ASN	2.2
1	G	255	LEU	2.2
2	B	372	ASP	2.2
1	A	812	HIS	2.2
2	B	584	ASP	2.2
1	C	359	MET	2.2
1	G	347	SER	2.2
2	B	361	TYR	2.2
2	B	811	GLY	2.2
2	D	681	LEU	2.2
1	C	579	THR	2.2
2	H	914	GLY	2.2
1	G	317	LEU	2.2
1	C	239	PHE	2.1
2	F	896	PHE	2.1
2	H	761	GLN	2.1
1	G	515	LEU	2.1
1	C	560	ALA	2.1
2	F	270	ARG	2.1
2	B	915	SER	2.1
1	A	330	VAL	2.1
2	B	444	VAL	2.1
2	B	619	PRO	2.1
1	C	795	ASP	2.1
2	H	334	ARG	2.1
2	B	891	ALA	2.1
2	H	892	ALA	2.1
2	B	316	SER	2.1
1	G	805	LEU	2.1
1	E	623	GLY	2.1
1	C	707	THR	2.1
2	B	356	ALA	2.1
1	G	962	TYR	2.1
2	B	643	MET	2.0
2	B	582	PRO	2.0
2	D	582	PRO	2.0
1	C	557	PHE	2.0
1	C	794	ILE	2.0
2	H	940	ILE	2.0
1	A	454	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	398	ALA	2.0
1	G	920	GLU	2.0
2	F	245	GLU	2.0
1	C	821	LYS	2.0
1	C	326	VAL	2.0
1	C	519	PRO	2.0
1	G	762	PHE	2.0
1	A	313	THR	2.0
2	B	441	THR	2.0
1	G	210	VAL	2.0
2	B	297	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

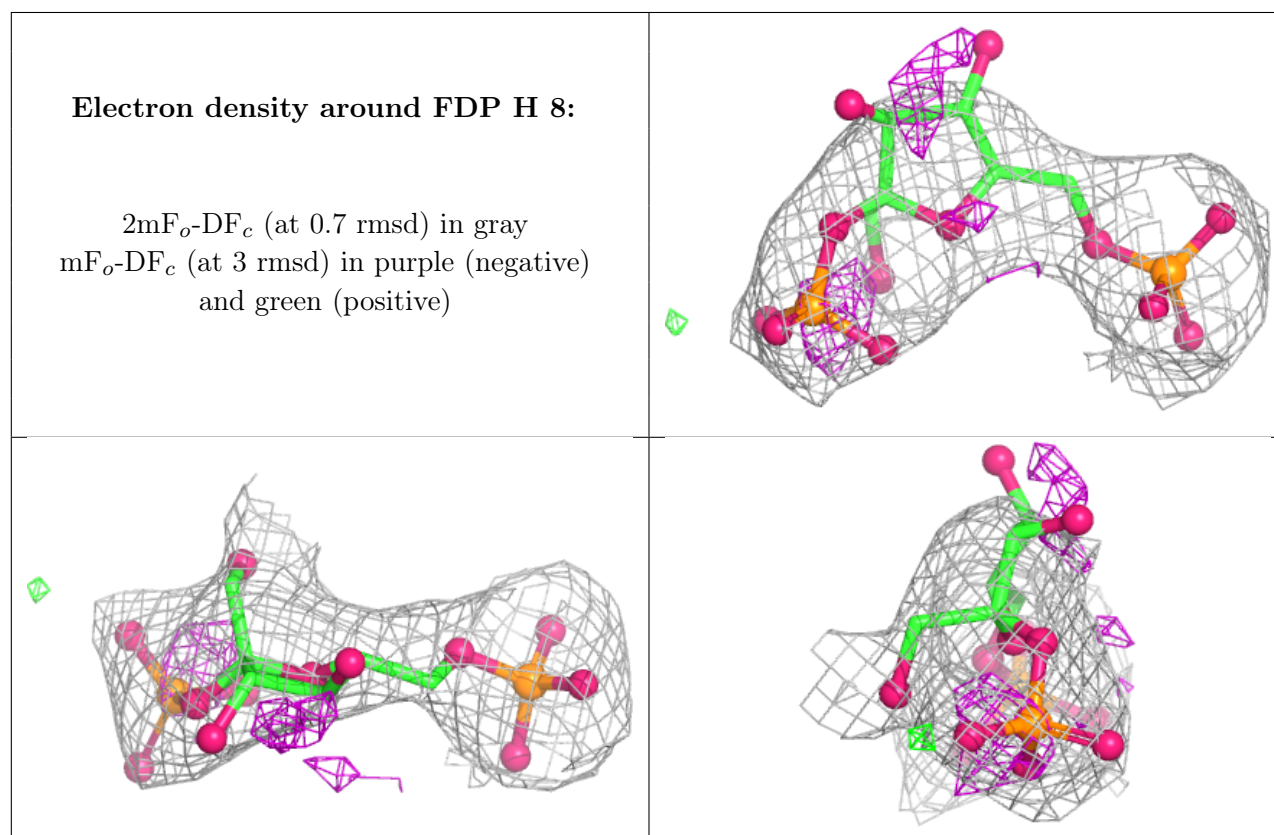
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	FDP	H	8	20/20	0.71	0.12	81,82,82,82	0
4	FDP	C	3	20/20	0.73	0.14	79,82,82,82	0
4	FDP	F	6	20/20	0.75	0.11	81,82,82,82	0
3	F6P	A	988	16/16	0.79	0.12	79,82,82,82	0
3	F6P	B	980	16/16	0.85	0.11	77,80,82,82	0
3	F6P	C	988	16/16	0.86	0.15	75,78,80,80	0
4	FDP	A	1	20/20	0.88	0.10	77,82,82,82	0
3	F6P	E	988	16/16	0.89	0.11	62,66,66,68	0
4	FDP	G	7	20/20	0.90	0.09	80,82,82,82	0
3	F6P	G	988	16/16	0.91	0.12	61,62,64,68	0
3	F6P	F	984	16/16	0.91	0.11	56,57,63,64	0
3	F6P	D	982	16/16	0.92	0.11	65,67,70,71	0

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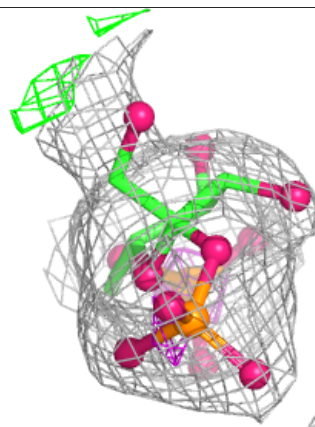
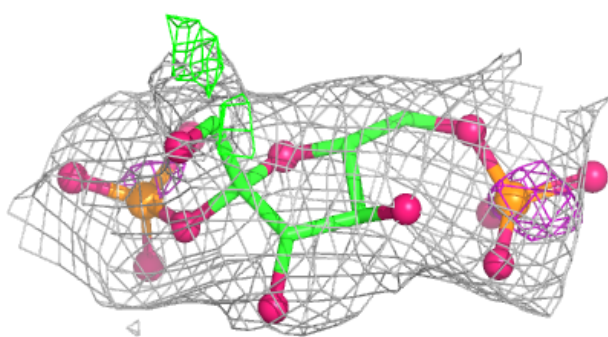
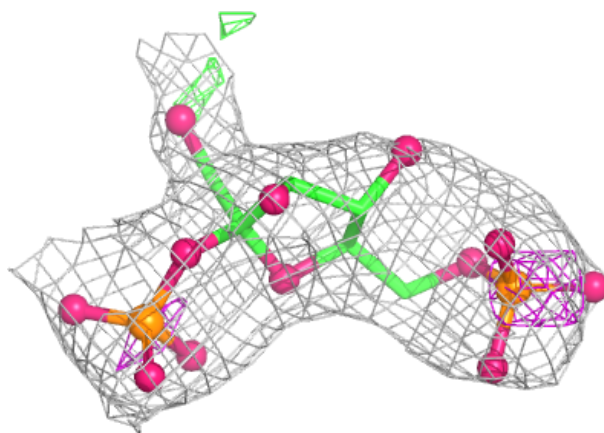
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FDP	B	2	20/20	0.93	0.12	65,68,70,71	0
4	FDP	E	5	20/20	0.94	0.08	66,70,74,74	0
3	F6P	H	986	16/16	0.95	0.08	41,47,47,49	0
4	FDP	D	4	20/20	0.97	0.06	52,54,56,57	0

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.

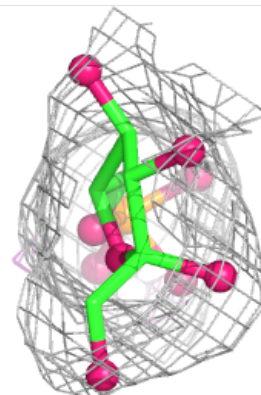
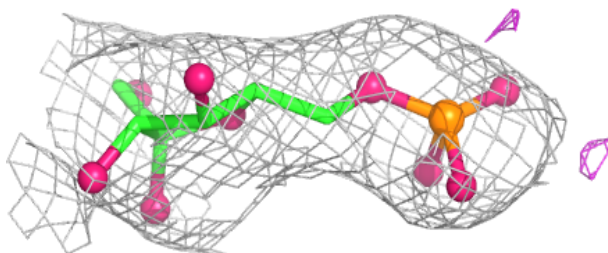
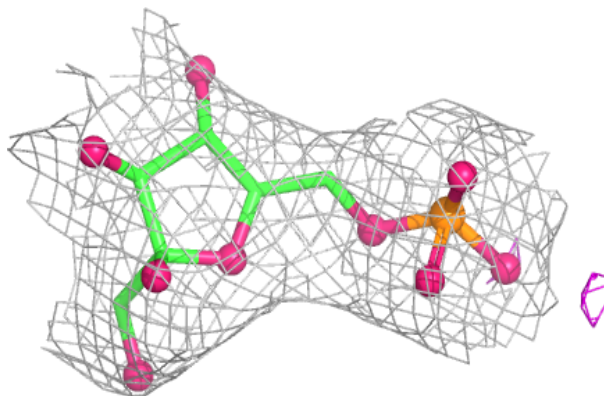


Electron density around FDP F 6:

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

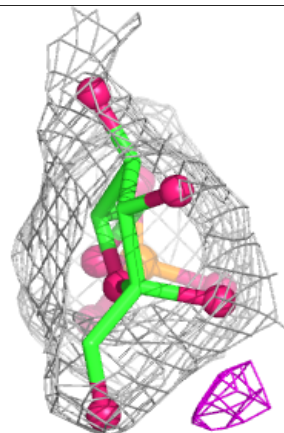
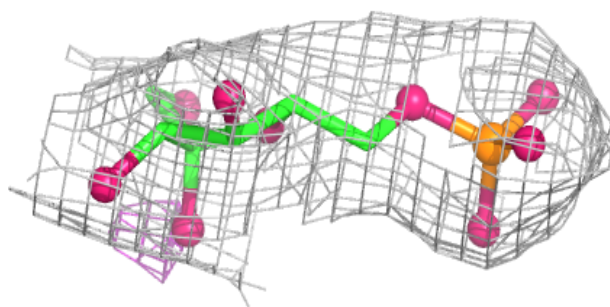
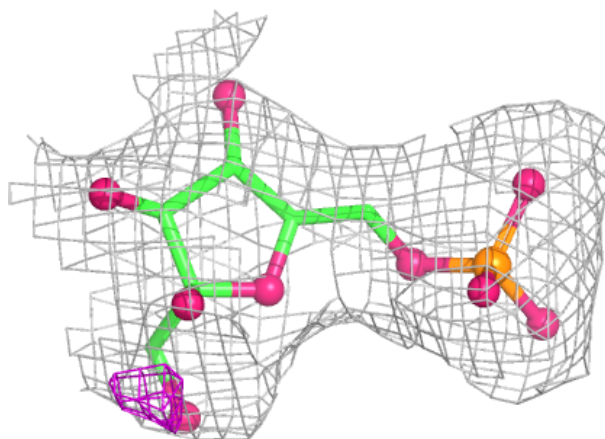
**Electron density around F6P A 988:**

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



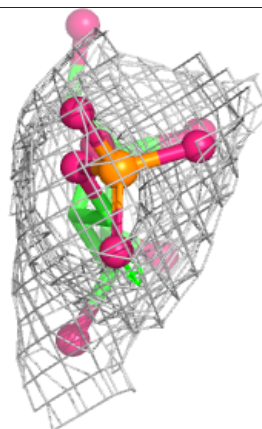
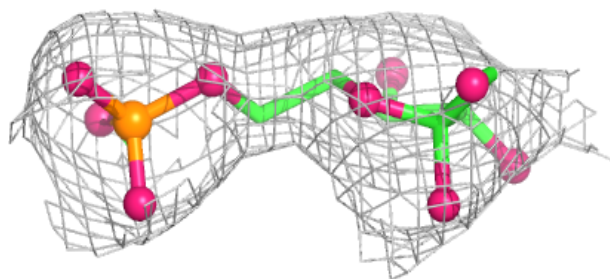
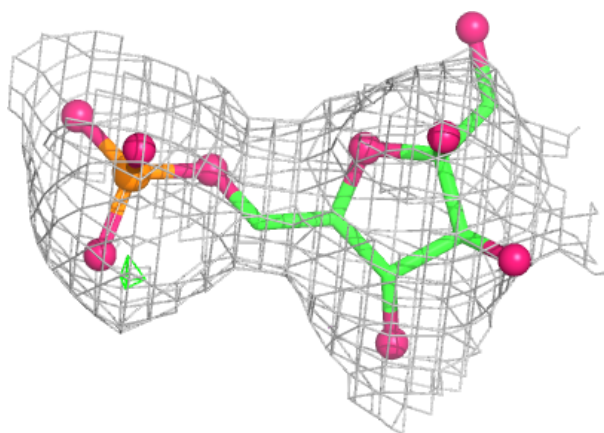
Electron density around F6P B 980:

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



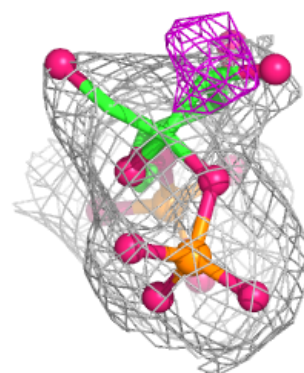
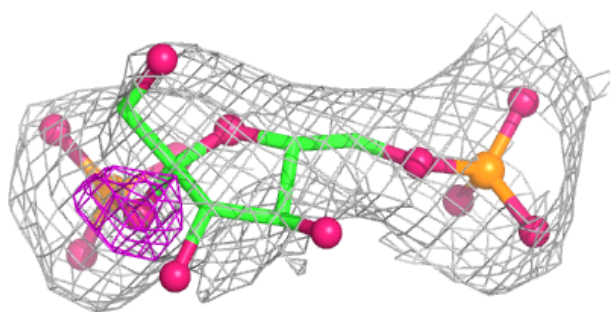
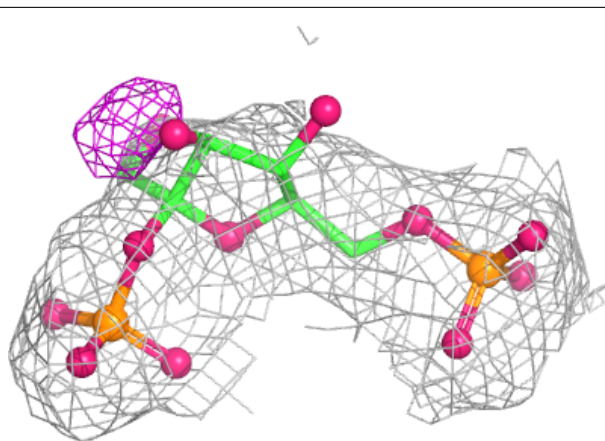
Electron density around F6P C 988:

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



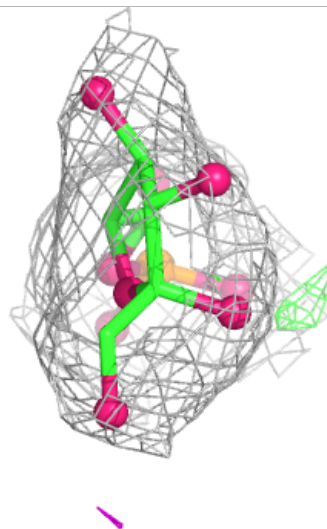
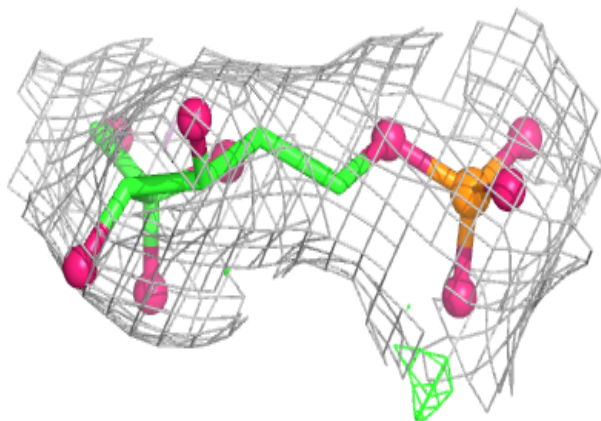
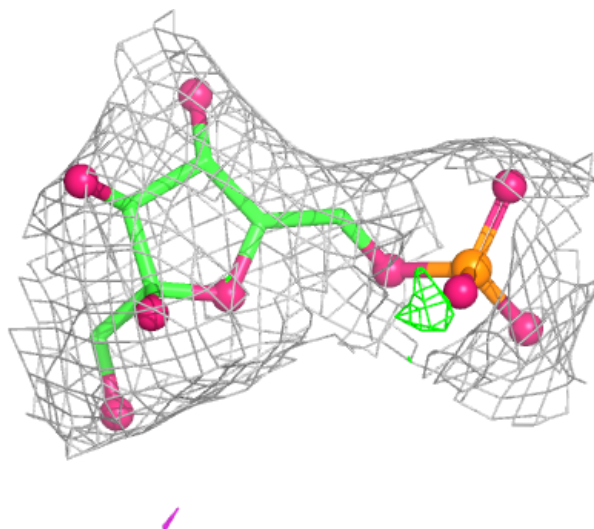
Electron density around FDP A 1:

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



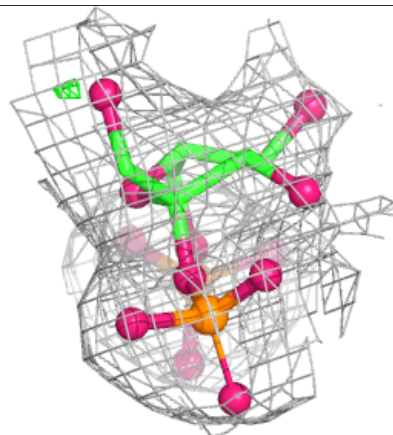
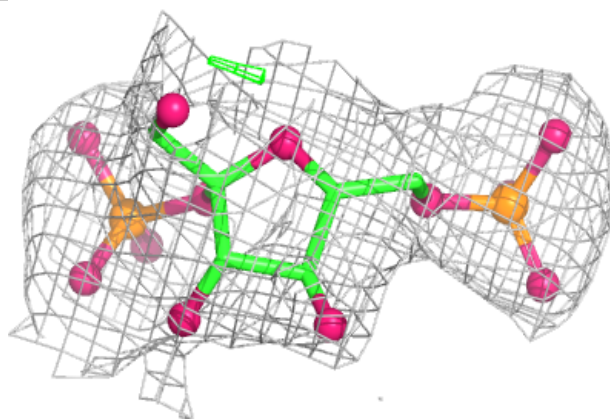
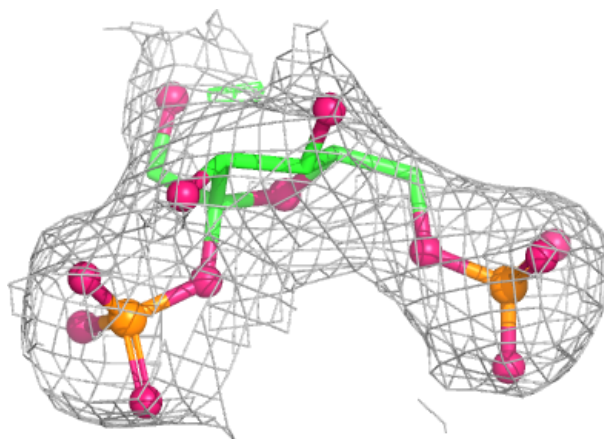
Electron density around F6P E 988:

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



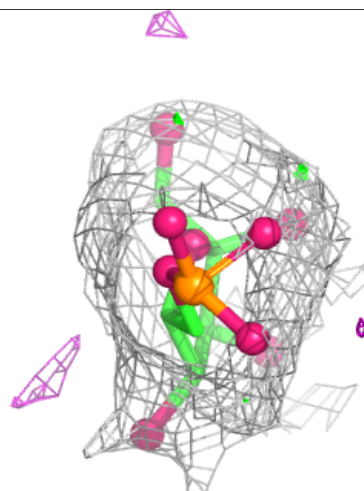
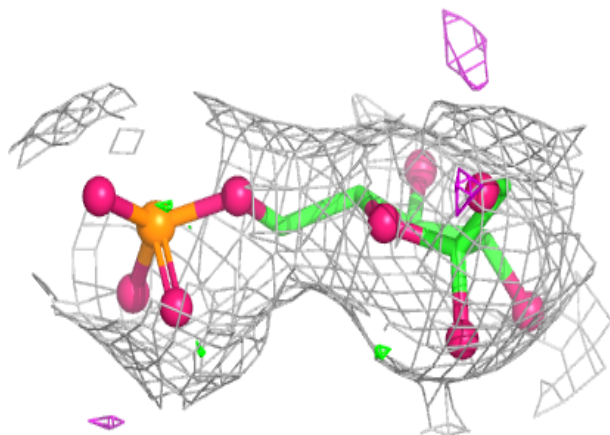
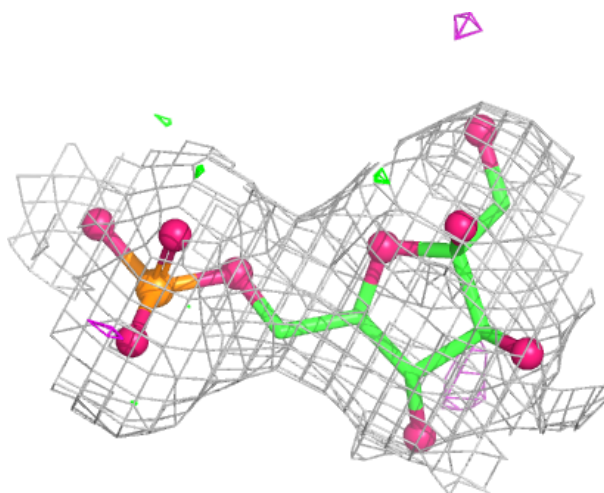
Electron density around FDP G 7:

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



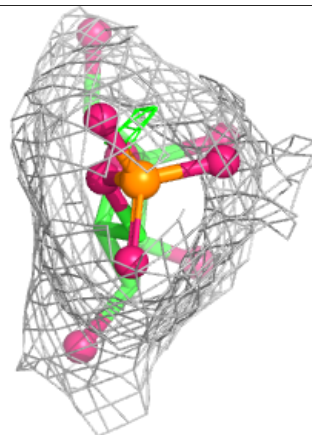
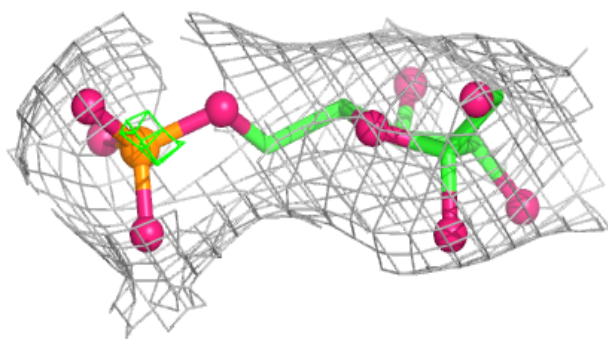
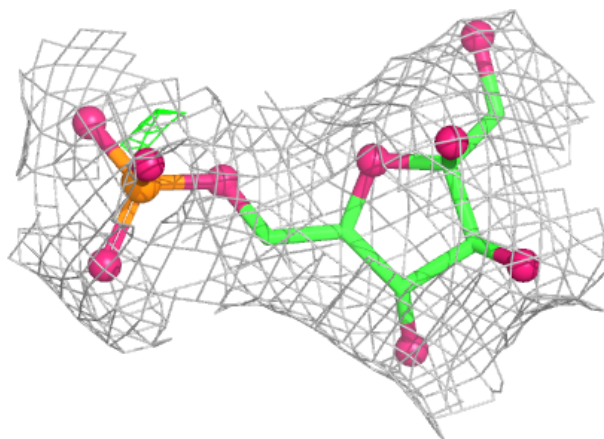
Electron density around F6P G 988:

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



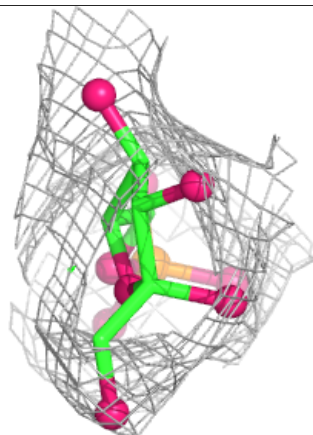
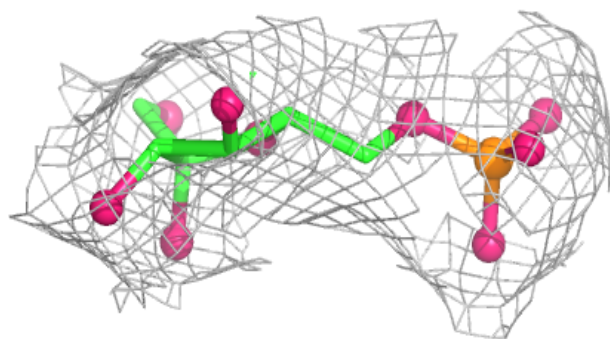
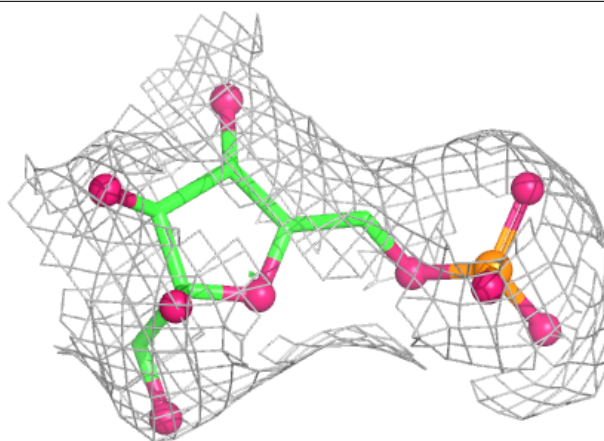
Electron density around F6P F 984:

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



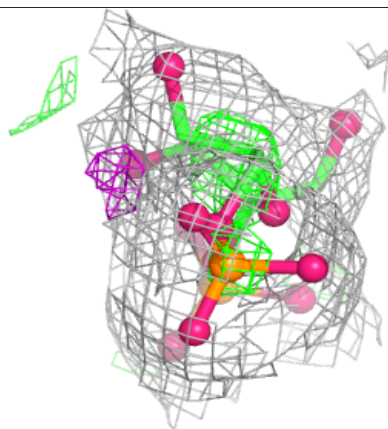
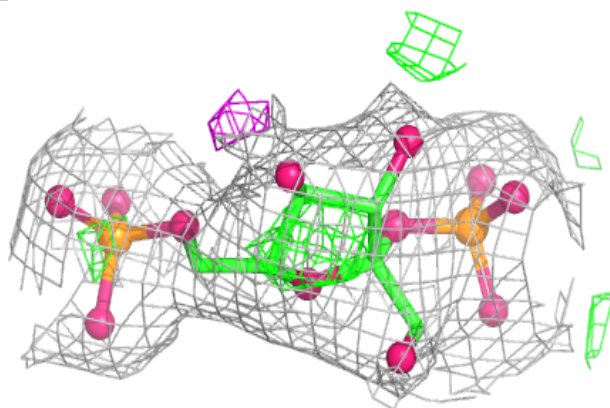
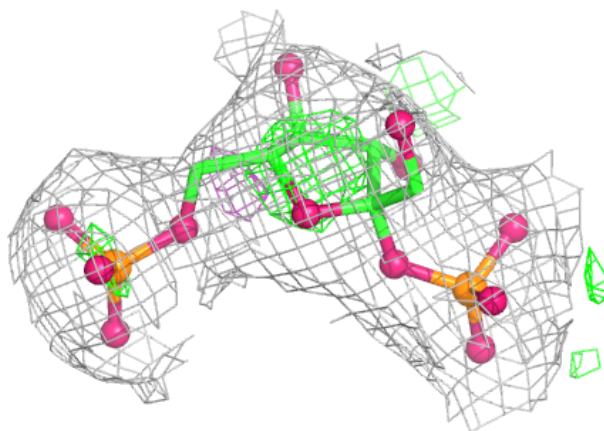
Electron density around F6P D 982:

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



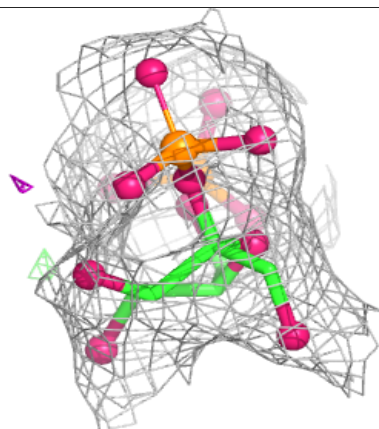
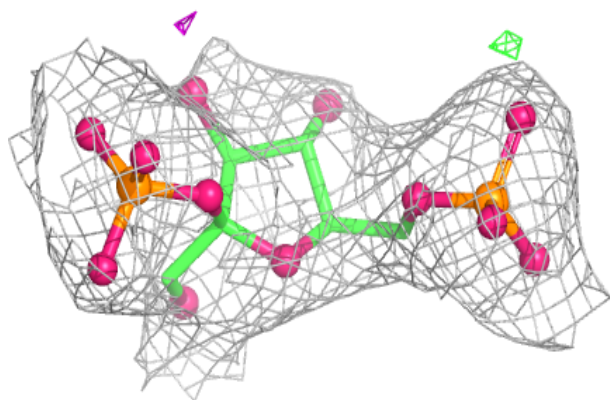
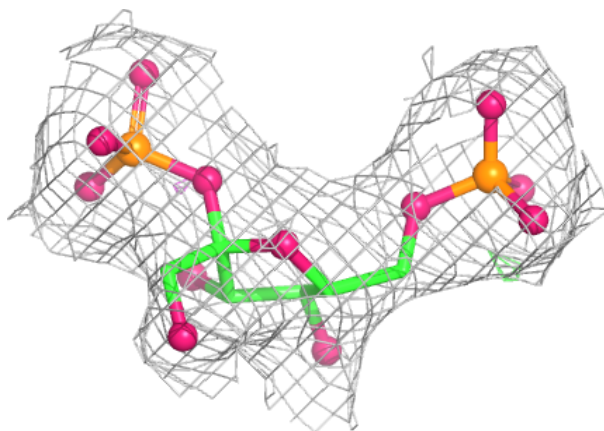
Electron density around FDP B 2:

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



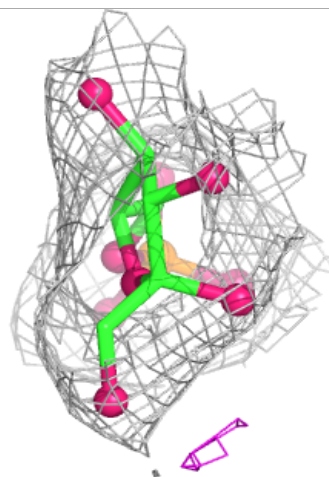
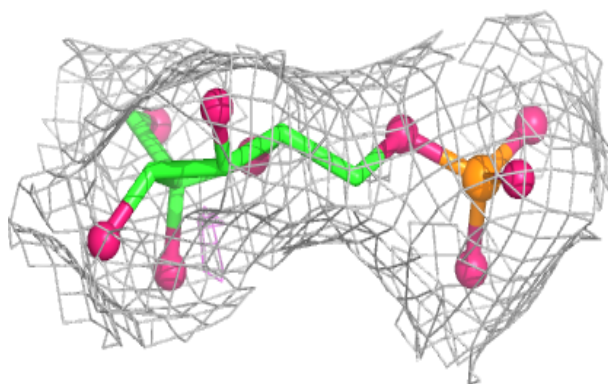
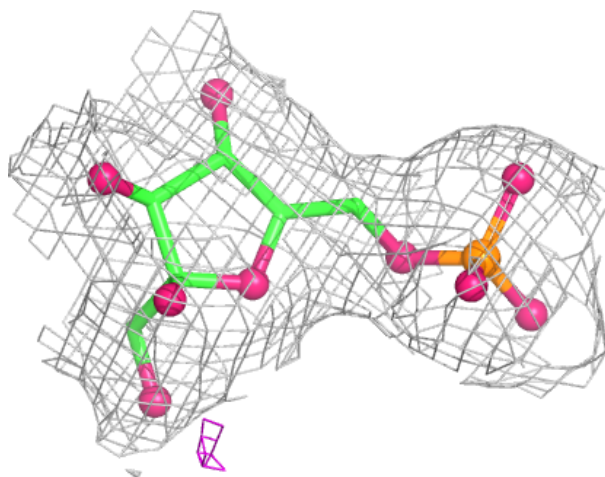
Electron density around FDP E 5:

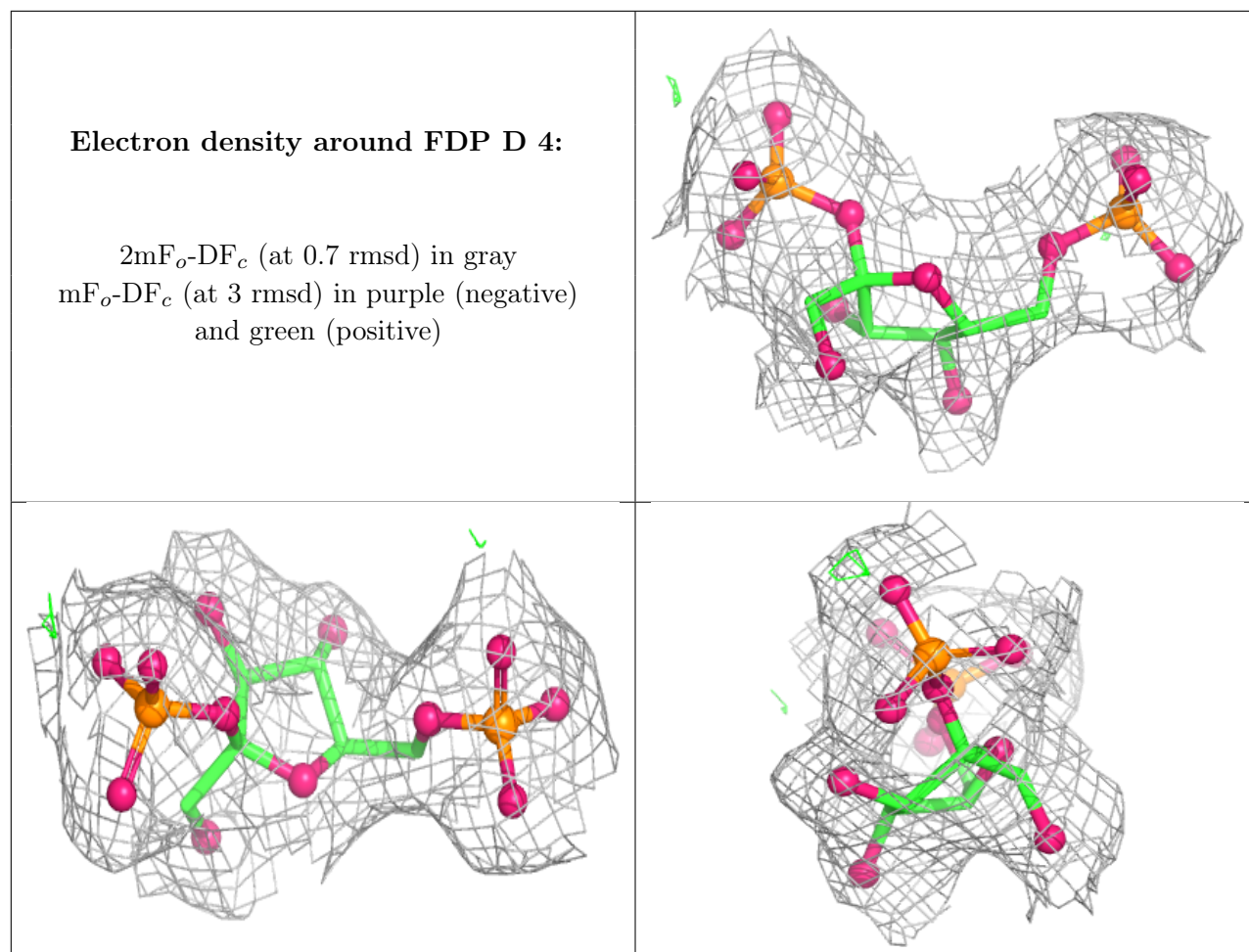
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around F6P 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.