Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:20 am BST

PDB ID	:	2VPX
Title	:	Polysulfide reductase with bound quinone (UQ1)
Authors	:	Jormakka, M.; Yokoyama, K.; Yano, T.; Tamakoshi, M.; Akimoto, S.; Shimamura, T.; Curmi, P.; Iwata, S.
Deposited on	:	2008-03-09
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

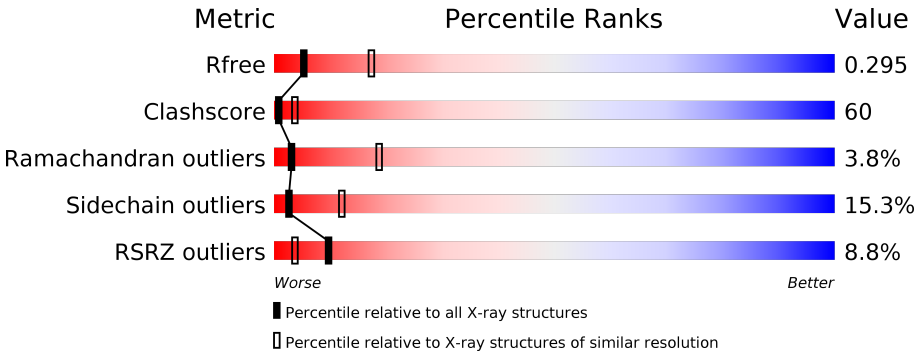
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.10 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	765	9% 30% 49% 15%
1	E	765	10% 33% 45% 15%
2	B	195	3% 37% 51% 10%
2	F	195	9% 38% 48% 11%
3	C	253	5% 49% 40% 9%
3	G	253	12% 40% 49% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	A	1764	-	-	X	-
4	SF4	B	1194	-	-	X	-
4	SF4	B	1195	-	-	X	-
4	SF4	B	1196	-	-	X	-
4	SF4	F	1194	-	-	X	-
4	SF4	F	1195	-	-	X	-
7	UQ1	C	1252	-	-	X	-
7	UQ1	G	1251	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20229 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 THIOSULFATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			
1	E	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			

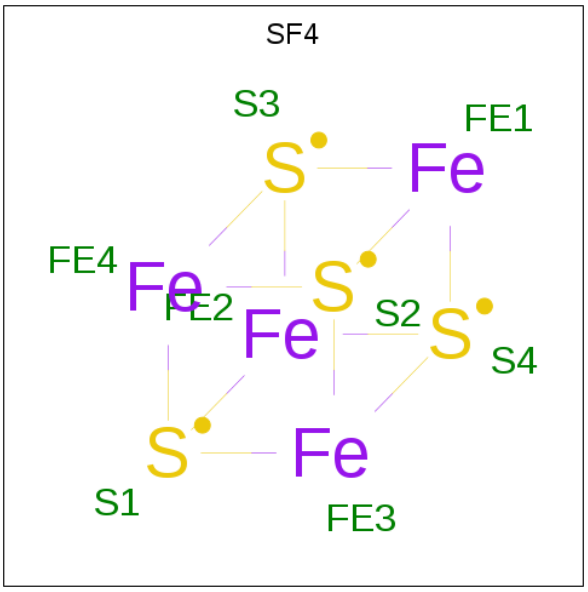
- Molecule 2 is a protein called NRFC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			
2	F	194	Total	C	N	O	S	0	0	1
			1475	930	256	269	20			

- Molecule 3 is a protein called HYPOTHETICAL MEMBRANE SPANNING PROTEIN.

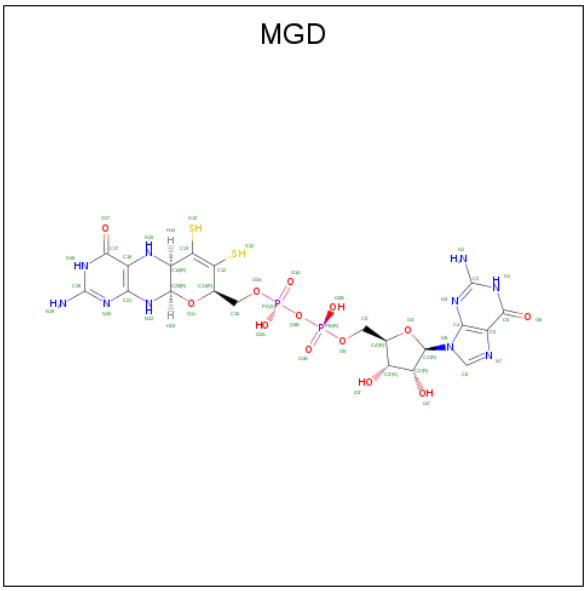
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			
3	G	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	E	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 8 4 4	0	0

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).

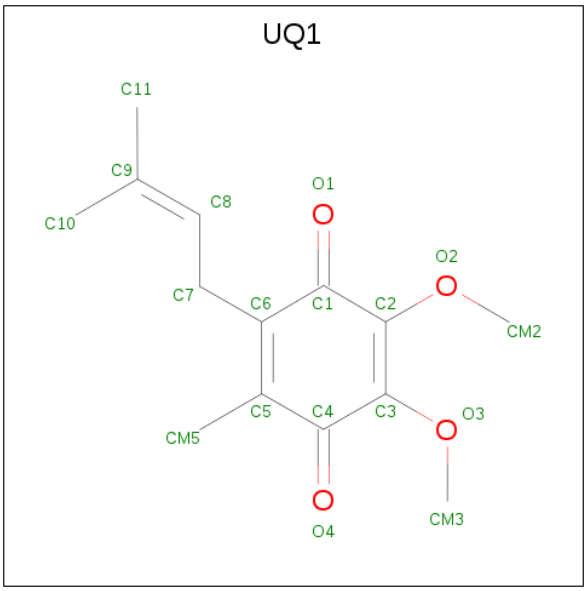


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 6 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		
6	E	1	Total	Mo	0	0
			1	1		

- Molecule 7 is UBIQUINONE-1 (three-letter code: UQ1) (formula: $C_{14}H_{18}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 18 14 4	0	0
7	G	1	Total C O 18 14 4	0	0

- Molecule 8 is water.

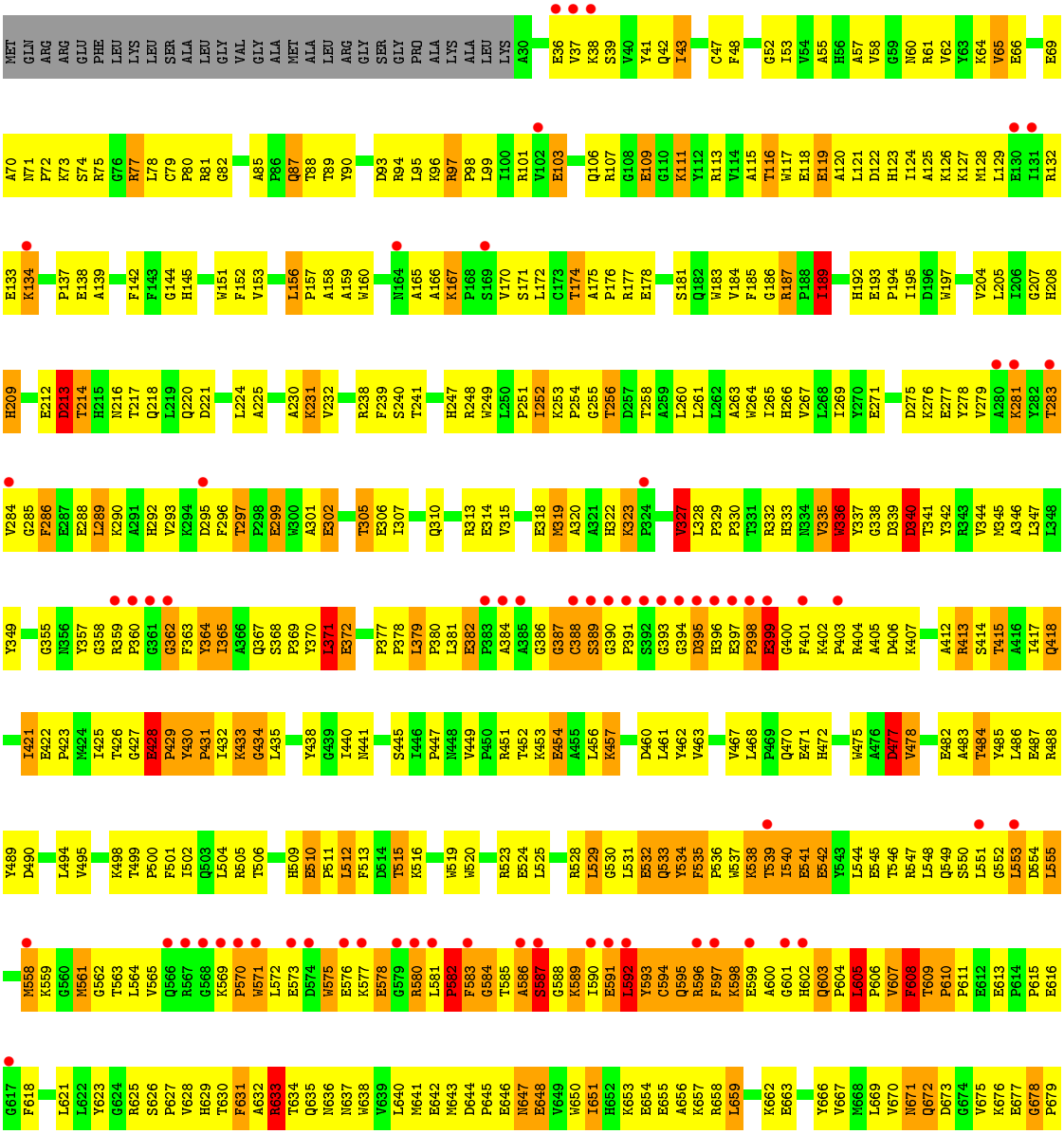
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	387	Total O 387 387	0	0
8	B	149	Total O 149 149	0	0
8	C	90	Total O 90 90	0	0
8	E	452	Total O 452 452	0	0
8	F	130	Total O 130 130	0	0
8	G	77	Total O 77 77	0	0

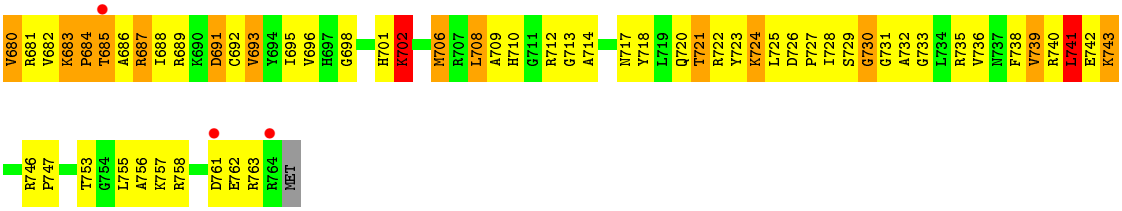
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: THIOSULFATE REDUCTASE

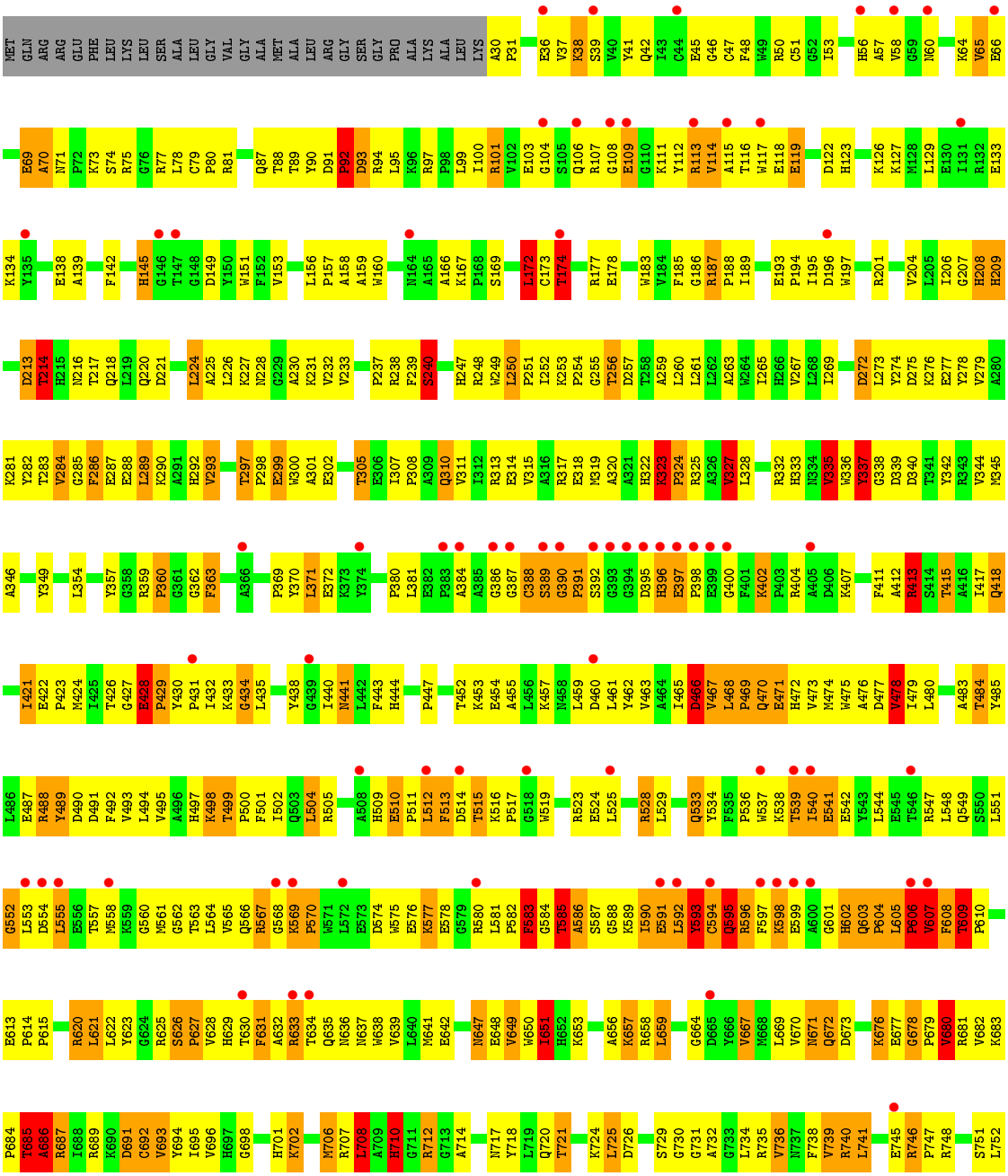
Chain A:

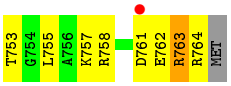




• Molecule 1: THIOSULFATE REDUCTASE

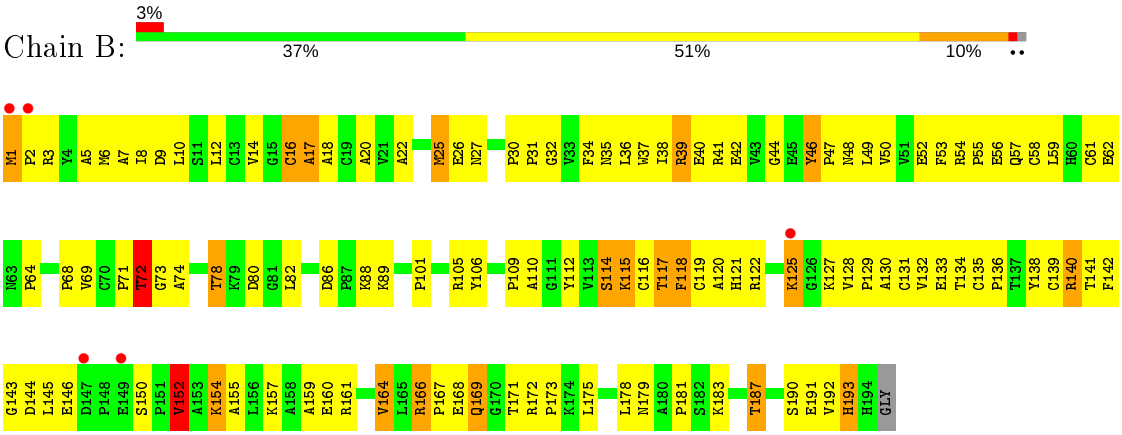
Chain E:





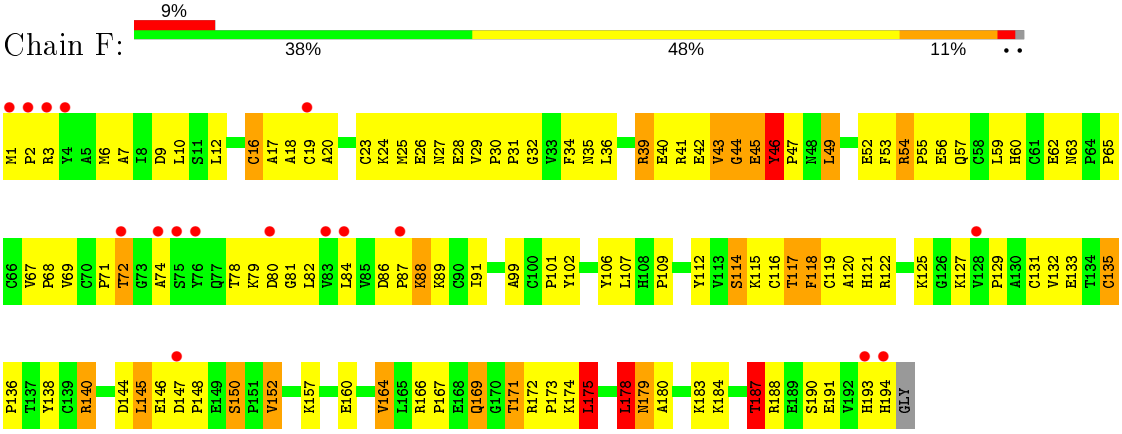
• Molecule 2: NRFC PROTEIN

Chain B:



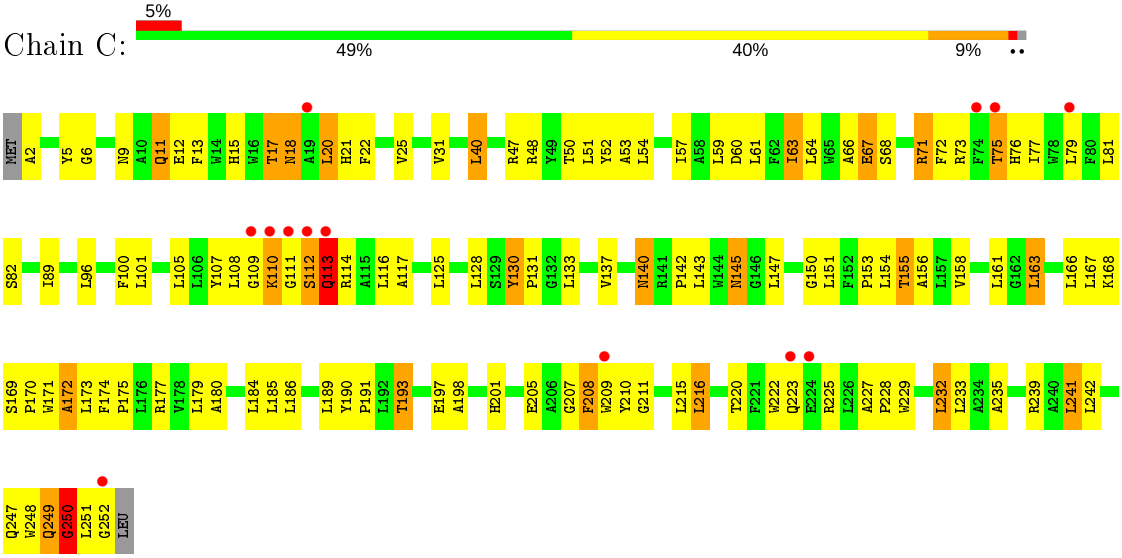
• Molecule 2: NRFC PROTEIN

Chain F:



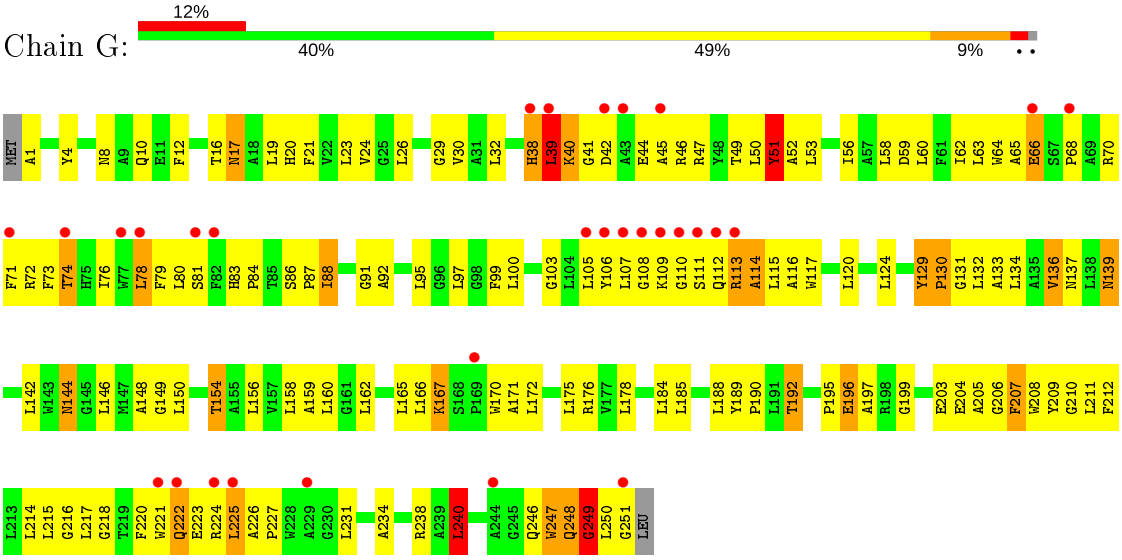
• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN

Chain C:



• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.59Å 161.16Å 239.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.10 40.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.00-3.10) 99.3 (40.00-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.301 , 0.314 0.293 , 0.295	Depositor DCC
R_{free} test set	1642 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å^2)	75.2	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 99.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	20229	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: UQ1, SF4, MO, MGD

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	0.82	6/6079 (0.1%)	1.09	30/8267 (0.4%)
1	E	0.92	9/6079 (0.1%)	1.27	66/8267 (0.8%)
2	B	0.97	1/1512 (0.1%)	1.22	9/2058 (0.4%)
2	F	0.94	2/1512 (0.1%)	1.24	16/2058 (0.8%)
3	C	0.76	3/2016 (0.1%)	0.91	6/2764 (0.2%)
3	G	0.79	1/2016 (0.0%)	1.13	13/2764 (0.5%)
All	All	0.87	22/19214 (0.1%)	1.16	140/26178 (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
1	E	0	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	592	LEU	CG-CD1	14.31	2.04	1.51
2	F	135	CYS	CB-SG	9.28	1.98	1.82
1	A	336	TRP	CB-CG	-7.84	1.36	1.50
3	C	114	ARG	NE-CZ	7.78	1.43	1.33
3	C	114	ARG	CZ-NH1	7.58	1.42	1.33
1	A	648	GLU	CB-CG	7.37	1.66	1.52
1	E	387	GLY	C-N	-7.12	1.17	1.34
2	F	16	CYS	CB-SG	7.03	1.94	1.82
1	E	692	CYS	CB-SG	-6.90	1.70	1.82
1	A	399	GLU	CD-OE2	-6.42	1.18	1.25
3	G	247	TRP	CB-CG	-6.33	1.38	1.50
1	E	363	PHE	CB-CG	-5.83	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	388	CYS	CB-SG	-5.66	1.72	1.81
1	A	364	TYR	C-O	-5.64	1.12	1.23
2	B	135	CYS	CB-SG	5.38	1.91	1.82
3	C	114	ARG	CD-NE	5.33	1.55	1.46
1	E	323	LYS	C-N	5.30	1.44	1.34
1	E	595	GLN	CB-CG	-5.30	1.38	1.52
1	A	575	TRP	CB-CG	-5.26	1.40	1.50
1	E	388	CYS	N-CA	-5.24	1.35	1.46
1	A	372	GLU	CB-CG	-5.16	1.42	1.52
1	E	231	LYS	CB-CG	-5.04	1.39	1.52

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	323	LYS	C-N-CD	-16.02	85.35	120.60
1	E	240	SER	N-CA-CB	-11.26	93.61	110.50
1	A	401	PHE	N-CA-C	11.10	140.98	111.00
3	G	249	GLY	N-CA-C	10.77	140.04	113.10
1	E	595	GLN	N-CA-CB	-10.62	91.49	110.60
1	E	172	LEU	CA-CB-CG	-10.00	92.30	115.30
2	F	171	THR	N-CA-C	9.88	137.68	111.00
2	B	46	TYR	N-CA-C	9.23	135.93	111.00
1	E	185	PHE	N-CA-C	-9.03	86.62	111.00
1	A	691	ASP	CB-CA-C	-9.02	92.36	110.40
2	F	44	GLY	N-CA-C	8.95	135.48	113.10
1	E	593	TYR	CB-CA-C	-8.70	92.99	110.40
1	E	583	PHE	N-CA-CB	-8.57	95.17	110.60
2	B	169	GLN	N-CA-C	-8.40	88.33	111.00
1	E	323	LYS	C-N-CA	8.36	157.13	122.00
1	E	583	PHE	N-CA-C	8.35	133.54	111.00
1	E	680	VAL	CB-CA-C	-8.27	95.69	111.40
2	B	46	TYR	CB-CA-C	-8.25	93.90	110.40
3	G	207	PHE	CB-CA-C	-8.12	94.17	110.40
1	A	592	LEU	N-CA-C	8.09	132.83	111.00
1	E	388	CYS	N-CA-C	8.05	132.74	111.00
3	G	114	ALA	N-CA-C	-8.00	89.41	111.00
1	E	323	LYS	CB-CA-C	7.84	126.07	110.40
1	E	659	LEU	N-CA-C	-7.79	89.98	111.00
1	E	582	PRO	N-CA-C	7.66	132.02	112.10
1	E	327	VAL	CB-CA-C	-7.58	97.01	111.40
1	E	390	GLY	N-CA-C	-7.55	94.23	113.10
1	E	585	THR	CB-CA-C	7.49	131.82	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	207	PHE	CB-CG-CD1	-7.45	115.59	120.80
3	G	78	LEU	CB-CG-CD2	-7.44	98.36	111.00
1	E	324	PRO	N-CD-CG	-7.43	92.05	103.20
1	E	231	LYS	N-CA-CB	-7.43	97.23	110.60
3	G	131	GLY	N-CA-C	-7.41	94.58	113.10
1	E	686	ALA	N-CA-C	7.38	130.93	111.00
1	E	725	LEU	CA-CB-CG	7.35	132.20	115.30
1	A	327	VAL	CB-CA-C	-7.27	97.59	111.40
1	E	593	TYR	CB-CG-CD1	-7.26	116.64	121.00
1	E	594	CYS	N-CA-CB	-7.25	97.54	110.60
3	G	225	LEU	N-CA-C	-7.25	91.42	111.00
1	E	585	THR	CA-CB-CG2	-7.01	102.58	112.40
2	B	72	THR	N-CA-C	-6.97	92.19	111.00
1	E	323	LYS	CA-CB-CG	-6.96	98.09	113.40
1	A	583	PHE	CA-C-N	-6.90	102.40	116.20
1	E	685	THR	C-N-CA	6.86	138.85	121.70
3	G	240	LEU	CA-CB-CG	6.81	130.97	115.30
1	A	213	ASP	N-CA-C	-6.81	92.62	111.00
2	F	16	CYS	N-CA-C	-6.79	92.68	111.00
1	E	593	TYR	N-CA-C	-6.72	92.85	111.00
1	E	324	PRO	CA-N-CD	-6.65	102.19	111.50
1	E	213	ASP	N-CA-C	-6.65	93.05	111.00
1	A	185	PHE	C-N-CA	-6.64	108.35	122.30
1	E	467	VAL	N-CA-C	6.64	128.94	111.00
1	A	477	ASP	N-CA-C	-6.54	93.35	111.00
1	E	710	HIS	C-N-CA	-6.53	108.58	122.30
1	A	571	TRP	N-CA-CB	-6.53	98.85	110.60
1	E	92	PRO	N-CA-C	-6.52	95.14	112.10
3	G	248	GLN	N-CA-CB	-6.48	98.93	110.60
2	F	152	VAL	CB-CA-C	-6.43	99.19	111.40
1	E	400	GLY	N-CA-C	-6.41	97.09	113.10
2	F	54	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	E	731	GLY	N-CA-C	6.39	129.07	113.10
3	G	4	TYR	N-CA-C	-6.33	93.90	111.00
1	A	648	GLU	N-CA-CB	-6.29	99.27	110.60
2	F	43	VAL	N-CA-C	-6.28	94.05	111.00
1	E	207	GLY	N-CA-C	-6.24	97.51	113.10
1	E	594	CYS	N-CA-C	6.23	127.83	111.00
2	F	39	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	B	152	VAL	CB-CA-C	-6.20	99.62	111.40
1	A	340	ASP	N-CA-C	6.20	127.73	111.00
1	E	590	ILE	CB-CA-C	-6.15	99.29	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	6	GLY	N-CA-C	-6.09	97.86	113.10
1	E	324	PRO	N-CA-C	-6.08	96.29	112.10
2	B	169	GLN	C-N-CA	-6.07	109.56	122.30
3	G	130	PRO	N-CA-C	-6.04	96.40	112.10
1	E	478	VAL	N-CA-C	-6.02	94.73	111.00
3	G	207	PHE	CB-CG-CD2	6.02	125.02	120.80
2	F	46	TYR	N-CA-C	6.02	127.24	111.00
2	F	16	CYS	C-N-CA	-5.97	106.77	121.70
1	A	109	GLU	N-CA-C	-5.97	94.89	111.00
1	A	433	LYS	N-CA-C	-5.96	94.92	111.00
1	E	593	TYR	N-CA-CB	5.88	121.19	110.60
3	C	113	GLN	N-CA-C	5.88	126.86	111.00
1	E	603	GLN	N-CA-C	5.84	126.76	111.00
1	E	708	LEU	CA-CB-CG	5.83	128.72	115.30
1	E	606	PRO	N-CA-C	-5.81	96.99	112.10
1	A	659	LEU	N-CA-C	-5.81	95.32	111.00
1	E	593	TYR	CB-CG-CD2	5.75	124.45	121.00
1	E	38	LYS	N-CA-C	-5.74	95.50	111.00
3	C	114	ARG	N-CA-C	-5.72	95.57	111.00
1	E	706	MET	N-CA-C	-5.69	95.64	111.00
1	E	712	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	E	687	ARG	CB-CG-CD	-5.64	96.94	111.60
1	E	335	VAL	CB-CA-C	5.63	122.09	111.40
3	G	51	TYR	N-CA-C	-5.62	95.81	111.00
1	A	741	LEU	CA-CB-CG	5.62	128.22	115.30
1	E	710	HIS	N-CA-C	5.60	126.12	111.00
1	A	534	TYR	N-CA-C	-5.55	96.02	111.00
1	E	214	THR	N-CA-CB	-5.55	99.76	110.30
2	B	16	CYS	N-CA-C	-5.54	96.05	111.00
1	A	365	ILE	N-CA-CB	5.51	123.47	110.80
1	A	371	LEU	N-CA-C	-5.50	96.14	111.00
1	E	387	GLY	C-N-CA	-5.49	107.98	121.70
1	E	413	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	E	189	ILE	N-CA-C	-5.46	96.26	111.00
1	E	174	THR	N-CA-CB	-5.46	99.93	110.30
1	A	583	PHE	O-C-N	5.45	132.47	123.20
3	C	5	TYR	N-CA-C	-5.45	96.29	111.00
1	E	323	LYS	O-C-N	-5.43	110.79	121.10
2	F	175	LEU	N-CA-C	-5.42	96.37	111.00
2	B	72	THR	N-CA-CB	-5.40	100.04	110.30
2	F	178	LEU	CA-CB-CG	-5.38	102.92	115.30
1	E	335	VAL	N-CA-CB	-5.38	99.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	741	LEU	CB-CG-CD1	-5.38	101.86	111.00
1	E	651	ILE	CB-CA-C	-5.35	100.91	111.60
1	A	98	PRO	CA-N-CD	-5.34	104.02	111.50
1	E	185	PHE	C-N-CA	-5.34	111.08	122.30
1	A	702	LYS	N-CA-C	-5.31	96.67	111.00
1	A	706	MET	N-CA-C	-5.29	96.71	111.00
2	F	187	THR	N-CA-CB	-5.28	100.27	110.30
3	C	250	GLY	N-CA-C	5.27	126.28	113.10
1	A	583	PHE	C-N-CA	5.26	133.36	122.30
2	F	140	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	F	188	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	F	145	LEU	CA-CB-CG	5.20	127.26	115.30
1	A	189	ILE	N-CA-C	-5.20	96.96	111.00
1	A	583	PHE	CB-CA-C	-5.20	100.01	110.40
1	A	364	TYR	N-CA-C	5.18	124.99	111.00
3	C	52	TYR	CB-CG-CD1	-5.17	117.89	121.00
1	E	692	CYS	CB-CA-C	-5.11	100.19	110.40
2	F	169	GLN	C-N-CA	-5.09	111.61	122.30
1	E	478	VAL	CB-CA-C	5.07	121.04	111.40
1	A	582	PRO	N-CA-C	5.06	125.25	112.10
1	E	586	ALA	N-CA-CB	-5.05	103.02	110.10
1	E	337	TYR	N-CA-C	5.05	124.64	111.00
1	A	608	PHE	N-CA-C	-5.04	97.39	111.00
1	E	489	TYR	CB-CA-C	-5.01	100.37	110.40
1	A	319	MET	CA-CB-CG	5.01	121.81	113.30
1	E	741	LEU	CA-CB-CG	5.01	126.82	115.30
1	E	736	VAL	N-CA-CB	-5.00	100.49	111.50
2	B	166	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	323	LYS	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5896	0	5814	816	3
1	E	5896	0	5815	764	3
2	B	1475	0	1453	181	0
2	F	1475	0	1453	159	0
3	C	1948	0	2001	177	0
3	G	1948	0	2004	203	0
4	A	8	0	0	2	0
4	B	32	0	0	8	0
4	E	8	0	0	1	0
4	F	32	0	0	6	0
5	A	94	0	43	12	0
5	E	94	0	43	23	0
6	A	1	0	0	0	0
6	E	1	0	0	1	0
7	C	18	0	18	26	0
7	G	18	0	18	22	0
8	A	387	0	0	104	0
8	B	149	0	0	41	0
8	C	90	0	0	10	0
8	E	452	0	0	141	0
8	F	130	0	0	31	0
8	G	77	0	0	35	0
All	All	20229	0	18662	2247	3

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 60.

All (2247) 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:A:602:HIS:CE1	1:A:606:PRO:HG3	1.48	1.46
3:G:78:LEU:HD21	7:G:1251:UQ1:C7	1.49	1.43
1:E:592:LEU:HA	1:E:603:GLN:NE2	1.19	1.41
1:E:605:LEU:CD2	1:E:605:LEU:H	1.30	1.39
1:A:186:GLY:HA3	1:A:583:PHE:C	1.40	1.36
1:A:591:GLU:OE2	1:A:604:PRO:HG3	1.22	1.36
1:A:184:VAL:CG2	1:A:592:LEU:HD23	1.58	1.33
1:E:388:CYS:HB2	1:E:593:TYR:OH	1.30	1.27
2:B:41:ARG:HH11	2:B:187:THR:CG2	1.47	1.27
1:A:582:PRO:HB2	8:A:2093:HOH:O	1.27	1.27
2:B:46:TYR:HB2	8:B:2034:HOH:O	1.34	1.27
1:A:604:PRO:O	1:A:606:PRO:HD2	1.33	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:602:HIS:CE1	1:E:606:PRO:HG3	1.70	1.24
2:F:57:GLN:NE2	2:F:140:ARG:HH22	1.34	1.23
3:G:207:PHE:CE2	3:G:211:LEU:HD13	1.71	1.23
1:A:97:ARG:HH21	1:A:763:ARG:NH2	1.36	1.23
1:A:601:GLY:HA2	8:A:2281:HOH:O	1.06	1.23
1:E:591:GLU:OE1	1:E:604:PRO:HB3	1.30	1.22
1:E:592:LEU:CA	1:E:603:GLN:HE21	1.49	1.22
3:C:171:TRP:CE3	3:C:171:TRP:O	1.95	1.20
1:E:605:LEU:HD23	1:E:605:LEU:N	1.40	1.19
1:A:583:PHE:CE2	1:A:588:GLY:N	2.10	1.19
1:A:395:ASP:O	1:A:399:GLU:HB2	1.39	1.19
1:A:337:TYR:O	1:A:340:ASP:OD2	1.57	1.19
1:E:477:ASP:O	1:E:478:VAL:HG23	1.35	1.18
1:E:116:THR:HG22	1:E:119:GLU:HB3	1.19	1.17
1:E:36:GLU:O	1:E:58:VAL:CG2	1.93	1.17
1:A:288:GLU:HB3	1:A:591:GLU:HG3	1.27	1.17
1:E:602:HIS:CD2	1:E:604:PRO:HD2	1.78	1.16
1:A:395:ASP:HA	1:A:399:GLU:CG	1.74	1.16
1:A:42:GLN:O	1:A:53:ILE:HG13	1.45	1.15
2:F:57:GLN:HE22	2:F:140:ARG:NH2	1.43	1.15
1:A:284:VAL:O	1:A:590:ILE:HG22	1.44	1.14
1:A:77:ARG:NH1	2:B:138:TYR:HE2	1.43	1.14
1:E:36:GLU:O	1:E:58:VAL:HG22	0.98	1.14
1:E:323:LYS:HD3	1:E:354:LEU:CA	1.77	1.14
1:A:584:GLY:HA2	8:A:2274:HOH:O	0.98	1.14
1:A:428:GLU:HB3	1:A:429:PRO:HD2	1.29	1.14
1:A:97:ARG:NH2	1:A:763:ARG:HH22	1.44	1.13
3:G:1:ALA:HB1	8:G:2001:HOH:O	1.48	1.13
1:E:477:ASP:O	1:E:478:VAL:CG2	1.96	1.13
1:E:511:PRO:HB3	1:E:515:THR:HG22	1.30	1.12
3:G:78:LEU:HD21	7:G:1251:UQ1:C8	1.79	1.12
1:A:184:VAL:HG23	1:A:592:LEU:CD2	1.80	1.12
1:E:339:ASP:HB2	1:E:607:VAL:HG11	1.30	1.11
1:E:602:HIS:NE2	1:E:604:PRO:HD2	1.65	1.11
1:E:607:VAL:O	1:E:607:VAL:HG12	1.45	1.11
3:G:78:LEU:HD21	7:G:1251:UQ1:H71	1.28	1.11
1:E:592:LEU:CA	1:E:603:GLN:NE2	2.11	1.10
1:A:604:PRO:O	1:A:606:PRO:CD	2.00	1.10
1:E:97:ARG:HG3	8:E:2028:HOH:O	1.50	1.09
1:A:397:GLU:HB3	1:A:398:PRO:HD3	1.12	1.09
2:B:134:THR:HG23	2:B:134:THR:O	1.51	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:562:GLY:O	8:E:2314:HOH:O	1.66	1.09
3:G:154:THR:CG2	3:G:238:ARG:HE	1.66	1.09
1:A:69:GLU:O	8:A:2032:HOH:O	1.69	1.09
1:E:607:VAL:O	1:E:607:VAL:CG1	1.98	1.08
1:E:592:LEU:HD23	1:E:603:GLN:HE22	1.19	1.08
1:E:763:ARG:HG2	8:E:2441:HOH:O	1.53	1.08
1:E:116:THR:CG2	1:E:119:GLU:H	1.66	1.08
2:B:41:ARG:HD2	2:B:187:THR:CG2	1.83	1.08
1:E:602:HIS:HE1	1:E:606:PRO:CG	1.67	1.08
1:A:632:ALA:O	1:A:635:GLN:HG2	1.54	1.08
1:A:395:ASP:CA	1:A:399:GLU:HG3	1.81	1.07
1:E:591:GLU:OE1	1:E:604:PRO:CB	2.02	1.07
1:A:279:VAL:HG13	1:A:283:THR:HG21	1.33	1.07
3:C:22:PHE:O	3:C:239:ARG:NH1	1.86	1.07
1:E:47:CYS:HB2	8:E:2450:HOH:O	1.52	1.07
1:A:467:VAL:HB	8:A:2226:HOH:O	1.54	1.07
1:A:591:GLU:OE2	1:A:604:PRO:CG	2.02	1.07
2:F:57:GLN:NE2	2:F:140:ARG:NH2	2.01	1.07
1:E:95:LEU:HD12	1:E:466:ASP:O	1.53	1.06
1:E:626:SER:HB2	8:E:2347:HOH:O	1.54	1.06
1:A:43:ILE:HG13	1:A:505:ARG:HB3	1.14	1.06
1:A:592:LEU:O	1:A:593:TYR:HB2	1.52	1.06
1:E:605:LEU:N	1:E:605:LEU:CD2	1.92	1.06
1:E:591:GLU:CD	1:E:604:PRO:HB3	1.76	1.06
1:E:230:ALA:O	8:E:2138:HOH:O	1.71	1.06
1:E:653:LYS:HD2	1:E:686:ALA:HB2	1.34	1.06
2:B:134:THR:O	2:B:134:THR:CG2	1.99	1.05
1:A:685:THR:HB	2:B:42:GLU:OE2	1.56	1.05
3:C:17:THR:CG2	3:C:67:GLU:HG3	1.85	1.05
1:A:172:LEU:HD13	1:A:445:SER:O	1.56	1.05
1:A:186:GLY:HA3	1:A:583:PHE:O	1.57	1.05
1:E:342:TYR:CD1	1:E:607:VAL:HB	1.91	1.05
1:E:413:ARG:HD3	8:E:2248:HOH:O	1.57	1.05
1:E:429:PRO:HD2	8:E:2257:HOH:O	1.54	1.05
3:G:38:HIS:HD2	3:G:45:ALA:HB1	1.15	1.05
1:A:165:ALA:O	1:A:415:THR:HG21	1.55	1.04
1:A:651:ILE:HD11	1:A:682:VAL:HG13	1.39	1.04
2:B:41:ARG:HH11	2:B:187:THR:HG22	1.17	1.04
1:A:602:HIS:CE1	1:A:606:PRO:CG	2.40	1.04
1:E:224:LEU:HD12	8:E:2132:HOH:O	1.56	1.04
1:A:170:VAL:O	1:A:175:ALA:HB2	1.56	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:TYR:CD1	8:B:2034:HOH:O	2.10	1.03
2:B:41:ARG:HD2	2:B:187:THR:HG21	1.32	1.03
1:E:598:LYS:HD2	8:E:2330:HOH:O	1.58	1.03
2:F:41:ARG:HD2	2:F:187:THR:CG2	1.89	1.02
1:A:116:THR:HG22	1:A:119:GLU:H	1.17	1.02
3:G:221:TRP:HE3	3:G:225:LEU:HD22	1.19	1.01
3:C:155:THR:HG22	3:C:239:ARG:HE	1.24	1.01
3:C:171:TRP:CD2	3:C:171:TRP:O	2.14	1.01
1:A:583:PHE:HE2	1:A:588:GLY:N	1.53	1.00
1:A:763:ARG:HG2	8:A:2379:HOH:O	1.58	1.00
1:A:186:GLY:CA	1:A:583:PHE:C	2.29	1.00
1:A:632:ALA:O	1:A:635:GLN:CG	2.09	1.00
1:A:591:GLU:HB3	1:A:603:GLN:NE2	1.77	0.99
1:E:533:GLN:HE21	1:E:533:GLN:H	1.07	0.99
1:A:603:GLN:HB3	1:A:604:PRO:HD3	1.38	0.99
3:G:221:TRP:CE3	3:G:225:LEU:HD22	1.98	0.99
3:G:38:HIS:CD2	3:G:45:ALA:HB1	1.97	0.99
2:B:192:VAL:HG21	8:B:2017:HOH:O	1.63	0.99
1:A:116:THR:CG2	1:A:119:GLU:H	1.74	0.99
1:A:531:LEU:O	1:A:534:TYR:O	1.80	0.98
1:A:580:ARG:HH11	1:A:580:ARG:CB	1.77	0.98
1:A:729:SER:O	1:A:731:GLY:N	1.96	0.98
1:A:42:GLN:O	1:A:53:ILE:CG1	2.11	0.98
2:B:72:THR:HG22	2:B:74:ALA:H	1.22	0.98
1:E:764:ARG:N	8:E:2445:HOH:O	1.96	0.98
1:A:434:GLY:HA2	1:A:461:LEU:O	1.62	0.98
1:E:349:TYR:OH	1:E:591:GLU:HA	1.63	0.98
2:F:41:ARG:HD2	2:F:187:THR:HG23	1.41	0.98
1:E:92:PRO:O	1:E:94:ARG:N	1.95	0.98
1:A:569:LYS:O	8:A:2269:HOH:O	1.82	0.98
1:E:635:GLN:O	1:E:641:MET:HG3	1.64	0.97
1:A:335:VAL:O	1:A:733:GLY:HA2	1.64	0.97
3:G:111:SER:HB3	8:G:2032:HOH:O	1.62	0.97
1:A:585:THR:O	1:A:586:ALA:HB3	1.64	0.97
3:G:207:PHE:HE2	3:G:211:LEU:HD13	1.09	0.97
2:B:46:TYR:CE2	8:B:2031:HOH:O	2.17	0.97
3:C:207:GLY:O	3:C:210:TYR:N	1.97	0.97
1:A:360:PRO:HD3	1:A:571:TRP:CE3	1.99	0.96
1:A:680:VAL:HG11	8:A:2311:HOH:O	1.64	0.96
2:B:160:GLU:H	2:B:179:ASN:HD21	1.06	0.96
1:E:323:LYS:CD	1:E:354:LEU:HA	1.94	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:551:LEU:O	1:E:553:LEU:N	1.98	0.96
1:E:608:PHE:O	8:E:2335:HOH:O	1.82	0.96
1:A:284:VAL:HG23	1:A:587:SER:HB3	1.47	0.96
1:E:323:LYS:HD3	1:E:354:LEU:HA	0.97	0.96
2:F:41:ARG:HH11	2:F:187:THR:CG2	1.79	0.96
2:F:46:TYR:HB3	8:F:2034:HOH:O	1.64	0.96
1:E:428:GLU:O	1:E:430:TYR:N	1.97	0.96
1:E:209:HIS:HE1	1:E:625:ARG:H	1.12	0.96
1:E:635:GLN:O	1:E:641:MET:CG	2.13	0.96
1:A:314:GLU:O	1:A:318:GLU:HG3	1.65	0.95
1:E:112:TYR:OH	1:E:474:MET:O	1.84	0.95
1:E:397:GLU:HB3	1:E:398:PRO:HD3	1.48	0.95
1:E:606:PRO:O	1:E:608:PHE:N	1.98	0.95
3:G:206:GLY:O	3:G:209:TYR:N	1.99	0.95
1:A:591:GLU:CD	1:A:604:PRO:HG3	1.87	0.95
1:E:116:THR:HG23	1:E:119:GLU:H	1.30	0.95
2:F:2:PRO:HD2	2:F:80:ASP:OD2	1.67	0.94
1:A:599:GLU:O	8:A:2280:HOH:O	1.85	0.94
1:E:324:PRO:HD3	8:E:2167:HOH:O	1.66	0.94
1:A:763:ARG:HB2	8:A:2382:HOH:O	1.66	0.94
1:E:297:THR:HG22	1:E:300:TRP:H	1.31	0.94
1:A:349:TYR:OH	1:A:591:GLU:O	1.86	0.93
1:A:183:TRP:CH2	1:A:596:ARG:HD3	2.01	0.93
3:C:140:ASN:HD22	3:C:140:ASN:H	1.16	0.93
1:A:276:LYS:HA	8:A:2148:HOH:O	1.68	0.93
1:E:569:LYS:HD2	8:E:2320:HOH:O	1.66	0.93
1:A:629:HIS:ND1	1:A:634:THR:HG23	1.82	0.93
1:E:95:LEU:CD1	1:E:466:ASP:O	2.16	0.93
3:C:17:THR:HG21	3:C:67:GLU:HG3	1.49	0.93
1:A:395:ASP:HA	1:A:399:GLU:HG3	0.93	0.93
1:A:397:GLU:HB3	1:A:398:PRO:CD	1.99	0.93
3:G:20:HIS:ND1	3:G:59:ASP:OD2	2.00	0.93
1:A:42:GLN:NE2	1:A:505:ARG:HD3	1.83	0.92
1:E:493:VAL:HG13	8:E:2013:HOH:O	1.68	0.92
2:B:41:ARG:NH1	2:B:187:THR:CG2	2.32	0.92
2:B:25:MET:CE	2:B:25:MET:HA	2.00	0.92
2:B:16:CYS:O	2:B:16:CYS:SG	2.27	0.92
3:C:108:LEU:O	3:C:110:LYS:HG2	1.68	0.92
1:A:42:GLN:NE2	1:A:485:TYR:O	2.03	0.92
1:A:335:VAL:CG1	1:A:732:ALA:O	2.18	0.92
1:A:519:TRP:CE2	1:A:540:ILE:HG12	2.05	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:ALA:O	2:F:183:LYS:HE2	1.70	0.92
3:G:129:TYR:OH	7:G:1251:UQ1:O4	1.88	0.92
3:G:139:ASN:HD22	3:G:139:ASN:H	1.17	0.92
1:E:604:PRO:O	1:E:606:PRO:HD3	1.69	0.91
3:G:206:GLY:O	3:G:210:GLY:N	2.01	0.91
1:A:97:ARG:NH2	1:A:763:ARG:NH2	2.08	0.91
1:E:301:ALA:O	1:E:305:THR:HB	1.71	0.91
3:C:128:LEU:HB3	8:C:2063:HOH:O	1.68	0.91
7:G:1251:UQ1:C8	7:G:1251:UQ1:HM51	2.00	0.91
1:E:602:HIS:HE1	1:E:606:PRO:HG3	0.78	0.91
1:E:614:PRO:HG2	8:E:2341:HOH:O	1.70	0.91
1:A:608:PHE:CD1	1:A:608:PHE:O	2.23	0.91
3:C:53:ALA:O	3:C:57:ILE:HG13	1.70	0.91
1:E:305:THR:HG22	1:E:307:ILE:H	1.35	0.91
1:A:607:VAL:HG12	1:A:607:VAL:O	1.71	0.90
2:F:47:PRO:HD2	8:F:2034:HOH:O	1.69	0.90
1:E:494:LEU:HD22	1:E:502:ILE:HG12	1.54	0.90
7:C:1252:UQ1:C8	7:C:1252:UQ1:HM51	2.00	0.90
1:E:116:THR:CG2	1:E:119:GLU:HB3	2.01	0.90
1:E:388:CYS:SG	1:E:413:ARG:NE	2.44	0.90
1:A:397:GLU:CB	1:A:398:PRO:HD3	2.02	0.90
1:A:602:HIS:ND1	1:A:606:PRO:HG3	1.86	0.90
1:E:590:ILE:HG13	8:E:2178:HOH:O	1.72	0.90
1:A:653:LYS:HG3	1:A:684:PRO:O	1.72	0.90
1:A:186:GLY:HA3	1:A:584:GLY:N	1.87	0.90
2:F:65:PRO:HD2	4:F:1196:SF4:S4	2.11	0.90
2:F:160:GLU:H	2:F:179:ASN:HD21	1.10	0.90
7:C:1252:UQ1:H8	7:C:1252:UQ1:HM51	1.54	0.89
3:C:172:ALA:HA	3:C:175:PRO:HG2	1.54	0.89
3:G:154:THR:HG22	3:G:238:ARG:HE	1.35	0.89
1:A:413:ARG:CD	1:A:413:ARG:H	1.86	0.89
1:E:305:THR:CG2	1:E:307:ILE:H	1.85	0.89
1:E:648:GLU:HG2	1:E:681:ARG:HH12	1.36	0.89
2:F:72:THR:HG22	2:F:74:ALA:H	1.36	0.89
1:A:97:ARG:HH21	1:A:763:ARG:HH22	0.93	0.89
1:E:510:GLU:HG3	8:E:2299:HOH:O	1.71	0.89
1:A:93:ASP:OD1	1:A:758:ARG:NH2	2.04	0.89
1:A:256:THR:HG21	1:A:305:THR:HA	1.55	0.89
1:A:400:GLY:HA3	8:A:2192:HOH:O	1.73	0.89
1:E:116:THR:HG22	1:E:119:GLU:CB	2.01	0.89
1:E:608:PHE:CD1	1:E:608:PHE:O	2.26	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:GLU:HG2	8:B:2110:HOH:O	1.73	0.88
1:A:607:VAL:HG13	1:A:609:THR:OG1	1.72	0.88
1:E:81:ARG:HG2	1:E:628:VAL:O	1.73	0.88
1:A:207:GLY:O	5:A:1766:MGD:O5'	1.92	0.88
7:C:1252:UQ1:O2	7:C:1252:UQ1:HM32	1.74	0.88
3:C:168:LYS:HE2	8:C:2065:HOH:O	1.72	0.88
3:G:78:LEU:CD2	7:G:1251:UQ1:C8	2.52	0.88
1:A:602:HIS:HE1	1:A:606:PRO:HG3	1.07	0.88
1:A:183:TRP:HE1	1:A:413:ARG:HH22	1.22	0.88
1:A:183:TRP:HH2	1:A:596:ARG:HD3	1.36	0.87
1:A:604:PRO:C	1:A:606:PRO:CD	2.43	0.87
3:C:64:LEU:HB3	7:C:1252:UQ1:H113	1.53	0.87
2:B:117:THR:HG21	8:B:2095:HOH:O	1.75	0.87
1:A:672:GLN:NE2	1:A:738:PHE:H	1.73	0.87
1:E:256:THR:HG21	1:E:305:THR:HA	1.55	0.87
1:E:488:ARG:HD3	1:E:490:ASP:OD2	1.74	0.87
2:B:41:ARG:NH1	2:B:187:THR:HG22	1.89	0.87
1:A:116:THR:HG22	1:A:119:GLU:HB3	1.54	0.87
7:G:1251:UQ1:HM51	7:G:1251:UQ1:H8	1.54	0.87
1:A:209:HIS:HE1	1:A:625:ARG:H	1.23	0.87
3:C:155:THR:CG2	3:C:239:ARG:HE	1.88	0.87
3:G:78:LEU:CD2	7:G:1251:UQ1:C7	2.46	0.87
1:A:580:ARG:HH11	1:A:580:ARG:HB3	1.38	0.86
2:F:146:GLU:HG2	8:F:2003:HOH:O	1.73	0.86
1:A:153:VAL:HG11	1:A:167:LYS:HE2	1.57	0.86
3:G:196:GLU:HG2	8:G:2055:HOH:O	1.72	0.86
1:A:75:ARG:HD2	1:A:220:GLN:HE22	1.37	0.86
1:A:335:VAL:HG11	1:A:732:ALA:O	1.73	0.86
7:G:1251:UQ1:HM32	7:G:1251:UQ1:O2	1.74	0.86
1:E:283:THR:HG22	8:E:2179:HOH:O	1.73	0.86
1:A:591:GLU:HB3	1:A:603:GLN:HE22	1.37	0.86
1:E:629:HIS:ND1	1:E:634:THR:HG23	1.90	0.86
1:A:591:GLU:O	1:A:592:LEU:HD12	1.75	0.86
2:B:57:GLN:HE22	2:B:140:ARG:HH22	1.21	0.86
2:B:46:TYR:HD1	8:B:2034:HOH:O	1.48	0.86
1:E:428:GLU:O	1:E:429:PRO:C	2.08	0.86
1:A:77:ARG:NH1	2:B:138:TYR:CE2	2.28	0.86
1:E:498:LYS:HE2	8:E:2119:HOH:O	1.76	0.86
1:E:342:TYR:HD1	1:E:607:VAL:HB	1.36	0.86
2:B:160:GLU:H	2:B:179:ASN:ND2	1.72	0.86
1:A:651:ILE:HD11	1:A:682:VAL:CG1	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:GLY:CA	8:A:2281:HOH:O	1.73	0.85
1:E:592:LEU:CD2	1:E:603:GLN:HE22	1.89	0.85
1:A:393:GLY:HA3	1:A:407:LYS:CE	2.07	0.85
2:F:117:THR:HG23	2:F:120:ALA:H	1.41	0.85
3:G:111:SER:O	3:G:115:LEU:HD12	1.76	0.85
1:A:184:VAL:HG23	1:A:592:LEU:HD23	0.86	0.85
1:A:629:HIS:HA	1:A:634:THR:HG21	1.58	0.85
8:B:2145:HOH:O	3:C:251:LEU:HD11	1.75	0.85
1:E:308:PRO:HB2	8:E:2195:HOH:O	1.77	0.85
1:E:89:THR:OG1	1:E:484:THR:HG21	1.77	0.85
1:A:48:PHE:CE1	1:A:145:HIS:CE1	2.65	0.84
1:A:605:LEU:H	1:A:605:LEU:CD2	1.90	0.84
1:E:277:GLU:O	1:E:281:LYS:HG2	1.76	0.84
1:A:342:TYR:CD1	1:A:607:VAL:HB	2.13	0.84
1:A:186:GLY:CA	1:A:583:PHE:O	2.26	0.84
1:A:390:GLY:H	1:A:595:GLN:HE22	1.26	0.84
1:E:511:PRO:HB3	1:E:515:THR:CG2	2.08	0.84
3:G:234:ALA:O	3:G:238:ARG:HG3	1.76	0.84
1:A:686:ALA:HB3	8:A:2331:HOH:O	1.77	0.83
1:A:75:ARG:HH11	1:A:220:GLN:NE2	1.76	0.83
1:A:320:ALA:O	1:A:323:LYS:HG2	1.78	0.83
3:C:235:ALA:O	3:C:239:ARG:HG3	1.78	0.83
1:A:138:GLU:OE2	1:A:402:LYS:HB2	1.78	0.83
2:F:1:MET:HA	8:F:2058:HOH:O	1.78	0.83
1:A:231:LYS:HA	1:A:247:HIS:CD2	2.13	0.83
1:A:42:GLN:HE22	1:A:505:ARG:HD3	1.42	0.83
1:A:721:THR:HG22	1:A:722:ARG:HG3	1.60	0.83
1:E:109:GLU:HG3	8:E:2067:HOH:O	1.77	0.83
1:E:297:THR:CG2	1:E:299:GLU:H	1.90	0.83
3:C:64:LEU:HD21	7:C:1252:UQ1:C3	2.08	0.83
1:E:473:VAL:HG11	8:E:2276:HOH:O	1.79	0.83
1:E:592:LEU:HD23	1:E:603:GLN:NE2	1.92	0.83
1:A:740:ARG:NH1	8:A:2361:HOH:O	2.09	0.83
1:E:539:THR:HG23	1:E:542:GLU:H	1.44	0.83
1:E:590:ILE:CG1	8:E:2178:HOH:O	2.25	0.83
1:A:377:PRO:HG2	1:A:533:GLN:HG3	1.61	0.82
1:A:429:PRO:O	1:A:430:TYR:CD2	2.31	0.82
1:E:685:THR:HG22	2:F:42:GLU:CD	1.99	0.82
1:A:279:VAL:HG13	1:A:283:THR:CG2	2.07	0.82
3:G:222:GLN:HA	3:G:222:GLN:OE1	1.80	0.82
1:A:633:ARG:HD2	5:A:1765:MGD:O2B	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:155:THR:HG21	3:C:239:ARG:HG2	1.62	0.82
2:F:72:THR:HG23	2:F:89:LYS:HB3	1.62	0.82
2:B:46:TYR:CB	8:B:2034:HOH:O	2.04	0.82
1:E:562:GLY:C	8:E:2314:HOH:O	2.09	0.82
1:A:393:GLY:HA3	1:A:407:LYS:HE3	1.59	0.82
2:F:67:VAL:HB	2:F:68:PRO:HD3	1.60	0.82
1:E:239:PHE:HB3	1:E:687:ARG:HB3	1.62	0.81
1:A:388:CYS:HA	1:A:593:TYR:OH	1.79	0.81
1:E:232:VAL:H	1:E:247:HIS:CD2	1.98	0.81
1:E:88:THR:HG23	1:E:468:LEU:HD21	1.61	0.81
3:G:76:ILE:O	3:G:80:LEU:HG	1.80	0.81
1:E:635:GLN:H	1:E:635:GLN:NE2	1.79	0.81
2:B:46:TYR:HE2	8:B:2031:HOH:O	1.58	0.81
1:E:339:ASP:CB	1:E:607:VAL:HG11	2.10	0.81
2:F:57:GLN:HE22	2:F:140:ARG:HH22	1.03	0.81
3:C:173:LEU:HG	3:C:173:LEU:O	1.80	0.81
1:E:453:LYS:HG2	1:E:475:TRP:CH2	2.15	0.81
3:G:21:PHE:O	3:G:238:ARG:NH1	2.14	0.81
1:E:75:ARG:HH11	1:E:220:GLN:NE2	1.77	0.81
1:E:469:PRO:O	1:E:706:MET:HG3	1.80	0.81
3:C:140:ASN:ND2	3:C:140:ASN:H	1.73	0.81
1:A:605:LEU:HD23	1:A:605:LEU:H	1.44	0.81
1:A:393:GLY:HA3	1:A:407:LYS:NZ	1.95	0.81
1:A:585:THR:O	1:A:586:ALA:CB	2.28	0.81
1:E:297:THR:HG23	1:E:299:GLU:H	1.43	0.81
1:E:438:TYR:HD2	8:E:2092:HOH:O	1.63	0.81
3:C:207:GLY:O	3:C:209:TRP:N	2.14	0.80
1:E:209:HIS:HE1	1:E:625:ARG:N	1.79	0.80
1:A:677:GLU:O	1:A:678:GLY:O	1.99	0.80
1:E:397:GLU:HB3	1:E:398:PRO:CD	2.11	0.80
1:E:604:PRO:O	1:E:606:PRO:CD	2.29	0.80
3:G:107:LEU:O	3:G:109:LYS:N	2.13	0.80
1:A:390:GLY:N	1:A:595:GLN:HE22	1.79	0.80
1:E:113:ARG:NH1	1:E:114:VAL:HG13	1.96	0.80
1:E:75:ARG:HH11	1:E:220:GLN:HE21	1.27	0.80
1:E:232:VAL:H	1:E:247:HIS:HD2	1.30	0.80
3:G:139:ASN:ND2	3:G:139:ASN:H	1.80	0.80
1:A:457:LYS:HA	8:A:2221:HOH:O	1.80	0.80
1:A:604:PRO:C	1:A:606:PRO:HD3	2.01	0.80
1:A:170:VAL:O	1:A:175:ALA:CB	2.30	0.80
1:E:431:PRO:HD2	8:E:2260:HOH:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:VAL:H	1:A:247:HIS:HD2	1.25	0.80
1:A:395:ASP:O	1:A:399:GLU:CB	2.25	0.80
3:C:155:THR:HG21	3:C:239:ARG:CG	2.12	0.80
1:E:183:TRP:CH2	1:E:596:ARG:HD3	2.17	0.80
1:A:561:MET:O	1:A:563:THR:N	2.14	0.80
1:A:647:ASN:C	1:A:648:GLU:HG3	2.00	0.80
1:E:539:THR:HG22	1:E:542:GLU:CB	2.12	0.80
1:A:342:TYR:HD1	1:A:607:VAL:HB	1.47	0.79
1:E:183:TRP:HH2	1:E:596:ARG:HD3	1.45	0.79
1:E:311:VAL:HB	8:E:2195:HOH:O	1.80	0.79
1:E:71:ASN:HD22	1:E:74:SER:H	1.29	0.79
1:E:109:GLU:CG	8:E:2067:HOH:O	2.29	0.79
1:E:95:LEU:HD21	8:E:2276:HOH:O	1.82	0.79
1:E:100:ILE:HG12	1:E:478:VAL:HG22	1.63	0.79
3:G:78:LEU:HD21	7:G:1251:UQ1:H72	1.62	0.79
2:B:16:CYS:O	2:B:18:ALA:N	2.14	0.79
1:E:605:LEU:N	1:E:605:LEU:HD22	1.94	0.79
1:E:648:GLU:HG2	1:E:681:ARG:NH1	1.97	0.79
1:E:717:ASN:HD22	5:E:1765:MGD:H192	1.30	0.79
1:E:95:LEU:HD11	8:E:2276:HOH:O	1.80	0.79
1:E:97:ARG:NH2	1:E:763:ARG:HD2	1.97	0.79
1:A:625:ARG:HH22	5:A:1765:MGD:H15	1.31	0.79
1:A:519:TRP:NE1	1:A:540:ILE:HG12	1.96	0.79
3:C:171:TRP:O	3:C:172:ALA:HB2	1.82	0.79
1:A:285:GLY:O	1:A:590:ILE:HG23	1.83	0.79
1:A:605:LEU:HD23	1:A:605:LEU:N	1.97	0.79
3:G:206:GLY:O	3:G:207:PHE:C	2.21	0.79
1:A:583:PHE:HE2	1:A:588:GLY:H	1.25	0.78
1:E:297:THR:CG2	1:E:299:GLU:HG2	2.13	0.78
1:A:629:HIS:CA	1:A:634:THR:HG21	2.13	0.78
1:E:139:ALA:O	1:E:433:LYS:O	2.02	0.78
1:E:746:ARG:HG3	1:E:746:ARG:HH11	1.48	0.78
1:A:673:ASP:OD2	1:A:721:THR:HG21	1.84	0.78
1:E:673:ASP:OD2	1:E:721:THR:CG2	2.32	0.78
1:A:651:ILE:HD13	1:A:656:ALA:HB2	1.63	0.78
2:B:41:ARG:HH11	2:B:187:THR:HG23	1.48	0.78
1:E:608:PHE:CD1	1:E:608:PHE:C	2.52	0.78
1:E:589:LYS:HB3	1:E:592:LEU:HB2	1.65	0.78
1:A:209:HIS:O	1:A:213:ASP:HB3	1.83	0.78
1:A:510:GLU:HG3	8:A:2022:HOH:O	1.84	0.78
2:F:41:ARG:HH11	2:F:187:THR:HG23	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:GLU:O	1:A:58:VAL:HG22	1.84	0.78
1:E:397:GLU:CB	1:E:398:PRO:HD3	2.14	0.78
1:A:301:ALA:O	1:A:305:THR:HB	1.84	0.78
1:A:367:GLN:HG3	8:A:2268:HOH:O	1.83	0.78
3:G:12:PHE:CZ	3:G:246:GLN:HG2	2.18	0.78
1:A:174:THR:HG23	1:A:178:GLU:HG2	1.66	0.77
1:A:70:ALA:O	8:A:2035:HOH:O	1.99	0.77
3:C:241:LEU:C	3:C:241:LEU:HD12	2.04	0.77
1:E:339:ASP:HB2	1:E:607:VAL:CG1	2.13	0.77
2:F:55:PRO:HG2	4:F:1194:SF4:S2	2.23	0.77
1:A:483:ALA:HA	1:A:515:THR:CG2	2.14	0.77
1:E:38:LYS:HG3	8:E:2019:HOH:O	1.84	0.77
1:A:339:ASP:HB3	1:A:607:VAL:HG11	1.65	0.77
1:A:428:GLU:HB3	1:A:429:PRO:CD	2.10	0.77
2:F:3:ARG:HD2	2:F:62:GLU:OE2	1.84	0.77
1:A:382:GLU:HA	8:A:2184:HOH:O	1.83	0.77
1:E:386:GLY:O	1:E:388:CYS:SG	2.40	0.77
1:E:424:MET:HG2	1:E:459:LEU:HD21	1.67	0.77
2:F:40:GLU:HB2	8:F:2020:HOH:O	1.85	0.77
1:A:396:HIS:HB3	1:A:403:PRO:HB3	1.66	0.77
1:E:116:THR:HG21	8:E:2072:HOH:O	1.84	0.77
1:E:602:HIS:CD2	1:E:604:PRO:CD	2.62	0.77
2:F:57:GLN:HE21	2:F:140:ARG:HH22	1.33	0.77
1:A:428:GLU:O	1:A:429:PRO:C	2.20	0.77
2:B:190:SER:HB3	3:C:252:GLY:N	1.98	0.77
1:A:116:THR:HG22	1:A:119:GLU:N	1.97	0.77
1:E:483:ALA:N	1:E:516:LYS:O	2.16	0.77
3:G:88:ILE:CD1	7:G:1251:UQ1:HM33	2.14	0.77
1:A:647:ASN:H	1:A:647:ASN:HD22	1.33	0.76
2:B:25:MET:HE2	2:B:25:MET:HA	1.67	0.76
1:E:762:GLU:HB2	8:E:2444:HOH:O	1.84	0.76
2:F:160:GLU:H	2:F:179:ASN:ND2	1.83	0.76
1:E:259:ALA:HB3	8:E:2193:HOH:O	1.85	0.76
2:B:41:ARG:HD2	2:B:187:THR:HG23	1.68	0.76
1:A:578:GLU:HB3	1:A:580:ARG:HD3	1.66	0.76
3:C:108:LEU:O	3:C:110:LYS:CG	2.34	0.76
1:E:421:ILE:O	1:E:421:ILE:CG2	2.33	0.76
1:E:100:ILE:HG23	1:E:478:VAL:HG22	1.67	0.76
1:E:671:ASN:C	1:E:671:ASN:HD22	1.89	0.76
1:E:651:ILE:HD11	1:E:682:VAL:CG1	2.16	0.76
1:A:422:GLU:HB3	1:A:423:PRO:HD3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:VAL:HG11	1:E:167:LYS:HE2	1.68	0.76
1:E:642:GLU:OE2	2:F:32:GLY:N	2.15	0.76
3:G:150:LEU:O	3:G:154:THR:HB	1.86	0.76
1:A:595:GLN:CG	1:A:595:GLN:O	2.34	0.76
2:F:3:ARG:HG2	8:F:2002:HOH:O	1.85	0.76
3:G:206:GLY:HA2	3:G:209:TYR:HB3	1.67	0.76
1:A:152:PHE:O	1:A:157:PRO:HD3	1.85	0.76
1:A:284:VAL:O	1:A:590:ILE:CG2	2.31	0.76
1:E:434:GLY:HA2	1:E:461:LEU:O	1.85	0.76
1:A:184:VAL:CG2	1:A:592:LEU:CD2	2.49	0.75
1:A:73:LYS:NZ	1:A:192:HIS:HD2	1.83	0.75
1:A:305:THR:HG22	1:A:307:ILE:H	1.51	0.75
1:A:139:ALA:O	1:A:433:LYS:O	2.03	0.75
1:A:286:PHE:HA	1:A:590:ILE:HG21	1.68	0.75
1:A:653:LYS:HD2	1:A:686:ALA:H	1.48	0.75
1:E:577:LYS:HE2	8:E:2321:HOH:O	1.85	0.75
1:A:467:VAL:HG13	8:A:2047:HOH:O	1.86	0.75
1:A:606:PRO:O	1:A:608:PHE:N	2.18	0.75
2:B:6:MET:HE3	8:B:2046:HOH:O	1.87	0.75
1:E:488:ARG:HB2	1:E:517:PRO:HB3	1.67	0.75
1:E:673:ASP:OD2	1:E:721:THR:HG21	1.86	0.75
3:G:225:LEU:HB3	8:G:2068:HOH:O	1.85	0.75
1:A:232:VAL:H	1:A:247:HIS:CD2	2.04	0.75
2:B:17:ALA:HB1	2:B:20:ALA:HB3	1.68	0.75
1:E:118:GLU:HG3	8:E:2305:HOH:O	1.87	0.75
1:E:69:GLU:O	1:E:70:ALA:HB3	1.84	0.75
1:A:427:GLY:O	1:A:428:GLU:O	2.03	0.75
1:A:642:GLU:HG2	2:B:34:PHE:HZ	1.52	0.75
1:A:511:PRO:HB3	1:A:515:THR:HG22	1.67	0.75
1:A:611:PRO:HB3	8:A:2136:HOH:O	1.85	0.75
8:A:2013:HOH:O	2:B:25:MET:HE1	1.86	0.75
1:E:253:LYS:O	1:E:256:THR:HB	1.86	0.75
1:A:346:ALA:HB2	1:A:605:LEU:CD1	2.15	0.75
1:E:174:THR:HG23	1:E:178:GLU:HG2	1.68	0.75
3:C:101:LEU:O	3:C:105:LEU:HD12	1.86	0.75
1:E:318:GLU:O	1:E:322:HIS:HD2	1.70	0.75
1:A:595:GLN:HG3	1:A:595:GLN:O	1.85	0.75
3:C:197:GLU:HG2	8:C:2075:HOH:O	1.85	0.75
3:C:61:LEU:HD22	7:C:1252:UQ1:H101	1.68	0.75
1:E:305:THR:HG23	1:E:307:ILE:HG12	1.68	0.75
2:F:169:GLN:NE2	8:F:2107:HOH:O	2.19	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:THR:CG2	1:E:119:GLU:N	2.48	0.74
1:E:591:GLU:OE2	1:E:604:PRO:HG3	1.87	0.74
3:G:154:THR:CG2	3:G:238:ARG:NE	2.46	0.74
1:A:99:LEU:O	1:A:478:VAL:HA	1.88	0.74
1:A:89:THR:OG1	1:A:484:THR:HG21	1.88	0.74
1:A:349:TYR:HE1	1:A:605:LEU:HD21	1.52	0.74
3:C:64:LEU:HD22	7:C:1252:UQ1:C1	2.17	0.74
1:A:330:PRO:HD2	8:A:2164:HOH:O	1.86	0.74
1:A:484:THR:HG22	1:A:487:GLU:HG3	1.69	0.74
1:E:209:HIS:CE1	1:E:625:ARG:H	2.02	0.74
1:A:336:TRP:HD1	1:A:336:TRP:H	1.34	0.74
1:A:672:GLN:HE22	1:A:738:PHE:H	1.32	0.74
1:E:575:TRP:O	1:E:578:GLU:HB2	1.86	0.74
1:E:75:ARG:HD2	1:E:220:GLN:HE22	1.53	0.74
3:G:129:TYR:CD2	3:G:130:PRO:HD3	2.22	0.74
1:A:592:LEU:O	1:A:593:TYR:CB	2.33	0.74
1:A:75:ARG:HH11	1:A:220:GLN:HE21	1.35	0.74
1:A:687:ARG:NH2	2:B:40:GLU:OE2	2.20	0.74
1:E:597:PHE:HB3	8:E:2325:HOH:O	1.86	0.74
1:E:720:GLN:HB3	8:E:2418:HOH:O	1.88	0.74
1:E:391:PRO:O	1:E:413:ARG:HG2	1.87	0.73
1:A:186:GLY:H	1:A:583:PHE:HA	1.53	0.73
1:A:349:TYR:CE2	1:A:590:ILE:O	2.41	0.73
3:C:145:ASN:HD22	3:C:145:ASN:C	1.89	0.73
2:F:117:THR:HG21	8:F:2077:HOH:O	1.86	0.73
2:B:47:PRO:O	2:B:48:ASN:OD1	2.07	0.73
1:E:69:GLU:O	1:E:70:ALA:CB	2.36	0.73
2:F:78:THR:HG21	8:F:2059:HOH:O	1.88	0.73
1:A:488:ARG:NH2	5:A:1765:MGD:O6	2.21	0.73
1:A:195:ILE:HA	1:A:362:GLY:O	1.88	0.73
2:B:46:TYR:O	8:B:2033:HOH:O	2.06	0.73
1:A:519:TRP:CE2	1:A:540:ILE:CG1	2.71	0.73
1:A:604:PRO:C	1:A:606:PRO:HD2	2.06	0.73
2:B:121:HIS:O	2:B:125:LYS:HE2	1.89	0.73
3:G:78:LEU:CD2	7:G:1251:UQ1:H71	2.14	0.73
3:C:21:HIS:CE1	3:C:64:LEU:HD11	2.24	0.73
1:E:284:VAL:HG12	1:E:592:LEU:CD1	2.19	0.73
2:F:78:THR:HG22	2:F:80:ASP:H	1.52	0.73
1:A:153:VAL:CG1	1:A:167:LYS:HE2	2.19	0.73
1:A:400:GLY:CA	8:A:2192:HOH:O	2.31	0.73
1:A:631:PHE:O	1:A:698:GLY:HA3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:MET:HA	2:B:25:MET:HE3	1.69	0.73
1:E:346:ALA:N	1:E:605:LEU:HD12	2.04	0.73
1:E:708:LEU:HA	8:E:2406:HOH:O	1.89	0.73
1:E:91:ASP:O	1:E:92:PRO:O	2.07	0.73
1:A:413:ARG:HD2	1:A:413:ARG:H	1.52	0.73
1:A:71:ASN:HD22	1:A:74:SER:H	1.33	0.73
1:E:421:ILE:O	1:E:421:ILE:HG23	1.87	0.72
1:E:511:PRO:CB	1:E:515:THR:HG22	2.14	0.72
1:E:438:TYR:CD2	8:E:2092:HOH:O	2.40	0.72
1:E:551:LEU:O	1:E:553:LEU:HB2	1.89	0.72
1:E:734:LEU:HD22	8:E:2418:HOH:O	1.89	0.72
1:A:391:PRO:O	1:A:413:ARG:HB3	1.89	0.72
2:B:47:PRO:HD3	8:B:2036:HOH:O	1.89	0.72
1:E:470:GLN:HG2	1:E:706:MET:SD	2.29	0.72
3:G:115:LEU:HD13	8:G:2031:HOH:O	1.89	0.72
3:G:154:THR:HG21	3:G:238:ARG:HG2	1.72	0.72
3:G:51:TYR:N	8:G:2015:HOH:O	2.23	0.72
1:A:395:ASP:C	1:A:399:GLU:HB2	2.09	0.72
1:E:672:GLN:NE2	1:E:738:PHE:H	1.87	0.72
1:E:639:VAL:HG11	2:F:25:MET:HE3	1.70	0.72
1:E:465:ILE:O	1:E:466:ASP:HB3	1.88	0.72
1:E:622:LEU:HD22	5:E:1766:MGD:H8	1.70	0.72
3:C:222:TRP:CG	3:C:223:GLN:N	2.54	0.72
1:E:553:LEU:HD21	1:E:557:THR:HG21	1.72	0.72
1:E:605:LEU:HD23	1:E:605:LEU:H	0.58	0.72
1:A:166:ALA:HB2	1:A:415:THR:HG23	1.70	0.72
1:A:413:ARG:NE	1:A:413:ARG:H	1.86	0.72
2:F:47:PRO:CD	8:F:2034:HOH:O	2.32	0.72
3:G:221:TRP:HZ3	3:G:225:LEU:HD13	1.54	0.72
1:A:299:GLU:OE2	1:A:313:ARG:NH2	2.17	0.71
1:A:601:GLY:N	8:A:2281:HOH:O	2.00	0.71
1:A:632:ALA:O	1:A:635:GLN:HG3	1.89	0.71
1:A:338:GLY:O	1:A:726:ASP:HA	1.90	0.71
1:E:299:GLU:OE2	1:E:313:ARG:NH2	2.15	0.71
1:E:589:LYS:HG2	1:E:592:LEU:HD12	1.72	0.71
1:E:708:LEU:O	1:E:712:ARG:HD2	1.91	0.71
2:F:45:GLU:HB2	8:F:2027:HOH:O	1.89	0.71
1:A:79:CYS:HB2	1:A:80:PRO:HD2	1.72	0.71
1:A:305:THR:O	1:A:306:GLU:HB2	1.89	0.71
2:B:117:THR:HG22	2:B:119:CYS:N	2.04	0.71
2:B:72:THR:HG21	2:B:89:LYS:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:ILE:HG23	1:E:478:VAL:CG2	2.20	0.71
1:A:183:TRP:CB	1:A:592:LEU:HD22	2.20	0.71
2:B:27:ASN:HD21	2:B:121:HIS:CE1	2.08	0.71
3:C:47:ARG:NH1	3:C:107:TYR:O	2.24	0.71
2:F:43:VAL:HG23	8:F:2122:HOH:O	1.91	0.71
1:A:387:GLY:O	1:A:593:TYR:CE1	2.44	0.71
1:A:349:TYR:CE1	1:A:605:LEU:HD21	2.26	0.71
1:A:729:SER:OG	1:A:729:SER:O	2.00	0.71
2:B:78:THR:HG21	8:B:2068:HOH:O	1.91	0.71
2:F:117:THR:HG22	2:F:119:CYS:H	1.55	0.71
1:A:152:PHE:O	1:A:157:PRO:CD	2.39	0.71
1:A:37:VAL:HG12	1:A:38:LYS:N	2.05	0.71
1:A:121:LEU:HD13	1:A:524:GLU:HB3	1.72	0.71
2:F:88:LYS:O	3:G:74:THR:HG22	1.91	0.71
1:A:539:THR:CG2	1:A:541:GLU:HG2	2.21	0.71
1:E:585:THR:OG1	1:E:589:LYS:HE3	1.90	0.71
3:G:206:GLY:HA2	3:G:209:TYR:CB	2.21	0.71
1:A:635:GLN:HG3	1:A:701:HIS:NE2	2.06	0.70
3:G:105:LEU:HG	8:G:2031:HOH:O	1.89	0.70
1:A:642:GLU:HG2	2:B:34:PHE:CZ	2.25	0.70
1:A:95:LEU:HD11	1:A:468:LEU:O	1.90	0.70
1:A:495:VAL:HG13	8:A:2018:HOH:O	1.90	0.70
1:E:311:VAL:CB	8:E:2195:HOH:O	2.38	0.70
1:A:314:GLU:HG2	8:A:2161:HOH:O	1.91	0.70
2:B:46:TYR:CE2	8:B:2035:HOH:O	2.45	0.70
1:E:97:ARG:HH21	1:E:763:ARG:NH1	1.88	0.70
1:A:388:CYS:HA	1:A:593:TYR:CE1	2.26	0.70
1:A:594:CYS:O	1:A:598:LYS:HG3	1.91	0.70
2:B:117:THR:CG2	2:B:120:ALA:H	2.04	0.70
3:C:61:LEU:HD22	7:C:1252:UQ1:C10	2.21	0.70
1:E:670:VAL:HG22	1:E:676:LYS:HG3	1.73	0.70
1:A:231:LYS:HA	1:A:247:HIS:NE2	2.06	0.70
1:A:580:ARG:CB	1:A:580:ARG:NH1	2.52	0.70
2:F:41:ARG:HD2	2:F:187:THR:HG21	1.70	0.70
1:E:539:THR:CG2	1:E:542:GLU:H	2.04	0.70
1:E:647:ASN:H	1:E:647:ASN:HD22	1.38	0.70
2:F:41:ARG:HH11	2:F:187:THR:HG22	1.57	0.70
1:A:755:LEU:O	1:A:758:ARG:HD3	1.92	0.69
1:E:418:GLN:H	1:E:418:GLN:NE2	1.89	0.69
1:E:465:ILE:O	1:E:466:ASP:CB	2.40	0.69
1:E:490:ASP:O	8:E:2288:HOH:O	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:588:GLY:HA3	8:E:2174:HOH:O	1.90	0.69
2:F:72:THR:HG21	2:F:89:LYS:O	1.91	0.69
3:C:59:LEU:O	3:C:63:ILE:HG23	1.92	0.69
1:E:282:TYR:O	1:E:587:SER:HB3	1.92	0.69
2:B:22:ALA:HB2	2:B:134:THR:HG21	1.75	0.69
2:B:72:THR:HG23	2:B:89:LYS:HB3	1.75	0.69
1:E:342:TYR:HD1	1:E:607:VAL:CB	2.06	0.69
1:A:238:ARG:HG3	1:A:688:ILE:HD12	1.73	0.69
1:A:293:VAL:O	1:A:293:VAL:HG13	1.91	0.69
1:E:606:PRO:CD	1:E:607:VAL:H	2.04	0.69
1:E:669:LEU:CD2	1:E:741:LEU:HD22	2.22	0.69
1:A:708:LEU:HD22	1:A:755:LEU:HB3	1.74	0.69
3:G:105:LEU:HB3	8:G:2011:HOH:O	1.92	0.69
1:A:127:LYS:HE2	8:A:2223:HOH:O	1.93	0.69
1:A:602:HIS:ND1	1:A:606:PRO:CG	2.51	0.69
1:A:685:THR:HB	2:B:42:GLU:CD	2.13	0.69
2:B:44:GLY:O	2:B:49:LEU:HD13	1.93	0.69
1:E:90:TYR:OH	1:E:509:HIS:HE1	1.76	0.69
1:E:591:GLU:O	1:E:591:GLU:HG3	1.90	0.69
1:A:345:MET:HE3	1:A:592:LEU:HD11	1.75	0.68
2:B:44:GLY:O	2:B:49:LEU:CD1	2.40	0.68
1:E:116:THR:HG22	1:E:119:GLU:H	1.49	0.68
1:A:642:GLU:OE2	2:B:31:PRO:O	2.11	0.68
1:E:649:VAL:HG13	1:E:695:ILE:CG2	2.23	0.68
1:A:134:LYS:HE2	8:A:2075:HOH:O	1.92	0.68
2:F:164:VAL:HG22	2:F:173:PRO:HB2	1.75	0.68
1:A:109:GLU:OE2	1:A:111:LYS:HE2	1.93	0.68
1:A:710:HIS:O	8:A:2345:HOH:O	2.12	0.68
1:E:687:ARG:NH2	2:F:40:GLU:OE2	2.27	0.68
1:A:608:PHE:C	1:A:608:PHE:CD1	2.62	0.68
3:G:207:PHE:HE2	3:G:211:LEU:CD1	1.97	0.68
1:A:429:PRO:O	1:A:430:TYR:CG	2.46	0.68
1:E:539:THR:HG22	1:E:542:GLU:HB2	1.76	0.68
1:E:740:ARG:NH1	8:E:2426:HOH:O	2.26	0.68
1:E:391:PRO:HG3	1:E:411:PHE:CZ	2.29	0.68
1:A:603:GLN:HB3	1:A:604:PRO:CD	2.20	0.68
1:E:284:VAL:HG12	1:E:592:LEU:HD12	1.74	0.68
1:E:30:ALA:HB3	8:E:2002:HOH:O	1.92	0.68
1:E:671:ASN:ND2	1:E:673:ASP:H	1.91	0.68
1:A:53:ILE:HD12	1:A:65:VAL:HG22	1.76	0.67
1:A:256:THR:CG2	1:A:305:THR:HA	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:GLN:HE22	2:B:140:ARG:NH2	1.90	0.67
1:E:632:ALA:O	1:E:635:GLN:NE2	2.27	0.67
8:E:2383:HOH:O	2:F:49:LEU:HD11	1.94	0.67
1:A:95:LEU:HD12	1:A:467:VAL:C	2.15	0.67
3:C:239:ARG:NH2	8:C:2084:HOH:O	2.26	0.67
1:E:633:ARG:HD2	5:E:1765:MGD:O2B	1.94	0.67
1:E:479:ILE:O	1:E:480:LEU:HD23	1.95	0.67
1:A:380:PRO:HD3	1:A:534:TYR:OH	1.94	0.67
1:A:653:LYS:CG	1:A:684:PRO:O	2.42	0.67
3:C:18:ASN:OD1	3:C:67:GLU:OE2	2.11	0.67
1:E:686:ALA:HB1	8:E:2383:HOH:O	1.94	0.67
1:A:183:TRP:HB2	1:A:592:LEU:HD22	1.77	0.67
1:E:208:HIS:HE1	1:E:218:GLN:NE2	1.92	0.67
1:E:267:VAL:HG22	8:E:2197:HOH:O	1.94	0.67
1:E:297:THR:HG21	8:E:2189:HOH:O	1.94	0.67
1:E:81:ARG:NH1	1:E:630:THR:OG1	2.27	0.67
1:A:204:VAL:HB	1:A:328:LEU:HG	1.76	0.67
3:C:21:HIS:HE1	3:C:64:LEU:HD11	1.59	0.67
1:E:310:GLN:NE2	1:E:314:GLU:OE2	2.27	0.67
1:A:382:GLU:HB3	8:A:2185:HOH:O	1.94	0.67
3:C:112:SER:O	3:C:113:GLN:HG2	1.95	0.67
1:A:558:MET:HE2	1:A:558:MET:HA	1.75	0.67
3:G:208:TRP:CE3	3:G:208:TRP:HA	2.30	0.67
1:A:120:ALA:HB3	8:A:2065:HOH:O	1.94	0.67
1:A:428:GLU:O	1:A:430:TYR:N	2.28	0.67
1:A:292:HIS:NE2	1:A:604:PRO:HB2	2.10	0.67
2:B:88:LYS:O	3:C:75:THR:HG22	1.94	0.67
1:E:108:GLY:HA3	8:E:2065:HOH:O	1.95	0.67
1:E:129:LEU:O	1:E:133:GLU:HG2	1.95	0.67
1:E:478:VAL:HG23	8:E:2281:HOH:O	1.94	0.67
1:A:630:THR:H	1:A:634:THR:HG21	1.59	0.66
1:A:166:ALA:HB2	1:A:415:THR:CG2	2.24	0.66
2:B:47:PRO:CD	8:B:2036:HOH:O	2.42	0.66
1:E:204:VAL:HB	1:E:328:LEU:HG	1.77	0.66
3:C:155:THR:CG2	3:C:239:ARG:NE	2.58	0.66
1:E:589:LYS:HG2	1:E:592:LEU:CD1	2.25	0.66
2:F:193:HIS:HB2	8:F:2130:HOH:O	1.94	0.66
1:A:239:PHE:HB3	1:A:687:ARG:HB3	1.78	0.66
2:B:3:ARG:HG2	8:B:2001:HOH:O	1.95	0.66
3:C:197:GLU:CD	3:C:197:GLU:H	1.99	0.66
1:E:297:THR:HG23	1:E:299:GLU:HG2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:MET:HG2	1:A:592:LEU:HD21	1.78	0.66
1:A:428:GLU:CB	1:A:429:PRO:HD2	2.17	0.66
1:E:635:GLN:N	1:E:635:GLN:NE2	2.43	0.66
1:A:252:ILE:CD1	1:A:256:THR:HG22	2.25	0.66
3:C:171:TRP:O	3:C:172:ALA:CB	2.42	0.66
1:E:396:HIS:CE1	1:E:404:ARG:H	2.14	0.66
1:E:539:THR:HG23	1:E:541:GLU:HG2	1.78	0.66
1:E:679:PRO:HG2	1:E:747:PRO:HB3	1.77	0.66
1:A:602:HIS:CD2	1:A:604:PRO:HD2	2.31	0.66
1:E:539:THR:HG22	1:E:542:GLU:HB3	1.77	0.66
2:F:166:ARG:HH22	3:G:248:GLN:HE21	1.44	0.66
1:A:357:TYR:HA	1:A:363:PHE:HB2	1.77	0.66
1:A:580:ARG:HH11	1:A:580:ARG:HB2	1.58	0.66
1:A:483:ALA:HA	1:A:515:THR:HG21	1.78	0.66
1:A:583:PHE:HE2	1:A:588:GLY:CA	2.08	0.65
2:B:192:VAL:HG12	2:B:193:HIS:N	2.12	0.65
1:E:93:ASP:OD1	1:E:758:ARG:NH2	2.29	0.65
1:A:293:VAL:CG1	1:A:293:VAL:O	2.43	0.65
3:G:206:GLY:O	3:G:209:TYR:CA	2.43	0.65
1:A:319:MET:CE	1:A:328:LEU:HD11	2.25	0.65
2:B:57:GLN:NE2	2:B:140:ARG:HH22	1.91	0.65
3:C:17:THR:CG2	3:C:67:GLU:CG	2.69	0.65
1:E:495:VAL:CG2	8:E:2296:HOH:O	2.45	0.65
3:G:39:LEU:HD13	3:G:116:ALA:HB3	1.79	0.65
1:A:428:GLU:O	1:A:430:TYR:O	2.14	0.65
1:A:583:PHE:CE2	1:A:587:SER:C	2.69	0.65
2:B:166:ARG:NH2	3:C:249:GLN:NE2	2.43	0.65
3:G:196:GLU:CD	3:G:196:GLU:H	1.97	0.65
2:B:117:THR:HB	8:B:2010:HOH:O	1.96	0.65
1:E:589:LYS:NZ	8:E:2324:HOH:O	2.23	0.65
1:E:647:ASN:HD21	1:E:714:ALA:H	1.45	0.65
3:G:156:LEU:HD12	3:G:178:LEU:HD13	1.79	0.65
3:G:20:HIS:CE1	3:G:63:LEU:HD21	2.31	0.65
3:G:189:TYR:O	3:G:192:THR:HB	1.97	0.65
1:E:116:THR:HG23	1:E:119:GLU:N	2.09	0.65
1:A:122:ASP:OD1	1:A:528:ARG:NH1	2.29	0.65
1:A:75:ARG:NH1	1:A:220:GLN:NE2	2.44	0.65
1:A:107:ARG:HG2	1:A:475:TRP:O	1.97	0.65
1:A:346:ALA:HB2	1:A:605:LEU:HD13	1.78	0.65
2:B:2:PRO:HB3	2:B:144:ASP:CG	2.17	0.65
3:C:241:LEU:C	3:C:241:LEU:CD1	2.64	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:NH2	1:A:367:GLN:NE2	2.45	0.64
1:A:591:GLU:CB	1:A:603:GLN:HE22	2.10	0.64
1:A:604:PRO:O	1:A:606:PRO:HD3	1.94	0.64
1:E:279:VAL:O	1:E:283:THR:HB	1.96	0.64
1:E:590:ILE:O	1:E:592:LEU:HG	1.97	0.64
1:E:79:CYS:HB2	1:E:80:PRO:HD2	1.79	0.64
2:F:194:HIS:N	8:F:2129:HOH:O	2.29	0.64
3:G:38:HIS:CE1	8:G:2011:HOH:O	2.50	0.64
1:A:540:ILE:O	1:A:544:LEU:HG	1.97	0.64
3:C:130:TYR:CD2	3:C:131:PRO:HD3	2.32	0.64
1:A:364:TYR:HB2	1:A:570:PRO:HB3	1.78	0.64
1:A:471:GLU:HG2	1:A:471:GLU:O	1.98	0.64
1:A:525:LEU:O	1:A:529:LEU:HG	1.98	0.64
1:A:581:LEU:HD11	8:A:2272:HOH:O	1.97	0.64
1:A:671:ASN:HD21	1:A:675:VAL:H	1.46	0.64
1:E:256:THR:CG2	1:E:305:THR:HA	2.28	0.64
1:E:388:CYS:HB2	1:E:593:TYR:HH	1.55	0.64
1:A:39:SER:HB2	8:A:2005:HOH:O	1.97	0.64
1:A:427:GLY:O	1:A:430:TYR:O	2.15	0.64
1:A:581:LEU:CD1	8:A:2272:HOH:O	2.45	0.64
1:A:689:ARG:NH2	1:A:691:ASP:OD2	2.31	0.64
2:B:166:ARG:HH22	3:C:249:GLN:NE2	1.94	0.64
2:B:72:THR:CG2	2:B:74:ALA:H	2.05	0.64
3:G:207:PHE:O	3:G:211:LEU:N	2.31	0.64
1:A:558:MET:CE	1:A:561:MET:SD	2.86	0.64
1:E:77:ARG:NE	8:E:2044:HOH:O	2.30	0.64
3:G:30:VAL:HG12	3:G:52:ALA:HB2	1.80	0.64
3:G:76:ILE:HG12	3:G:80:LEU:HD11	1.80	0.64
1:A:335:VAL:HG13	1:A:732:ALA:C	2.17	0.64
1:A:519:TRP:CZ2	1:A:540:ILE:HG13	2.33	0.64
3:C:140:ASN:HD22	3:C:140:ASN:N	1.93	0.64
1:E:467:VAL:HG12	1:E:468:LEU:HG	1.80	0.64
2:F:43:VAL:CG2	8:F:2122:HOH:O	2.46	0.64
1:A:364:TYR:HB2	1:A:570:PRO:CB	2.28	0.64
1:A:388:CYS:HA	1:A:593:TYR:CZ	2.33	0.64
1:E:396:HIS:HB3	1:E:407:LYS:HE3	1.80	0.64
1:E:569:LYS:CD	8:E:2320:HOH:O	2.35	0.64
1:E:642:GLU:HG3	8:E:2435:HOH:O	1.97	0.64
1:E:81:ARG:HE	1:E:214:THR:HG22	1.62	0.63
2:B:36:LEU:HD11	8:B:2105:HOH:O	1.98	0.63
3:C:21:HIS:CE1	3:C:64:LEU:HG	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:GLN:HG3	8:E:2311:HOH:O	1.98	0.63
2:F:72:THR:HG22	2:F:74:ALA:N	2.09	0.63
1:A:367:GLN:O	1:A:500:PRO:HG3	1.96	0.63
2:B:142:PHE:C	2:B:152:VAL:HG22	2.18	0.63
1:E:519:TRP:CE2	1:E:540:ILE:CG1	2.81	0.63
3:G:49:THR:HG21	8:G:2011:HOH:O	1.97	0.63
1:A:633:ARG:CD	5:A:1765:MGD:O2B	2.46	0.63
1:E:651:ILE:HD13	1:E:656:ALA:HB2	1.80	0.63
1:A:195:ILE:HG12	1:A:329:PRO:HB3	1.81	0.63
1:A:335:VAL:HG13	1:A:732:ALA:O	1.97	0.63
8:B:2029:HOH:O	3:C:2:ALA:HB1	1.98	0.63
1:E:88:THR:HG21	1:E:467:VAL:HG11	1.79	0.63
3:G:220:PHE:HD1	8:G:2063:HOH:O	1.81	0.63
1:A:151:TRP:O	1:A:156:LEU:HB2	1.99	0.63
1:A:609:THR:O	1:A:610:PRO:C	2.37	0.63
3:C:21:HIS:ND1	3:C:64:LEU:HG	2.13	0.63
7:G:1251:UQ1:CM3	7:G:1251:UQ1:O2	2.46	0.63
1:A:73:LYS:NZ	1:A:192:HIS:CD2	2.67	0.63
1:E:186:GLY:HA3	1:E:584:GLY:N	2.14	0.63
1:E:621:LEU:HD22	1:E:622:LEU:O	1.98	0.63
1:A:286:PHE:CA	1:A:590:ILE:HG21	2.29	0.62
1:A:360:PRO:HD3	1:A:571:TRP:CZ3	2.34	0.62
1:A:603:GLN:CB	1:A:604:PRO:HD3	2.22	0.62
1:E:591:GLU:O	1:E:603:GLN:NE2	2.32	0.62
1:A:426:THR:HG23	8:A:2049:HOH:O	1.98	0.62
1:A:80:PRO:HD3	2:B:18:ALA:HB2	1.81	0.62
2:B:140:ARG:NH2	8:B:2046:HOH:O	2.32	0.62
3:C:64:LEU:HD22	7:C:1252:UQ1:C6	2.29	0.62
1:A:96:LYS:HB3	1:A:513:PHE:HB3	1.81	0.62
1:E:553:LEU:CD2	1:E:557:THR:HG21	2.29	0.62
1:E:635:GLN:HE21	1:E:635:GLN:H	1.46	0.62
1:A:607:VAL:HG13	1:A:609:THR:CB	2.29	0.62
3:C:207:GLY:O	3:C:208:PHE:C	2.35	0.62
1:E:186:GLY:H	1:E:583:PHE:HA	1.63	0.62
1:E:418:GLN:H	1:E:418:GLN:HE21	1.44	0.62
1:E:470:GLN:NE2	8:E:2277:HOH:O	2.32	0.62
2:F:115:LYS:HG3	2:F:116:CYS:O	2.00	0.62
1:A:71:ASN:HD21	1:A:73:LYS:HB2	1.64	0.62
2:B:57:GLN:O	2:B:58:CYS:C	2.37	0.62
1:E:512:LEU:O	1:E:515:THR:HB	2.00	0.62
2:F:91:ILE:HD12	7:G:1251:UQ1:O1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:PRO:HG2	1:A:537:TRP:H	1.65	0.62
2:B:134:THR:O	2:B:134:THR:HG22	1.93	0.62
1:E:607:VAL:HG23	8:E:2145:HOH:O	2.00	0.62
1:A:630:THR:N	1:A:634:THR:HG21	2.15	0.62
1:A:635:GLN:O	1:A:709:ALA:HB2	1.98	0.62
1:A:53:ILE:HD12	1:A:65:VAL:CG2	2.29	0.62
7:C:1252:UQ1:O2	7:C:1252:UQ1:CM3	2.46	0.62
2:F:41:ARG:CD	2:F:187:THR:HG23	2.23	0.62
3:G:172:LEU:O	3:G:176:ARG:HG3	2.00	0.62
2:B:2:PRO:HB3	2:B:144:ASP:HB2	1.82	0.62
1:A:483:ALA:CA	1:A:515:THR:HG23	2.29	0.62
1:A:523:ARG:HG3	1:A:535:PHE:HB3	1.81	0.62
1:A:646:GLU:O	1:A:648:GLU:OE2	2.18	0.62
1:E:297:THR:HG22	1:E:300:TRP:N	2.10	0.62
1:E:604:PRO:C	1:E:606:PRO:HD3	2.20	0.62
3:G:139:ASN:N	3:G:139:ASN:HD22	1.95	0.62
1:A:345:MET:CE	1:A:592:LEU:HD11	2.30	0.62
1:A:37:VAL:HG13	1:A:57:ALA:O	2.00	0.62
1:E:311:VAL:CG2	8:E:2195:HOH:O	2.48	0.62
1:E:701:HIS:O	1:E:710:HIS:O	2.16	0.62
2:F:44:GLY:O	2:F:45:GLU:HB2	2.00	0.62
1:A:580:ARG:NH1	1:A:580:ARG:HB2	2.14	0.61
3:C:171:TRP:CG	3:C:171:TRP:O	2.53	0.61
3:C:172:ALA:CA	3:C:175:PRO:HG2	2.29	0.61
1:E:359:ARG:HD3	8:E:2222:HOH:O	1.98	0.61
1:E:533:GLN:HE21	1:E:533:GLN:N	1.89	0.61
1:A:152:PHE:O	1:A:157:PRO:CG	2.48	0.61
3:G:20:HIS:NE2	3:G:63:LEU:HD21	2.14	0.61
1:A:284:VAL:CG2	1:A:587:SER:HB3	2.25	0.61
1:A:42:GLN:O	1:A:53:ILE:HG12	2.00	0.61
1:A:535:PHE:N	1:A:536:PRO:CD	2.62	0.61
3:C:128:LEU:HD22	8:C:2063:HOH:O	2.00	0.61
1:E:591:GLU:OE1	1:E:604:PRO:CA	2.48	0.61
1:E:627:PRO:HB2	2:F:16:CYS:HA	1.83	0.61
1:E:724:LYS:HG2	8:E:2423:HOH:O	2.00	0.61
3:C:207:GLY:HA2	3:C:210:TYR:HB3	1.83	0.61
3:C:248:TRP:CE2	3:C:250:GLY:HA3	2.35	0.61
1:E:315:VAL:HG12	1:E:319:MET:HE3	1.83	0.61
3:G:226:ALA:HB3	3:G:227:PRO:HD3	1.82	0.61
1:A:335:VAL:HG13	1:A:733:GLY:HA2	1.82	0.61
1:A:627:PRO:HB2	2:B:16:CYS:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:519:TRP:CE2	1:E:540:ILE:HG13	2.35	0.61
1:E:598:LYS:HB3	1:E:599:GLU:OE1	2.01	0.61
1:E:345:MET:HB2	1:E:605:LEU:HD13	1.82	0.61
1:E:99:LEU:O	1:E:478:VAL:HA	2.01	0.61
1:A:388:CYS:O	1:A:391:PRO:HD3	2.01	0.61
1:A:39:SER:OG	8:A:2004:HOH:O	2.16	0.61
1:A:534:TYR:O	1:A:535:PHE:HB2	1.99	0.61
1:A:320:ALA:O	1:A:323:LYS:CG	2.48	0.61
1:E:281:LYS:HG3	1:E:282:TYR:CE1	2.36	0.61
1:A:336:TRP:O	1:A:735:ARG:HB2	2.00	0.61
1:A:346:ALA:HB2	1:A:605:LEU:HD12	1.83	0.61
3:G:115:LEU:HB3	8:G:2031:HOH:O	2.00	0.61
1:A:319:MET:HE1	1:A:328:LEU:HD11	1.80	0.61
1:A:358:GLY:O	1:A:571:TRP:HA	2.00	0.61
2:B:114:SER:O	2:B:115:LYS:HB3	2.00	0.61
2:B:2:PRO:HD2	2:B:80:ASP:OD2	2.01	0.61
1:E:81:ARG:HE	1:E:214:THR:CG2	2.14	0.61
1:E:286:PHE:CB	8:E:2178:HOH:O	2.49	0.61
1:E:686:ALA:CB	8:E:2383:HOH:O	2.48	0.61
1:E:689:ARG:NH2	1:E:691:ASP:OD2	2.21	0.61
7:G:1251:UQ1:C8	7:G:1251:UQ1:CM5	2.78	0.61
1:A:572:LEU:HD22	8:A:2272:HOH:O	2.01	0.61
1:E:336:TRP:O	1:E:340:ASP:OD1	2.19	0.61
2:F:2:PRO:HB3	2:F:144:ASP:CG	2.21	0.61
3:G:70:ARG:HG2	3:G:71:PHE:H	1.65	0.61
1:A:239:PHE:O	1:A:687:ARG:HD2	2.01	0.60
2:B:121:HIS:O	2:B:125:LYS:CE	2.48	0.60
3:C:64:LEU:CD2	7:C:1252:UQ1:C2	2.79	0.60
1:E:608:PHE:C	8:E:2335:HOH:O	2.30	0.60
3:G:144:ASN:OD1	3:G:192:THR:CG2	2.49	0.60
2:B:122:ARG:HB3	2:B:127:LYS:HB2	1.82	0.60
8:E:2165:HOH:O	2:F:46:TYR:HB2	2.00	0.60
1:A:396:HIS:CB	1:A:403:PRO:HB3	2.30	0.60
1:A:721:THR:OG1	8:A:2353:HOH:O	2.16	0.60
1:E:209:HIS:CG	5:E:1766:MGD:H5'1	2.36	0.60
1:E:81:ARG:NE	1:E:214:THR:HG22	2.15	0.60
3:G:227:PRO:O	3:G:231:LEU:HB2	2.01	0.60
3:G:38:HIS:CE1	3:G:105:LEU:HD22	2.35	0.60
1:A:295:ASP:HB2	8:A:2156:HOH:O	2.01	0.60
1:A:384:ALA:N	8:A:2186:HOH:O	2.25	0.60
3:C:140:ASN:O	3:C:142:PRO:HD3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:ASP:C	1:E:478:VAL:HG23	2.14	0.60
2:B:27:ASN:HD21	2:B:121:HIS:HE1	1.48	0.60
3:C:21:HIS:ND1	3:C:60:ASP:OD1	2.34	0.60
1:A:658:ARG:C	1:A:659:LEU:O	2.34	0.60
3:C:67:GLU:O	3:C:67:GLU:HG2	2.01	0.60
3:C:77:ILE:HG12	3:C:81:LEU:HD11	1.83	0.60
2:F:39:ARG:HD2	2:F:56:GLU:OE2	2.00	0.60
1:A:42:GLN:CD	1:A:505:ARG:HB2	2.21	0.60
2:B:2:PRO:HB3	2:B:144:ASP:CB	2.31	0.60
1:E:391:PRO:HG2	1:E:392:SER:H	1.65	0.60
1:E:81:ARG:HD2	1:E:630:THR:OG1	2.02	0.60
1:E:93:ASP:O	1:E:469:PRO:HD3	2.01	0.60
1:A:101:ARG:HB2	1:A:477:ASP:HA	1.84	0.60
1:A:81:ARG:HE	1:A:214:THR:HG22	1.66	0.60
1:A:36:GLU:HG2	1:A:36:GLU:O	2.02	0.60
2:B:183:LYS:HE3	8:B:2142:HOH:O	2.02	0.60
1:E:342:TYR:CE1	1:E:607:VAL:HB	2.34	0.60
1:A:305:THR:HG23	1:A:307:ILE:HD12	1.83	0.60
3:C:151:LEU:O	3:C:155:THR:HB	2.02	0.60
3:C:64:LEU:HD21	7:C:1252:UQ1:C4	2.32	0.60
1:E:371:LEU:HD13	1:E:547:ARG:CZ	2.31	0.60
1:E:606:PRO:HG2	1:E:607:VAL:N	2.17	0.60
1:A:708:LEU:N	1:A:708:LEU:HD23	2.17	0.59
1:E:519:TRP:NE1	1:E:540:ILE:HG12	2.17	0.59
3:G:249:GLY:O	8:G:2075:HOH:O	2.16	0.59
1:A:336:TRP:CD1	1:A:336:TRP:N	2.60	0.59
1:A:209:HIS:CE1	1:A:625:ARG:H	2.11	0.59
3:C:20:LEU:HD13	3:C:63:ILE:HD13	1.83	0.59
1:A:81:ARG:HE	1:A:214:THR:CG2	2.15	0.59
1:A:558:MET:HE2	1:A:561:MET:SD	2.43	0.59
3:G:225:LEU:CB	8:G:2068:HOH:O	2.48	0.59
1:A:583:PHE:CE2	1:A:588:GLY:CA	2.83	0.59
1:A:595:GLN:HA	1:A:598:LYS:HD2	1.85	0.59
1:E:313:ARG:HD3	1:E:317:ARG:NH2	2.18	0.59
3:G:206:GLY:C	3:G:209:TYR:H	2.04	0.59
1:A:193:GLU:HG2	8:A:2118:HOH:O	2.03	0.59
1:E:466:ASP:HA	5:E:1765:MGD:N2	2.17	0.59
1:E:97:ARG:HH22	1:E:763:ARG:HD2	1.66	0.59
3:G:66:GLU:HG2	3:G:66:GLU:O	2.03	0.59
1:A:519:TRP:CD1	1:A:540:ILE:HG21	2.37	0.59
1:E:252:ILE:HG12	1:E:256:THR:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:474:MET:HE2	8:E:2069:HOH:O	2.02	0.59
1:A:413:ARG:N	1:A:413:ARG:HD2	2.16	0.59
1:A:421:ILE:HG22	1:A:421:ILE:O	2.01	0.59
1:E:346:ALA:H	1:E:605:LEU:HD12	1.67	0.59
3:G:221:TRP:HD1	8:G:2065:HOH:O	1.86	0.59
1:A:428:GLU:OE2	1:A:428:GLU:HA	1.94	0.59
1:A:183:TRP:HB3	1:A:592:LEU:O	2.02	0.59
8:B:2075:HOH:O	3:C:82:SER:HB3	2.02	0.59
1:E:273:LEU:O	1:E:323:LYS:NZ	2.24	0.59
1:E:635:GLN:O	1:E:641:MET:HG2	1.99	0.59
1:E:755:LEU:O	1:E:758:ARG:HD3	2.02	0.59
1:A:284:VAL:HG23	1:A:587:SER:CB	2.30	0.59
1:A:415:THR:HG22	8:A:2200:HOH:O	2.03	0.59
1:A:483:ALA:HA	1:A:515:THR:HG23	1.82	0.59
1:E:197:TRP:CG	1:E:221:ASP:HB3	2.38	0.59
1:E:37:VAL:HA	1:E:57:ALA:O	2.03	0.59
1:E:568:GLY:O	1:E:570:PRO:HD3	2.03	0.59
1:A:554:ASP:N	1:A:554:ASP:OD2	2.36	0.59
1:A:673:ASP:OD2	1:A:721:THR:CG2	2.49	0.59
3:C:79:LEU:HD21	7:C:1252:UQ1:C8	2.33	0.59
1:E:397:GLU:CG	1:E:398:PRO:HD3	2.33	0.59
1:E:41:TYR:HE1	1:E:560:GLY:O	1.86	0.59
1:E:623:TYR:HA	1:E:695:ILE:O	2.02	0.59
1:A:422:GLU:HB2	8:A:2202:HOH:O	2.02	0.58
1:E:590:ILE:HB	8:E:2178:HOH:O	2.03	0.58
3:G:60:LEU:HD22	7:G:1251:UQ1:H101	1.84	0.58
1:A:454:GLU:HG2	8:A:2099:HOH:O	2.03	0.58
2:B:117:THR:HG22	2:B:119:CYS:H	1.68	0.58
1:E:606:PRO:CG	1:E:607:VAL:N	2.66	0.58
3:G:132:LEU:O	3:G:136:VAL:HB	2.03	0.58
1:A:231:LYS:CA	1:A:247:HIS:CD2	2.85	0.58
1:A:232:VAL:N	1:A:247:HIS:HD2	1.96	0.58
1:A:519:TRP:CZ2	1:A:540:ILE:CG1	2.87	0.58
1:A:599:GLU:HB2	8:A:2277:HOH:O	2.04	0.58
2:B:78:THR:HG22	2:B:80:ASP:H	1.69	0.58
1:E:263:ALA:HB2	1:E:301:ALA:HB2	1.85	0.58
1:E:658:ARG:C	1:E:659:LEU:O	2.30	0.58
1:A:186:GLY:C	1:A:583:PHE:O	2.41	0.58
3:C:174:PHE:H	3:C:175:PRO:HD2	1.68	0.58
1:E:380:PRO:HD3	1:E:534:TYR:OH	2.03	0.58
1:E:630:THR:HG23	8:E:2450:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HD12	1:A:590:ILE:HD11	1.86	0.58
1:A:519:TRP:CG	1:A:540:ILE:HG21	2.38	0.58
3:C:68:SER:O	3:C:71:ARG:HB3	2.03	0.58
1:E:173:CYS:SG	5:E:1766:MGD:S12	3.01	0.58
2:F:35:ASN:ND2	2:F:106:TYR:HE2	2.02	0.58
3:G:160:LEU:HB3	3:G:175:LEU:HB2	1.84	0.58
1:A:183:TRP:HB3	1:A:592:LEU:HD22	1.84	0.58
1:A:548:LEU:HD13	1:A:558:MET:HB2	1.86	0.58
1:A:64:LYS:HE2	2:B:26:GLU:HB2	1.85	0.58
1:E:551:LEU:O	1:E:552:GLY:C	2.42	0.58
1:E:647:ASN:HD22	1:E:647:ASN:N	1.95	0.58
1:E:239:PHE:O	1:E:687:ARG:HD2	2.03	0.58
3:G:189:TYR:HB3	3:G:190:PRO:HD3	1.86	0.58
1:A:214:THR:O	1:A:214:THR:HG23	2.04	0.58
8:A:2039:HOH:O	2:B:133:GLU:HG3	2.04	0.58
2:B:86:ASP:OD1	2:B:88:LYS:HB2	2.03	0.58
3:C:57:ILE:HG21	3:C:100:PHE:HB2	1.85	0.58
1:E:647:ASN:H	1:E:647:ASN:ND2	2.02	0.58
2:B:57:GLN:NE2	8:B:2046:HOH:O	2.36	0.58
1:E:142:PHE:CG	1:E:157:PRO:HG3	2.38	0.58
1:A:558:MET:HE1	1:A:561:MET:SD	2.44	0.58
1:A:583:PHE:CZ	1:A:587:SER:HA	2.39	0.58
1:A:75:ARG:HD2	1:A:220:GLN:NE2	2.13	0.58
2:B:32:GLY:N	8:B:2011:HOH:O	2.35	0.58
1:E:335:VAL:HG13	1:E:732:ALA:O	2.04	0.58
1:E:45:GLU:HG3	8:E:2011:HOH:O	2.03	0.58
1:A:93:ASP:CG	1:A:758:ARG:HH22	2.06	0.58
1:E:412:ALA:HB1	1:E:413:ARG:NH1	2.19	0.58
1:E:651:ILE:HD11	1:E:682:VAL:HG12	1.86	0.58
3:G:16:THR:HG21	3:G:66:GLU:HB2	1.86	0.58
3:G:88:ILE:HD13	7:G:1251:UQ1:HM33	1.85	0.58
1:A:187:ARG:HH22	1:A:367:GLN:NE2	2.02	0.57
1:A:629:HIS:NE2	1:A:644:ASP:O	2.31	0.57
3:C:89:ILE:HD11	7:C:1252:UQ1:HM33	1.85	0.57
2:F:190:SER:O	2:F:194:HIS:N	2.36	0.57
1:A:379:LEU:O	1:A:380:PRO:C	2.42	0.57
1:A:647:ASN:HD22	1:A:647:ASN:N	1.95	0.57
3:G:247:TRP:CE2	3:G:249:GLY:HA3	2.39	0.57
1:A:183:TRP:HH2	1:A:596:ARG:CD	2.14	0.57
1:E:345:MET:CB	1:E:605:LEU:HD13	2.34	0.57
1:E:632:ALA:C	1:E:635:GLN:NE2	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:19:CYS:HB2	2:F:131:CYS:HB2	1.86	0.57
1:A:81:ARG:HH21	1:A:214:THR:HG22	1.69	0.57
2:B:160:GLU:N	2:B:179:ASN:HD21	1.89	0.57
3:C:145:ASN:ND2	3:C:145:ASN:C	2.55	0.57
1:E:265:ILE:HD11	1:E:349:TYR:HB2	1.86	0.57
1:E:36:GLU:HB3	8:E:2005:HOH:O	2.04	0.57
3:G:46:ARG:HG3	8:G:2014:HOH:O	2.02	0.57
1:A:231:LYS:HB2	1:A:247:HIS:CD2	2.40	0.57
1:A:671:ASN:ND2	1:A:675:VAL:H	2.02	0.57
2:B:139:CYS:SG	4:B:1194:SF4:S3	3.02	0.57
1:E:574:ASP:HA	1:E:577:LYS:HD3	1.85	0.57
1:A:623:TYR:HA	1:A:695:ILE:O	2.04	0.57
7:C:1252:UQ1:C8	7:C:1252:UQ1:CM5	2.78	0.57
1:E:109:GLU:HG2	8:E:2067:HOH:O	1.99	0.57
1:E:100:ILE:HG12	1:E:478:VAL:HG13	1.86	0.57
1:E:519:TRP:CE2	1:E:540:ILE:HG12	2.39	0.57
2:F:35:ASN:HD22	2:F:106:TYR:HE2	1.52	0.57
3:G:206:GLY:CA	3:G:209:TYR:CB	2.82	0.57
2:F:166:ARG:HH22	3:G:248:GLN:NE2	2.01	0.57
1:A:647:ASN:HD21	1:A:714:ALA:H	1.52	0.57
2:B:155:ALA:HB1	8:B:2114:HOH:O	2.04	0.57
1:E:100:ILE:HG12	1:E:478:VAL:CG2	2.33	0.57
3:G:240:LEU:HD12	3:G:240:LEU:C	2.24	0.57
1:A:124:ILE:HD11	1:A:478:VAL:HG11	1.87	0.57
1:A:134:LYS:CE	8:A:2075:HOH:O	2.50	0.57
3:C:50:THR:O	3:C:54:LEU:HG	2.05	0.57
1:E:602:HIS:NE2	1:E:604:PRO:CD	2.56	0.57
1:E:607:VAL:O	1:E:607:VAL:HG13	2.00	0.57
1:E:651:ILE:HD11	1:E:682:VAL:HG13	1.86	0.57
1:A:118:GLU:CD	1:A:118:GLU:H	2.07	0.57
1:A:64:LYS:CE	2:B:26:GLU:HB2	2.34	0.57
1:E:153:VAL:CG1	1:E:167:LYS:HE2	2.35	0.57
2:F:147:ASP:O	2:F:150:SER:HB2	2.04	0.57
3:G:70:ARG:HG2	3:G:71:PHE:N	2.19	0.57
1:A:457:LYS:HD3	8:A:2220:HOH:O	2.05	0.56
3:C:79:LEU:HD21	7:C:1252:UQ1:H71	1.87	0.56
3:G:207:PHE:CD2	3:G:207:PHE:C	2.77	0.56
1:A:483:ALA:CA	1:A:515:THR:CG2	2.81	0.56
1:A:184:VAL:HG22	1:A:592:LEU:HD23	1.73	0.56
3:C:21:HIS:CE1	3:C:64:LEU:CD1	2.88	0.56
1:E:81:ARG:HB2	4:E:1764:SF4:S3	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:601:GLY:HA2	8:E:2332:HOH:O	2.04	0.56
3:G:40:LYS:O	3:G:40:LYS:HG3	2.05	0.56
3:G:70:ARG:CG	3:G:71:PHE:N	2.67	0.56
1:A:427:GLY:C	1:A:428:GLU:O	2.44	0.56
1:A:512:LEU:O	1:A:515:THR:HB	2.04	0.56
1:A:519:TRP:CD2	1:A:540:ILE:HG23	2.39	0.56
1:A:678:GLY:HA3	8:A:2329:HOH:O	2.06	0.56
2:B:129:PRO:HB3	4:B:1195:SF4:S3	2.46	0.56
3:C:207:GLY:C	3:C:209:TRP:N	2.58	0.56
3:C:89:ILE:CD1	7:C:1252:UQ1:HM33	2.35	0.56
1:E:286:PHE:C	1:E:288:GLU:H	2.07	0.56
1:E:323:LYS:CD	1:E:354:LEU:CA	2.69	0.56
1:E:422:GLU:H	1:E:423:PRO:HD2	1.70	0.56
1:E:586:ALA:HB3	8:E:2324:HOH:O	2.04	0.56
1:A:231:LYS:HB2	1:A:247:HIS:CG	2.40	0.56
1:A:585:THR:HG22	1:A:585:THR:O	2.03	0.56
2:B:191:GLU:HG3	8:B:2144:HOH:O	2.05	0.56
1:E:209:HIS:CD2	5:E:1766:MGD:H5'1	2.41	0.56
1:E:247:HIS:CE1	8:E:2146:HOH:O	2.58	0.56
1:A:369:PRO:HG2	1:A:494:LEU:HB3	1.86	0.56
1:A:284:VAL:HB	1:A:589:LYS:HA	1.87	0.56
1:E:275:ASP:N	1:E:323:LYS:HE3	2.20	0.56
1:E:590:ILE:CB	8:E:2178:HOH:O	2.53	0.56
1:A:647:ASN:H	1:A:647:ASN:ND2	1.99	0.56
3:C:172:ALA:HA	3:C:175:PRO:CG	2.33	0.56
3:C:17:THR:HG22	3:C:18:ASN:N	2.21	0.56
1:A:391:PRO:O	1:A:413:ARG:CB	2.54	0.56
2:B:112:TYR:HB3	3:C:73:ARG:NH2	2.20	0.56
2:B:192:VAL:HG12	2:B:193:HIS:H	1.70	0.56
1:E:454:GLU:HG2	8:E:2272:HOH:O	2.05	0.56
1:E:433:LYS:HB3	1:E:460:ASP:HB2	1.87	0.56
1:E:651:ILE:HD12	1:E:684:PRO:HA	1.87	0.56
2:F:57:GLN:HE22	2:F:140:ARG:HH21	1.47	0.56
1:A:183:TRP:HE1	1:A:413:ARG:NH2	1.98	0.56
1:A:277:GLU:HB3	1:A:281:LYS:HZ2	1.71	0.56
1:A:159:ALA:HA	1:A:380:PRO:HD2	1.88	0.56
3:C:108:LEU:HB3	3:C:110:LYS:HG3	1.88	0.56
1:A:103:GLU:OE1	1:A:103:GLU:HA	2.06	0.56
1:A:116:THR:HG23	1:A:118:GLU:N	2.21	0.56
1:A:390:GLY:H	1:A:595:GLN:NE2	1.99	0.56
1:A:555:LEU:O	1:A:559:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:THR:HG21	1:E:627:PRO:O	2.04	0.56
1:A:75:ARG:NH1	1:A:220:GLN:HE21	2.00	0.56
1:E:622:LEU:HD22	8:E:2425:HOH:O	2.05	0.56
1:A:305:THR:CG2	1:A:307:ILE:HB	2.36	0.55
1:A:342:TYR:CD2	1:A:605:LEU:HA	2.41	0.55
3:C:185:LEU:O	3:C:189:LEU:HG	2.06	0.55
1:E:428:GLU:OE1	1:E:428:GLU:HA	2.05	0.55
1:A:195:ILE:N	1:A:195:ILE:HD12	2.20	0.55
1:A:404:ARG:HG3	1:A:406:ASP:OD2	2.07	0.55
1:E:173:CYS:SG	5:E:1765:MGD:S13	3.03	0.55
1:E:305:THR:HG23	1:E:307:ILE:H	1.69	0.55
1:E:315:VAL:HG12	1:E:319:MET:CE	2.37	0.55
1:E:620:ARG:HB3	8:E:2389:HOH:O	2.06	0.55
1:E:671:ASN:ND2	1:E:671:ASN:C	2.58	0.55
1:A:107:ARG:HB2	8:A:2221:HOH:O	2.05	0.55
1:A:124:ILE:O	1:A:128:MET:HG3	2.06	0.55
1:A:519:TRP:CG	1:A:540:ILE:CG2	2.89	0.55
1:A:582:PRO:C	8:A:2093:HOH:O	2.44	0.55
2:B:36:LEU:CD1	8:B:2105:HOH:O	2.54	0.55
3:C:229:TRP:O	3:C:233:LEU:HG	2.06	0.55
1:E:297:THR:HG22	1:E:299:GLU:H	1.70	0.55
2:F:117:THR:HG22	2:F:119:CYS:N	2.21	0.55
2:F:172:ARG:N	2:F:173:PRO:HD3	2.22	0.55
1:E:519:TRP:CZ2	1:E:540:ILE:HG13	2.42	0.55
2:F:27:ASN:HD21	2:F:121:HIS:HE1	1.55	0.55
2:F:67:VAL:CB	2:F:68:PRO:HD3	2.33	0.55
1:A:449:VAL:O	1:A:453:LYS:HG3	2.06	0.55
1:A:467:VAL:CG2	8:A:2226:HOH:O	2.54	0.55
1:E:166:ALA:HB2	1:E:415:THR:CG2	2.36	0.55
1:A:422:GLU:HB3	1:A:423:PRO:CD	2.36	0.55
1:A:254:PRO:HG2	1:A:692:CYS:SG	2.46	0.55
3:C:21:HIS:CE1	3:C:64:LEU:CG	2.90	0.55
1:E:345:MET:HB3	1:E:605:LEU:CD1	2.37	0.55
1:E:327:VAL:HG13	1:E:362:GLY:HA2	1.87	0.55
1:E:412:ALA:HB1	1:E:413:ARG:HH12	1.71	0.55
1:E:97:ARG:NH2	1:E:763:ARG:NH1	2.55	0.55
1:E:97:ARG:HH21	1:E:763:ARG:CZ	2.20	0.55
1:A:575:TRP:O	1:A:580:ARG:HG2	2.07	0.55
3:C:190:TYR:HB3	3:C:191:PRO:HD3	1.89	0.55
1:E:169:SER:O	1:E:174:THR:HB	2.06	0.55
1:E:287:GLU:N	1:E:287:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:ALA:O	1:E:323:LYS:HB2	2.06	0.55
1:A:654:GLU:HG3	8:A:2316:HOH:O	2.06	0.55
3:C:186:LEU:HD22	3:G:149:GLY:HA2	1.89	0.55
1:E:553:LEU:HD21	1:E:557:THR:CG2	2.37	0.55
1:A:113:ARG:NH2	8:A:2063:HOH:O	2.40	0.55
1:A:285:GLY:C	1:A:590:ILE:HG23	2.27	0.55
1:A:79:CYS:CB	1:A:80:PRO:HD2	2.37	0.55
1:E:336:TRP:O	1:E:338:GLY:N	2.40	0.55
1:E:497:HIS:O	1:E:498:LYS:C	2.45	0.55
1:E:672:GLN:H	1:E:672:GLN:NE2	2.05	0.55
3:G:60:LEU:HD23	3:G:63:LEU:HD12	1.88	0.55
1:A:501:PHE:HA	1:A:564:LEU:O	2.07	0.54
1:E:499:THR:HA	1:E:567:ARG:O	2.08	0.54
1:E:677:GLU:O	1:E:678:GLY:O	2.24	0.54
3:G:91:GLY:O	3:G:95:LEU:HD12	2.07	0.54
1:A:429:PRO:C	1:A:430:TYR:CD2	2.79	0.54
1:A:186:GLY:N	1:A:583:PHE:HA	2.23	0.54
1:E:609:THR:HG23	8:E:2336:HOH:O	2.07	0.54
3:G:139:ASN:ND2	8:G:2039:HOH:O	2.40	0.54
1:A:305:THR:CG2	1:A:307:ILE:H	2.18	0.54
1:A:488:ARG:HD3	1:A:490:ASP:OD2	2.07	0.54
1:E:75:ARG:NH1	1:E:220:GLN:HE21	2.00	0.54
1:E:297:THR:HG21	1:E:299:GLU:HG2	1.88	0.54
1:E:158:ALA:HB1	1:E:381:LEU:O	2.06	0.54
2:F:88:LYS:O	3:G:74:THR:CG2	2.54	0.54
1:A:310:GLN:HG3	8:A:2160:HOH:O	2.08	0.54
1:A:596:ARG:O	1:A:600:ALA:N	2.33	0.54
1:A:602:HIS:HE1	1:A:606:PRO:CG	1.99	0.54
2:B:117:THR:CG2	2:B:117:THR:O	2.55	0.54
2:B:55:PRO:HB2	8:B:2105:HOH:O	2.06	0.54
1:E:421:ILE:HD11	1:E:452:THR:HG23	1.90	0.54
1:E:684:PRO:O	1:E:685:THR:C	2.43	0.54
2:F:91:ILE:CD1	7:G:1251:UQ1:O1	2.56	0.54
3:G:205:ALA:HB1	3:G:240:LEU:CD2	2.37	0.54
1:A:48:PHE:HE1	1:A:145:HIS:CE1	2.25	0.54
1:A:530:GLY:HA2	1:A:532:GLU:OE2	2.07	0.54
1:A:341:THR:OG1	1:A:729:SER:HB3	2.07	0.54
1:E:248:ARG:NH1	1:E:318:GLU:OE2	2.41	0.54
1:E:311:VAL:HG23	8:E:2195:HOH:O	2.05	0.54
3:G:100:LEU:HB3	8:G:2030:HOH:O	2.07	0.54
1:A:212:GLU:OE1	1:A:240:SER:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:GLY:HA2	1:A:337:TYR:CE1	2.42	0.54
1:E:53:ILE:HD12	1:E:65:VAL:HG22	1.90	0.54
1:E:492:PHE:HZ	1:E:548:LEU:HG	1.73	0.54
1:E:639:VAL:HG21	2:F:25:MET:HE3	1.89	0.54
2:F:129:PRO:HB3	4:F:1195:SF4:S2	2.48	0.54
1:A:428:GLU:CB	1:A:429:PRO:CD	2.82	0.54
3:C:133:LEU:O	3:C:137:VAL:HG22	2.07	0.54
1:E:536:PRO:O	8:E:2308:HOH:O	2.19	0.54
1:A:194:PRO:O	1:A:363:PHE:HA	2.08	0.54
1:A:533:GLN:HG2	1:A:534:TYR:N	2.22	0.54
2:B:106:TYR:CE1	2:B:114:SER:HB3	2.42	0.54
1:E:250:LEU:HD13	1:E:307:ILE:HG21	1.90	0.54
1:E:606:PRO:CG	1:E:607:VAL:H	2.21	0.54
1:E:708:LEU:HD22	1:E:755:LEU:HB3	1.90	0.54
1:E:627:PRO:CB	2:F:16:CYS:HA	2.38	0.54
2:F:78:THR:CG2	2:F:79:LYS:N	2.71	0.54
1:A:116:THR:HG22	1:A:119:GLU:CB	2.32	0.54
1:A:541:GLU:O	1:A:545:GLU:HG2	2.07	0.54
1:E:424:MET:CE	1:E:455:ALA:HB1	2.38	0.54
1:E:48:PHE:CZ	1:E:145:HIS:CE1	2.96	0.54
1:E:524:GLU:OE1	1:E:528:ARG:NH2	2.41	0.54
3:G:52:ALA:O	3:G:56:ILE:HG13	2.08	0.54
1:A:490:ASP:OD2	1:A:505:ARG:NH1	2.40	0.54
1:A:592:LEU:O	1:A:592:LEU:HD13	2.08	0.54
2:B:190:SER:CB	3:C:252:GLY:N	2.70	0.54
3:C:64:LEU:CD2	7:C:1252:UQ1:C3	2.82	0.54
1:E:39:SER:OG	1:E:56:HIS:ND1	2.31	0.54
1:E:606:PRO:CD	1:E:607:VAL:N	2.70	0.54
2:F:46:TYR:C	2:F:46:TYR:CD1	2.79	0.54
1:A:345:MET:HE1	1:A:605:LEU:CD2	2.37	0.53
1:E:453:LYS:HG2	1:E:475:TRP:CZ2	2.43	0.53
2:F:16:CYS:O	4:F:1194:SF4:S3	2.66	0.53
1:A:115:ALA:HB1	1:A:119:GLU:HG2	1.89	0.53
1:E:227:LYS:HE2	2:F:12:LEU:HD11	1.89	0.53
1:E:345:MET:CB	1:E:605:LEU:CD1	2.86	0.53
1:E:69:GLU:HA	8:E:2038:HOH:O	2.07	0.53
2:F:107:LEU:HD21	3:G:68:PRO:HG2	1.90	0.53
1:A:753:THR:CG2	1:A:757:LYS:HE2	2.38	0.53
3:C:64:LEU:CB	7:C:1252:UQ1:H113	2.32	0.53
1:E:48:PHE:CE1	1:E:145:HIS:CE1	2.96	0.53
2:F:9:ASP:HA	2:F:178:LEU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:PHE:HA	1:A:590:ILE:CG2	2.36	0.53
1:A:596:ARG:NH1	1:A:600:ALA:CB	2.71	0.53
1:E:717:ASN:ND2	5:E:1765:MGD:H192	2.02	0.53
1:E:201:ARG:HD3	8:E:2123:HOH:O	2.08	0.53
1:E:239:PHE:CB	1:E:687:ARG:HB3	2.36	0.53
2:F:190:SER:N	3:G:251:GLY:N	2.56	0.53
1:A:288:GLU:HB3	1:A:591:GLU:CG	2.19	0.53
1:A:37:VAL:CG1	1:A:38:LYS:N	2.70	0.53
1:A:689:ARG:NE	1:A:691:ASP:OD2	2.40	0.53
2:B:46:TYR:CD2	8:B:2035:HOH:O	2.61	0.53
2:B:47:PRO:CG	8:B:2036:HOH:O	2.57	0.53
1:E:346:ALA:N	1:E:605:LEU:CD1	2.70	0.53
1:E:724:LYS:CG	8:E:2423:HOH:O	2.56	0.53
2:B:168:GLU:C	2:B:169:GLN:O	2.44	0.53
3:G:206:GLY:CA	3:G:209:TYR:HB3	2.38	0.53
1:A:193:GLU:CG	8:A:2118:HOH:O	2.55	0.53
1:A:682:VAL:HG12	1:A:684:PRO:HD3	1.90	0.53
3:C:155:THR:CG2	3:C:239:ARG:CG	2.86	0.53
1:E:575:TRP:HB3	1:E:580:ARG:O	2.08	0.53
1:E:388:CYS:CB	1:E:593:TYR:OH	2.26	0.53
2:F:35:ASN:ND2	2:F:106:TYR:CE2	2.75	0.53
1:A:276:LYS:CA	8:A:2148:HOH:O	2.42	0.53
1:E:225:ALA:O	1:E:230:ALA:HB3	2.09	0.53
1:E:539:THR:CG2	1:E:541:GLU:HG2	2.38	0.53
1:E:592:LEU:HA	1:E:603:GLN:HE22	1.55	0.53
2:F:122:ARG:HG2	2:F:127:LYS:HE3	1.91	0.53
1:A:158:ALA:HB1	1:A:381:LEU:O	2.09	0.53
1:A:589:LYS:O	1:A:592:LEU:CA	2.57	0.53
1:A:96:LYS:HB3	1:A:513:PHE:CB	2.38	0.53
1:E:638:TRP:O	1:E:642:GLU:HB2	2.09	0.53
1:A:43:ILE:HB	1:A:505:ARG:HH21	1.74	0.53
2:B:117:THR:O	2:B:117:THR:HG23	2.09	0.53
2:B:5:ALA:HB3	2:B:145:LEU:HD13	1.91	0.53
1:E:272:ASP:OD2	1:E:276:LYS:NZ	2.20	0.53
3:G:208:TRP:HE3	3:G:208:TRP:HA	1.74	0.53
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.91	0.52
1:A:209:HIS:HD2	5:A:1766:MGD:O2A	1.91	0.52
1:A:285:GLY:C	1:A:590:ILE:CG2	2.78	0.52
1:A:335:VAL:HG13	1:A:733:GLY:CA	2.38	0.52
1:A:482:GLU:HG2	1:A:483:ALA:H	1.75	0.52
1:A:647:ASN:C	1:A:648:GLU:CG	2.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:GLU:HB3	8:E:2239:HOH:O	2.09	0.52
1:E:428:GLU:O	1:E:430:TYR:CA	2.57	0.52
1:E:591:GLU:CD	1:E:604:PRO:CB	2.60	0.52
1:E:622:LEU:HB2	1:E:693:VAL:O	2.09	0.52
1:E:669:LEU:HD23	1:E:741:LEU:HD22	1.90	0.52
1:A:295:ASP:O	1:A:297:THR:HG22	2.09	0.52
1:A:651:ILE:HG23	1:A:693:VAL:HG23	1.90	0.52
1:E:112:TYR:CZ	1:E:474:MET:O	2.61	0.52
1:E:112:TYR:OH	1:E:476:ALA:O	2.27	0.52
1:E:632:ALA:C	1:E:635:GLN:HE22	2.13	0.52
3:G:17:ASN:O	3:G:21:PHE:HD1	1.91	0.52
1:A:241:THR:HG21	2:B:14:VAL:HB	1.91	0.52
1:A:605:LEU:N	1:A:606:PRO:CD	2.70	0.52
2:B:50:VAL:HG13	2:B:181:PRO:HB2	1.90	0.52
2:B:71:PRO:HB2	3:C:79:LEU:CD1	2.39	0.52
1:E:397:GLU:CB	1:E:398:PRO:CD	2.80	0.52
1:E:484:THR:HB	1:E:487:GLU:OE1	2.09	0.52
1:E:283:THR:HG23	1:E:590:ILE:HG13	1.92	0.52
1:E:88:THR:CG2	1:E:467:VAL:HG11	2.39	0.52
2:F:55:PRO:CG	4:F:1194:SF4:S2	2.96	0.52
1:A:85:ALA:HA	8:A:2041:HOH:O	2.09	0.52
1:E:160:TRP:O	1:E:160:TRP:CG	2.63	0.52
2:F:16:CYS:O	2:F:16:CYS:SG	2.67	0.52
2:F:67:VAL:HB	2:F:68:PRO:CD	2.37	0.52
1:A:73:LYS:HZ3	1:A:192:HIS:CD2	2.27	0.52
1:A:116:THR:HG23	1:A:118:GLU:H	1.73	0.52
1:A:370:TYR:CD2	1:A:551:LEU:HD21	2.45	0.52
1:A:81:ARG:HH21	1:A:214:THR:CG2	2.23	0.52
2:B:132:VAL:HA	2:B:140:ARG:HG3	1.92	0.52
1:E:204:VAL:HG21	1:E:319:MET:CE	2.39	0.52
1:E:469:PRO:O	1:E:706:MET:CG	2.55	0.52
1:E:95:LEU:CD2	8:E:2276:HOH:O	2.50	0.52
2:F:125:LYS:HE2	8:F:2078:HOH:O	2.10	0.52
2:F:44:GLY:HA3	8:F:2024:HOH:O	2.09	0.52
3:G:195:PRO:HD2	3:G:196:GLU:OE2	2.09	0.52
1:A:591:GLU:O	1:A:592:LEU:CD1	2.53	0.52
2:B:88:LYS:O	3:C:75:THR:CG2	2.57	0.52
1:E:116:THR:HG22	1:E:119:GLU:N	2.19	0.52
1:E:149:ASP:CB	8:E:2092:HOH:O	2.57	0.52
1:E:305:THR:HG23	1:E:307:ILE:CG1	2.40	0.52
1:E:324:PRO:HD2	8:E:2210:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ILE:HD12	1:E:65:VAL:CG2	2.39	0.52
1:E:492:PHE:CZ	1:E:548:LEU:HG	2.45	0.52
3:G:144:ASN:C	3:G:144:ASN:HD22	2.12	0.52
1:A:345:MET:HE1	1:A:605:LEU:HD22	1.91	0.52
1:A:655:GLU:CD	1:A:658:ARG:HH22	2.13	0.52
1:A:702:LYS:HG3	8:A:2229:HOH:O	2.09	0.52
1:A:676:LYS:NZ	1:A:742:GLU:OE1	2.42	0.52
2:B:3:ARG:HD2	2:B:62:GLU:OE2	2.09	0.52
3:C:155:THR:HG22	3:C:239:ARG:NE	2.08	0.52
1:A:132:ARG:CD	8:A:2073:HOH:O	2.56	0.52
1:A:430:TYR:HB2	1:A:431:PRO:HD3	1.92	0.52
2:B:164:VAL:HG22	2:B:173:PRO:HB2	1.91	0.52
3:C:12:GLU:OE1	3:C:15:HIS:ND1	2.39	0.52
1:E:497:HIS:HB3	1:E:499:THR:O	2.10	0.52
3:G:44:GLU:OE1	3:G:47:ARG:NH1	2.42	0.52
1:A:583:PHE:CZ	1:A:587:SER:CA	2.93	0.52
1:A:587:SER:O	1:A:589:LYS:HE2	2.09	0.52
1:E:101:ARG:HB2	1:E:477:ASP:HA	1.92	0.52
1:E:494:LEU:HD23	1:E:502:ILE:HG23	1.91	0.52
1:E:495:VAL:HG21	8:E:2296:HOH:O	2.08	0.52
1:E:391:PRO:HD2	1:E:595:GLN:OE1	2.10	0.52
1:E:71:ASN:HD21	1:E:73:LYS:HB2	1.75	0.52
1:A:43:ILE:HB	1:A:505:ARG:NH2	2.25	0.51
1:E:142:PHE:CD1	1:E:157:PRO:HB3	2.45	0.51
1:E:447:PRO:HB3	8:E:2418:HOH:O	2.09	0.51
3:G:148:ALA:HA	8:G:2045:HOH:O	2.10	0.51
3:G:205:ALA:HB1	3:G:240:LEU:HD22	1.91	0.51
1:A:386:GLY:HA3	1:A:391:PRO:HB2	1.90	0.51
2:B:72:THR:CG2	2:B:73:GLY:N	2.73	0.51
3:C:222:TRP:CD1	3:C:223:GLN:N	2.78	0.51
1:E:149:ASP:HA	8:E:2092:HOH:O	2.10	0.51
1:E:504:LEU:HD22	1:E:505:ARG:N	2.26	0.51
8:E:2132:HOH:O	2:F:138:TYR:CD1	2.54	0.51
2:F:63:ASN:HB2	8:F:2110:HOH:O	2.09	0.51
3:G:20:HIS:CE1	3:G:59:ASP:OD1	2.64	0.51
1:A:258:THR:HB	1:A:608:PHE:HA	1.92	0.51
1:E:548:LEU:CD1	1:E:555:LEU:HA	2.40	0.51
1:E:730:GLY:HA3	8:E:2250:HOH:O	2.10	0.51
3:G:39:LEU:HD13	3:G:116:ALA:CB	2.40	0.51
3:G:42:ASP:OD1	3:G:44:GLU:HG3	2.10	0.51
1:E:197:TRP:CB	1:E:221:ASP:HB3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:488:ARG:HG3	8:E:2287:HOH:O	2.09	0.51
1:E:620:ARG:HA	1:E:738:PHE:HD2	1.75	0.51
2:F:164:VAL:CG2	2:F:173:PRO:HB2	2.40	0.51
3:G:20:HIS:HE1	3:G:59:ASP:OD1	1.92	0.51
1:A:43:ILE:CG1	1:A:505:ARG:HB3	2.10	0.51
1:A:592:LEU:HD13	1:A:592:LEU:C	2.30	0.51
1:A:680:VAL:HG22	1:A:714:ALA:HB2	1.92	0.51
1:A:635:GLN:C	1:A:709:ALA:HB2	2.30	0.51
3:C:145:ASN:OD1	3:C:193:THR:CG2	2.57	0.51
1:E:683:LYS:HE2	1:E:685:THR:HB	1.90	0.51
1:E:650:TRP:HB2	1:E:694:TYR:HB3	1.92	0.51
1:A:284:VAL:HG12	1:A:285:GLY:N	2.25	0.51
1:A:499:THR:HB	1:A:565:VAL:CG1	2.40	0.51
1:A:65:VAL:HG13	1:A:78:LEU:HD21	1.92	0.51
2:B:64:PRO:HB3	4:B:1196:SF4:S3	2.51	0.51
3:C:143:LEU:CD2	3:C:198:ALA:HB1	2.41	0.51
1:E:342:TYR:CD1	1:E:607:VAL:CB	2.77	0.51
1:E:397:GLU:CB	8:E:2239:HOH:O	2.58	0.51
1:E:636:ASN:HA	1:E:708:LEU:HB2	1.91	0.51
1:E:648:GLU:CG	1:E:681:ARG:NH1	2.71	0.51
1:E:91:ASP:C	1:E:92:PRO:O	2.49	0.51
3:G:222:GLN:CA	3:G:222:GLN:OE1	2.54	0.51
1:E:308:PRO:CB	8:E:2195:HOH:O	2.46	0.51
1:E:591:GLU:O	1:E:591:GLU:CG	2.57	0.51
3:G:107:LEU:C	3:G:109:LYS:H	2.13	0.51
3:G:222:GLN:C	8:G:2068:HOH:O	2.47	0.51
1:A:72:PRO:HG2	1:A:501:PHE:CD2	2.45	0.51
2:B:117:THR:HG23	2:B:120:ALA:H	1.74	0.51
1:E:166:ALA:HB2	1:E:415:THR:HG21	1.93	0.51
1:E:100:ILE:CG1	1:E:478:VAL:HG22	2.38	0.51
1:E:369:PRO:HG2	1:E:494:LEU:HB3	1.93	0.51
1:A:193:GLU:HB2	1:A:195:ILE:CD1	2.41	0.51
1:A:418:GLN:NE2	1:A:730:GLY:O	2.43	0.51
1:A:462:TYR:OH	1:A:472:HIS:O	2.22	0.51
2:B:166:ARG:HG2	8:B:2145:HOH:O	2.11	0.51
1:E:93:ASP:CG	1:E:758:ARG:HH22	2.14	0.51
1:A:42:GLN:NE2	1:A:505:ARG:CD	2.66	0.51
1:A:488:ARG:CD	1:A:490:ASP:OD2	2.59	0.51
1:A:548:LEU:C	1:A:553:LEU:O	2.50	0.51
1:A:345:MET:CE	1:A:605:LEU:HD22	2.41	0.51
1:A:607:VAL:CG1	1:A:607:VAL:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:LEU:HD22	4:F:1195:SF4:S4	2.51	0.51
1:A:279:VAL:HA	1:A:283:THR:HB	1.94	0.50
1:A:423:PRO:HB2	1:A:432:ILE:HD12	1.92	0.50
2:B:41:ARG:CD	2:B:187:THR:HG23	2.39	0.50
8:B:2025:HOH:O	3:C:251:LEU:HD11	2.11	0.50
1:E:553:LEU:CD2	1:E:557:THR:CG2	2.89	0.50
1:E:625:ARG:HD2	5:E:1766:MGD:C17	2.41	0.50
1:E:671:ASN:ND2	1:E:673:ASP:N	2.59	0.50
1:E:746:ARG:CG	1:E:746:ARG:HH11	2.22	0.50
1:A:81:ARG:NE	1:A:214:THR:HG22	2.25	0.50
1:A:337:TYR:O	1:A:340:ASP:CG	2.41	0.50
1:A:494:LEU:HD22	1:A:502:ILE:HG12	1.91	0.50
1:A:666:TYR:CZ	1:A:681:ARG:HG3	2.46	0.50
1:A:336:TRP:HA	1:A:735:ARG:HG3	1.93	0.50
3:C:228:PRO:O	3:C:232:LEU:HD12	2.12	0.50
1:E:119:GLU:HG2	8:E:2075:HOH:O	2.11	0.50
1:E:302:GLU:HG2	1:E:302:GLU:O	2.11	0.50
1:E:60:ASN:ND2	8:E:2022:HOH:O	2.43	0.50
8:E:2132:HOH:O	2:F:138:TYR:CE1	2.64	0.50
1:A:252:ILE:HG13	1:A:307:ILE:HD11	1.92	0.50
1:A:548:LEU:O	1:A:553:LEU:O	2.29	0.50
1:A:581:LEU:HD23	1:A:583:PHE:HE1	1.76	0.50
1:A:90:TYR:OH	1:A:509:HIS:HE1	1.94	0.50
1:E:233:VAL:HG13	1:E:248:ARG:HB2	1.93	0.50
1:E:39:SER:HG	1:E:56:HIS:HD1	1.57	0.50
3:G:206:GLY:CA	3:G:209:TYR:HB2	2.42	0.50
1:E:204:VAL:HG21	1:E:319:MET:HE1	1.93	0.50
1:E:591:GLU:OE2	1:E:604:PRO:CG	2.58	0.50
1:E:685:THR:HG22	2:F:42:GLU:OE2	2.11	0.50
1:A:561:MET:O	1:A:563:THR:O	2.29	0.50
1:E:113:ARG:HB3	8:E:2042:HOH:O	2.12	0.50
1:E:123:HIS:CE1	8:E:2080:HOH:O	2.65	0.50
1:E:247:HIS:N	1:E:247:HIS:CD2	2.78	0.50
1:E:435:LEU:HB3	1:E:459:LEU:CD1	2.42	0.50
3:G:208:TRP:O	3:G:212:PHE:CD2	2.64	0.50
1:A:339:ASP:HB3	1:A:607:VAL:CG1	2.38	0.50
1:A:65:VAL:CG1	1:A:78:LEU:HD21	2.42	0.50
3:C:150:GLY:HA2	3:G:185:LEU:HD22	1.93	0.50
1:E:256:THR:HG23	8:E:2193:HOH:O	2.11	0.50
1:E:591:GLU:OE2	1:E:604:PRO:HB3	2.09	0.50
1:E:620:ARG:CG	1:E:620:ARG:O	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:O	1:A:133:GLU:HG2	2.12	0.50
1:A:435:LEU:O	1:A:462:TYR:HA	2.12	0.50
1:A:596:ARG:CZ	1:A:600:ALA:HB1	2.42	0.50
1:A:647:ASN:ND2	1:A:713:GLY:HA3	2.26	0.50
1:E:634:THR:H	1:E:635:GLN:NE2	2.09	0.50
2:F:166:ARG:HD2	8:F:2105:HOH:O	2.11	0.50
3:G:65:ALA:O	3:G:70:ARG:NH1	2.45	0.50
1:A:628:VAL:HG13	1:A:640:LEU:HD22	1.94	0.50
1:E:370:TYR:OH	1:E:372:GLU:HG3	2.11	0.50
1:E:462:TYR:CE1	1:E:463:VAL:O	2.65	0.50
1:E:79:CYS:CB	1:E:80:PRO:HD2	2.42	0.50
2:F:117:THR:O	2:F:117:THR:HG23	2.10	0.50
1:A:174:THR:HG23	1:A:178:GLU:CG	2.39	0.50
1:A:422:GLU:N	1:A:423:PRO:HD2	2.27	0.50
1:A:77:ARG:NH2	8:A:2039:HOH:O	2.33	0.50
1:E:391:PRO:HD3	1:E:595:GLN:CD	2.32	0.50
2:F:106:TYR:CE1	2:F:114:SER:HB3	2.47	0.50
1:A:66:GLU:HG3	8:A:2038:HOH:O	2.12	0.49
1:E:625:ARG:HH22	5:E:1765:MGD:H15	1.59	0.49
1:E:100:ILE:CG2	1:E:478:VAL:HG22	2.40	0.49
1:E:501:PHE:HB3	1:E:565:VAL:HG13	1.92	0.49
1:E:390:GLY:H	1:E:391:PRO:HD3	1.77	0.49
1:E:371:LEU:HD12	1:E:494:LEU:HD21	1.94	0.49
1:E:630:THR:H	1:E:634:THR:HG21	1.76	0.49
1:E:753:THR:HG22	1:E:757:LYS:HE3	1.93	0.49
2:F:160:GLU:N	2:F:179:ASN:HD21	1.94	0.49
3:G:92:ALA:CB	7:G:1251:UQ1:H8	2.42	0.49
1:A:430:TYR:HB2	1:A:431:PRO:CD	2.42	0.49
1:A:95:LEU:N	1:A:467:VAL:O	2.36	0.49
1:A:626:SER:HB2	1:A:696:VAL:HG11	1.94	0.49
2:B:57:GLN:CD	8:B:2046:HOH:O	2.51	0.49
3:C:161:LEU:CD1	3:C:179:LEU:HD12	2.42	0.49
1:E:626:SER:HB3	1:E:696:VAL:HG11	1.94	0.49
1:A:81:ARG:NH2	1:A:214:THR:HG22	2.26	0.49
1:A:393:GLY:HA3	1:A:407:LYS:HZ1	1.72	0.49
1:A:534:TYR:O	1:A:535:PHE:CB	2.61	0.49
2:B:159:ALA:O	2:F:183:LYS:CE	2.53	0.49
2:B:166:ARG:HH22	3:C:249:GLN:HE21	1.59	0.49
3:C:25:VAL:HG23	3:C:96:LEU:HD21	1.95	0.49
1:A:256:THR:O	1:A:256:THR:HG23	2.11	0.49
1:E:252:ILE:CG1	1:E:256:THR:HG22	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:206:GLY:O	3:G:209:TYR:CB	2.61	0.49
1:A:371:LEU:HD23	1:A:551:LEU:CD1	2.43	0.49
1:A:166:ALA:CB	1:A:415:THR:CG2	2.90	0.49
3:C:207:GLY:HA2	3:C:210:TYR:CB	2.42	0.49
3:C:222:TRP:CD1	3:C:222:TRP:C	2.85	0.49
2:F:166:ARG:NH2	3:G:248:GLN:HG3	2.27	0.49
1:A:122:ASP:HB2	8:A:2068:HOH:O	2.11	0.49
1:A:207:GLY:O	5:A:1766:MGD:PB	2.71	0.49
1:A:253:LYS:O	1:A:256:THR:HB	2.13	0.49
1:A:433:LYS:HD3	1:A:460:ASP:OD2	2.13	0.49
1:A:489:TYR:CD1	1:A:540:ILE:HD13	2.47	0.49
2:B:52:GLU:OE2	2:B:187:THR:HB	2.13	0.49
2:B:61:CYS:HB2	4:B:1196:SF4:S3	2.53	0.49
1:E:576:GLU:C	1:E:578:GLU:H	2.16	0.49
1:E:591:GLU:O	1:E:603:GLN:HG2	2.11	0.49
1:E:647:ASN:ND2	1:E:647:ASN:N	2.61	0.49
3:G:170:TRP:CE3	3:G:171:ALA:N	2.80	0.49
1:A:338:GLY:HA3	1:A:724:LYS:HG2	1.93	0.49
1:A:405:ALA:HB2	1:A:430:TYR:CZ	2.48	0.49
1:A:121:LEU:HD22	1:A:525:LEU:HG	1.94	0.49
1:A:349:TYR:OH	1:A:592:LEU:HG	2.12	0.49
1:A:253:LYS:NZ	1:A:613:GLU:OE2	2.34	0.49
1:E:614:PRO:HB3	1:E:738:PHE:CD2	2.47	0.49
1:A:73:LYS:HZ1	1:A:192:HIS:HD2	1.59	0.49
1:A:267:VAL:O	1:A:271:GLU:HB2	2.12	0.49
1:A:588:GLY:HA3	8:A:2152:HOH:O	2.13	0.49
1:E:117:TRP:CE2	1:E:516:LYS:HG3	2.48	0.49
1:E:630:THR:HA	5:E:1766:MGD:C17	2.42	0.49
1:E:186:GLY:HA3	1:E:583:PHE:C	2.33	0.49
1:E:297:THR:HG22	1:E:299:GLU:N	2.27	0.49
2:F:23:CYS:SG	2:F:35:ASN:HB2	2.52	0.49
1:A:434:GLY:CA	1:A:461:LEU:O	2.50	0.49
1:A:761:ASP:C	1:A:763:ARG:H	2.16	0.49
3:C:227:ALA:HB3	3:C:228:PRO:HD3	1.95	0.49
1:E:292:HIS:HD2	8:E:2084:HOH:O	1.94	0.49
1:A:138:GLU:CD	1:A:402:LYS:HB2	2.33	0.48
1:A:483:ALA:HB2	1:A:515:THR:CG2	2.43	0.48
2:B:190:SER:CA	3:C:252:GLY:N	2.76	0.48
1:E:369:PRO:CG	1:E:494:LEU:HB3	2.43	0.48
1:E:138:GLU:CD	1:E:402:LYS:HB2	2.33	0.48
1:E:708:LEU:HD22	8:E:2406:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:PRO:HD3	2:F:18:ALA:HB2	1.95	0.48
1:E:90:TYR:OH	1:E:509:HIS:CE1	2.62	0.48
2:F:146:GLU:O	2:F:148:PRO:HD3	2.13	0.48
3:C:13:PHE:CZ	3:C:247:GLN:HG2	2.48	0.48
1:E:293:VAL:HG13	1:E:293:VAL:O	2.12	0.48
1:E:314:GLU:HG3	8:E:2199:HOH:O	2.12	0.48
1:E:423:PRO:HB2	1:E:432:ILE:HG13	1.94	0.48
1:E:672:GLN:HE22	1:E:738:PHE:H	1.62	0.48
2:F:117:THR:CG2	2:F:119:CYS:N	2.75	0.48
3:G:32:LEU:HD12	3:G:120:LEU:HD12	1.95	0.48
3:G:73:PHE:HA	8:G:2021:HOH:O	2.13	0.48
1:A:170:VAL:HG12	1:A:171:SER:N	2.28	0.48
1:A:184:VAL:HG22	1:A:592:LEU:CB	2.43	0.48
1:A:389:SER:CA	1:A:595:GLN:HE22	2.27	0.48
1:A:618:PHE:CZ	1:A:740:ARG:HD3	2.48	0.48
1:A:88:THR:HG23	1:A:468:LEU:HD21	1.95	0.48
2:B:150:SER:O	2:B:154:LYS:HG2	2.14	0.48
2:B:39:ARG:HD2	2:B:56:GLU:OE2	2.14	0.48
3:C:143:LEU:HD23	3:C:198:ALA:HB1	1.96	0.48
1:E:53:ILE:HG22	1:E:78:LEU:HD11	1.95	0.48
3:G:134:LEU:HG	8:G:2034:HOH:O	2.13	0.48
1:A:113:ARG:NE	8:A:2063:HOH:O	2.47	0.48
1:A:506:THR:CG2	8:A:2244:HOH:O	2.61	0.48
1:A:753:THR:HG22	1:A:757:LYS:HE2	1.94	0.48
3:C:71:ARG:HG2	3:C:72:PHE:N	2.28	0.48
1:E:172:LEU:HB3	5:E:1765:MGD:H23	1.95	0.48
1:E:468:LEU:HB3	1:E:469:PRO:HD2	1.94	0.48
1:E:186:GLY:HA3	1:E:584:GLY:CA	2.43	0.48
1:A:355:GLY:O	1:A:359:ARG:HG3	2.13	0.48
1:A:573:GLU:O	1:A:577:LYS:HG3	2.13	0.48
1:E:107:ARG:O	1:E:108:GLY:C	2.52	0.48
1:A:586:ALA:O	1:A:587:SER:CB	2.61	0.48
3:C:173:LEU:CG	3:C:173:LEU:O	2.58	0.48
3:C:174:PHE:N	3:C:175:PRO:HD2	2.29	0.48
1:A:483:ALA:CB	1:A:515:THR:CG2	2.92	0.48
2:B:57:GLN:O	2:B:59:LEU:HD23	2.14	0.48
1:E:596:ARG:CZ	1:E:601:GLY:HA3	2.44	0.48
1:E:669:LEU:HD21	1:E:741:LEU:HD22	1.93	0.48
1:A:449:VAL:CG1	1:A:453:LYS:HE3	2.44	0.48
1:A:629:HIS:ND1	1:A:634:THR:CG2	2.66	0.48
1:A:667:VAL:HG11	1:A:741:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:ASP:O	1:E:344:VAL:HG23	2.13	0.48
1:E:195:ILE:CD1	1:E:363:PHE:CE2	2.97	0.48
1:E:589:LYS:CB	1:E:592:LEU:HB2	2.40	0.48
2:F:72:THR:CG2	2:F:89:LYS:HB3	2.39	0.48
1:A:388:CYS:HA	1:A:593:TYR:HE1	1.74	0.48
1:E:174:THR:HG23	1:E:178:GLU:CG	2.41	0.48
1:E:422:GLU:HG3	8:E:2104:HOH:O	2.12	0.48
1:E:494:LEU:CD2	1:E:502:ILE:HG23	2.44	0.48
2:F:99:ALA:HB2	3:G:137:ASN:ND2	2.28	0.48
3:G:165:LEU:C	3:G:167:LYS:H	2.17	0.48
1:A:232:VAL:N	1:A:247:HIS:CD2	2.76	0.48
1:A:248:ARG:HB3	8:A:2133:HOH:O	2.13	0.48
1:A:263:ALA:O	1:A:267:VAL:HG23	2.14	0.48
1:A:712:ARG:NH2	8:A:2347:HOH:O	2.46	0.48
3:C:208:PHE:CD2	3:C:208:PHE:C	2.86	0.48
1:E:30:ALA:N	1:E:31:PRO:CD	2.77	0.48
1:E:595:GLN:HG3	1:E:595:GLN:O	2.10	0.48
1:A:249:TRP:O	1:A:251:PRO:HD3	2.14	0.47
3:C:63:ILE:O	3:C:67:GLU:HB3	2.13	0.47
1:E:500:PRO:O	1:E:566:GLN:N	2.33	0.47
1:E:540:ILE:O	1:E:544:LEU:HG	2.14	0.47
1:E:630:THR:HA	5:E:1766:MGD:N18	2.29	0.47
1:E:636:ASN:HB2	1:E:706:MET:HE3	1.95	0.47
3:G:38:HIS:O	3:G:41:GLY:N	2.25	0.47
1:A:156:LEU:HB3	1:A:157:PRO:HD3	1.96	0.47
1:A:277:GLU:HB3	1:A:281:LYS:NZ	2.28	0.47
1:A:319:MET:CE	1:A:328:LEU:CD1	2.92	0.47
1:A:393:GLY:CA	1:A:407:LYS:HE3	2.39	0.47
1:A:488:ARG:HG2	1:A:489:TYR:O	2.14	0.47
1:A:184:VAL:HG22	1:A:592:LEU:CG	2.43	0.47
1:A:743:LYS:HG3	8:A:2365:HOH:O	2.14	0.47
2:B:117:THR:HG22	2:B:119:CYS:CA	2.43	0.47
1:E:159:ALA:HA	1:E:380:PRO:HD2	1.96	0.47
1:E:208:HIS:HE1	1:E:218:GLN:HE22	1.62	0.47
1:E:325:ARG:NH1	8:E:2211:HOH:O	2.28	0.47
1:E:622:LEU:HD22	5:E:1766:MGD:C8	2.43	0.47
1:E:734:LEU:CD2	8:E:2418:HOH:O	2.56	0.47
1:E:77:ARG:NH1	2:F:135:CYS:O	2.47	0.47
3:G:207:PHE:HB3	3:G:208:TRP:H	1.37	0.47
2:F:166:ARG:NH2	3:G:248:GLN:NE2	2.61	0.47
3:G:47:ARG:HH21	3:G:166:LEU:HB3	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LYS:HD2	8:A:2221:HOH:O	2.14	0.47
1:A:686:ALA:O	1:A:687:ARG:HG2	2.14	0.47
1:A:71:ASN:ND2	1:A:73:LYS:HB2	2.29	0.47
1:E:285:GLY:HA3	1:E:592:LEU:HD11	1.96	0.47
1:E:426:THR:C	1:E:428:GLU:N	2.67	0.47
1:E:634:THR:H	1:E:635:GLN:HE22	1.62	0.47
1:E:650:TRP:O	1:E:693:VAL:HG22	2.14	0.47
1:A:578:GLU:HB3	1:A:580:ARG:CD	2.42	0.47
1:A:87:GLN:HG3	1:A:637:ASN:CG	2.35	0.47
1:A:647:ASN:HD21	1:A:713:GLY:CA	2.27	0.47
1:A:69:GLU:C	8:A:2032:HOH:O	2.37	0.47
1:A:722:ARG:NE	8:A:2356:HOH:O	2.48	0.47
2:B:36:LEU:HD12	2:B:37:TRP:N	2.30	0.47
2:B:71:PRO:HB2	3:C:79:LEU:HD11	1.95	0.47
1:E:288:GLU:HG3	8:E:2183:HOH:O	2.14	0.47
1:E:339:ASP:CB	1:E:607:VAL:CG1	2.85	0.47
1:A:318:GLU:O	1:A:322:HIS:HD2	1.97	0.47
2:B:192:VAL:CG1	2:B:193:HIS:N	2.77	0.47
1:E:384:ALA:HB1	8:E:2237:HOH:O	2.15	0.47
1:E:502:ILE:O	1:E:563:THR:HA	2.13	0.47
1:A:183:TRP:CH2	1:A:596:ARG:CD	2.85	0.47
1:A:42:GLN:OE1	1:A:506:THR:N	2.47	0.47
1:A:628:VAL:HG11	1:A:643:MET:HB2	1.96	0.47
1:A:651:ILE:HG23	1:A:693:VAL:CG2	2.44	0.47
2:B:161:ARG:HG2	2:B:179:ASN:HA	1.94	0.47
1:E:177:ARG:HA	1:E:344:VAL:HG11	1.96	0.47
1:E:238:ARG:NH2	1:E:240:SER:HB2	2.29	0.47
1:E:289:LEU:HD12	1:E:590:ILE:HG21	1.95	0.47
1:E:583:PHE:CD2	1:E:583:PHE:N	2.75	0.47
3:G:206:GLY:H	3:G:209:TYR:HB2	1.79	0.47
3:G:47:ARG:O	3:G:50:LEU:O	2.31	0.47
1:A:193:GLU:OE2	1:A:332:ARG:NH1	2.47	0.47
1:A:509:HIS:HD2	1:A:510:GLU:O	1.97	0.47
1:E:201:ARG:CD	8:E:2123:HOH:O	2.62	0.47
1:E:302:GLU:HG3	1:E:307:ILE:O	2.14	0.47
1:E:670:VAL:HB	1:E:740:ARG:HG3	1.96	0.47
2:F:174:LYS:HE2	8:F:2046:HOH:O	2.14	0.47
2:F:6:MET:HG2	2:F:175:LEU:HD22	1.97	0.47
3:G:112:GLN:N	8:G:2032:HOH:O	2.47	0.47
3:G:206:GLY:HA2	3:G:209:TYR:HB2	1.95	0.47
3:G:86:SER:O	3:G:87:PRO:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:53:LEU:O	3:G:99:PHE:HE1	1.97	0.47
1:A:548:LEU:HD22	1:A:553:LEU:HD12	1.97	0.47
1:A:587:SER:O	1:A:589:LYS:CE	2.62	0.47
1:A:615:PRO:O	1:A:618:PHE:HB2	2.15	0.47
1:A:630:THR:H	1:A:634:THR:CG2	2.26	0.47
2:B:157:LYS:HD3	8:F:2038:HOH:O	2.15	0.47
1:E:500:PRO:HD3	1:E:567:ARG:O	2.14	0.47
1:E:602:HIS:CE1	1:E:606:PRO:CG	2.58	0.47
1:E:48:PHE:CE1	1:E:631:PHE:CE1	3.03	0.47
1:E:649:VAL:HG13	1:E:695:ILE:HG23	1.95	0.47
1:E:669:LEU:CD2	1:E:741:LEU:CD2	2.91	0.47
1:E:648:GLU:CG	1:E:681:ARG:HH12	2.16	0.47
2:F:72:THR:HG21	2:F:89:LYS:C	2.34	0.47
3:G:247:TRP:CZ2	3:G:249:GLY:HA3	2.49	0.47
3:G:26:LEU:HG	3:G:158:LEU:HB3	1.97	0.47
1:A:132:ARG:O	1:A:132:ARG:HG2	2.14	0.47
1:A:686:ALA:CB	8:A:2331:HOH:O	2.49	0.47
3:C:201:HIS:CE1	3:C:205:GLU:HG3	2.50	0.47
1:A:422:GLU:N	1:A:423:PRO:CD	2.78	0.47
1:A:653:LYS:HD3	8:B:2026:HOH:O	2.15	0.47
1:E:95:LEU:CD1	8:E:2276:HOH:O	2.53	0.47
3:G:240:LEU:CD1	3:G:240:LEU:C	2.83	0.47
3:G:20:HIS:CE1	3:G:59:ASP:OD2	2.67	0.47
8:F:2075:HOH:O	3:G:72:ARG:HD3	2.15	0.47
1:E:322:HIS:O	1:E:323:LYS:C	2.53	0.47
1:E:523:ARG:HG2	1:E:523:ARG:HH11	1.80	0.47
1:E:680:VAL:HG22	1:E:714:ALA:HB2	1.97	0.47
2:F:87:PRO:HB3	2:F:112:TYR:CD1	2.50	0.47
1:A:647:ASN:HD21	1:A:713:GLY:HA3	1.80	0.46
3:C:76:HIS:O	3:C:79:LEU:HB2	2.15	0.46
1:E:196:ASP:OD1	1:E:360:PRO:HA	2.14	0.46
1:E:462:TYR:CD2	1:E:476:ALA:HA	2.50	0.46
3:G:142:LEU:HD21	3:G:197:ALA:O	2.14	0.46
1:A:263:ALA:HB2	1:A:301:ALA:HB2	1.96	0.46
1:A:358:GLY:N	1:A:363:PHE:O	2.46	0.46
1:A:717:ASN:HA	1:A:720:GLN:OE1	2.15	0.46
3:C:128:LEU:HA	8:C:2049:HOH:O	2.15	0.46
1:E:606:PRO:HG2	1:E:607:VAL:H	1.79	0.46
1:E:621:LEU:HD22	1:E:622:LEU:N	2.30	0.46
1:A:117:TRP:CE2	1:A:516:LYS:HG3	2.50	0.46
1:A:209:HIS:H	1:A:209:HIS:CD2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:HIS:CD2	1:A:403:PRO:CB	2.98	0.46
3:C:79:LEU:HD21	7:C:1252:UQ1:C7	2.45	0.46
1:E:106:GLN:NE2	8:E:2062:HOH:O	2.49	0.46
1:E:491:ASP:OD1	1:E:492:PHE:N	2.48	0.46
8:E:2383:HOH:O	2:F:49:LEU:CD1	2.60	0.46
1:A:482:GLU:HG2	1:A:483:ALA:N	2.30	0.46
1:A:555:LEU:HA	1:A:555:LEU:HD23	1.72	0.46
3:C:145:ASN:OD1	3:C:193:THR:HG23	2.16	0.46
1:E:113:ARG:CB	8:E:2042:HOH:O	2.63	0.46
1:E:500:PRO:CD	1:E:567:ARG:O	2.64	0.46
2:F:27:ASN:O	2:F:28:GLU:C	2.53	0.46
8:F:2028:HOH:O	3:G:250:LEU:HD12	2.14	0.46
1:A:264:TRP:CZ2	1:A:315:VAL:HG11	2.50	0.46
1:A:389:SER:HA	1:A:595:GLN:NE2	2.30	0.46
1:A:107:ARG:O	1:A:457:LYS:HE3	2.16	0.46
2:B:117:THR:HG22	2:B:120:ALA:H	1.77	0.46
3:C:166:LEU:HD21	3:C:228:PRO:HB2	1.98	0.46
1:E:591:GLU:O	1:E:603:GLN:CD	2.53	0.46
1:E:708:LEU:O	1:E:712:ARG:CD	2.62	0.46
2:F:54:ARG:NH1	2:F:56:GLU:OE2	2.41	0.46
3:G:16:THR:CG2	3:G:66:GLU:HB2	2.45	0.46
1:A:666:TYR:CE1	1:A:681:ARG:HG3	2.51	0.46
1:A:712:ARG:NH1	8:A:2346:HOH:O	2.47	0.46
1:E:333:HIS:HB2	5:E:1766:MGD:S12	2.55	0.46
1:E:423:PRO:O	1:E:427:GLY:HA2	2.16	0.46
1:E:346:ALA:HB2	1:E:605:LEU:HD12	1.97	0.46
2:F:46:TYR:CG	2:F:47:PRO:N	2.83	0.46
3:G:19:LEU:O	3:G:19:LEU:HD23	2.15	0.46
3:G:50:LEU:O	3:G:51:TYR:CD2	2.69	0.46
1:A:502:ILE:N	1:A:564:LEU:O	2.44	0.46
1:A:602:HIS:CE1	1:A:606:PRO:CD	2.97	0.46
1:E:525:LEU:O	1:E:529:LEU:HG	2.16	0.46
1:E:64:LYS:HD2	8:E:2046:HOH:O	2.15	0.46
1:A:122:ASP:CB	8:A:2068:HOH:O	2.63	0.46
1:A:523:ARG:HG2	1:A:523:ARG:HH11	1.80	0.46
1:A:647:ASN:N	1:A:647:ASN:ND2	2.61	0.46
1:A:650:TRP:O	1:A:693:VAL:HA	2.15	0.46
2:B:35:ASN:ND2	2:B:106:TYR:OH	2.49	0.46
3:C:193:THR:HG23	3:C:193:THR:O	2.16	0.46
3:C:31:VAL:HG12	3:C:53:ALA:HB2	1.98	0.46
1:E:201:ARG:NH2	1:E:228:ASN:O	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:TRP:CZ2	1:E:251:PRO:HB3	2.50	0.46
1:E:75:ARG:HD2	1:E:220:GLN:NE2	2.24	0.46
3:G:134:LEU:N	8:G:2034:HOH:O	2.48	0.46
3:G:46:ARG:CG	8:G:2014:HOH:O	2.59	0.46
3:G:23:LEU:HD22	3:G:62:ILE:HD12	1.98	0.46
3:G:92:ALA:HB2	7:G:1251:UQ1:H8	1.98	0.46
1:A:231:LYS:HE3	1:A:231:LYS:HB3	1.60	0.46
1:A:339:ASP:CB	1:A:607:VAL:HG11	2.38	0.46
1:A:538:LYS:HE2	1:A:538:LYS:N	2.30	0.46
1:A:284:VAL:N	1:A:588:GLY:O	2.32	0.46
3:C:153:PRO:HB3	8:C:2063:HOH:O	2.14	0.46
1:E:193:GLU:H	1:E:193:GLU:CD	2.20	0.46
1:E:413:ARG:H	1:E:413:ARG:NH1	2.14	0.46
1:E:424:MET:HE2	1:E:455:ALA:HB1	1.97	0.46
1:E:466:ASP:OD1	1:E:473:VAL:HG21	2.16	0.46
1:E:604:PRO:O	1:E:606:PRO:HD2	2.13	0.46
3:G:223:GLU:N	8:G:2068:HOH:O	2.47	0.46
1:A:189:ILE:O	1:A:194:PRO:HD3	2.16	0.46
1:A:42:GLN:OE1	1:A:506:THR:O	2.34	0.46
1:A:504:LEU:HD22	1:A:505:ARG:N	2.30	0.46
1:A:536:PRO:HG2	1:A:537:TRP:N	2.29	0.46
1:A:647:ASN:O	1:A:648:GLU:HG3	2.16	0.46
3:C:130:TYR:CZ	7:C:1252:UQ1:O4	2.63	0.46
3:C:220:THR:HA	3:C:227:ALA:HA	1.97	0.46
1:E:45:GLU:HB2	1:E:485:TYR:HB3	1.96	0.46
1:E:209:HIS:CE1	1:E:625:ARG:N	2.71	0.46
1:E:237:PRO:CB	1:E:689:ARG:HD3	2.46	0.46
1:A:113:ARG:CZ	8:A:2063:HOH:O	2.65	0.45
1:A:116:THR:HG23	1:A:118:GLU:OE1	2.16	0.45
1:A:252:ILE:HD11	1:A:256:THR:HG22	1.94	0.45
1:A:753:THR:HG22	1:A:757:LYS:CE	2.46	0.45
3:C:155:THR:CG2	3:C:239:ARG:CD	2.94	0.45
2:F:117:THR:HB	8:F:2011:HOH:O	2.14	0.45
3:G:100:LEU:O	3:G:103:GLY:N	2.47	0.45
1:A:224:LEU:HB3	8:A:2124:HOH:O	2.16	0.45
1:A:266:HIS:HB2	1:A:293:VAL:HG13	1.97	0.45
1:A:144:GLY:HA2	1:A:438:TYR:O	2.16	0.45
2:B:54:ARG:NH2	2:B:187:THR:O	2.46	0.45
1:E:335:VAL:CG1	1:E:335:VAL:O	2.64	0.45
1:E:391:PRO:C	1:E:413:ARG:CG	2.85	0.45
1:E:533:GLN:O	1:E:536:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LYS:HB3	1:A:475:TRP:CH2	2.51	0.45
3:C:173:LEU:O	3:C:177:ARG:HG3	2.16	0.45
1:E:51:CYS:SG	1:E:216:ASN:HB3	2.57	0.45
1:E:255:GLY:HA2	1:E:337:TYR:CE1	2.52	0.45
1:E:45:GLU:HB2	1:E:485:TYR:CB	2.47	0.45
1:E:470:GLN:O	1:E:471:GLU:C	2.53	0.45
1:E:594:CYS:O	1:E:598:LYS:HB2	2.16	0.45
2:F:178:LEU:O	2:F:180:ALA:N	2.48	0.45
1:A:477:ASP:C	1:A:478:VAL:HG23	2.37	0.45
1:A:569:LYS:HA	1:A:570:PRO:HD3	1.71	0.45
1:A:412:ALA:HB2	1:A:728:ILE:O	2.15	0.45
2:B:143:GLY:N	2:B:152:VAL:CG2	2.79	0.45
1:E:422:GLU:HB2	8:E:2253:HOH:O	2.16	0.45
1:E:50:ARG:HD2	8:E:2013:HOH:O	2.16	0.45
1:E:183:TRP:CD1	1:E:593:TYR:CE1	3.04	0.45
1:E:702:LYS:HE3	1:E:718:TYR:CE2	2.51	0.45
1:E:97:ARG:HH21	1:E:763:ARG:HD2	1.77	0.45
1:A:265:ILE:CG2	1:A:293:VAL:HG21	2.46	0.45
1:A:349:TYR:CZ	1:A:590:ILE:O	2.69	0.45
1:A:604:PRO:HA	1:A:605:LEU:HD23	1.98	0.45
1:A:66:GLU:HB3	8:A:2016:HOH:O	2.16	0.45
2:B:50:VAL:CG1	2:B:181:PRO:HB2	2.47	0.45
3:C:108:LEU:O	3:C:109:GLY:C	2.55	0.45
1:E:75:ARG:NH1	1:E:220:GLN:NE2	2.55	0.45
1:E:422:GLU:N	1:E:423:PRO:CD	2.79	0.45
1:A:390:GLY:N	1:A:391:PRO:HD3	2.31	0.45
1:A:596:ARG:NH1	1:A:600:ALA:HB1	2.30	0.45
1:E:187:ARG:NH1	8:E:2108:HOH:O	2.46	0.45
1:A:532:GLU:HB3	8:A:2253:HOH:O	2.16	0.45
1:A:533:GLN:HE21	1:A:533:GLN:H	1.65	0.45
1:A:602:HIS:CD2	1:A:603:GLN:H	2.35	0.45
2:B:160:GLU:N	2:B:179:ASN:ND2	2.52	0.45
3:C:128:LEU:CD2	3:C:156:ALA:HB3	2.46	0.45
1:E:633:ARG:HB2	5:E:1765:MGD:H2'	1.99	0.45
1:E:345:MET:HB3	1:E:605:LEU:HD11	1.98	0.45
1:E:604:PRO:CA	1:E:605:LEU:HD23	2.47	0.45
2:F:10:LEU:HD22	2:F:53:PHE:O	2.16	0.45
3:G:53:LEU:HB2	8:G:2015:HOH:O	2.17	0.45
1:A:142:PHE:O	1:A:165:ALA:HA	2.17	0.45
3:C:128:LEU:HD23	3:C:156:ALA:CB	2.47	0.45
1:E:315:VAL:O	1:E:319:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:588:GLY:HA3	8:E:2107:HOH:O	2.17	0.45
2:F:191:GLU:HB2	8:F:2123:HOH:O	2.17	0.45
3:G:46:ARG:NH1	3:G:106:TYR:O	2.50	0.45
1:A:220:GLN:HA	2:B:136:PRO:O	2.16	0.45
1:A:523:ARG:HG2	1:A:523:ARG:NH1	2.31	0.45
1:A:41:TYR:HD1	1:A:559:LYS:O	1.98	0.45
1:A:73:LYS:HZ1	1:A:192:HIS:CD2	2.34	0.45
2:B:166:ARG:HD2	8:B:2124:HOH:O	2.16	0.45
2:B:192:VAL:CG1	2:B:193:HIS:H	2.30	0.45
1:E:115:ALA:HB1	1:E:119:GLU:HG2	1.98	0.45
1:E:183:TRP:CG	1:E:593:TYR:CD1	3.05	0.45
1:E:257:ASP:OD2	5:E:1766:MGD:N1	2.41	0.45
1:E:278:TYR:OH	1:E:357:TYR:HB3	2.17	0.45
1:E:590:ILE:HG22	1:E:591:GLU:N	2.31	0.45
1:E:726:ASP:O	1:E:729:SER:O	2.34	0.45
2:F:101:PRO:HD2	2:F:102:TYR:CD1	2.52	0.45
3:G:214:LEU:O	3:G:217:LEU:HB2	2.17	0.45
1:A:197:TRP:HB2	1:A:221:ASP:HB3	1.98	0.45
1:A:60:ASN:HB2	8:A:2021:HOH:O	2.16	0.45
1:A:683:LYS:HA	1:A:684:PRO:HD2	1.63	0.45
1:A:80:PRO:HG2	1:A:627:PRO:O	2.16	0.45
8:B:2025:HOH:O	3:C:251:LEU:CD1	2.63	0.45
1:E:427:GLY:O	1:E:428:GLU:O	2.35	0.45
1:E:606:PRO:HD2	1:E:607:VAL:H	1.80	0.45
3:G:206:GLY:O	3:G:209:TYR:HB3	2.16	0.45
1:A:327:VAL:HG13	1:A:362:GLY:HA3	1.99	0.44
1:A:655:GLU:OE2	1:A:658:ARG:NH2	2.49	0.44
1:A:657:LYS:O	1:A:659:LEU:O	2.34	0.44
1:A:65:VAL:CG1	1:A:78:LEU:CD2	2.94	0.44
3:C:17:THR:HG21	8:C:2014:HOH:O	2.16	0.44
3:C:61:LEU:HD22	7:C:1252:UQ1:H102	1.99	0.44
1:E:127:LYS:HD3	8:E:2083:HOH:O	2.17	0.44
1:E:707:ARG:NE	8:E:2403:HOH:O	2.48	0.44
1:A:648:GLU:HG2	1:A:681:ARG:NH1	2.33	0.44
1:A:73:LYS:HG3	1:A:501:PHE:HZ	1.81	0.44
2:B:130:ALA:HB3	4:B:1195:SF4:S2	2.57	0.44
2:B:167:PRO:O	2:B:169:GLN:O	2.36	0.44
2:B:183:LYS:NZ	2:F:157:LYS:O	2.50	0.44
3:C:108:LEU:HB3	3:C:110:LYS:CG	2.47	0.44
1:E:47:CYS:HB3	1:E:81:ARG:HH12	1.81	0.44
1:A:371:LEU:HG	1:A:502:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:C	8:A:2005:HOH:O	2.56	0.44
1:A:541:GLU:HB2	1:A:555:LEU:HD12	1.99	0.44
1:A:727:PRO:HA	8:A:2197:HOH:O	2.16	0.44
1:A:638:TRP:HB2	1:A:756:ALA:HB2	2.00	0.44
1:E:114:VAL:HG21	8:E:2054:HOH:O	2.17	0.44
1:E:138:GLU:OE2	1:E:402:LYS:HB2	2.16	0.44
1:E:664:GLY:N	8:E:2372:HOH:O	2.46	0.44
2:F:132:VAL:HA	2:F:140:ARG:HG3	2.00	0.44
2:F:82:LEU:HD12	2:F:84:LEU:HD11	1.98	0.44
1:A:133:GLU:HG3	8:A:2074:HOH:O	2.17	0.44
1:A:636:ASN:HB2	1:A:706:MET:HE3	1.99	0.44
1:E:252:ILE:CD1	1:E:256:THR:HG22	2.48	0.44
1:E:391:PRO:C	1:E:413:ARG:HG2	2.37	0.44
1:E:730:GLY:N	8:E:2251:HOH:O	2.43	0.44
1:E:74:SER:HB2	1:E:77:ARG:O	2.18	0.44
2:F:79:LYS:HD2	2:F:79:LYS:HA	1.72	0.44
1:A:394:GLY:CA	8:A:2188:HOH:O	2.65	0.44
1:A:418:GLN:HG3	1:A:418:GLN:H	1.39	0.44
1:A:447:PRO:HD3	8:A:2212:HOH:O	2.17	0.44
1:A:471:GLU:HB2	1:A:702:LYS:O	2.17	0.44
2:B:172:ARG:HD3	8:F:2127:HOH:O	2.18	0.44
2:B:9:ASP:HA	2:B:178:LEU:HB2	1.99	0.44
1:E:274:TYR:HA	1:E:323:LYS:NZ	2.33	0.44
1:E:336:TRP:HB3	1:E:735:ARG:HD2	2.00	0.44
1:E:159:ALA:O	1:E:380:PRO:HG2	2.17	0.44
1:E:642:GLU:OE2	2:F:31:PRO:HA	2.17	0.44
2:F:46:TYR:HB2	8:F:2033:HOH:O	2.17	0.44
1:A:252:ILE:HG13	1:A:307:ILE:CD1	2.48	0.44
2:B:41:ARG:NH1	2:B:187:THR:HG23	2.16	0.44
2:B:46:TYR:HE2	8:B:2035:HOH:O	1.91	0.44
2:B:78:THR:CG2	2:B:80:ASP:H	2.29	0.44
3:C:128:LEU:HD23	3:C:156:ALA:HB3	1.99	0.44
3:C:161:LEU:HD12	3:C:179:LEU:HD12	1.99	0.44
3:C:207:GLY:O	3:C:211:GLY:N	2.50	0.44
1:E:103:GLU:HG2	1:E:104:GLY:N	2.33	0.44
3:G:199:GLY:O	3:G:203:GLU:HG3	2.18	0.44
3:G:23:LEU:CD2	3:G:62:ILE:HD12	2.48	0.44
1:A:214:THR:HG21	1:A:627:PRO:O	2.18	0.44
1:A:38:LYS:HG2	8:A:2020:HOH:O	2.17	0.44
1:A:596:ARG:CZ	1:A:600:ALA:CB	2.95	0.44
1:A:638:TRP:HB2	1:A:756:ALA:CB	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:CYS:HB3	2:B:171:THR:O	2.17	0.44
1:E:512:LEU:O	1:E:513:PHE:HB2	2.18	0.44
1:E:557:THR:O	1:E:561:MET:HG3	2.18	0.44
1:E:569:LYS:HB2	1:E:575:TRP:HE1	1.83	0.44
1:E:349:TYR:CE1	1:E:605:LEU:HD11	2.52	0.44
1:E:630:THR:O	1:E:631:PHE:O	2.34	0.44
3:G:81:SER:HB2	3:G:83:HIS:CD2	2.53	0.44
1:A:638:TRP:HB3	1:A:708:LEU:HD11	1.99	0.44
2:B:116:CYS:HA	4:B:1195:SF4:S1	2.57	0.44
3:C:111:GLY:O	3:C:116:LEU:HD11	2.17	0.44
1:E:371:LEU:HD11	1:E:492:PHE:CD1	2.53	0.44
1:E:569:LYS:HB2	1:E:575:TRP:NE1	2.33	0.44
1:E:607:VAL:HG22	1:E:609:THR:OG1	2.18	0.44
2:F:106:TYR:CZ	2:F:114:SER:HB3	2.53	0.44
3:G:29:GLY:HA3	3:G:159:ALA:HB2	1.99	0.44
1:A:142:PHE:CG	1:A:157:PRO:HG3	2.53	0.44
1:A:266:HIS:C	1:A:266:HIS:CD2	2.91	0.44
1:A:371:LEU:HD13	1:A:547:ARG:CZ	2.47	0.44
1:A:548:LEU:HD23	1:A:548:LEU:HA	1.72	0.44
1:A:339:ASP:CB	1:A:607:VAL:CG1	2.95	0.44
1:A:669:LEU:HB3	1:A:739:VAL:HG21	2.00	0.44
2:B:7:ALA:HB3	2:B:141:THR:OG1	2.18	0.44
2:B:169:GLN:NE2	8:B:2128:HOH:O	2.33	0.44
3:C:171:TRP:HE3	3:C:171:TRP:O	1.83	0.44
1:E:630:THR:HA	5:E:1766:MGD:O17	2.17	0.44
1:E:292:HIS:HE1	1:E:605:LEU:O	2.01	0.44
1:E:510:GLU:HG3	1:E:510:GLU:H	1.46	0.44
1:E:512:LEU:HD12	1:E:512:LEU:HA	1.71	0.44
2:F:78:THR:HG23	2:F:79:LYS:N	2.32	0.44
1:A:302:GLU:HG3	1:A:302:GLU:O	2.17	0.43
1:A:625:ARG:HD2	5:A:1766:MGD:C17	2.48	0.43
1:A:632:ALA:HB3	5:A:1765:MGD:O1B	2.17	0.43
1:E:412:ALA:CB	1:E:413:ARG:HH12	2.30	0.43
1:E:349:TYR:HH	1:E:591:GLU:HA	1.78	0.43
1:E:683:LYS:O	1:E:683:LYS:HG2	2.16	0.43
2:F:44:GLY:O	2:F:45:GLU:CB	2.66	0.43
1:A:717:ASN:HD22	5:A:1765:MGD:H192	1.65	0.43
1:A:278:TYR:OH	1:A:357:TYR:HB3	2.18	0.43
1:A:648:GLU:HG2	1:A:681:ARG:HH12	1.82	0.43
1:A:693:VAL:HG21	1:A:741:LEU:HD21	1.99	0.43
2:B:106:TYR:CZ	2:B:114:SER:HB3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ALA:HB3	4:B:1194:SF4:S2	2.58	0.43
2:B:35:ASN:HB3	2:B:116:CYS:HB2	2.00	0.43
2:B:8:ILE:HD13	2:B:55:PRO:HG2	1.99	0.43
5:E:1766:MGD:H8	8:E:2425:HOH:O	2.18	0.43
1:E:407:LYS:HG3	1:E:407:LYS:O	2.18	0.43
3:G:133:ALA:HB3	8:G:2034:HOH:O	2.19	0.43
2:B:38:ILE:HD12	4:B:1194:SF4:S1	2.58	0.43
1:A:220:GLN:HG2	2:B:136:PRO:O	2.17	0.43
3:C:145:ASN:HD21	3:C:147:LEU:HB2	1.83	0.43
3:C:20:LEU:HD13	3:C:63:ILE:CD1	2.48	0.43
1:E:553:LEU:HD23	1:E:553:LEU:HA	1.72	0.43
2:F:184:LYS:HE2	8:F:2121:HOH:O	2.19	0.43
3:G:79:PHE:CZ	7:G:1251:UQ1:H103	2.52	0.43
1:A:116:THR:CG2	1:A:119:GLU:N	2.60	0.43
1:A:137:PRO:HD2	1:A:138:GLU:OE1	2.18	0.43
1:A:319:MET:HE1	1:A:328:LEU:CD1	2.47	0.43
1:A:471:GLU:OE2	1:A:718:TYR:OH	2.31	0.43
1:A:501:PHE:CA	1:A:564:LEU:O	2.67	0.43
1:A:597:PHE:HB3	1:A:598:LYS:H	1.61	0.43
2:B:1:MET:O	2:B:146:GLU:OE1	2.36	0.43
1:E:187:ARG:HB3	1:E:188:PRO:CD	2.48	0.43
1:E:613:GLU:HB3	1:E:614:PRO:HD2	2.00	0.43
2:F:1:MET:H3	2:F:2:PRO:CD	2.31	0.43
3:G:222:GLN:CB	8:G:2068:HOH:O	2.67	0.43
1:A:65:VAL:HG13	1:A:78:LEU:CD2	2.49	0.43
3:C:25:VAL:HB	3:C:60:ASP:OD2	2.19	0.43
3:C:77:ILE:HG12	3:C:81:LEU:CD1	2.47	0.43
1:E:115:ALA:HB1	1:E:119:GLU:CG	2.49	0.43
1:E:256:THR:HG23	1:E:256:THR:O	2.19	0.43
1:E:457:LYS:CD	8:E:2064:HOH:O	2.66	0.43
1:E:457:LYS:HD3	8:E:2064:HOH:O	2.17	0.43
1:E:717:ASN:ND2	8:E:2414:HOH:O	2.51	0.43
3:G:178:LEU:HD23	3:G:178:LEU:HA	1.81	0.43
1:A:181:SER:HB2	1:A:189:ILE:HD12	2.01	0.43
1:A:335:VAL:O	1:A:337:TYR:N	2.51	0.43
1:A:39:SER:CB	8:A:2005:HOH:O	2.63	0.43
1:A:539:THR:HG21	1:A:541:GLU:HG2	2.00	0.43
1:A:717:ASN:ND2	5:A:1765:MGD:H192	2.17	0.43
1:A:642:GLU:OE2	2:B:31:PRO:C	2.57	0.43
1:E:133:GLU:HB2	8:E:2087:HOH:O	2.18	0.43
1:E:252:ILE:HD11	1:E:256:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:ASP:C	1:E:275:ASP:OD1	2.56	0.43
1:E:281:LYS:HG3	1:E:282:TYR:CD1	2.54	0.43
1:E:422:GLU:N	1:E:423:PRO:HD2	2.33	0.43
1:E:494:LEU:CD2	1:E:502:ILE:HG12	2.38	0.43
1:E:69:GLU:HA	1:E:75:ARG:HA	1.99	0.43
2:F:59:LEU:O	2:F:60:HIS:C	2.57	0.43
3:G:206:GLY:N	3:G:209:TYR:HB2	2.34	0.43
1:A:435:LEU:N	1:A:461:LEU:O	2.51	0.43
2:B:41:ARG:CD	2:B:187:THR:CG2	2.75	0.43
3:C:51:LEU:O	3:C:54:LEU:HB2	2.19	0.43
3:C:79:LEU:HA	3:C:79:LEU:HD12	1.84	0.43
1:E:100:ILE:HA	1:E:478:VAL:HG22	2.00	0.43
1:E:633:ARG:CD	5:E:1765:MGD:O2B	2.66	0.43
1:E:472:HIS:HE1	8:E:2262:HOH:O	2.02	0.43
1:E:598:LYS:N	8:E:2325:HOH:O	2.51	0.43
3:G:38:HIS:CE1	3:G:105:LEU:HD13	2.53	0.43
3:G:63:LEU:HD22	7:G:1251:UQ1:C3	2.49	0.43
1:A:137:PRO:HB2	1:A:160:TRP:NE1	2.34	0.43
1:A:394:GLY:HA2	8:A:2189:HOH:O	2.18	0.43
1:A:395:ASP:CA	1:A:399:GLU:CG	2.63	0.43
1:A:635:GLN:HG2	1:A:635:GLN:H	1.32	0.43
1:A:94:ARG:O	1:A:94:ARG:HG3	2.19	0.43
3:C:241:LEU:HD12	3:C:242:LEU:N	2.33	0.43
1:E:466:ASP:OD1	1:E:473:VAL:CG2	2.67	0.43
2:F:29:VAL:HA	2:F:30:PRO:HD3	1.64	0.43
3:G:176:ARG:O	3:G:220:PHE:HE2	2.02	0.43
1:A:573:GLU:HG2	8:A:2271:HOH:O	2.18	0.43
1:E:274:TYR:H	1:E:274:TYR:HD2	1.64	0.43
1:E:569:LYS:HG2	1:E:569:LYS:H	1.45	0.43
1:E:346:ALA:CA	1:E:605:LEU:HD12	2.49	0.43
1:E:620:ARG:HD3	1:E:735:ARG:O	2.18	0.43
2:F:71:PRO:HB2	3:G:78:LEU:HD12	2.00	0.43
1:A:118:GLU:HG3	8:A:2252:HOH:O	2.18	0.43
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.88	0.43
1:A:523:ARG:HA	1:A:535:PHE:CD2	2.54	0.43
1:A:572:LEU:O	1:A:576:GLU:HB2	2.18	0.43
1:A:581:LEU:HD23	1:A:583:PHE:CE1	2.54	0.43
3:C:40:LEU:HD13	3:C:117:ALA:CB	2.48	0.43
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.86	0.43
1:E:305:THR:CG2	1:E:307:ILE:HB	2.49	0.43
1:E:630:THR:HA	5:E:1766:MGD:H18	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:LYS:HE3	2:F:26:GLU:HB2	2.01	0.43
2:B:25:MET:CE	2:B:25:MET:CA	2.81	0.42
2:B:64:PRO:O	2:B:68:PRO:HD2	2.18	0.42
1:E:206:ILE:CD1	1:E:261:LEU:HD21	2.48	0.42
1:E:548:LEU:HD12	1:E:555:LEU:HA	2.00	0.42
1:A:394:GLY:N	8:A:2188:HOH:O	2.53	0.42
1:A:87:GLN:HG3	1:A:637:ASN:ND2	2.34	0.42
1:E:195:ILE:HD13	1:E:363:PHE:CE2	2.54	0.42
1:E:495:VAL:HG13	8:E:2018:HOH:O	2.18	0.42
1:E:622:LEU:O	1:E:623:TYR:HB3	2.19	0.42
1:E:639:VAL:HG21	2:F:25:MET:CE	2.48	0.42
2:F:46:TYR:CD2	2:F:47:PRO:HD3	2.54	0.42
2:F:59:LEU:HD13	2:F:173:PRO:HB3	2.01	0.42
1:A:519:TRP:CG	1:A:540:ILE:HG23	2.54	0.42
1:E:117:TRP:CE2	1:E:516:LYS:CG	3.02	0.42
1:E:441:ASN:HD21	1:E:444:HIS:HD2	1.68	0.42
1:E:604:PRO:CA	1:E:605:LEU:CD2	2.97	0.42
1:E:647:ASN:C	1:E:648:GLU:HG3	2.40	0.42
2:F:35:ASN:ND2	2:F:106:TYR:OH	2.47	0.42
3:G:221:TRP:CZ3	3:G:225:LEU:HD13	2.44	0.42
1:A:327:VAL:CG1	1:A:362:GLY:HA3	2.49	0.42
1:A:677:GLU:C	1:A:678:GLY:O	2.58	0.42
3:C:11:GLN:NE2	3:C:11:GLN:H	2.18	0.42
1:E:614:PRO:HA	1:E:615:PRO:HD3	1.89	0.42
1:E:658:ARG:NH1	1:E:658:ARG:HB3	2.34	0.42
3:G:216:GLY:C	3:G:218:GLY:H	2.23	0.42
3:G:217:LEU:CD2	8:G:2063:HOH:O	2.67	0.42
1:A:499:THR:O	1:A:499:THR:OG1	2.37	0.42
1:A:535:PHE:N	1:A:536:PRO:HD3	2.34	0.42
1:A:743:LYS:CG	8:A:2365:HOH:O	2.68	0.42
3:C:166:LEU:C	3:C:168:LYS:H	2.22	0.42
1:E:173:CYS:HG	6:E:1767:MO:MO	1.56	0.42
1:E:297:THR:CG2	1:E:299:GLU:N	2.69	0.42
1:E:591:GLU:OE2	1:E:604:PRO:CB	2.67	0.42
1:E:745:GLU:HG3	8:E:2430:HOH:O	2.19	0.42
3:G:17:ASN:HB2	8:G:2010:HOH:O	2.19	0.42
3:G:58:LEU:HD12	3:G:58:LEU:O	2.20	0.42
3:G:70:ARG:HG3	3:G:71:PHE:CD2	2.54	0.42
1:A:671:ASN:HD22	1:A:671:ASN:C	2.22	0.42
1:A:81:ARG:HD2	1:A:630:THR:OG1	2.19	0.42
3:C:79:LEU:CD2	7:C:1252:UQ1:C8	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:SER:HA	3:C:170:PRO:HD3	1.82	0.42
1:E:151:TRP:O	1:E:156:LEU:HB3	2.19	0.42
1:E:428:GLU:C	1:E:430:TYR:N	2.69	0.42
1:E:673:ASP:OD2	1:E:721:THR:HG22	2.15	0.42
2:F:164:VAL:HG12	2:F:167:PRO:HB3	2.00	0.42
2:F:175:LEU:HD12	2:F:175:LEU:C	2.39	0.42
1:E:639:VAL:CG1	2:F:25:MET:HE3	2.44	0.42
1:A:310:GLN:CG	8:A:2160:HOH:O	2.67	0.42
1:A:47:CYS:HB3	1:A:81:ARG:HH12	1.84	0.42
1:A:52:GLY:H	1:A:71:ASN:ND2	2.18	0.42
3:C:154:LEU:O	3:C:158:VAL:HG23	2.20	0.42
1:E:576:GLU:C	1:E:578:GLU:N	2.72	0.42
1:E:632:ALA:HB2	1:E:698:GLY:HA2	2.02	0.42
3:G:117:TRP:CB	8:G:2033:HOH:O	2.68	0.42
1:A:349:TYR:HH	1:A:591:GLU:C	2.05	0.42
1:A:101:ARG:NH1	1:A:477:ASP:OD1	2.53	0.42
1:A:644:ASP:HA	1:A:645:PRO:HD3	1.67	0.42
1:A:641:MET:CE	1:A:645:PRO:HA	2.50	0.42
3:C:125:LEU:HD23	3:C:125:LEU:HA	1.87	0.42
1:E:160:TRP:CD1	1:E:160:TRP:O	2.73	0.42
1:E:177:ARG:NH1	1:E:332:ARG:HA	2.35	0.42
1:E:46:GLY:O	1:E:630:THR:HG21	2.19	0.42
1:E:548:LEU:HD23	1:E:548:LEU:HA	1.76	0.42
1:E:602:HIS:CE1	1:E:606:PRO:CD	3.02	0.42
3:G:154:THR:HG21	3:G:238:ARG:CG	2.45	0.42
3:G:184:LEU:O	3:G:188:LEU:HG	2.20	0.42
1:A:205:LEU:HB3	1:A:208:HIS:HB3	2.01	0.42
1:A:421:ILE:CG2	1:A:421:ILE:O	2.67	0.42
1:A:425:ILE:HD11	1:A:451:ARG:HG2	2.02	0.42
2:B:12:LEU:HB2	2:B:139:CYS:HB3	2.01	0.42
2:B:22:ALA:CB	2:B:134:THR:HG21	2.47	0.42
1:E:412:ALA:CB	1:E:413:ARG:NH1	2.82	0.42
1:E:488:ARG:HG2	1:E:489:TYR:N	2.34	0.42
1:E:626:SER:O	1:E:628:VAL:N	2.52	0.42
1:E:629:HIS:HA	1:E:634:THR:HG21	2.00	0.42
2:F:135:CYS:HA	2:F:136:PRO:HD3	1.71	0.42
3:G:142:LEU:HD23	3:G:197:ALA:HB1	2.02	0.42
3:G:165:LEU:HD22	3:G:224:ARG:HH11	1.83	0.42
8:F:2052:HOH:O	3:G:88:ILE:HG13	2.19	0.42
1:A:82:GLY:HA3	4:A:1764:SF4:S3	2.60	0.42
1:A:333:HIS:O	1:A:336:TRP:NE1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.87	0.42
1:A:591:GLU:HB3	1:A:603:GLN:HE21	1.76	0.42
1:A:678:GLY:N	8:A:2329:HOH:O	2.52	0.42
2:B:110:ALA:HB3	2:B:112:TYR:CE2	2.54	0.42
3:C:241:LEU:CD1	3:C:241:LEU:O	2.68	0.42
3:C:48:ARG:HD3	3:C:48:ARG:HH11	1.70	0.42
1:E:269:ILE:HG21	1:E:290:LYS:HG3	2.02	0.42
1:E:339:ASP:O	1:E:342:TYR:HB2	2.20	0.42
1:E:371:LEU:HD13	1:E:547:ARG:NH2	2.35	0.42
1:E:413:ARG:HH11	1:E:413:ARG:HD2	1.71	0.42
1:E:607:VAL:CG2	8:E:2145:HOH:O	2.61	0.42
8:F:2030:HOH:O	3:G:1:ALA:CB	2.66	0.42
1:A:346:ALA:CB	1:A:605:LEU:HD13	2.49	0.41
1:A:678:GLY:CA	8:A:2329:HOH:O	2.68	0.41
1:A:71:ASN:ND2	1:A:74:SER:H	2.08	0.41
1:A:95:LEU:HG	1:A:467:VAL:O	2.20	0.41
3:C:108:LEU:HB3	3:C:110:LYS:HD2	2.02	0.41
3:C:251:LEU:HD23	8:C:2087:HOH:O	2.20	0.41
1:E:391:PRO:CD	1:E:595:GLN:OE1	2.68	0.41
1:E:604:PRO:CB	1:E:605:LEU:HD23	2.50	0.41
1:E:636:ASN:HB2	1:E:706:MET:CE	2.50	0.41
1:E:87:GLN:OE1	1:E:637:ASN:HA	2.20	0.41
1:E:761:ASP:C	1:E:763:ARG:H	2.21	0.41
1:A:279:VAL:O	1:A:283:THR:HB	2.19	0.41
1:A:426:THR:CG2	8:A:2049:HOH:O	2.63	0.41
1:E:254:PRO:HG3	1:E:692:CYS:SG	2.60	0.41
1:E:69:GLU:HG2	1:E:69:GLU:H	1.59	0.41
3:G:124:LEU:HD23	3:G:124:LEU:HA	1.92	0.41
3:G:222:GLN:HB2	8:G:2068:HOH:O	2.20	0.41
1:A:335:VAL:HG13	1:A:733:GLY:N	2.35	0.41
1:A:498:LYS:HE3	8:A:2107:HOH:O	2.18	0.41
1:A:42:GLN:OE1	1:A:505:ARG:HB2	2.21	0.41
1:A:539:THR:HG22	1:A:542:GLU:H	1.85	0.41
1:A:283:THR:HA	1:A:588:GLY:O	2.20	0.41
1:A:723:TYR:CD1	1:A:732:ALA:HB1	2.56	0.41
1:E:310:GLN:O	1:E:314:GLU:HB2	2.20	0.41
3:G:144:ASN:C	3:G:144:ASN:ND2	2.74	0.41
3:G:146:LEU:HD23	3:G:146:LEU:HA	1.90	0.41
3:G:78:LEU:HG	3:G:92:ALA:CB	2.50	0.41
1:A:225:ALA:C	1:A:230:ALA:HB3	2.41	0.41
1:A:278:TYR:HD1	1:A:359:ARG:NH2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:SER:HA	1:A:595:GLN:HE22	1.85	0.41
1:E:281:LYS:HE2	1:E:281:LYS:HB3	1.89	0.41
1:E:651:ILE:O	1:E:684:PRO:O	2.39	0.41
2:F:117:THR:HG23	2:F:120:ALA:N	2.22	0.41
2:F:24:LYS:NZ	2:F:30:PRO:O	2.53	0.41
2:F:67:VAL:CB	2:F:68:PRO:CD	2.97	0.41
3:G:38:HIS:HE1	3:G:105:LEU:HD22	1.80	0.41
3:G:223:GLU:HB3	8:G:2069:HOH:O	2.19	0.41
1:A:342:TYR:CG	1:A:605:LEU:HA	2.56	0.41
1:A:722:ARG:HA	8:A:2352:HOH:O	2.20	0.41
2:B:128:VAL:HG11	8:B:2070:HOH:O	2.19	0.41
3:C:163:LEU:O	3:C:167:LEU:HG	2.20	0.41
3:C:180:ALA:O	3:C:184:LEU:HG	2.21	0.41
3:C:18:ASN:O	3:C:21:HIS:HB3	2.21	0.41
3:C:17:THR:HG22	3:C:67:GLU:HG3	1.91	0.41
1:E:160:TRP:CE3	1:E:529:LEU:HD13	2.55	0.41
1:E:595:GLN:HB2	1:E:595:GLN:HE21	1.48	0.41
1:E:77:ARG:NH2	2:F:138:TYR:CE2	2.88	0.41
3:G:52:ALA:O	3:G:56:ILE:CG1	2.68	0.41
1:A:371:LEU:HD23	1:A:371:LEU:HA	1.85	0.41
1:A:641:MET:HE3	1:A:645:PRO:HA	2.01	0.41
1:E:197:TRP:CD1	1:E:221:ASP:HB3	2.55	0.41
1:E:220:GLN:O	1:E:224:LEU:HB2	2.20	0.41
1:E:292:HIS:CD2	8:E:2084:HOH:O	2.71	0.41
1:E:430:TYR:HB2	1:E:431:PRO:CD	2.51	0.41
1:E:537:TRP:O	1:E:537:TRP:CE3	2.73	0.41
1:E:651:ILE:CD1	1:E:656:ALA:HB2	2.49	0.41
1:E:650:TRP:O	1:E:693:VAL:HA	2.20	0.41
3:G:97:LEU:HD23	3:G:97:LEU:HA	1.84	0.41
1:A:452:THR:O	1:A:456:LEU:HG	2.21	0.41
1:A:124:ILE:HG12	1:A:463:VAL:HG21	2.01	0.41
1:A:679:PRO:HG2	1:A:747:PRO:HB3	2.02	0.41
3:C:171:TRP:CE3	3:C:172:ALA:HB2	2.56	0.41
3:C:215:LEU:O	3:C:216:LEU:C	2.58	0.41
1:E:510:GLU:CG	8:E:2299:HOH:O	2.49	0.41
1:E:282:TYR:C	1:E:587:SER:HB3	2.40	0.41
1:E:657:LYS:HB2	1:E:657:LYS:HE2	1.77	0.41
2:F:52:GLU:CD	2:F:187:THR:HB	2.40	0.41
3:G:112:GLN:O	3:G:114:ALA:N	2.54	0.41
2:F:71:PRO:O	3:G:83:HIS:CD2	2.74	0.41
1:A:103:GLU:OE1	1:A:103:GLU:CA	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:HIS:CE1	8:A:2069:HOH:O	2.74	0.41
1:A:239:PHE:HB3	1:A:687:ARG:CB	2.49	0.41
1:A:275:ASP:OD1	1:A:275:ASP:C	2.59	0.41
1:A:519:TRP:CD2	1:A:540:ILE:CG2	3.03	0.41
1:A:539:THR:HG23	1:A:541:GLU:H	1.85	0.41
1:A:541:GLU:O	1:A:545:GLU:CG	2.69	0.41
3:C:64:LEU:HD23	7:C:1252:UQ1:HM22	2.03	0.41
3:C:64:LEU:HD13	7:C:1252:UQ1:HM52	2.03	0.41
1:E:183:TRP:HA	1:E:593:TYR:CE1	2.55	0.41
2:F:109:PRO:HG3	8:F:2014:HOH:O	2.19	0.41
1:A:81:ARG:HB2	4:A:1764:SF4:S1	2.61	0.41
1:A:37:VAL:HG12	1:A:38:LYS:H	1.83	0.41
1:A:498:LYS:HD2	8:A:2241:HOH:O	2.19	0.41
1:A:607:VAL:C	1:A:609:THR:N	2.71	0.41
2:B:10:LEU:HD22	2:B:53:PHE:O	2.21	0.41
2:B:48:ASN:ND2	2:F:157:LYS:HE2	2.36	0.41
2:B:72:THR:HG22	2:B:74:ALA:N	2.07	0.41
2:F:118:PHE:HA	2:F:118:PHE:HD1	1.55	0.41
2:F:81:GLY:O	2:F:174:LYS:NZ	2.47	0.41
3:G:117:TRP:HB3	8:G:2033:HOH:O	2.21	0.41
3:G:165:LEU:HG	3:G:227:PRO:HB2	2.03	0.41
1:A:213:ASP:OD2	1:A:218:GLN:NE2	2.53	0.41
1:A:520:TRP:O	1:A:524:GLU:HG2	2.20	0.41
1:A:502:ILE:HD12	1:A:564:LEU:HD22	2.03	0.41
2:B:118:PHE:HD1	2:B:118:PHE:HA	1.63	0.41
2:B:7:ALA:O	2:B:140:ARG:HA	2.21	0.41
3:C:66:ALA:O	3:C:71:ARG:NH1	2.54	0.41
1:E:100:ILE:HG12	1:E:478:VAL:CG1	2.51	0.41
2:F:86:ASP:OD1	2:F:88:LYS:HB2	2.21	0.41
1:A:269:ILE:HG21	1:A:290:LYS:HG3	2.02	0.41
1:A:261:LEU:HD22	1:A:347:LEU:HA	2.03	0.41
1:A:546:THR:O	1:A:549:GLN:HB2	2.21	0.41
1:A:591:GLU:OE2	1:A:604:PRO:HG2	2.11	0.41
1:A:77:ARG:HD2	2:B:138:TYR:CE2	2.56	0.41
1:A:77:ARG:HH12	2:B:138:TYR:HE2	1.54	0.41
1:E:417:ILE:HG23	1:E:418:GLN:N	2.36	0.41
1:E:64:LYS:NZ	1:E:66:GLU:OE1	2.54	0.41
1:E:97:ARG:NH2	1:E:763:ARG:HH11	2.18	0.41
3:G:38:HIS:O	3:G:40:LYS:N	2.54	0.41
3:G:24:VAL:CG2	3:G:95:LEU:HD11	2.51	0.41
1:A:477:ASP:HB3	8:A:2069:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG21	1:A:486:LEU:HD22	2.03	0.40
1:A:510:GLU:H	1:A:510:GLU:HG3	1.62	0.40
1:A:630:THR:O	1:A:631:PHE:C	2.60	0.40
2:B:78:THR:HB	2:B:82:LEU:O	2.21	0.40
3:C:17:THR:CG2	3:C:18:ASN:N	2.84	0.40
2:B:101:PRO:HA	3:C:249:GLN:HE22	1.84	0.40
1:E:122:ASP:OD1	1:E:528:ARG:HD3	2.21	0.40
1:E:322:HIS:O	1:E:323:LYS:O	2.38	0.40
1:E:342:TYR:HD1	1:E:607:VAL:CG1	2.34	0.40
1:E:421:ILE:O	1:E:421:ILE:HG22	2.18	0.40
1:E:47:CYS:HB3	1:E:81:ARG:NH1	2.36	0.40
2:F:34:PHE:H	3:G:8:ASN:HD21	1.69	0.40
1:A:177:ARG:HA	1:A:344:VAL:HG11	2.03	0.40
1:A:293:VAL:HA	1:A:296:PHE:CD1	2.57	0.40
1:A:319:MET:HE2	1:A:328:LEU:HD11	2.02	0.40
1:A:39:SER:HA	1:A:55:ALA:O	2.21	0.40
1:A:552:GLY:O	8:A:2261:HOH:O	2.22	0.40
1:A:685:THR:CG2	8:B:2028:HOH:O	2.68	0.40
1:A:412:ALA:CB	1:A:728:ILE:O	2.69	0.40
2:B:30:PRO:HG3	2:B:109:PRO:HD2	2.03	0.40
3:C:111:GLY:O	3:C:112:SER:HB3	2.21	0.40
1:E:116:THR:HG23	1:E:118:GLU:N	2.36	0.40
1:E:216:ASN:O	1:E:220:GLN:HG3	2.22	0.40
1:E:95:LEU:HG	1:E:468:LEU:O	2.21	0.40
1:E:97:ARG:HA	1:E:514:ASP:HB3	2.03	0.40
1:E:574:ASP:O	1:E:578:GLU:HG3	2.21	0.40
1:E:632:ALA:HA	1:E:635:GLN:NE2	2.37	0.40
2:F:2:PRO:HB3	2:F:144:ASP:HB2	2.04	0.40
2:F:17:ALA:HB1	2:F:20:ALA:HB3	2.02	0.40
2:F:7:ALA:HB1	2:F:178:LEU:HD11	2.03	0.40
2:F:72:THR:CG2	2:F:89:LYS:O	2.65	0.40
3:G:83:HIS:HA	3:G:84:PRO:HD2	1.87	0.40
1:A:286:PHE:CG	1:A:286:PHE:O	2.71	0.40
1:E:194:PRO:O	1:E:363:PHE:HA	2.21	0.40
1:E:443:PHE:CE1	1:E:472:HIS:HA	2.56	0.40
1:E:669:LEU:HD22	1:E:739:VAL:HG13	2.03	0.40
1:A:417:ILE:HG23	1:A:418:GLN:N	2.36	0.40
1:A:589:LYS:H	1:A:589:LYS:HG2	1.53	0.40
1:A:589:LYS:O	1:A:592:LEU:CB	2.69	0.40
1:A:629:HIS:CB	1:A:634:THR:HG21	2.50	0.40
2:B:3:ARG:O	2:B:145:LEU:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:LEU:CD2	7:C:1252:UQ1:C1	2.93	0.40
3:C:9:ASN:ND2	8:C:2009:HOH:O	2.39	0.40
1:E:145:HIS:HD1	5:E:1765:MGD:PA	2.44	0.40
1:E:36:GLU:O	1:E:58:VAL:CB	2.66	0.40
1:E:457:LYS:HE2	8:E:2061:HOH:O	2.21	0.40
1:E:42:GLN:CB	1:E:53:ILE:HG13	2.52	0.40
1:E:667:VAL:HG11	1:E:741:LEU:HD13	2.04	0.40
3:G:223:GLU:C	3:G:225:LEU:H	2.25	0.40
1:A:116:THR:CG2	1:A:118:GLU:HB2	2.51	0.40
1:A:125:ALA:O	1:A:129:LEU:HG	2.22	0.40
1:A:209:HIS:CD2	5:A:1766:MGD:O2A	2.72	0.40
1:A:177:ARG:NH2	1:A:193:GLU:OE1	2.52	0.40
1:A:292:HIS:CD2	1:A:604:PRO:HB2	2.57	0.40
1:A:647:ASN:ND2	1:A:713:GLY:CA	2.85	0.40
1:A:670:VAL:HA	1:A:675:VAL:O	2.22	0.40
2:B:35:ASN:HD22	2:B:106:TYR:HE2	1.68	0.40
1:E:156:LEU:HB3	1:E:157:PRO:HD3	2.03	0.40
1:E:187:ARG:HB3	1:E:188:PRO:HD2	2.03	0.40
1:E:621:LEU:HD22	1:E:622:LEU:H	1.85	0.40
1:E:88:THR:CG2	1:E:467:VAL:CG1	3.00	0.40
3:G:150:LEU:HA	3:G:150:LEU:HD23	1.77	0.40

All (3) 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)
1:A:399:GLU:OE2	1:E:133:GLU:C[2_674]	1.77	0.43
1:A:399:GLU:OE2	1:E:134:LYS:N[2_674]	1.83	0.37
1:A:399:GLU:OE2	1:E:133:GLU:O[2_674]	2.04	0.16

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	733/765 (96%)	653 (89%)	45 (6%)	35 (5%)	2 14
1	E	733/765 (96%)	639 (87%)	59 (8%)	35 (5%)	2 14
2	B	192/195 (98%)	178 (93%)	11 (6%)	3 (2%)	9 37
2	F	192/195 (98%)	179 (93%)	9 (5%)	4 (2%)	7 30
3	C	249/253 (98%)	233 (94%)	11 (4%)	5 (2%)	7 31
3	G	249/253 (98%)	220 (88%)	21 (8%)	8 (3%)	4 22
All	All	2348/2426 (97%)	2102 (90%)	156 (7%)	90 (4%)	3 19

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	TRP
1	A	340	ASP
1	A	428	GLU
1	A	429	PRO
1	A	431	PRO
1	A	535	PHE
1	A	562	GLY
1	A	570	PRO
1	A	586	ALA
1	A	587	SER
1	A	593	TYR
1	A	605	LEU
1	A	678	GLY
1	A	687	ARG
1	A	730	GLY
2	B	17	ALA
3	C	208	PHE
3	C	250	GLY
1	E	92	PRO
1	E	93	ASP
1	E	109	GLU
1	E	396	HIS
1	E	397	GLU
1	E	428	GLU
1	E	429	PRO
1	E	552	GLY
1	E	567	ARG
1	E	583	PHE
1	E	593	TYR
1	E	607	VAL

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Mol	Chain	Res	Type
1	E	631	PHE
1	E	678	GLY
1	E	686	ALA
2	F	46	TYR
3	G	108	GLY
3	G	113	ARG
3	G	222	GLN
1	A	365	ILE
1	A	399	GLU
1	A	430	TYR
1	A	434	GLY
1	A	582	PRO
1	A	592	LEU
1	A	607	VAL
1	A	631	PHE
1	A	633	ARG
2	B	193	HIS
3	C	112	SER
3	C	172	ALA
1	E	337	TYR
1	E	391	PRO
1	E	606	PRO
1	E	685	THR
2	F	179	ASN
3	G	39	LEU
3	G	51	TYR
3	G	249	GLY
1	A	216	ASN
1	A	389	SER
1	A	398	PRO
1	E	466	ASP
1	E	469	PRO
1	E	478	VAL
1	E	513	PHE
1	E	570	PRO
1	E	627	PRO
2	F	45	GLU
2	F	178	LEU
1	A	478	VAL
2	B	115	LYS
3	C	113	GLN
1	E	389	SER

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Mol	Chain	Res	Type
1	E	471	GLU
1	E	763	ARG
1	A	387	GLY
1	E	70	ALA
1	E	710	HIS
3	G	38	HIS
1	A	584	GLY
1	A	598	LYS
1	A	610	PRO
1	A	609	THR
1	A	684	PRO
1	E	434	GLY
1	E	610	PRO
3	G	110	GLY
1	E	468	LEU
1	E	604	PRO
1	A	362	GLY
1	E	609	THR

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	610/632 (96%)	499 (82%)	111 (18%)	1 7
1	E	610/632 (96%)	503 (82%)	107 (18%)	2 8
2	B	162/163 (99%)	144 (89%)	18 (11%)	6 24
2	F	162/163 (99%)	147 (91%)	15 (9%)	9 32
3	C	185/187 (99%)	164 (89%)	21 (11%)	5 23
3	G	185/187 (99%)	164 (89%)	21 (11%)	5 23
All	All	1914/1964 (98%)	1621 (85%)	293 (15%)	2 12

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	61	ARG
1	A	65	VAL
1	A	77	ARG
1	A	87	GLN
1	A	97	ARG
1	A	103	GLU
1	A	106	GLN
1	A	111	LYS
1	A	116	THR
1	A	119	GLU
1	A	126	LYS
1	A	134	LYS
1	A	156	LEU
1	A	167	LYS
1	A	174	THR
1	A	187	ARG
1	A	189	ILE
1	A	209	HIS
1	A	213	ASP
1	A	214	THR
1	A	217	THR
1	A	231	LYS
1	A	252	ILE
1	A	256	THR
1	A	260	LEU
1	A	281	LYS
1	A	283	THR
1	A	286	PHE
1	A	289	LEU
1	A	297	THR
1	A	299	GLU
1	A	302	GLU
1	A	305	THR
1	A	323	LYS
1	A	327	VAL
1	A	335	VAL
1	A	368	SER
1	A	371	LEU
1	A	372	GLU
1	A	378	PRO
1	A	379	LEU
1	A	382	GLU

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Mol	Chain	Res	Type
1	A	388	CYS
1	A	395	ASP
1	A	413	ARG
1	A	414	SER
1	A	415	THR
1	A	418	GLN
1	A	421	ILE
1	A	428	GLU
1	A	440	ILE
1	A	441	ASN
1	A	454	GLU
1	A	457	LYS
1	A	470	GLN
1	A	477	ASP
1	A	484	THR
1	A	510	GLU
1	A	512	LEU
1	A	515	THR
1	A	529	LEU
1	A	532	GLU
1	A	533	GLN
1	A	538	LYS
1	A	539	THR
1	A	540	ILE
1	A	541	GLU
1	A	542	GLU
1	A	550	SER
1	A	553	LEU
1	A	555	LEU
1	A	558	MET
1	A	561	MET
1	A	578	GLU
1	A	580	ARG
1	A	587	SER
1	A	589	LYS
1	A	591	GLU
1	A	592	LEU
1	A	594	CYS
1	A	595	GLN
1	A	596	ARG
1	A	597	PHE
1	A	603	GLN

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Mol	Chain	Res	Type
1	A	605	LEU
1	A	608	PHE
1	A	616	GLU
1	A	621	LEU
1	A	633	ARG
1	A	647	ASN
1	A	651	ILE
1	A	662	LYS
1	A	663	GLU
1	A	671	ASN
1	A	672	GLN
1	A	680	VAL
1	A	683	LYS
1	A	685	THR
1	A	693	VAL
1	A	702	LYS
1	A	708	LEU
1	A	721	THR
1	A	724	LYS
1	A	725	LEU
1	A	736	VAL
1	A	739	VAL
1	A	741	LEU
1	A	743	LYS
1	A	746	ARG
1	A	762	GLU
2	B	1	MET
2	B	25	MET
2	B	39	ARG
2	B	69	VAL
2	B	72	THR
2	B	78	THR
2	B	105	ARG
2	B	114	SER
2	B	117	THR
2	B	118	PHE
2	B	125	LYS
2	B	131	CYS
2	B	140	ARG
2	B	152	VAL
2	B	154	LYS
2	B	164	VAL

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Mol	Chain	Res	Type
2	B	175	LEU
2	B	187	THR
3	C	11	GLN
3	C	17	THR
3	C	18	ASN
3	C	20	LEU
3	C	40	LEU
3	C	63	ILE
3	C	67	GLU
3	C	71	ARG
3	C	75	THR
3	C	110	LYS
3	C	130	TYR
3	C	140	ASN
3	C	145	ASN
3	C	155	THR
3	C	163	LEU
3	C	193	THR
3	C	216	LEU
3	C	225	ARG
3	C	232	LEU
3	C	241	LEU
3	C	249	GLN
1	E	65	VAL
1	E	69	GLU
1	E	101	ARG
1	E	111	LYS
1	E	113	ARG
1	E	114	VAL
1	E	119	GLU
1	E	126	LYS
1	E	145	HIS
1	E	172	LEU
1	E	174	THR
1	E	187	ARG
1	E	208	HIS
1	E	209	HIS
1	E	213	ASP
1	E	214	THR
1	E	217	THR
1	E	224	LEU
1	E	240	SER

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Mol	Chain	Res	Type
1	E	250	LEU
1	E	256	THR
1	E	260	LEU
1	E	272	ASP
1	E	284	VAL
1	E	286	PHE
1	E	289	LEU
1	E	293	VAL
1	E	297	THR
1	E	298	PRO
1	E	299	GLU
1	E	305	THR
1	E	310	GLN
1	E	323	LYS
1	E	327	VAL
1	E	335	VAL
1	E	360	PRO
1	E	371	LEU
1	E	389	SER
1	E	395	ASP
1	E	402	LYS
1	E	413	ARG
1	E	415	THR
1	E	418	GLN
1	E	421	ILE
1	E	428	GLU
1	E	440	ILE
1	E	441	ASN
1	E	466	ASP
1	E	470	GLN
1	E	484	THR
1	E	488	ARG
1	E	498	LYS
1	E	499	THR
1	E	504	LEU
1	E	510	GLU
1	E	512	LEU
1	E	515	THR
1	E	528	ARG
1	E	533	GLN
1	E	538	LYS
1	E	539	THR

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Mol	Chain	Res	Type
1	E	540	ILE
1	E	541	GLU
1	E	554	ASP
1	E	555	LEU
1	E	558	MET
1	E	564	LEU
1	E	569	LYS
1	E	577	LYS
1	E	581	LEU
1	E	585	THR
1	E	591	GLU
1	E	595	GLN
1	E	596	ARG
1	E	598	LYS
1	E	602	HIS
1	E	605	LEU
1	E	607	VAL
1	E	608	PHE
1	E	609	THR
1	E	620	ARG
1	E	621	LEU
1	E	626	SER
1	E	633	ARG
1	E	647	ASN
1	E	649	VAL
1	E	651	ILE
1	E	657	LYS
1	E	667	VAL
1	E	671	ASN
1	E	672	GLN
1	E	676	LYS
1	E	680	VAL
1	E	685	THR
1	E	691	ASP
1	E	693	VAL
1	E	702	LYS
1	E	708	LEU
1	E	721	THR
1	E	725	LEU
1	E	736	VAL
1	E	739	VAL
1	E	740	ARG

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Mol	Chain	Res	Type
1	E	746	ARG
1	E	748	ARG
1	E	751	SER
1	E	752	LEU
2	F	49	LEU
2	F	69	VAL
2	F	72	THR
2	F	88	LYS
2	F	114	SER
2	F	117	THR
2	F	118	PHE
2	F	133	GLU
2	F	145	LEU
2	F	150	SER
2	F	152	VAL
2	F	164	VAL
2	F	171	THR
2	F	175	LEU
2	F	187	THR
3	G	10	GLN
3	G	17	ASN
3	G	39	LEU
3	G	40	LYS
3	G	64	TRP
3	G	66	GLU
3	G	74	THR
3	G	88	ILE
3	G	113	ARG
3	G	129	TYR
3	G	136	VAL
3	G	139	ASN
3	G	144	ASN
3	G	154	THR
3	G	162	LEU
3	G	167	LYS
3	G	192	THR
3	G	196	GLU
3	G	204	GLU
3	G	215	LEU
3	G	240	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	71	ASN
1	A	83	GLN
1	A	192	HIS
1	A	209	HIS
1	A	220	GLN
1	A	247	HIS
1	A	322	HIS
1	A	367	GLN
1	A	441	ASN
1	A	470	GLN
1	A	472	HIS
1	A	509	HIS
1	A	533	GLN
1	A	595	GLN
1	A	602	HIS
1	A	603	GLN
1	A	647	ASN
1	A	671	ASN
1	A	672	GLN
1	A	717	ASN
2	B	27	ASN
2	B	35	ASN
2	B	48	ASN
2	B	57	GLN
2	B	77	GLN
2	B	179	ASN
3	C	9	ASN
3	C	11	GLN
3	C	39	HIS
3	C	84	HIS
3	C	113	GLN
3	C	140	ASN
3	C	145	ASN
3	C	201	HIS
3	C	249	GLN
1	E	60	ASN
1	E	71	ASN
1	E	83	GLN
1	E	123	HIS
1	E	192	HIS
1	E	208	HIS
1	E	209	HIS

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Mol	Chain	Res	Type
1	E	218	GLN
1	E	220	GLN
1	E	247	HIS
1	E	292	HIS
1	E	322	HIS
1	E	396	HIS
1	E	418	GLN
1	E	441	ASN
1	E	444	HIS
1	E	470	GLN
1	E	509	HIS
1	E	533	GLN
1	E	595	GLN
1	E	602	HIS
1	E	603	GLN
1	E	635	GLN
1	E	647	ASN
1	E	671	ASN
1	E	672	GLN
1	E	717	ASN
2	F	27	ASN
2	F	35	ASN
2	F	57	GLN
2	F	77	GLN
2	F	179	ASN
3	G	8	ASN
3	G	38	HIS
3	G	137	ASN
3	G	139	ASN
3	G	248	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SF4	F	1195	2	0,12,12	0.00	-	-		
4	SF4	B	1196	2	0,12,12	0.00	-	-		
4	SF4	E	1764	1	0,12,12	0.00	-	-		
4	SF4	F	1196	2	0,12,12	0.00	-	-		
5	MGD	E	1766	6	41,52,52	2.46	15 (36%)	43,81,81	2.40	13 (30%)
4	SF4	F	1194	2	0,12,12	0.00	-	-		
4	SF4	B	1197	2	0,12,12	0.00	-	-		
7	UQ1	G	1251	-	18,18,18	1.09	2 (11%)	22,25,25	1.66	6 (27%)
4	SF4	A	1764	1	0,12,12	0.00	-	-		
4	SF4	F	1197	2	0,12,12	0.00	-	-		
5	MGD	E	1765	6	41,52,52	2.61	22 (53%)	43,81,81	3.28	19 (44%)
5	MGD	A	1765	6	41,52,52	2.60	16 (39%)	43,81,81	3.66	20 (46%)
5	MGD	A	1766	6	41,52,52	2.53	15 (36%)	43,81,81	3.07	11 (25%)
4	SF4	B	1194	2	0,12,12	0.00	-	-		
7	UQ1	C	1252	3	18,18,18	1.09	2 (11%)	22,25,25	1.66	6 (27%)
4	SF4	B	1195	2	0,12,12	0.00	-	-		

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
7	UQ1	G	1251	-	-	3/9/33/33	0/1/1/1
4	SF4	B	1196	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	E	1764	1	-	-	0/6/5/5
4	SF4	F	1195	2	-	-	0/6/5/5
7	UQ1	C	1252	3	-	3/9/33/33	0/1/1/1
5	MGD	E	1766	6	-	1/18/66/66	0/6/6/6
4	SF4	F	1194	2	-	-	0/6/5/5
4	SF4	B	1197	2	-	-	0/6/5/5
5	MGD	A	1766	6	-	1/18/66/66	0/6/6/6
4	SF4	A	1764	1	-	-	0/6/5/5
4	SF4	F	1197	2	-	-	0/6/5/5
5	MGD	E	1765	6	-	2/18/66/66	0/6/6/6
5	MGD	A	1765	6	-	6/18/66/66	0/6/6/6
4	SF4	B	1194	2	-	-	0/6/5/5
4	SF4	F	1196	2	-	-	0/6/5/5
4	SF4	B	1195	2	-	-	0/6/5/5

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1765	MGD	C23-C14	-9.87	1.45	1.53
5	A	1766	MGD	C23-C14	-7.36	1.47	1.53
5	E	1765	MGD	C23-C14	-7.11	1.48	1.53
5	E	1766	MGD	C23-C14	-6.64	1.48	1.53
5	E	1765	MGD	C10-C11	-6.38	1.43	1.52
5	A	1766	MGD	C14-N15	-5.53	1.37	1.45
5	E	1765	MGD	C2'-C1'	-5.23	1.45	1.53
5	A	1765	MGD	C10-C11	-5.22	1.44	1.52
5	E	1766	MGD	O11-C11	-4.89	1.37	1.43
5	A	1766	MGD	C10-C11	-4.89	1.45	1.52
5	A	1766	MGD	C2'-C1'	-4.82	1.46	1.53
5	E	1766	MGD	C19-N19	-4.72	1.24	1.33
5	E	1766	MGD	C16-N15	-4.72	1.28	1.38
5	E	1766	MGD	C14-N15	-4.51	1.38	1.45
5	A	1765	MGD	C6-C5	4.42	1.49	1.41
5	E	1766	MGD	C19-N18	-4.36	1.27	1.35
5	E	1766	MGD	O4'-C4'	-3.73	1.36	1.45
5	E	1765	MGD	O11-C11	-3.71	1.38	1.43
5	E	1765	MGD	C2-N1	-3.68	1.28	1.35
5	A	1765	MGD	O11-C11	-3.65	1.38	1.43
5	E	1765	MGD	C3'-C4'	-3.52	1.44	1.53
5	A	1766	MGD	C17-C16	3.47	1.46	1.41
5	E	1765	MGD	C19-N18	-3.45	1.29	1.35
5	E	1765	MGD	C19-N20	-3.33	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1765	MGD	C23-N22	-3.30	1.38	1.44
5	A	1766	MGD	O4'-C4'	-3.23	1.37	1.45
5	A	1766	MGD	PB-O2B	-3.22	1.40	1.55
5	A	1766	MGD	C23-N22	-3.18	1.38	1.44
5	A	1765	MGD	O11-C23	-3.17	1.39	1.43
5	A	1766	MGD	O11-C11	-3.13	1.39	1.43
5	E	1766	MGD	C4-N3	-3.05	1.30	1.35
5	A	1765	MGD	C2'-C1'	-3.03	1.49	1.53
5	E	1765	MGD	O3'-C3'	-2.97	1.36	1.43
5	A	1765	MGD	C19-N20	-2.94	1.30	1.35
5	A	1766	MGD	PA-O2A	-2.90	1.41	1.55
5	A	1765	MGD	O4'-C4'	-2.90	1.38	1.45
5	A	1765	MGD	C21-N20	-2.86	1.29	1.34
5	A	1765	MGD	O2'-C2'	-2.86	1.36	1.43
5	E	1766	MGD	C2'-C1'	-2.86	1.49	1.53
5	E	1766	MGD	C23-N22	-2.82	1.39	1.44
5	A	1766	MGD	C19-N19	-2.81	1.28	1.33
5	E	1766	MGD	C10-C11	-2.68	1.48	1.52
5	E	1765	MGD	O11-C23	-2.66	1.39	1.43
5	A	1765	MGD	C3'-C4'	-2.62	1.46	1.53
5	A	1766	MGD	PA-O1A	-2.58	1.41	1.50
5	E	1765	MGD	C23-N22	-2.57	1.39	1.44
5	E	1766	MGD	PA-O1A	-2.42	1.42	1.50
5	E	1765	MGD	O4'-C4'	-2.40	1.39	1.45
5	E	1765	MGD	O2'-C2'	-2.39	1.37	1.43
5	E	1765	MGD	C17-C16	2.35	1.44	1.41
5	E	1765	MGD	C4-N3	-2.34	1.32	1.35
5	A	1765	MGD	C19-N18	-2.33	1.31	1.35
5	E	1766	MGD	O17-C17	-2.31	1.18	1.24
5	E	1765	MGD	PB-O1B	-2.30	1.42	1.50
5	E	1765	MGD	C14-N15	-2.28	1.42	1.45
7	G	1251	UQ1	C6-C5	2.28	1.39	1.35
7	C	1252	UQ1	C6-C5	2.28	1.39	1.35
5	E	1765	MGD	O3A-C10	-2.27	1.36	1.44
5	A	1765	MGD	PA-O2A	-2.22	1.44	1.55
5	E	1765	MGD	C16-C21	2.21	1.45	1.41
5	E	1765	MGD	PA-O2A	-2.20	1.45	1.55
5	E	1766	MGD	O3'-C3'	2.19	1.48	1.43
5	A	1766	MGD	C16-N15	-2.17	1.33	1.38
5	A	1766	MGD	C4-N3	-2.14	1.32	1.35
5	A	1765	MGD	C16-N15	-2.12	1.33	1.38
7	C	1252	UQ1	O1-C1	-2.11	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1766	MGD	C5-C4	2.09	1.46	1.40
7	G	1251	UQ1	O1-C1	-2.07	1.18	1.23
5	E	1765	MGD	O6-C6	-2.07	1.19	1.24
5	E	1765	MGD	C2'-C3'	-2.07	1.47	1.53
5	A	1765	MGD	PB-O2B	-2.06	1.45	1.55
5	A	1766	MGD	PB-O1B	-2.00	1.43	1.50

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1766	MGD	O11-C23-C14	14.24	118.46	108.96
5	A	1765	MGD	O11-C23-C14	12.67	117.42	108.96
5	E	1766	MGD	O11-C23-C14	10.85	116.20	108.96
5	E	1765	MGD	O11-C23-N22	-9.77	98.53	108.57
5	A	1765	MGD	C17-C16-N15	9.25	126.88	119.12
5	A	1765	MGD	C2-N3-C4	8.33	124.88	115.36
5	E	1765	MGD	C17-C16-N15	7.84	125.70	119.12
5	E	1765	MGD	C2-N3-C4	7.27	123.66	115.36
5	A	1766	MGD	C17-C16-N15	7.07	125.06	119.12
5	E	1765	MGD	O11-C23-C14	-6.77	104.45	108.96
5	A	1765	MGD	C5-C6-N1	-5.45	115.98	123.43
5	A	1765	MGD	C6-N1-C2	5.30	124.35	115.93
5	A	1765	MGD	N3-C2-N1	-5.21	120.27	127.22
5	E	1765	MGD	C4-C5-N7	-5.20	103.98	109.40
5	A	1766	MGD	C2-N3-C4	5.13	121.22	115.36
5	E	1765	MGD	C6-C5-C4	-4.88	116.14	120.80
5	A	1765	MGD	C17-N18-C19	4.72	123.42	115.93
5	E	1766	MGD	C2-N3-C4	4.47	120.47	115.36
5	E	1765	MGD	C6-N1-C2	4.42	122.96	115.93
5	A	1765	MGD	C4-C5-N7	-4.31	104.91	109.40
5	A	1766	MGD	C6-C5-C4	-4.24	116.75	120.80
5	E	1765	MGD	N3-C2-N1	-4.16	121.67	127.22
5	E	1765	MGD	C19-N20-C21	4.10	123.74	114.54
5	A	1765	MGD	O4'-C1'-C2'	-4.02	101.05	106.93
5	E	1765	MGD	C5-C6-N1	-3.95	118.03	123.43
5	A	1765	MGD	N2-C2-N1	3.91	123.33	117.25
5	A	1766	MGD	C6-N1-C2	3.86	122.06	115.93
5	E	1766	MGD	C5-C6-N1	-3.83	118.19	123.43
5	A	1765	MGD	C19-N20-C21	3.78	123.01	114.54
5	A	1766	MGD	O11-C23-N22	3.74	112.41	108.57
5	A	1766	MGD	N3-C2-N1	-3.73	122.25	127.22
5	A	1765	MGD	C6-C5-C4	-3.55	117.40	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	1251	UQ1	C10-C9-C8	-3.45	112.66	122.65
7	C	1252	UQ1	C10-C9-C8	-3.45	112.69	122.65
5	E	1765	MGD	C1'-N9-C4	-3.20	121.02	126.64
5	E	1765	MGD	C17-N18-C19	3.19	121.00	115.93
5	A	1766	MGD	C5-C6-N1	-3.11	119.18	123.43
5	A	1765	MGD	N19-C19-N18	3.04	121.99	117.25
5	A	1765	MGD	C16-C21-N22	3.03	120.90	118.13
5	A	1765	MGD	N18-C19-N20	-2.98	120.74	125.42
5	E	1765	MGD	C16-C21-N22	2.94	120.82	118.13
5	E	1766	MGD	O2A-PA-O1A	2.88	126.49	112.24
7	G	1251	UQ1	C5-C6-C1	-2.83	116.92	119.58
7	C	1252	UQ1	C5-C6-C1	-2.81	116.93	119.58
5	E	1765	MGD	O4'-C1'-C2'	-2.76	102.89	106.93
5	E	1766	MGD	C17-N18-C19	2.73	120.27	115.93
5	E	1766	MGD	O11-C23-N22	-2.71	105.78	108.57
5	E	1765	MGD	O3'-C3'-C4'	-2.71	103.21	111.05
5	A	1766	MGD	O5'-C5'-C4'	-2.71	99.67	108.99
5	E	1766	MGD	O3'-C3'-C4'	2.68	118.81	111.05
5	E	1766	MGD	C4-C5-N7	-2.68	106.61	109.40
7	C	1252	UQ1	O1-C1-C6	-2.63	116.94	121.55
5	E	1766	MGD	C6-N1-C2	2.63	120.10	115.93
7	G	1251	UQ1	O1-C1-C6	-2.63	116.94	121.55
5	E	1766	MGD	C19-N20-C21	2.60	120.36	114.54
5	A	1765	MGD	O4'-C4'-C5'	-2.53	101.04	109.37
5	E	1765	MGD	N2-C2-N1	2.53	121.19	117.25
7	C	1252	UQ1	C11-C9-C8	2.53	129.96	122.65
7	G	1251	UQ1	C11-C9-C8	2.53	129.96	122.65
5	E	1766	MGD	N19-C19-N20	2.51	121.16	117.25
5	E	1765	MGD	O2B-PB-O1B	2.38	123.98	112.24
5	A	1765	MGD	C23-C14-C13	-2.37	105.21	110.53
7	C	1252	UQ1	C6-C5-C4	2.36	121.05	119.18
7	G	1251	UQ1	C6-C5-C4	2.33	121.02	119.18
5	A	1766	MGD	C16-C21-N22	-2.30	116.03	118.13
5	A	1765	MGD	PA-O3B-PB	2.29	140.70	132.83
5	A	1766	MGD	O4'-C4'-C5'	-2.29	101.84	109.37
5	E	1765	MGD	C16-N15-C14	-2.23	111.92	120.00
7	G	1251	UQ1	CM3-O3-C3	-2.20	108.69	116.47
7	C	1252	UQ1	CM3-O3-C3	-2.18	108.73	116.47
5	A	1765	MGD	C16-C17-N18	-2.16	117.88	124.01
5	E	1765	MGD	O2A-PA-O1A	2.12	122.72	112.24
5	E	1766	MGD	C17-C16-N15	2.05	120.84	119.12
5	E	1766	MGD	C6-C5-C4	-2.04	118.85	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1765	MGD	C17-C16-C21	2.01	116.36	114.57

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	1251	UQ1	C1-C6-C7-C8
7	G	1251	UQ1	C5-C6-C7-C8
5	E	1765	MGD	O4'-C4'-C5'-O5'
5	A	1765	MGD	C5'-O5'-PB-O2B
7	C	1252	UQ1	C1-C6-C7-C8
7	C	1252	UQ1	C5-C6-C7-C8
5	E	1765	MGD	PA-O3B-PB-O5'
5	A	1765	MGD	PA-O3B-PB-O5'
5	A	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	C5'-O5'-PB-O3B
5	E	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	C5'-O5'-PB-O1B
5	A	1765	MGD	PA-O3B-PB-O1B
7	G	1251	UQ1	C4-C3-O3-CM3
7	C	1252	UQ1	C4-C3-O3-CM3
5	A	1765	MGD	O4'-C4'-C5'-O5'

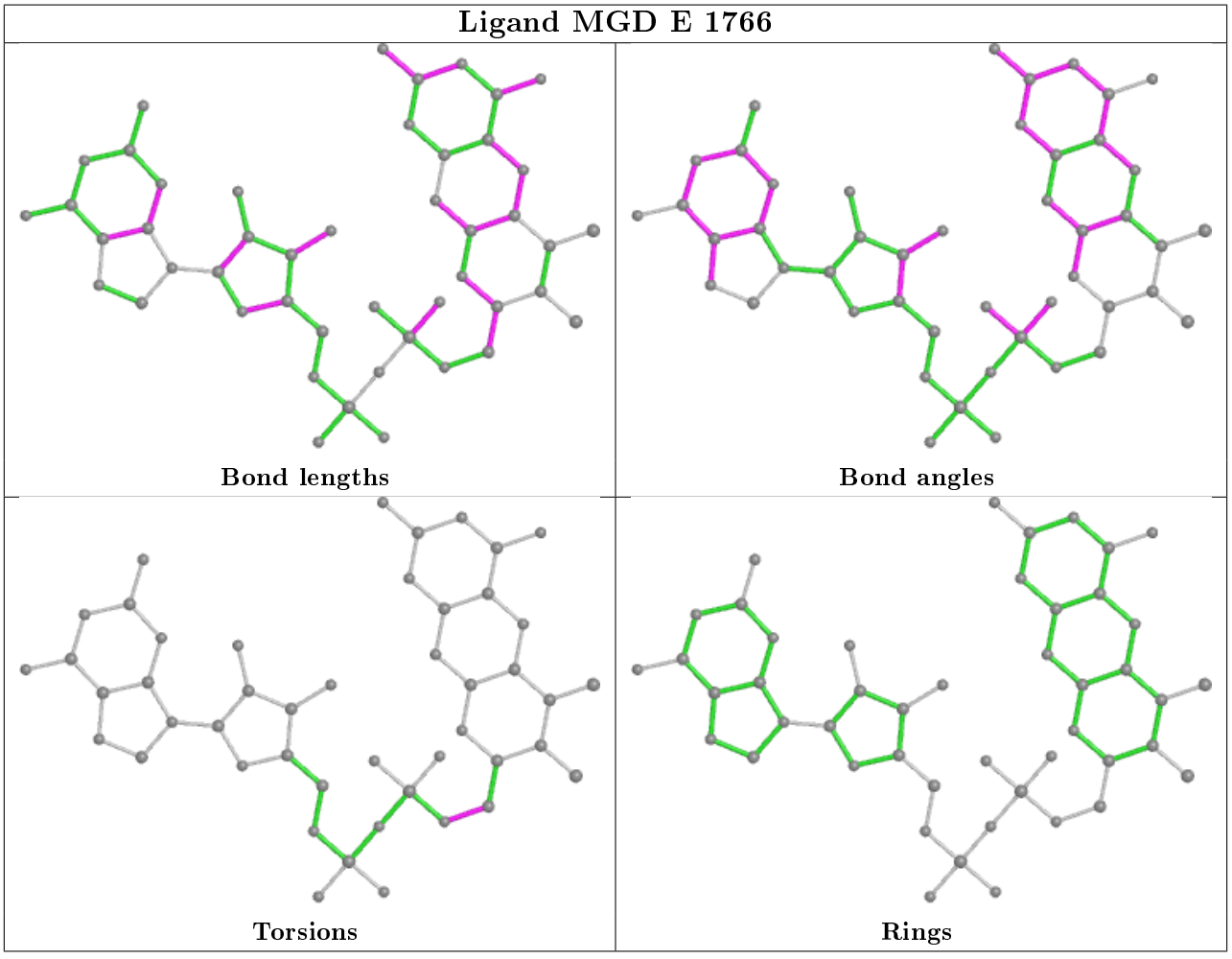
There are no ring outliers.

14 monomers are involved in 100 short contacts:

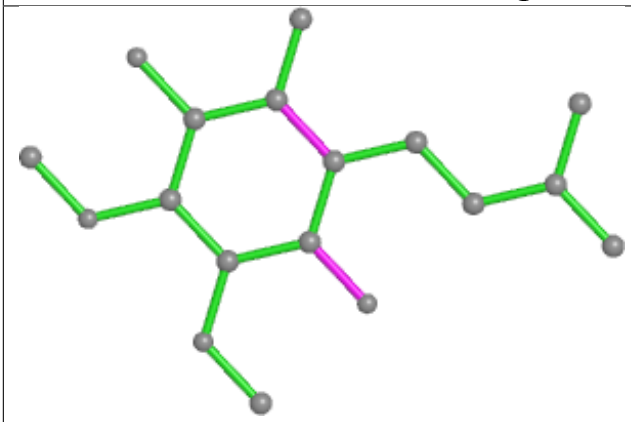
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1195	SF4	2	0
4	B	1196	SF4	2	0
4	E	1764	SF4	1	0
4	F	1196	SF4	1	0
5	E	1766	MGD	13	0
4	F	1194	SF4	3	0
7	G	1251	UQ1	22	0
4	A	1764	SF4	2	0
5	E	1765	MGD	10	0
5	A	1765	MGD	7	0
5	A	1766	MGD	5	0
4	B	1194	SF4	3	0
7	C	1252	UQ1	26	0
4	B	1195	SF4	3	0

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 then 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.

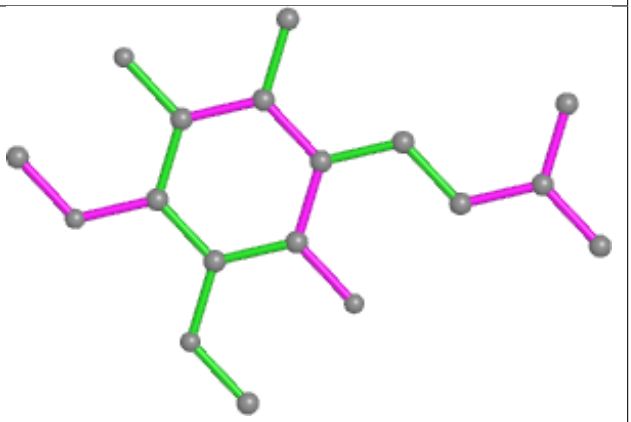
Ligand MGD E 1766



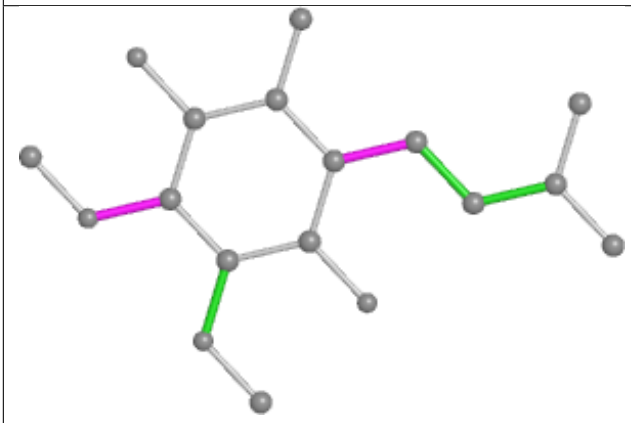
Ligand UQ1 G 1251



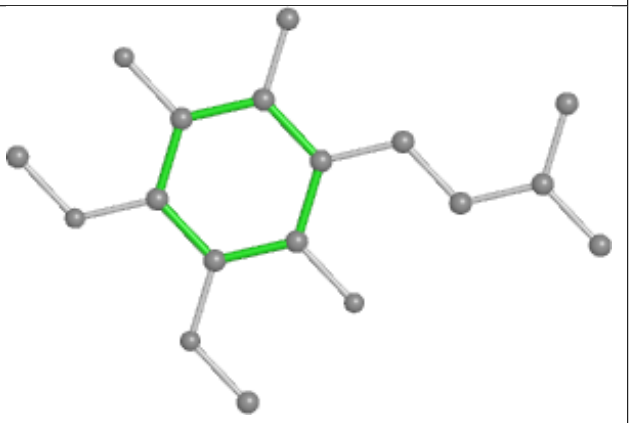
Bond lengths



Bond angles

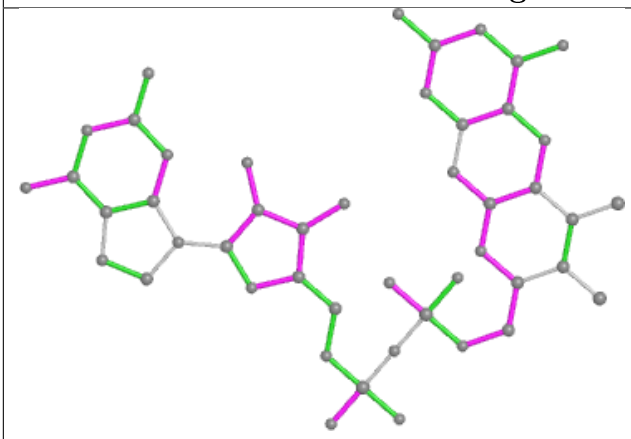


Torsions

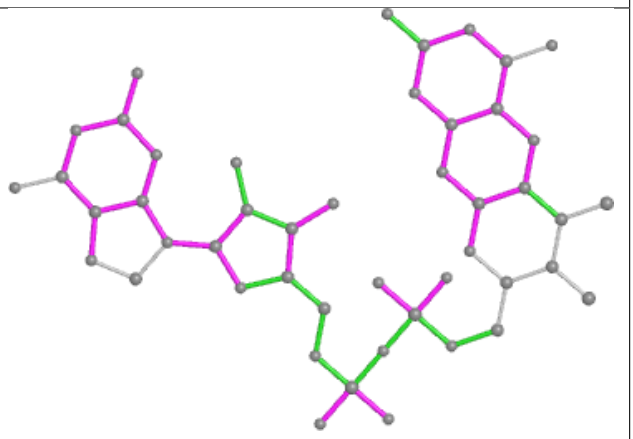


Rings

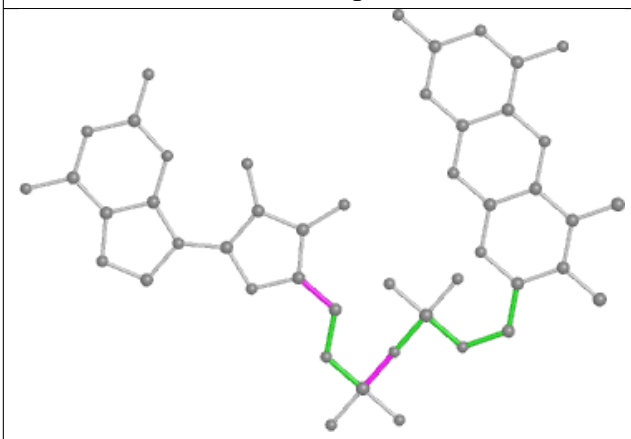
Ligand MGD E 1765



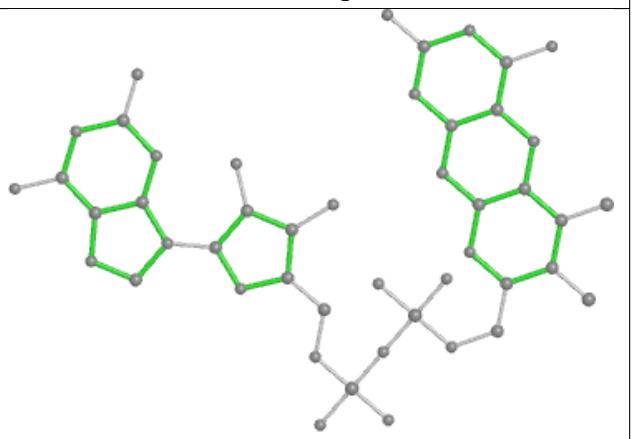
Bond lengths



Bond angles

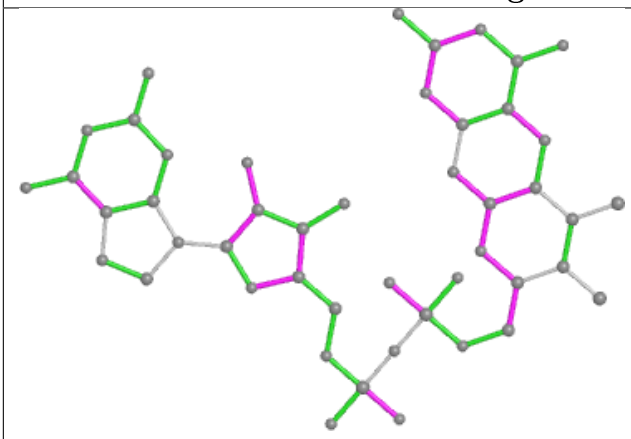


Torsions

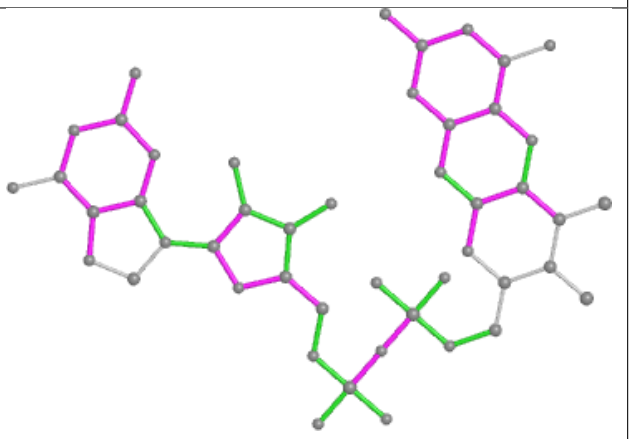


Rings

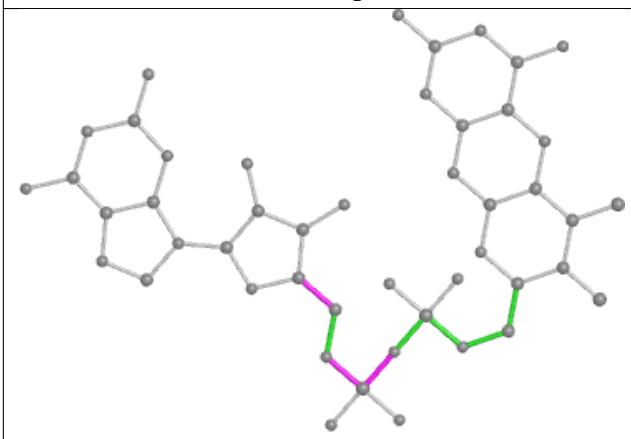
Ligand MGD A 1765



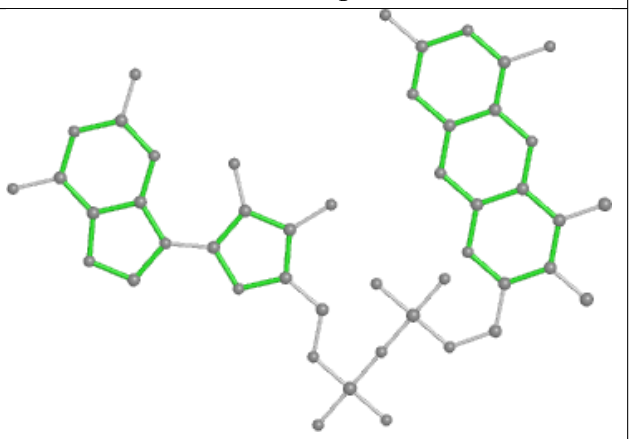
Bond lengths



Bond angles

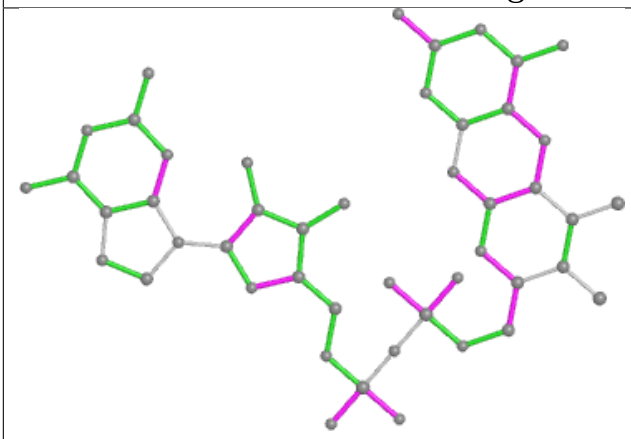


Torsions

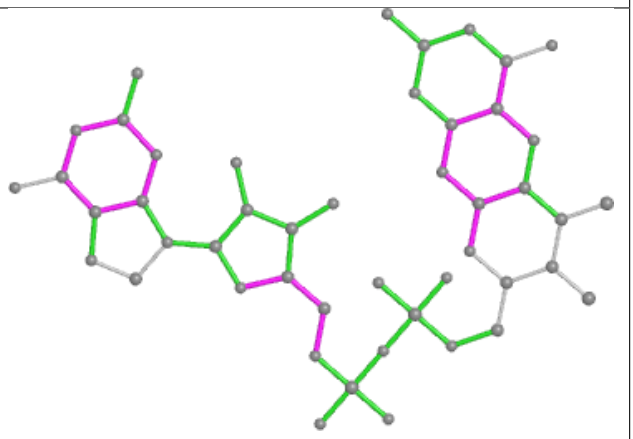


Rings

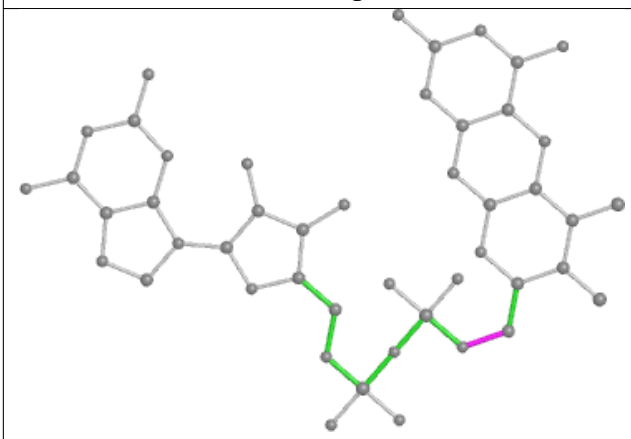
Ligand MGD A 1766



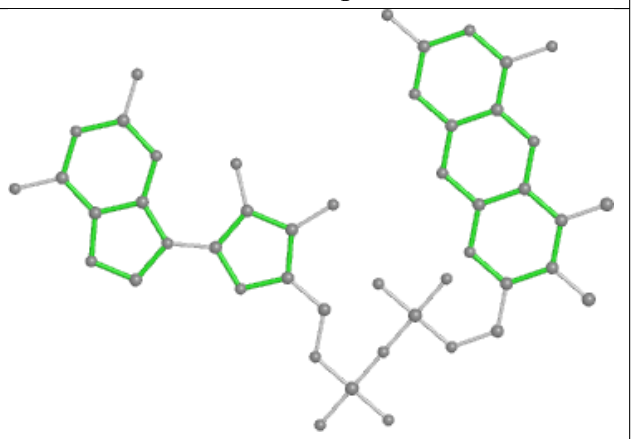
Bond lengths



Bond angles

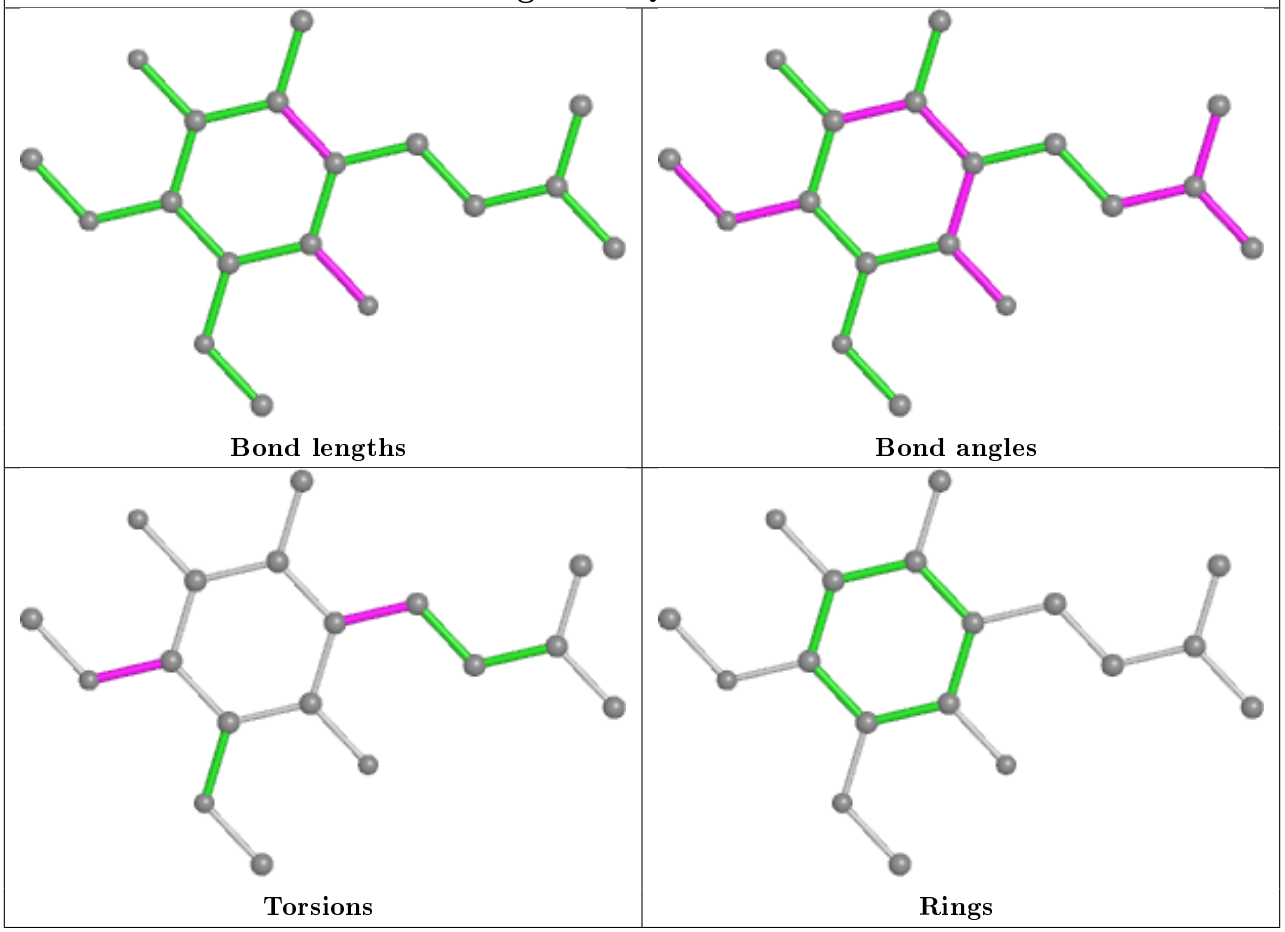


Torsions



Rings

Ligand UQ1 C 1252



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	387:GLY	C	388:CYS	N	1.17

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, 95^{th} 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	735/765 (96%)	0.59	68 (9%) 8 3	42, 73, 106, 157	0
1	E	735/765 (96%)	0.70	74 (10%) 7 2	44, 75, 104, 157	0
2	B	194/195 (99%)	0.06	5 (2%) 56 33	43, 61, 83, 106	0
2	F	194/195 (99%)	0.62	17 (8%) 10 4	50, 73, 91, 109	0
3	C	251/253 (99%)	0.27	13 (5%) 27 12	45, 75, 103, 119	0
3	G	251/253 (99%)	0.65	30 (11%) 4 2	55, 86, 115, 132	0
All	All	2360/2426 (97%)	0.55	207 (8%) 10 4	42, 74, 106, 157	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	251	GLY	11.4
1	A	396	HIS	10.5
3	C	111	GLY	10.1
1	A	392	SER	10.0
1	E	394	GLY	7.7
1	A	397	GLU	7.4
1	A	389	SER	7.2
1	A	384	ALA	6.7
1	A	393	GLY	6.3
1	E	390	GLY	6.2
1	E	396	HIS	6.2
1	E	393	GLY	6.1
1	A	764	ARG	5.6
1	E	397	GLU	5.6
1	E	398	PRO	5.5
1	A	398	PRO	5.3
3	C	110	LYS	5.3
1	A	388	CYS	5.1
2	F	1	MET	5.0

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Mol	Chain	Res	Type	RSRZ
1	E	389	SER	4.9
3	C	224	GLU	4.7
3	G	74	THR	4.7
3	G	111	SER	4.6
3	G	110	GLY	4.6
1	E	592	LEU	4.5
1	E	392	SER	4.5
1	A	394	GLY	4.5
1	E	555	LEU	4.4
1	E	395	ASP	4.4
3	C	112	SER	4.3
1	A	581	LEU	4.3
3	G	42	ASP	4.3
1	A	390	GLY	4.1
1	E	386	GLY	4.1
1	E	594	CYS	4.1
1	A	576	GLU	4.1
3	G	78	LEU	4.1
2	B	1	MET	4.0
1	E	399	GLU	4.0
3	G	81	SER	4.0
1	E	599	GLU	4.0
1	A	567	ARG	4.0
1	A	385	ALA	3.9
1	A	391	PRO	3.8
3	G	109	LYS	3.7
1	A	570	PRO	3.7
2	F	193	HIS	3.7
3	G	107	LEU	3.6
1	E	374	TYR	3.6
1	E	606	PRO	3.6
2	F	75	SER	3.5
3	G	224	ARG	3.5
3	C	223	GLN	3.5
1	E	60	ASN	3.4
1	A	591	GLU	3.4
1	E	36	GLU	3.4
3	G	221	TRP	3.3
1	A	599	GLU	3.3
3	G	77	TRP	3.3
2	B	2	PRO	3.2
1	A	362	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	539	THR	3.2
1	A	401	PHE	3.2
1	E	518	GLY	3.1
1	E	113	ARG	3.1
1	E	56	HIS	3.1
1	A	281	LYS	3.1
3	G	113	ARG	3.1
1	A	571	TRP	3.0
1	E	546	THR	3.0
1	E	569	LYS	3.0
3	C	75	THR	3.0
1	A	579	GLY	2.9
1	E	539	THR	2.9
1	A	295	ASP	2.9
1	E	761	ASP	2.9
1	A	617	GLY	2.9
3	G	225	LEU	2.9
3	G	106	TYR	2.9
2	F	194	HIS	2.9
1	E	106	GLN	2.8
3	G	43	ALA	2.8
1	A	551	LEU	2.7
1	A	395	ASP	2.7
1	E	44	CYS	2.7
1	A	169	SER	2.7
1	A	580	ARG	2.7
3	C	19	ALA	2.7
1	E	387	GLY	2.7
3	C	113	GLN	2.7
1	E	164	ASN	2.6
1	A	577	LYS	2.6
1	E	66	GLU	2.6
1	A	566	GLN	2.6
1	E	39	SER	2.6
1	A	685	THR	2.6
1	A	284	VAL	2.6
3	C	79	LEU	2.6
1	E	591	GLU	2.6
3	C	252	GLY	2.5
1	E	537	TRP	2.5
3	G	112	GLN	2.5
1	A	583	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	280	ALA	2.5
1	E	554	ASP	2.5
2	F	87	PRO	2.5
1	E	383	PRO	2.5
1	A	601	GLY	2.5
1	E	607	VAL	2.5
1	E	135	TYR	2.5
1	E	665	ASP	2.5
2	F	80	ASP	2.5
1	E	580	ARG	2.5
1	A	38	LYS	2.5
1	E	745	GLU	2.5
1	A	360	PRO	2.4
1	E	431	PRO	2.4
3	C	209	TRP	2.4
1	E	108	GLY	2.4
1	E	597	PHE	2.4
2	F	72	THR	2.4
1	A	592	LEU	2.4
1	E	514	ASP	2.4
1	E	366	ALA	2.4
1	A	164	ASN	2.4
1	A	131	ILE	2.4
1	E	104	GLY	2.4
1	A	383	PRO	2.4
1	E	400	GLY	2.4
1	A	586	ALA	2.4
1	A	590	ILE	2.4
1	A	568	GLY	2.3
2	B	149	GLU	2.3
3	G	68	PRO	2.3
3	G	229	ALA	2.3
1	A	37	VAL	2.3
1	E	508	ALA	2.3
1	A	596	ARG	2.3
2	F	84	LEU	2.3
2	F	3	ARG	2.3
1	E	58	VAL	2.3
1	A	587	SER	2.3
2	F	76	TYR	2.3
1	E	540	ILE	2.3
3	G	82	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	147	ASP	2.3
1	E	598	LYS	2.3
3	G	222	GLN	2.3
1	E	460	ASP	2.2
2	F	128	VAL	2.2
3	G	38	HIS	2.2
1	E	439	GLY	2.2
1	A	36	GLU	2.2
1	A	324	PRO	2.2
1	E	117	TRP	2.2
1	A	102	VAL	2.2
3	G	169	PRO	2.2
1	E	558	MET	2.2
1	A	558	MET	2.2
1	A	573	GLU	2.2
1	A	134	LYS	2.2
1	E	630	THR	2.2
1	E	115	ALA	2.1
1	A	403	PRO	2.1
1	E	572	LEU	2.1
3	G	105	LEU	2.1
2	F	2	PRO	2.1
3	G	39	LEU	2.1
1	A	283	THR	2.1
1	A	597	PHE	2.1
1	E	405	ALA	2.1
2	F	4	TYR	2.1
1	E	174	THR	2.1
1	E	146	GLY	2.1
2	B	147	ASP	2.1
1	A	361	GLY	2.1
1	E	512	LEU	2.1
3	G	244	ALA	2.1
1	A	761	ASP	2.1
1	E	131	ILE	2.1
1	E	147	THR	2.1
3	G	66	GLU	2.1
1	A	574	ASP	2.1
1	A	359	ARG	2.1
1	E	633	ARG	2.1
1	A	399	GLU	2.1
1	A	553	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	634	THR	2.1
1	E	553	LEU	2.1
2	F	19	CYS	2.1
2	B	125	LYS	2.1
1	E	384	ALA	2.1
1	E	525	LEU	2.1
1	A	569	LYS	2.0
2	F	83	VAL	2.0
3	C	109	GLY	2.0
3	C	74	PHE	2.0
1	E	196	ASP	2.0
3	G	108	GLY	2.0
1	E	109	GLU	2.0
3	G	45	ALA	2.0
1	A	602	HIS	2.0
1	E	568	GLY	2.0
1	E	600	ALA	2.0
2	F	74	ALA	2.0
3	G	71	PHE	2.0
1	A	130	GLU	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 carbohydrates 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, 95^{th} 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
6	MO	E	1767	1/1	0.72	0.17	60,60,60,60	0
7	UQ1	G	1251	18/18	0.83	0.33	82,86,87,88	0
6	MO	A	1767	1/1	0.84	0.17	55,55,55,55	0

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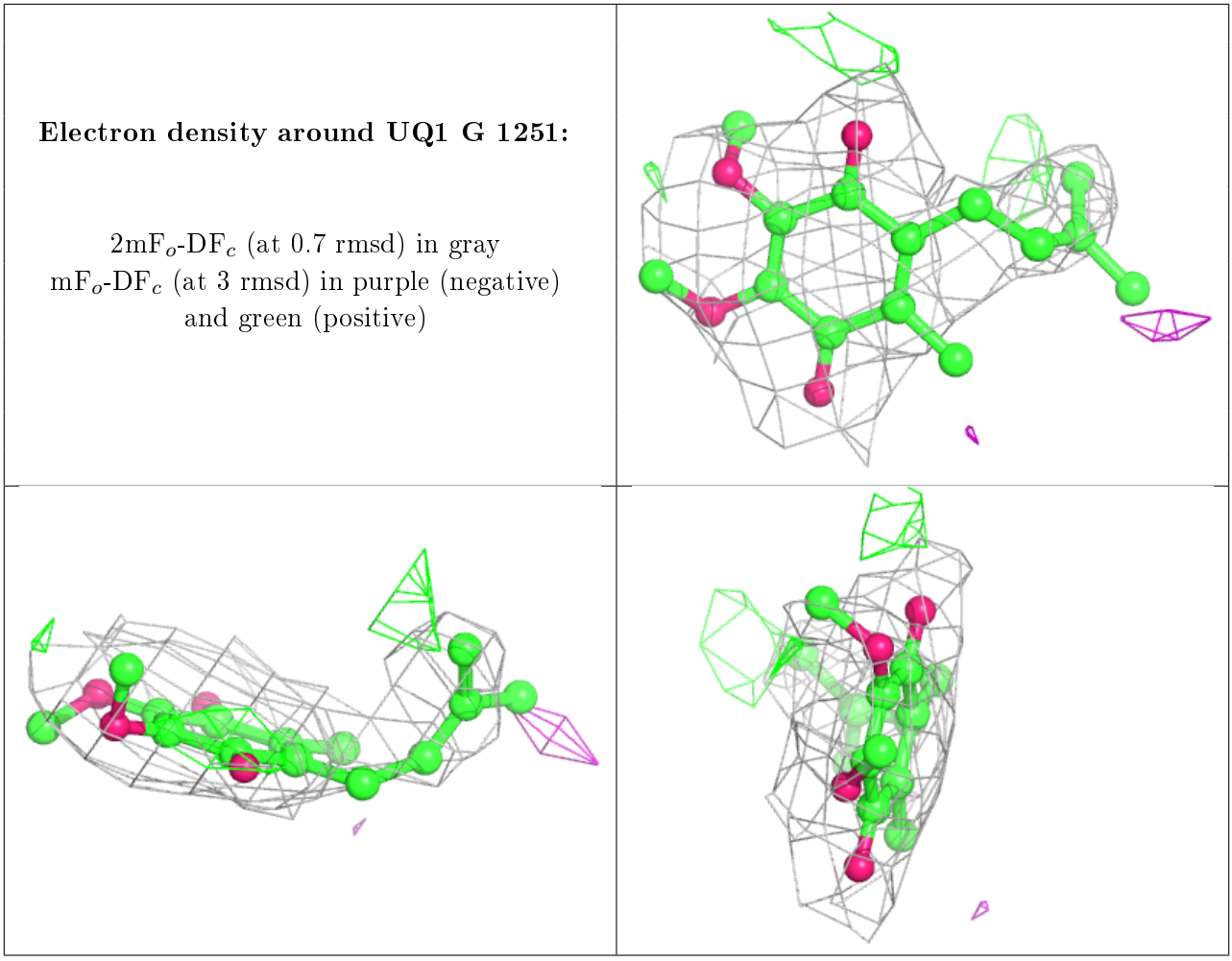
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SF4	F	1195	8/8	0.90	0.18	56,63,69,69	0
4	SF4	E	1764	8/8	0.91	0.21	60,69,74,77	0
4	SF4	F	1197	8/8	0.91	0.14	77,82,85,86	0
4	SF4	F	1194	8/8	0.92	0.13	67,71,72,73	0
4	SF4	F	1196	8/8	0.92	0.18	66,72,74,79	0
4	SF4	B	1196	8/8	0.93	0.17	48,56,63,63	0
5	MGD	E	1766	47/47	0.93	0.28	45,54,61,62	0
5	MGD	E	1765	47/47	0.93	0.30	50,61,75,76	0
5	MGD	A	1766	47/47	0.94	0.25	46,50,63,64	0
7	UQ1	C	1252	18/18	0.94	0.28	75,77,80,80	0
5	MGD	A	1765	47/47	0.95	0.23	52,55,58,59	0
4	SF4	B	1194	8/8	0.97	0.09	62,65,67,68	0
4	SF4	A	1764	8/8	0.97	0.18	50,54,57,57	0
4	SF4	B	1197	8/8	0.98	0.11	52,55,56,57	0
4	SF4	B	1195	8/8	0.98	0.11	60,61,63,65	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.

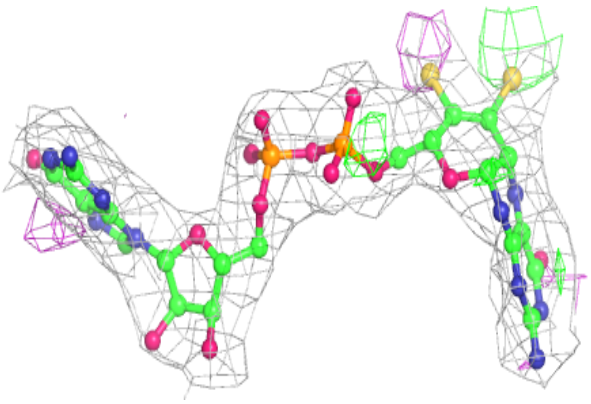
Electron density around UQ1 G 1251:

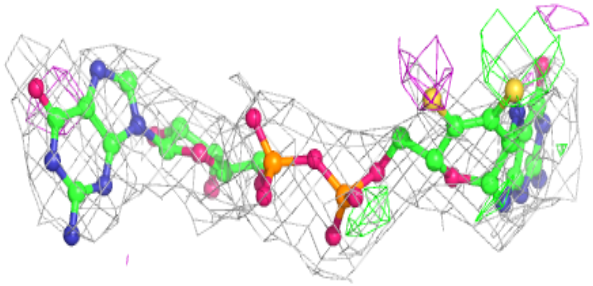
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

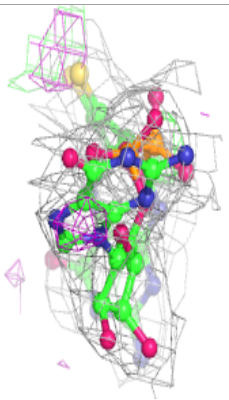


Electron density around MGD E 1766:

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

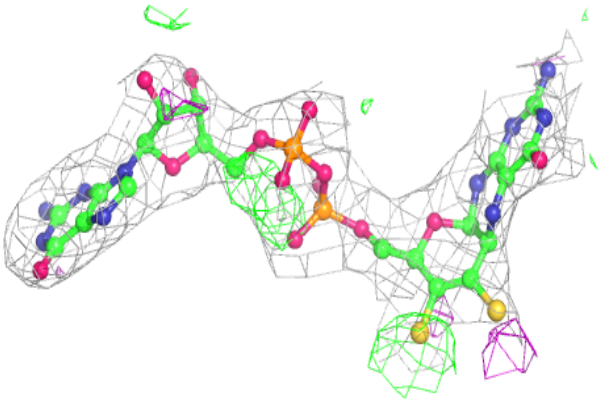


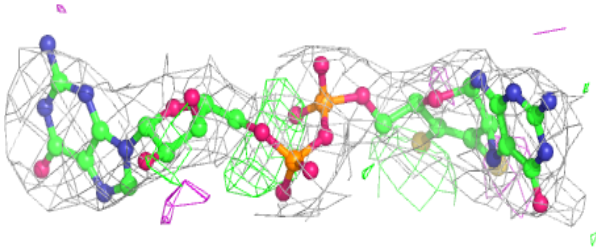




Electron density around MGD E 1765:

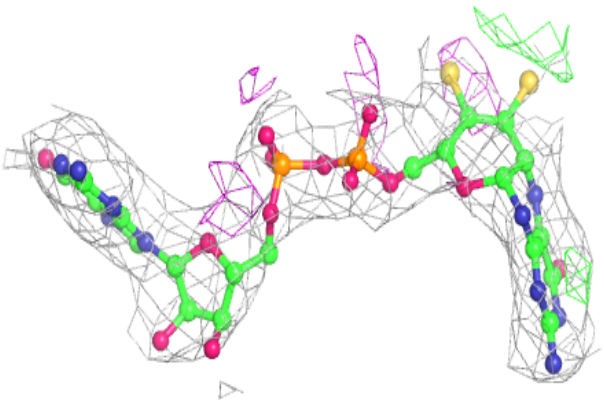
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

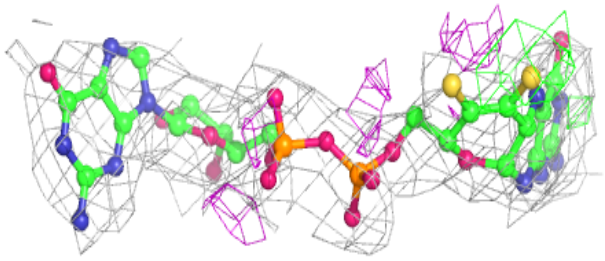


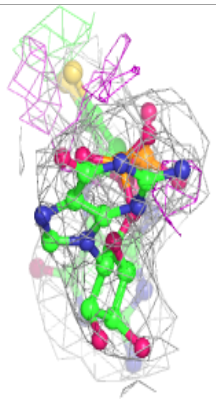


Electron density around MGD A 1766:

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

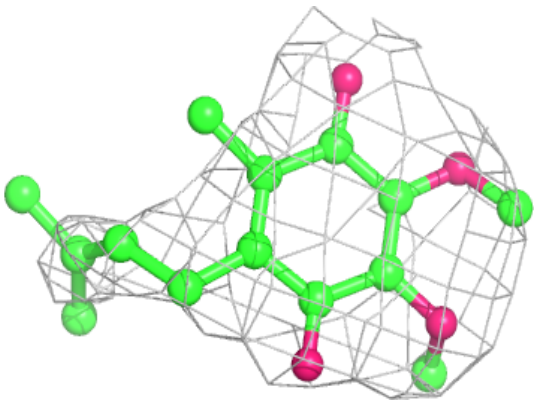


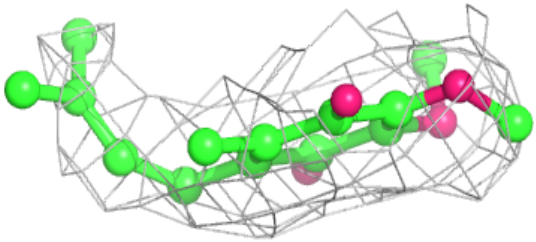


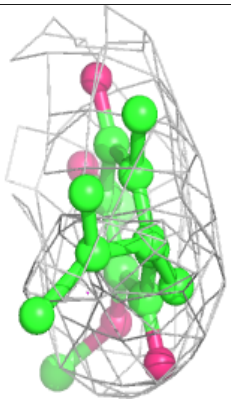


Electron density around UQ1 C 1252:

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

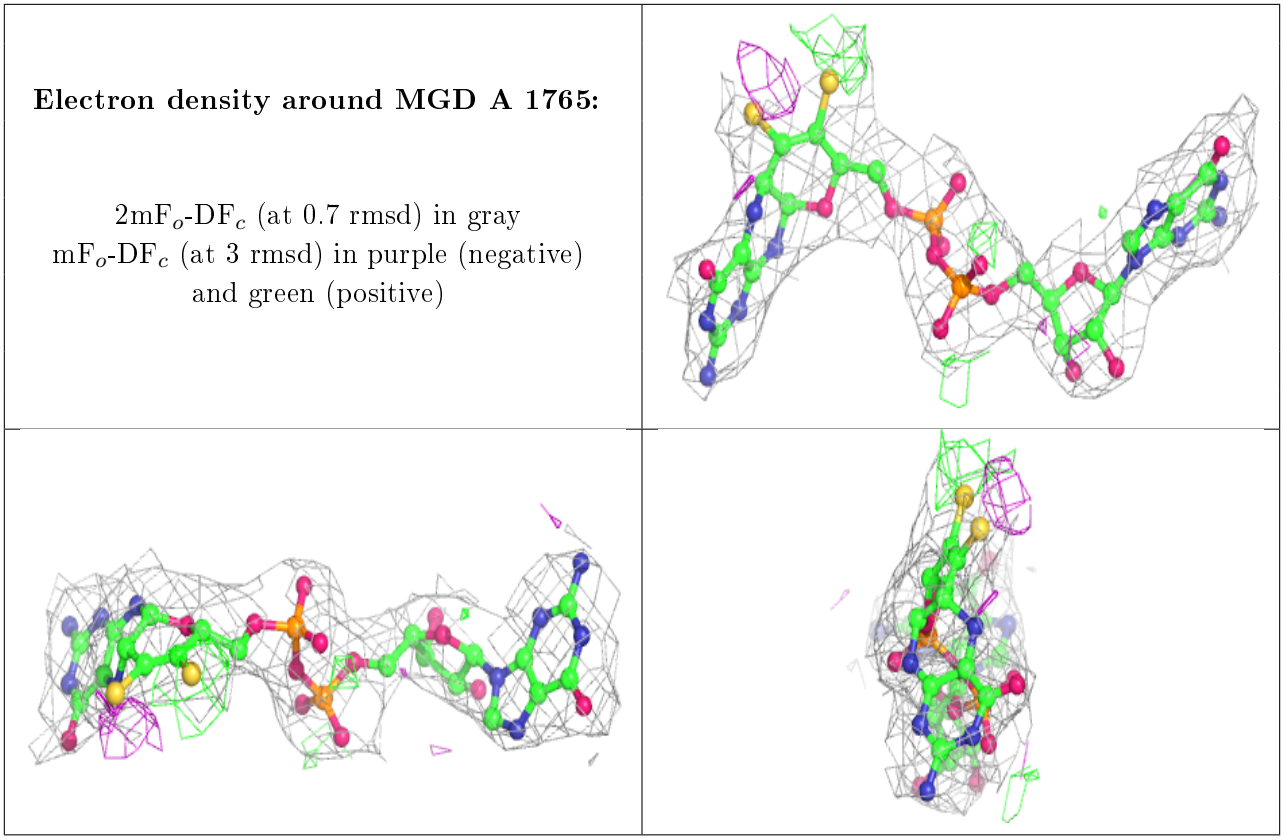






Electron density around MGD A 1765:

$2mF_o$-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.