



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:22 AM UTC

PDB ID : 2VPW / pdb_00002vpw
Title : Polysulfide reductase with bound menaquinone
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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 types of validation reports are described at

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

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

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

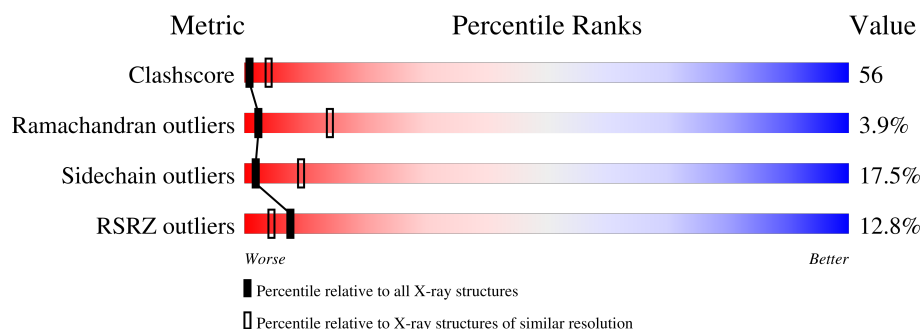
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	765	12% 31% 43% 17% 5% .
1	E	765	10% 32% 41% 17% 6% .
2	B	195	8% 38% 44% 13% . .
2	F	195	14% 36% 47% 13% . .
3	C	253	9% 49% 38% 11% . .
3	G	253	28% 43% 40% 13% . .

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	B	1194	-	-	X	-
4	SF4	B	1195	-	-	X	-
4	SF4	B	1196	-	-	X	-
4	SF4	F	1194	-	-	X	-
4	SF4	F	1195	-	-	X	-
7	MQ7	C	1252	-	-	-	X
7	MQ7	G	1251	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20223 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.

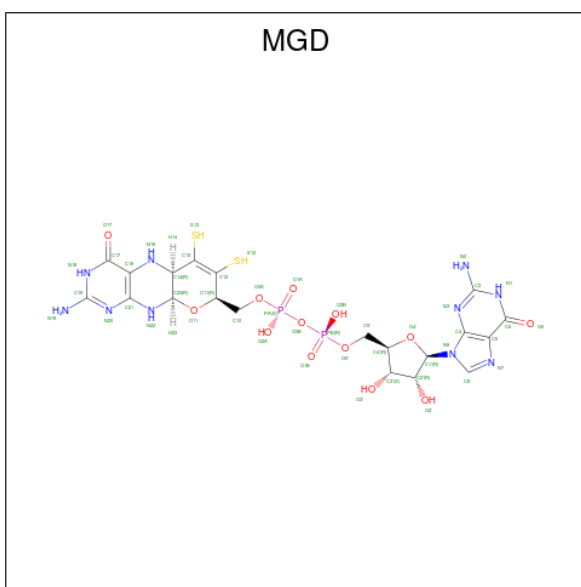
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			
3	G	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- 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 (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

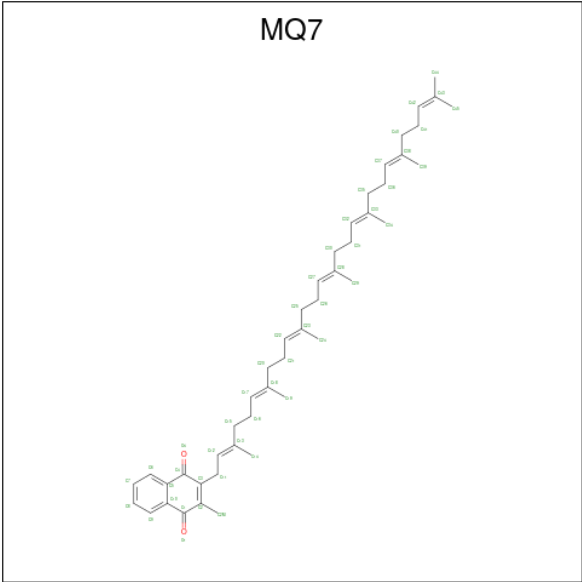


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	A	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
5	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 6 is MOLYBDENUM ATOM (CCD ID: 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		

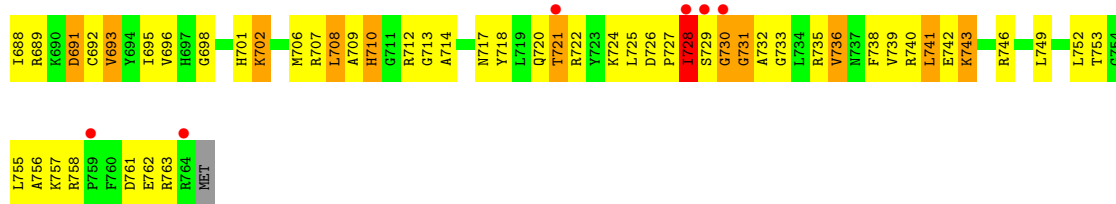
- Molecule 7 is MENAQUINONE-7 (CCD ID: MQ7) (formula: C₄₆H₆₄O₂).



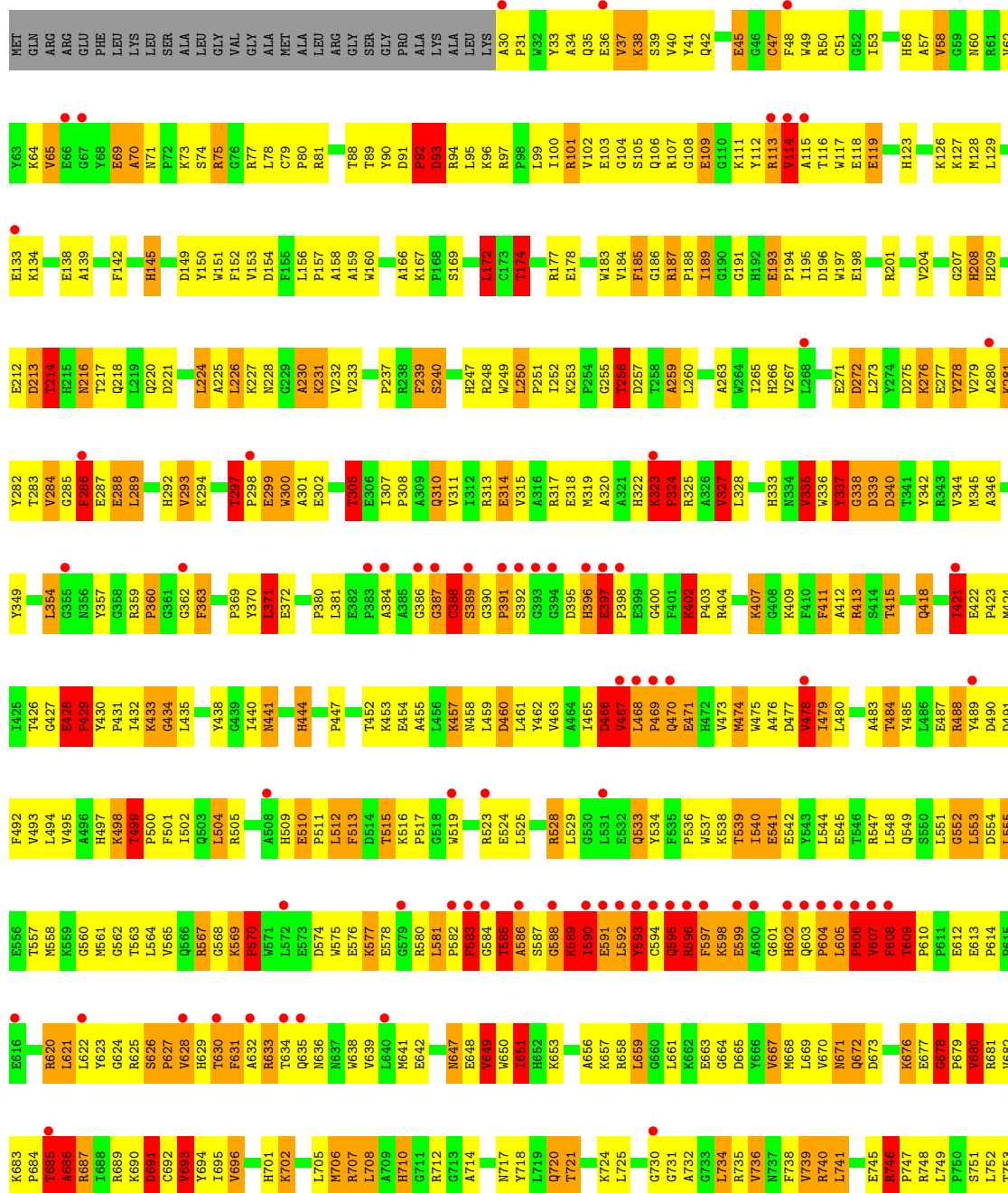
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			15	13	2		
7	G	1	Total	C	O	0	0
			15	13	2		

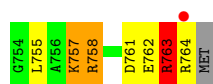
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	386	Total	O	0	0
			386	386		
8	B	149	Total	O	0	0
			149	149		
8	C	90	Total	O	0	0
			90	90		
8	E	453	Total	O	0	0
			453	453		
8	F	129	Total	O	0	0
			129	129		
8	G	78	Total	O	0	0
			78	78		

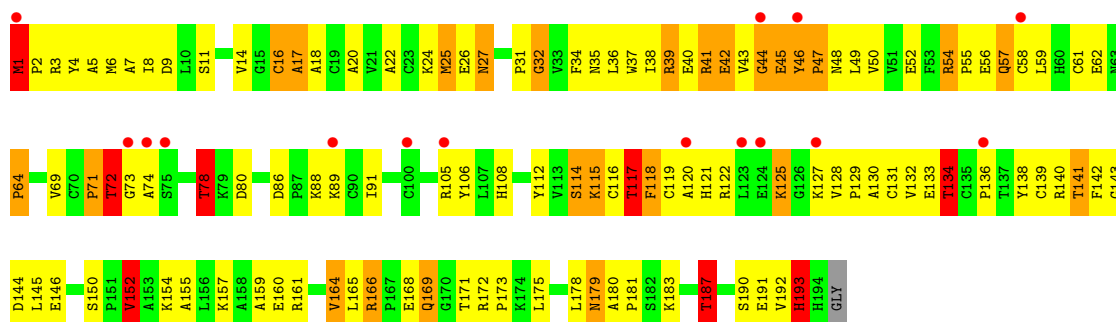


● Molecule 1: THIOSULFATE REDUCTASE

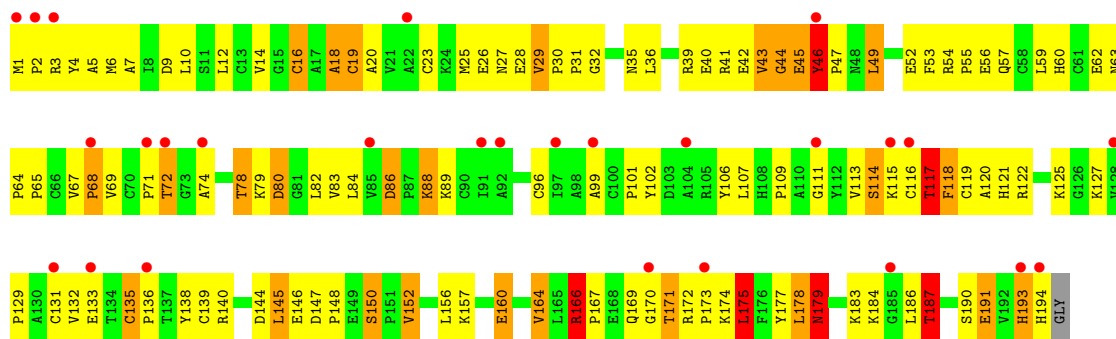




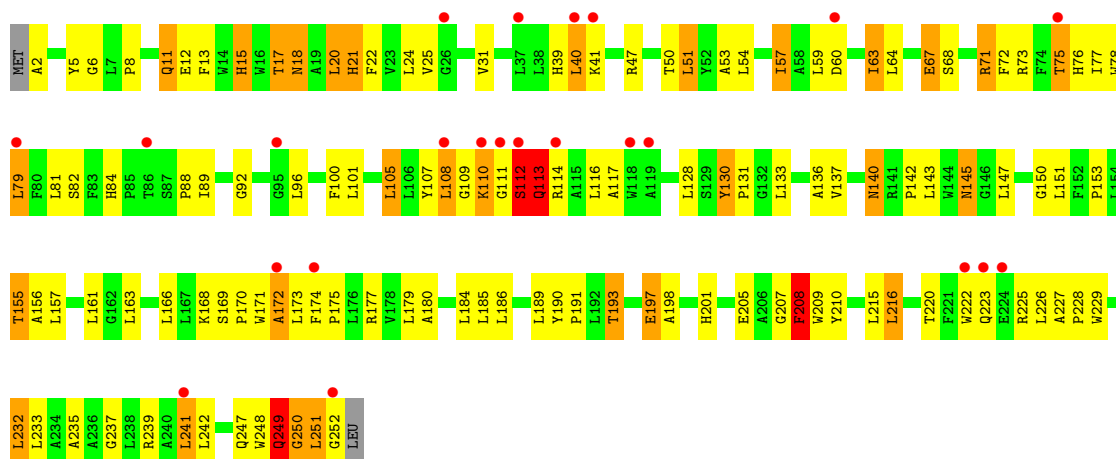
● Molecule 2: NRFC PROTEIN



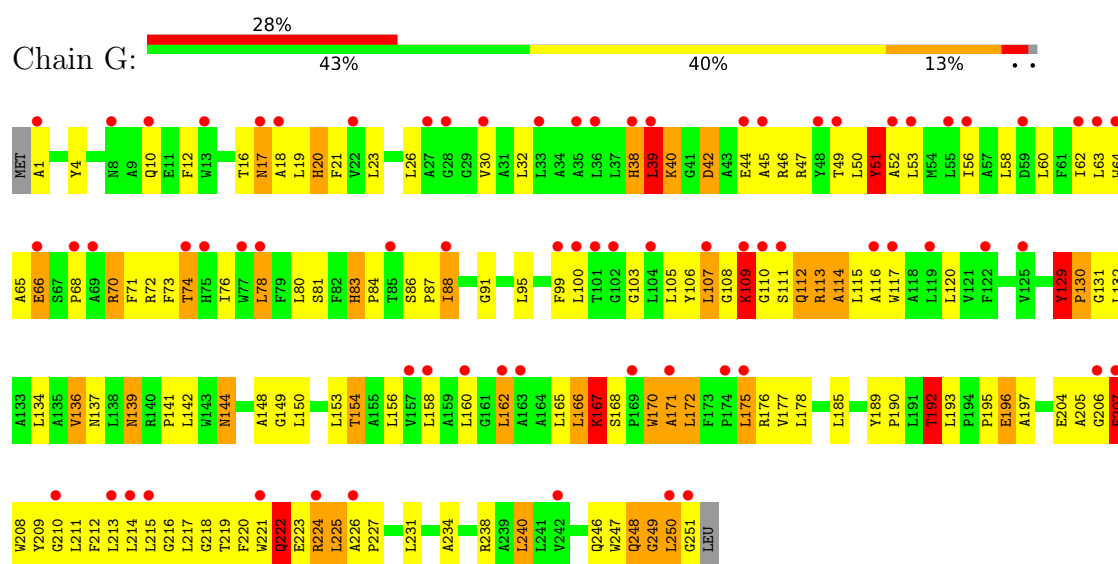
● Molecule 2: NRFC PROTEIN



● Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN



● Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.38Å 163.58Å 238.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.82 – 3.10 39.82 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.82-3.10) 95.9 (39.82-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.271 , 0.275 0.263 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20223	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MGD, MQ7, SF4, MO

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.15	16/6079 (0.3%)	1.64	120/8267 (1.5%)
1	E	1.32	18/6079 (0.3%)	1.95	193/8267 (2.3%)
2	B	1.17	3/1512 (0.2%)	1.68	33/2058 (1.6%)
2	F	1.19	5/1512 (0.3%)	1.77	40/2058 (1.9%)
3	C	0.96	3/2016 (0.1%)	1.38	23/2764 (0.8%)
3	G	1.08	4/2016 (0.2%)	1.59	37/2764 (1.3%)
All	All	1.19	49/19214 (0.3%)	1.73	446/26178 (1.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	E	1	5
3	G	0	1
All	All	2	8

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	387	GLY	C-N	-48.15	0.66	1.33
1	A	583	PHE	C-N	25.89	1.71	1.33
3	G	109	LYS	C-N	-19.12	1.05	1.33
1	E	323	LYS	C-N	14.06	1.66	1.33
1	E	388	CYS	C-N	11.30	1.49	1.33
1	E	685	THR	CA-C	10.03	1.66	1.52
1	E	585	THR	C-N	-9.71	1.22	1.33
1	A	365	ILE	N-CA	8.17	1.56	1.46
2	F	135	CYS	CB-SG	7.70	2.06	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	648	GLU	N-CA	-7.58	1.36	1.46
1	E	589	LYS	N-CA	-6.97	1.37	1.46
1	E	324	PRO	N-CA	6.96	1.56	1.47
3	G	112	GLN	C-N	6.86	1.43	1.33
2	F	44	GLY	CA-C	-6.57	1.45	1.52
1	E	588	GLY	C-N	-6.56	1.24	1.33
1	E	763	ARG	C-N	-6.53	1.24	1.33
1	A	602	HIS	CB-CG	6.29	1.58	1.50
1	A	667	VAL	N-CA	-6.29	1.38	1.46
1	A	360	PRO	N-CA	-6.17	1.40	1.47
1	A	666	TYR	C-N	-6.12	1.27	1.33
1	E	114	VAL	CA-CB	6.11	1.61	1.54
1	A	647	ASN	C-N	-6.09	1.25	1.33
3	C	113	GLN	N-CA	5.98	1.53	1.46
2	F	193	HIS	C-N	-5.88	1.25	1.33
3	C	251	LEU	C-N	-5.82	1.25	1.33
1	E	288	GLU	N-CA	-5.81	1.38	1.46
2	F	64	PRO	CA-C	-5.80	1.46	1.52
3	G	248	GLN	CA-C	-5.72	1.45	1.52
2	F	177	TYR	CA-C	-5.72	1.45	1.52
1	A	648	GLU	CA-C	5.68	1.59	1.52
1	E	421	ILE	N-CA	5.65	1.53	1.46
1	A	483	ALA	C-N	-5.59	1.25	1.33
2	B	193	HIS	C-N	-5.49	1.25	1.33
3	C	112	SER	N-CA	5.49	1.53	1.46
1	A	582	PRO	CA-C	5.49	1.60	1.52
2	B	46	TYR	N-CA	5.48	1.53	1.46
1	E	259	ALA	CA-CB	-5.47	1.44	1.53
2	B	43	VAL	N-CA	-5.42	1.38	1.46
1	E	421	ILE	C-N	-5.40	1.22	1.33
1	E	606	PRO	N-CA	-5.40	1.40	1.47
1	A	529	LEU	N-CA	5.32	1.52	1.46
1	A	582	PRO	N-CA	5.29	1.54	1.47
1	E	37	VAL	N-CA	-5.24	1.40	1.46
3	G	250	LEU	C-N	-5.23	1.26	1.33
1	A	528	ARG	CA-C	5.11	1.59	1.52
1	A	208	HIS	N-CA	-5.09	1.40	1.46
1	E	590	ILE	CA-C	-5.06	1.46	1.52
1	E	720	GLN	CA-C	-5.06	1.47	1.53
1	A	185	PHE	C-N	-5.01	1.25	1.33

All (446) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	240	SER	N-CA-CB	-26.20	62.28	109.18
1	E	595	GLN	N-CA-CB	-25.15	74.10	110.57
1	E	594	CYS	N-CA-C	25.02	137.84	111.07
1	E	387	GLY	O-C-N	-24.26	91.16	122.70
1	E	421	ILE	N-CA-CB	-23.23	81.38	112.28
1	E	323	LYS	CA-C-N	21.73	147.00	119.84
1	E	323	LYS	C-N-CA	21.73	147.00	119.84
1	A	401	PHE	N-CA-C	21.11	155.76	110.80
1	E	231	LYS	N-CA-CB	-21.01	77.23	110.85
1	E	185	PHE	N-CA-C	-20.75	79.61	108.86
1	E	585	THR	CB-CA-C	20.74	145.43	117.23
2	F	171	THR	N-CA-C	20.15	137.62	112.23
3	G	114	ALA	N-CA-C	-18.35	91.26	114.56
1	E	583	PHE	N-CA-CB	-17.82	80.37	110.49
1	E	594	CYS	N-CA-CB	-17.80	84.20	110.01
1	E	467	VAL	N-CA-C	17.29	127.02	110.42
1	E	582	PRO	N-CA-C	16.49	140.50	113.78
2	F	44	GLY	N-CA-C	15.64	134.39	112.81
1	E	421	ILE	O-C-N	-15.61	105.66	122.05
1	E	593	TYR	CB-CA-C	-15.16	80.26	110.42
2	B	169	GLN	N-CA-C	-14.34	90.56	110.35
1	A	571	TRP	N-CA-CB	-14.31	83.78	109.10
3	G	225	LEU	N-CA-C	-14.21	93.08	112.12
1	E	363	PHE	N-CA-CB	-14.15	85.61	111.37
1	E	189	ILE	N-CA-C	-14.02	98.41	111.45
1	A	189	ILE	N-CA-C	-13.85	99.90	111.81
1	A	583	PHE	O-C-N	13.80	140.94	122.59
1	A	402	LYS	O-C-N	-13.14	106.21	121.32
1	E	421	ILE	N-CA-C	-13.13	99.69	112.17
3	G	109	LYS	CA-C-N	12.93	146.75	121.41
3	G	109	LYS	C-N-CA	12.93	146.75	121.41
1	A	570	PRO	N-CA-C	12.89	139.02	112.47
1	E	659	LEU	N-CA-C	-12.45	90.55	109.60
3	G	249	GLY	N-CA-C	12.14	141.96	113.18
1	E	583	PHE	N-CA-C	11.68	135.68	110.80
2	F	16	CYS	N-CA-C	-11.59	94.16	110.50
2	B	72	THR	N-CA-C	-11.46	92.09	109.86
2	F	16	CYS	CA-C-N	-11.42	105.57	122.24
2	F	16	CYS	C-N-CA	-11.42	105.57	122.24
1	E	324	PRO	CA-N-CD	-11.35	96.11	112.00
3	C	114	ARG	N-CA-C	-11.26	98.21	113.18
1	E	585	THR	O-C-N	-11.08	107.37	121.33
3	G	18	ALA	N-CA-C	-10.87	100.15	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	193	LEU	CA-C-N	-10.75	109.31	120.38
3	G	193	LEU	C-N-CA	-10.75	109.31	120.38
1	E	583	PHE	CA-C-N	10.62	128.87	121.65
1	E	583	PHE	C-N-CA	10.62	128.87	121.65
3	G	171	ALA	N-CA-C	10.58	123.88	111.71
2	B	46	TYR	N-CA-C	10.50	133.01	109.81
1	A	691	ASP	CB-CA-C	-10.39	89.27	109.95
1	E	686	ALA	N-CA-C	10.39	132.93	110.80
1	E	478	VAL	CB-CA-C	10.36	128.28	111.29
1	E	680	VAL	CB-CA-C	-10.30	95.27	110.62
2	B	1	MET	CA-C-N	-10.29	106.97	119.84
2	B	1	MET	C-N-CA	-10.29	106.97	119.84
1	E	590	ILE	CB-CA-C	-10.27	96.88	110.84
1	E	340	ASP	N-CA-C	10.10	123.33	111.71
2	F	152	VAL	CB-CA-C	-10.10	98.51	112.14
1	A	98	PRO	CA-N-CD	-9.99	98.01	112.00
1	E	594	CYS	CB-CA-C	9.65	126.03	110.88
1	A	731	GLY	N-CA-C	9.63	122.62	111.36
1	E	593	TYR	N-CA-C	-9.60	90.35	110.80
2	F	64	PRO	N-CA-C	9.53	122.33	110.70
1	E	736	VAL	N-CA-CB	-9.48	99.67	112.28
1	E	216	ASN	N-CA-C	9.44	121.25	110.97
1	E	323	LYS	C-N-CD	-9.33	86.74	125.00
1	E	665	ASP	N-CA-C	9.27	123.58	110.50
2	F	43	VAL	N-CA-C	-9.21	94.14	107.77
1	A	736	VAL	N-CA-CB	-9.11	100.51	112.26
2	B	152	VAL	CB-CA-C	-9.08	99.69	112.22
1	E	388	CYS	CA-C-N	-9.08	104.20	121.54
1	E	388	CYS	C-N-CA	-9.08	104.20	121.54
1	A	364	TYR	N-CA-C	8.94	123.44	112.54
1	A	247	HIS	CA-CB-CG	-8.90	104.90	113.80
1	E	213	ASP	N-CA-C	-8.85	95.71	109.25
1	E	588	GLY	CA-C-N	-8.83	110.37	122.30
1	E	588	GLY	C-N-CA	-8.83	110.37	122.30
1	E	685	THR	CA-C-N	8.82	138.38	121.54
1	E	685	THR	C-N-CA	8.82	138.38	121.54
3	G	207	PHE	CB-CA-C	-8.81	92.88	110.42
1	E	212	GLU	N-CA-C	-8.77	101.01	112.68
3	C	84	HIS	CA-CB-CG	-8.75	105.05	113.80
1	A	570	PRO	CA-N-CD	-8.70	99.83	112.00
1	E	184	VAL	N-CA-C	8.69	123.08	111.44
1	E	150	TYR	N-CA-C	-8.68	101.89	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	652	HIS	CA-CB-CG	-8.65	105.15	113.80
1	A	608	PHE	N-CA-C	-8.64	101.99	112.54
1	A	364	TYR	CA-C-N	8.58	137.41	121.97
1	A	364	TYR	C-N-CA	8.58	137.41	121.97
1	E	34	ALA	CA-C-N	8.57	137.91	121.54
1	E	34	ALA	C-N-CA	8.57	137.91	121.54
1	A	109	GLU	N-CA-C	-8.55	99.12	110.24
3	C	226	LEU	N-CA-C	-8.53	103.00	113.41
2	B	134	THR	CB-CA-C	-8.49	96.70	111.05
1	E	390	GLY	N-CA-C	-8.45	95.10	112.34
1	E	207	GLY	N-CA-C	-8.36	98.78	111.24
3	G	109	LYS	O-C-N	-8.35	114.19	123.13
2	F	43	VAL	CA-C-N	-8.34	114.02	122.69
2	F	43	VAL	C-N-CA	-8.34	114.02	122.69
1	A	327	VAL	CB-CA-C	-8.26	97.78	110.50
1	A	644	ASP	CA-C-N	8.24	128.94	120.04
1	A	644	ASP	C-N-CA	8.24	128.94	120.04
1	A	328	LEU	CA-C-N	-8.23	111.91	120.38
1	A	328	LEU	C-N-CA	-8.23	111.91	120.38
1	A	535	PHE	CA-CB-CG	-8.22	105.58	113.80
2	B	46	TYR	CB-CA-C	-8.18	94.06	110.17
1	E	92	PRO	N-CA-C	-8.16	95.66	112.47
1	E	278	TYR	N-CA-C	-8.16	102.32	111.14
2	F	29	VAL	CA-C-N	8.12	128.74	120.38
2	F	29	VAL	C-N-CA	8.12	128.74	120.38
1	E	327	VAL	CB-CA-C	-8.10	97.73	110.69
1	E	323	LYS	CB-CA-C	8.08	122.80	109.56
1	E	595	GLN	N-CA-C	8.06	122.48	113.21
3	G	83	HIS	CA-C-N	8.05	129.90	119.84
3	G	83	HIS	C-N-CA	8.05	129.90	119.84
3	C	88	PRO	CA-N-CD	-8.03	100.76	112.00
1	E	214	THR	N-CA-CB	-7.99	98.07	111.17
1	A	431	PRO	CA-N-CD	-7.97	100.84	112.00
1	E	402	LYS	CA-C-N	-7.96	112.51	120.31
1	E	402	LYS	C-N-CA	-7.96	112.51	120.31
1	A	359	ARG	CA-C-N	-7.86	110.56	120.23
1	A	359	ARG	C-N-CA	-7.86	110.56	120.23
3	G	131	GLY	N-CA-C	-7.86	94.56	113.18
1	A	648	GLU	CB-CA-C	7.85	123.39	109.65
3	G	4	TYR	N-CA-C	-7.83	95.64	108.41
3	G	166	LEU	N-CA-C	-7.81	104.69	112.97
1	A	649	VAL	CB-CA-C	-7.81	101.94	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	72	THR	N-CA-CB	-7.80	97.98	110.39
1	E	586	ALA	N-CA-CB	-7.74	95.60	111.00
3	G	207	PHE	CA-CB-CG	-7.74	106.06	113.80
2	F	46	TYR	N-CA-C	7.71	126.86	109.81
1	E	678	GLY	CA-C-N	-7.66	111.56	119.83
1	E	678	GLY	C-N-CA	-7.66	111.56	119.83
1	E	710	HIS	CA-C-N	-7.64	106.43	121.41
1	E	710	HIS	C-N-CA	-7.64	106.43	121.41
3	C	6	GLY	N-CA-C	-7.58	98.42	112.37
3	G	248	GLN	N-CA-CB	-7.57	99.52	110.65
1	A	152	PHE	CA-CB-CG	-7.56	106.24	113.80
1	A	628	VAL	N-CA-CB	-7.55	103.91	112.21
2	F	18	ALA	N-CA-C	7.55	119.59	111.36
1	E	187	ARG	CA-C-N	7.54	127.70	120.31
1	E	187	ARG	C-N-CA	7.54	127.70	120.31
1	E	239	PHE	CB-CA-C	-7.51	99.02	111.41
1	E	590	ILE	N-CA-CB	7.46	119.94	110.99
1	A	433	LYS	N-CA-C	-7.44	99.45	110.46
1	A	340	ASP	N-CA-C	7.38	126.52	110.80
1	E	335	VAL	N-CA-CB	-7.38	99.06	111.23
1	A	213	ASP	N-CA-C	-7.37	97.98	109.25
1	A	360	PRO	CA-N-CD	-7.37	101.69	112.00
1	E	409	LYS	N-CA-C	7.31	122.02	113.18
2	B	27	ASN	CA-CB-CG	-7.30	105.30	112.60
1	E	35	GLN	CA-C-N	7.24	131.40	121.05
1	E	35	GLN	C-N-CA	7.24	131.40	121.05
2	B	180	ALA	CA-C-N	7.22	127.07	119.05
2	B	180	ALA	C-N-CA	7.22	127.07	119.05
1	A	582	PRO	CA-C-N	7.21	135.31	121.54
1	A	582	PRO	C-N-CA	7.21	135.31	121.54
3	C	113	GLN	N-CA-C	7.19	126.12	110.80
1	A	683	LYS	O-C-N	7.19	127.28	121.17
3	G	130	PRO	N-CA-C	-7.18	97.55	111.69
1	A	592	LEU	N-CA-C	7.17	126.07	110.80
1	A	421	ILE	CB-CA-C	-7.15	100.37	110.95
1	E	499	THR	CB-CA-C	-7.13	101.72	109.85
1	E	337	TYR	N-CA-C	7.12	125.97	110.80
1	E	466	ASP	CA-CB-CG	7.09	119.69	112.60
2	B	71	PRO	N-CA-C	7.08	122.89	113.40
1	E	214	THR	CB-CA-C	7.05	122.49	111.13
3	G	51	TYR	N-CA-C	-7.04	95.80	110.80
1	A	467	VAL	CB-CA-C	-7.02	104.03	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	692	CYS	N-CA-C	7.02	119.59	109.14
1	E	731	GLY	N-CA-C	7.01	129.79	113.18
1	A	601	GLY	CA-C-N	-7.01	111.81	122.81
1	A	601	GLY	C-N-CA	-7.01	111.81	122.81
1	E	608	PHE	CA-CB-CG	-7.00	106.81	113.80
1	A	360	PRO	N-CA-CB	6.99	108.89	103.30
1	A	477	ASP	N-CA-C	-6.99	97.15	108.41
2	F	187	THR	N-CA-CB	-6.99	99.28	109.83
1	E	96	LYS	N-CA-C	6.96	122.31	113.55
1	A	208	HIS	CA-CB-CG	6.95	120.75	113.80
1	E	281	LYS	N-CA-C	6.92	122.02	113.50
1	A	472	HIS	CA-CB-CG	-6.91	106.89	113.80
2	F	14	VAL	N-CA-C	-6.89	106.28	112.90
1	A	570	PRO	CB-CA-C	-6.89	100.19	111.56
1	E	608	PHE	N-CA-C	-6.88	103.80	111.71
1	A	401	PHE	CB-CA-C	-6.86	96.76	110.42
1	E	710	HIS	N-CA-C	6.78	125.25	110.80
1	E	172	LEU	CA-CB-CG	-6.78	92.57	116.30
1	E	411	PHE	N-CA-C	6.76	118.73	111.36
1	A	648	GLU	N-CA-CB	-6.76	99.45	110.81
2	B	57	GLN	CA-CB-CG	-6.75	100.59	114.10
2	B	45	GLU	CB-CG-CD	-6.75	101.12	112.60
3	C	113	GLN	CB-CA-C	-6.75	96.98	110.42
1	E	354	LEU	N-CA-C	-6.74	104.67	113.17
1	E	288	GLU	N-CA-C	-6.74	104.94	113.43
1	E	489	TYR	CB-CA-C	-6.73	98.64	109.75
2	F	152	VAL	N-CA-CB	6.73	119.69	110.54
1	E	174	THR	N-CA-C	6.72	121.57	113.23
1	A	608	PHE	CA-CB-CG	-6.72	107.08	113.80
1	A	581	LEU	O-C-N	-6.71	116.75	121.65
3	G	168	SER	N-CA-C	-6.71	99.90	109.62
1	A	212	GLU	N-CA-C	-6.70	103.77	112.68
2	F	16	CYS	O-C-N	-6.69	114.97	122.86
1	E	388	CYS	N-CA-C	6.68	125.02	110.80
1	E	37	VAL	CB-CA-C	6.67	120.69	110.55
1	E	707	ARG	N-CA-C	6.67	119.38	111.71
2	B	169	GLN	CA-C-N	-6.67	108.34	121.41
2	B	169	GLN	C-N-CA	-6.67	108.34	121.41
1	A	150	TYR	N-CA-C	-6.65	103.95	111.07
1	E	458	ASN	CA-CB-CG	-6.65	105.95	112.60
1	A	371	LEU	N-CA-C	-6.64	96.70	108.13
1	A	334	ASN	N-CA-C	6.63	121.03	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	478	VAL	N-CA-C	-6.63	95.55	109.34
1	E	335	VAL	CB-CA-C	6.59	122.10	111.29
1	E	256	THR	N-CA-CB	-6.59	100.98	110.80
1	A	680	VAL	CB-CA-C	-6.58	100.69	110.82
1	E	174	THR	N-CA-CB	-6.58	100.18	110.44
2	F	156	LEU	N-CA-C	-6.57	104.04	111.07
1	E	687	ARG	CB-CG-CD	-6.56	96.21	111.30
3	G	170	TRP	N-CA-C	6.55	119.25	111.71
1	A	427	GLY	N-CA-C	-6.54	105.89	115.30
2	F	83	VAL	N-CA-C	-6.53	99.02	108.36
3	C	8	PRO	N-CA-C	-6.51	101.68	111.57
1	A	684	PRO	CA-C-N	-6.46	113.81	122.72
1	A	684	PRO	C-N-CA	-6.46	113.81	122.72
1	E	47	CYS	N-CA-C	-6.45	99.72	108.24
2	B	44	GLY	N-CA-C	6.45	119.51	112.29
1	A	374	TYR	N-CA-C	-6.43	101.55	109.65
1	E	338	GLY	N-CA-C	6.42	124.23	115.30
1	A	513	PHE	CB-CA-C	-6.41	109.19	116.63
1	A	683	LYS	CA-C-N	6.40	127.84	119.84
1	A	683	LYS	C-N-CA	6.40	127.84	119.84
1	A	232	VAL	N-CA-C	6.39	117.07	107.80
1	A	591	GLU	N-CA-C	-6.39	104.32	111.28
1	A	359	ARG	O-C-N	6.37	127.75	121.57
2	F	160	GLU	N-CA-C	-6.37	104.21	112.23
1	A	663	GLU	N-CA-C	6.36	118.74	111.11
3	C	249	GLN	CA-C-N	6.36	133.87	121.41
3	C	249	GLN	C-N-CA	6.36	133.87	121.41
1	E	339	ASP	N-CA-C	-6.35	102.80	111.56
1	E	152	PHE	N-CA-C	6.35	120.88	113.20
1	A	736	VAL	N-CA-C	-6.34	106.81	112.90
2	B	16	CYS	N-CA-C	-6.32	96.86	107.99
2	B	4	TYR	N-CA-C	6.30	119.61	110.28
1	A	534	TYR	N-CA-C	-6.29	99.02	109.46
2	B	64	PRO	N-CA-C	6.28	118.36	110.70
1	E	33	TYR	CA-C-N	6.25	131.82	123.20
1	E	33	TYR	C-N-CA	6.25	131.82	123.20
1	E	466	ASP	CA-C-N	6.23	128.41	120.56
1	E	466	ASP	C-N-CA	6.23	128.41	120.56
2	F	117	THR	N-CA-CB	-6.21	100.95	111.27
1	E	34	ALA	N-CA-C	-6.21	99.79	108.54
1	E	585	THR	CA-C-N	6.19	129.81	122.44
1	E	585	THR	C-N-CA	6.19	129.81	122.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	400	GLY	N-CA-C	-6.17	98.56	113.18
2	B	108	HIS	N-CA-C	-6.14	101.27	110.24
1	A	193	GLU	CA-C-N	6.12	127.49	119.84
1	A	193	GLU	C-N-CA	6.12	127.49	119.84
1	A	277	GLU	CB-CA-C	-6.12	101.27	110.88
1	A	407	LYS	CA-C-N	-6.12	113.00	122.30
1	A	407	LYS	C-N-CA	-6.12	113.00	122.30
2	F	29	VAL	N-CA-C	-6.12	102.96	108.95
1	E	429	PRO	CA-N-CD	-6.10	103.46	112.00
1	E	185	PHE	O-C-N	-6.04	114.74	122.78
2	F	175	LEU	N-CA-C	-6.03	98.45	108.34
1	E	226	LEU	N-CA-C	-6.01	104.81	111.36
1	A	736	VAL	CB-CA-C	5.97	118.60	111.20
1	E	323	LYS	O-C-N	5.96	127.06	121.27
1	E	444	HIS	CA-CB-CG	-5.96	107.84	113.80
1	E	690	LYS	CA-C-N	5.96	131.57	121.14
1	E	690	LYS	C-N-CA	5.96	131.57	121.14
1	E	230	ALA	CA-C-O	-5.95	114.27	121.05
1	E	592	LEU	CB-CA-C	-5.95	99.06	110.24
1	E	668	MET	N-CA-C	-5.94	100.50	109.95
2	F	19	CYS	N-CA-C	-5.92	104.74	111.14
1	E	297	THR	N-CA-CB	-5.92	100.28	110.10
2	B	42	GLU	O-C-N	5.91	129.89	123.10
2	F	135	CYS	CA-C-N	5.91	125.61	119.05
2	F	135	CYS	C-N-CA	5.91	125.61	119.05
2	F	4	TYR	N-CA-C	5.90	118.82	109.96
1	E	93	ASP	N-CA-C	5.90	123.37	110.80
1	A	336	TRP	CB-CA-C	-5.90	98.68	110.42
2	F	64	PRO	CA-C-N	-5.88	113.76	119.87
2	F	64	PRO	C-N-CA	-5.88	113.76	119.87
1	E	749	LEU	CA-C-N	-5.88	114.21	120.03
1	E	749	LEU	C-N-CA	-5.88	114.21	120.03
3	C	15	HIS	CA-CB-CG	-5.88	107.92	113.80
2	B	11	SER	N-CA-C	-5.87	105.61	112.89
1	A	571	TRP	N-CA-C	-5.87	99.83	109.80
1	E	300	TRP	N-CA-C	-5.86	104.81	111.14
3	G	78	LEU	N-CA-C	-5.82	105.01	111.71
1	E	562	GLY	CA-C-N	5.82	131.20	123.05
1	E	562	GLY	C-N-CA	5.82	131.20	123.05
3	C	249	GLN	CA-C-O	5.82	125.98	119.41
1	E	33	TYR	O-C-N	-5.81	113.94	122.43
1	E	429	PRO	N-CA-CB	5.81	109.35	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	185	PHE	CA-C-N	-5.80	110.04	121.41
1	E	185	PHE	C-N-CA	-5.80	110.04	121.41
1	A	489	TYR	N-CA-C	-5.80	100.83	110.17
1	E	185	PHE	N-CA-CB	-5.80	101.62	111.31
1	E	388	CYS	O-C-N	5.80	130.30	122.59
1	A	211	GLY	N-CA-C	-5.78	107.39	113.58
2	F	139	CYS	CA-C-N	-5.76	114.57	122.93
2	F	139	CYS	C-N-CA	-5.76	114.57	122.93
3	C	24	LEU	N-CA-C	5.76	117.36	111.14
1	E	239	PHE	CA-C-N	-5.75	110.63	122.82
1	E	239	PHE	C-N-CA	-5.75	110.63	122.82
3	G	219	THR	N-CA-C	-5.75	105.53	112.54
1	E	276	LYS	N-CA-C	5.75	117.62	111.36
1	A	365	ILE	N-CA-CB	5.74	120.71	111.23
1	E	38	LYS	N-CA-C	-5.74	98.14	108.48
1	A	409	LYS	N-CA-C	5.74	119.46	112.23
1	E	581	LEU	CA-C-N	5.74	125.21	119.24
1	E	581	LEU	C-N-CA	5.74	125.21	119.24
1	E	734	LEU	N-CA-C	5.74	120.35	113.23
1	A	214	THR	N-CA-CB	-5.71	102.47	111.39
2	F	186	LEU	CA-C-N	5.71	128.82	120.71
2	F	186	LEU	C-N-CA	5.71	128.82	120.71
2	B	46	TYR	CA-C-N	5.71	126.98	119.84
2	B	46	TYR	C-N-CA	5.71	126.98	119.84
1	A	707	ARG	CA-C-N	-5.70	113.53	122.65
1	A	707	ARG	C-N-CA	-5.70	113.53	122.65
2	F	179	ASN	N-CA-C	5.70	122.94	110.80
1	E	651	ILE	CB-CA-C	-5.69	100.53	110.71
1	E	191	GLY	N-CA-C	5.68	119.37	112.49
1	E	479	ILE	N-CA-CB	-5.67	99.35	111.37
2	F	86	ASP	N-CA-C	-5.66	98.50	108.69
1	A	569	LYS	CA-C-N	5.65	126.91	119.84
1	A	569	LYS	C-N-CA	5.65	126.91	119.84
1	E	388	CYS	CB-CA-C	-5.65	99.17	110.42
1	E	606	PRO	N-CA-C	-5.64	100.86	112.47
1	A	569	LYS	O-C-N	5.63	125.88	121.88
3	C	51	LEU	CA-C-N	5.63	127.83	120.28
3	C	51	LEU	C-N-CA	5.63	127.83	120.28
1	A	208	HIS	CA-C-N	-5.62	115.54	122.84
1	A	208	HIS	C-N-CA	-5.62	115.54	122.84
3	C	41	LYS	N-CA-C	-5.62	106.20	113.16
1	A	514	ASP	CA-CB-CG	-5.61	106.99	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	49	TRP	N-CA-C	-5.60	105.95	112.89
1	E	693	VAL	CB-CA-C	5.59	119.75	110.30
2	B	187	THR	N-CA-CB	-5.58	101.77	109.97
3	C	249	GLN	CB-CA-C	-5.58	99.47	109.24
3	G	42	ASP	N-CA-C	5.58	118.44	110.24
1	E	757	LYS	N-CA-C	5.57	119.80	112.89
1	A	75	ARG	CB-CA-C	-5.55	103.70	111.80
1	E	706	MET	N-CA-C	-5.55	96.81	107.57
1	A	566	GLN	CA-C-N	-5.54	113.88	122.09
1	A	566	GLN	C-N-CA	-5.54	113.88	122.09
1	E	630	THR	CB-CA-C	-5.54	101.92	110.78
3	C	136	ALA	N-CA-C	5.53	119.12	112.38
1	E	58	VAL	N-CA-C	-5.51	97.88	109.34
1	E	371	LEU	N-CA-C	-5.50	98.85	107.93
3	C	5	TYR	N-CA-C	-5.50	98.40	108.02
1	E	198	GLU	N-CA-C	5.48	118.02	111.71
1	E	651	ILE	N-CA-C	-5.48	99.93	108.81
1	A	189	ILE	CB-CA-C	5.46	117.83	111.55
2	B	179	ASN	N-CA-C	5.43	118.69	111.30
3	G	141	PRO	N-CA-C	5.43	121.69	113.81
3	G	248	GLN	O-C-N	5.43	129.03	122.35
1	E	75	ARG	CB-CG-CD	-5.43	98.80	111.30
2	B	78	THR	N-CA-CB	-5.42	102.21	110.45
1	E	280	ALA	N-CA-C	5.42	117.89	111.33
1	E	596	ARG	N-CA-C	-5.42	105.47	112.68
2	F	5	ALA	N-CA-C	5.42	117.30	109.07
1	A	98	PRO	N-CA-CB	5.41	108.36	103.33
1	E	685	THR	N-CA-CB	-5.41	101.35	110.49
1	A	590	ILE	N-CA-C	5.41	115.61	110.42
1	E	324	PRO	N-CA-CB	5.41	108.93	103.25
1	E	45	GLU	N-CA-C	-5.40	106.47	112.57
2	F	170	GLY	N-CA-C	5.40	120.61	114.67
1	A	710	HIS	CA-CB-CG	-5.39	108.41	113.80
1	E	599	GLU	CB-CA-C	5.39	120.34	109.68
1	E	608	PHE	CA-C-N	5.37	134.91	121.80
1	E	608	PHE	C-N-CA	5.37	134.91	121.80
1	A	356	ASN	N-CA-C	5.36	119.82	113.28
1	A	534	TYR	CB-CA-C	5.36	118.59	109.80
3	G	213	LEU	N-CA-C	-5.36	104.86	111.40
3	G	107	LEU	N-CA-C	-5.36	105.44	112.72
1	A	336	TRP	CB-CG-CD2	-5.35	119.31	126.80
1	E	271	GLU	N-CA-C	-5.33	106.45	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	GLY	N-CA-C	5.33	124.35	115.66
1	E	407	LYS	CA-C-N	-5.31	113.27	122.83
1	E	407	LYS	C-N-CA	-5.31	113.27	122.83
1	E	692	CYS	CB-CA-C	-5.30	98.84	110.67
3	G	192	THR	N-CA-CB	-5.30	102.63	110.53
3	G	224	ARG	N-CA-C	-5.29	106.20	113.56
1	A	649	VAL	N-CA-CB	5.29	116.87	110.95
1	E	433	LYS	N-CA-C	-5.28	101.09	109.59
1	E	649	VAL	CB-CA-C	-5.27	104.38	110.91
1	E	739	VAL	N-CA-CB	-5.27	102.07	111.92
1	E	305	THR	N-CA-CB	-5.26	102.42	110.26
1	E	691	ASP	N-CA-CB	-5.26	101.83	110.40
1	A	271	GLU	N-CA-C	-5.26	106.54	113.17
3	G	162	LEU	N-CA-C	-5.26	105.24	110.97
1	E	746	ARG	CA-C-N	-5.26	115.16	120.31
1	E	746	ARG	C-N-CA	-5.26	115.16	120.31
1	E	105	SER	CA-C-N	5.25	128.31	120.95
1	E	105	SER	C-N-CA	5.25	128.31	120.95
1	E	553	LEU	CA-C-N	-5.24	114.58	122.81
1	E	553	LEU	C-N-CA	-5.24	114.58	122.81
3	G	177	VAL	N-CA-C	-5.23	106.58	111.45
1	E	460	ASP	N-CA-C	-5.22	106.06	112.90
1	E	758	ARG	N-CA-C	-5.22	103.14	109.57
1	A	379	LEU	CA-C-N	-5.22	113.31	119.84
1	A	379	LEU	C-N-CA	-5.22	113.31	119.84
1	E	570	PRO	CA-N-CD	-5.21	104.70	112.00
3	G	70	ARG	N-CA-C	5.20	116.64	110.97
1	A	583	PHE	N-CA-C	5.20	121.87	110.80
1	A	728	ILE	CB-CA-C	-5.20	105.67	111.80
3	C	39	HIS	CA-CB-CG	-5.20	108.60	113.80
1	E	40	VAL	CB-CA-C	-5.20	104.11	111.38
2	F	111	GLY	N-CA-C	5.19	123.59	114.76
1	A	631	PHE	CA-CB-CG	-5.19	108.61	113.80
1	E	597	PHE	CA-C-N	5.18	127.48	120.44
1	E	597	PHE	C-N-CA	5.18	127.48	120.44
1	E	421	ILE	CB-CA-C	-5.18	105.28	111.85
1	E	581	LEU	CB-CA-C	-5.18	102.43	109.42
1	E	661	LEU	N-CA-C	5.17	117.91	109.59
1	E	592	LEU	N-CA-C	5.16	117.71	109.81
1	A	648	GLU	CB-CG-CD	5.15	121.36	112.60
1	A	749	LEU	CA-C-N	-5.14	115.27	120.21
1	A	749	LEU	C-N-CA	-5.14	115.27	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	117	THR	N-CA-CB	-5.14	102.77	110.73
1	E	397	GLU	N-CA-C	5.13	121.14	109.81
1	E	154	ASP	CB-CA-C	-5.12	100.74	109.65
1	A	659	LEU	N-CA-C	-5.11	99.91	110.80
3	G	172	LEU	N-CA-C	5.11	116.54	111.07
1	E	62	VAL	N-CA-C	-5.10	100.42	108.23
1	E	294	LYS	N-CA-C	5.10	117.50	111.33
3	G	129	TYR	CA-C-N	-5.10	113.36	120.25
3	G	129	TYR	C-N-CA	-5.10	113.36	120.25
3	C	108	LEU	CB-CA-C	-5.10	102.53	110.94
1	A	576	GLU	N-CA-C	5.08	116.82	111.28
2	F	166	ARG	CB-CA-C	-5.08	107.59	111.20
1	E	402	LYS	N-CA-C	5.07	116.27	109.83
1	A	525	LEU	N-CA-C	-5.07	106.26	112.90
1	A	645	PRO	CA-N-CD	-5.06	104.92	112.00
1	A	327	VAL	N-CA-C	5.06	116.00	108.46
1	A	139	ALA	N-CA-C	-5.05	106.96	113.02
1	A	616	GLU	CB-CA-C	5.05	117.78	109.90
3	C	237	GLY	N-CA-C	-5.05	106.64	112.50
3	C	208	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	590	ILE	CA-C-N	-5.04	113.53	120.28
1	A	590	ILE	C-N-CA	-5.04	113.53	120.28
2	B	16	CYS	CA-C-N	-5.01	111.96	121.54
2	B	16	CYS	C-N-CA	-5.01	111.96	121.54
1	E	286	PHE	CA-CB-CG	5.01	118.81	113.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	401	PHE	CA
1	E	585	THR	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	LYS	Mainchain
1	A	571	TRP	Mainchain
1	E	185	PHE	Mainchain
1	E	387	GLY	Mainchain
1	E	388	CYS	Mainchain
1	E	421	ILE	Mainchain
1	E	585	THR	Mainchain

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Mol	Chain	Res	Type	Group
3	G	109	LYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5896	0	5813	788	3
1	E	5896	0	5814	716	3
2	B	1475	0	1453	171	0
2	F	1475	0	1454	147	0
3	C	1948	0	2001	167	0
3	G	1948	0	2003	187	0
4	A	8	0	0	0	0
4	B	32	0	0	7	0
4	E	8	0	0	1	0
4	F	32	0	0	6	0
5	A	94	0	44	11	0
5	E	94	0	43	18	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	C	15	0	9	19	0
7	G	15	0	9	20	0
8	A	386	0	0	97	0
8	B	149	0	0	44	0
8	C	90	0	0	11	0
8	E	453	0	0	138	0
8	F	129	0	0	33	0
8	G	78	0	0	34	0
All	All	20223	0	18643	2122	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 56.

All (2122) 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	1.28	1.63
1:A:186:GLY:HA3	1:A:583:PHE:C	1.15	1.49
1:A:583:PHE:C	1:A:584:GLY:N	1.71	1.48
1:A:184:VAL:CG2	1:A:592:LEU:HD23	1.45	1.45
2:F:135:CYS:SG	2:F:135:CYS:CB	2.06	1.43
1:E:592:LEU:HA	1:E:603:GLN:NE2	1.08	1.39
1:E:605:LEU:H	1:E:605:LEU:CD2	1.01	1.38
3:C:171:TRP:O	3:C:171:TRP:CE3	1.79	1.34
1:E:36:GLU:O	1:E:58:VAL:CG2	1.75	1.34
1:E:477:ASP:O	1:E:478:VAL:HG23	1.16	1.32
1:E:602:HIS:CE1	1:E:606:PRO:HG3	1.64	1.32
1:A:583:PHE:CE2	1:A:588:GLY:N	1.98	1.32
3:G:207:PHE:CE2	3:G:211:LEU:HD13	1.64	1.30
1:A:591:GLU:OE2	1:A:604:PRO:HG3	1.13	1.30
1:A:604:PRO:O	1:A:606:PRO:CD	1.80	1.29
1:E:591:GLU:OE1	1:E:604:PRO:CB	1.81	1.28
1:A:604:PRO:O	1:A:606:PRO:HD2	1.25	1.28
1:E:592:LEU:CA	1:E:603:GLN:HE21	1.44	1.27
2:B:41:ARG:HH11	2:B:187:THR:CG2	1.46	1.27
1:E:477:ASP:O	1:E:478:VAL:CG2	1.80	1.27
2:B:134:THR:O	2:B:134:THR:CG2	1.76	1.27
1:E:388:CYS:HB2	1:E:593:TYR:OH	1.23	1.26
1:E:591:GLU:CD	1:E:604:PRO:HB3	1.57	1.26
1:A:395:ASP:O	1:A:399:GLU:HB2	1.32	1.26
1:A:186:GLY:CA	1:A:583:PHE:C	2.07	1.24
1:A:582:PRO:HB2	8:A:2274:HOH:O	1.08	1.24
1:A:42:GLN:O	1:A:53:ILE:HG13	1.33	1.24
1:A:602:HIS:CE1	1:A:606:PRO:CG	2.20	1.23
1:A:395:ASP:HA	1:A:399:GLU:CG	1.67	1.23
1:A:97:ARG:HH21	1:A:763:ARG:NH2	1.36	1.23
1:E:607:VAL:O	1:E:607:VAL:CG1	1.83	1.22
7:C:1252:MQ7:H2M3	7:C:1252:MQ7:C12	1.65	1.21
1:A:583:PHE:HB3	1:A:584:GLY:N	1.56	1.21
1:A:184:VAL:HG23	1:A:592:LEU:CD2	1.70	1.21
2:F:57:GLN:NE2	2:F:140:ARG:HH22	1.38	1.20
1:E:323:LYS:HD3	1:E:354:LEU:CA	1.71	1.20
1:A:284:VAL:O	1:A:590:ILE:HG22	1.35	1.20
1:A:569:LYS:O	8:A:2269:HOH:O	1.60	1.20
2:B:46:TYR:HB2	8:B:2028:HOH:O	1.04	1.20
1:E:591:GLU:OE1	1:E:604:PRO:HB3	1.04	1.20
3:G:1:ALA:HB1	8:G:2001:HOH:O	1.43	1.19
1:A:591:GLU:OE2	1:A:604:PRO:CG	1.90	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:592:LEU:CA	1:E:603:GLN:NE2	2.03	1.18
7:C:1252:MQ7:C12	7:C:1252:MQ7:C2M	2.22	1.16
1:E:590:ILE:HG13	8:E:2177:HOH:O	1.45	1.16
1:E:116:THR:HG22	1:E:119:GLU:HB3	1.21	1.16
1:A:583:PHE:CB	1:A:584:GLY:N	2.06	1.16
3:C:22:PHE:O	3:C:239:ARG:NH1	1.77	1.16
1:A:77:ARG:NH1	2:B:138:TYR:HE2	1.43	1.16
1:E:605:LEU:CD2	1:E:605:LEU:N	1.72	1.16
1:A:395:ASP:CA	1:A:399:GLU:HG3	1.73	1.15
2:B:46:TYR:CD1	8:B:2028:HOH:O	1.84	1.15
1:E:97:ARG:HG3	8:E:2191:HOH:O	1.43	1.15
1:E:626:SER:HB2	8:E:2348:HOH:O	1.44	1.14
1:E:608:PHE:O	8:E:2335:HOH:O	1.64	1.14
1:E:95:LEU:HD12	1:E:466:ASP:O	1.47	1.14
1:A:288:GLU:HB3	1:A:591:GLU:HG3	1.30	1.13
1:E:602:HIS:NE2	1:E:604:PRO:HD2	1.64	1.13
1:E:602:HIS:CD2	1:E:604:PRO:HD2	1.82	1.13
1:A:632:ALA:O	1:A:635:GLN:HG2	1.47	1.13
1:A:632:ALA:O	1:A:635:GLN:CG	1.96	1.13
1:A:467:VAL:HB	8:A:2226:HOH:O	1.49	1.13
1:E:602:HIS:HE1	1:E:606:PRO:CG	1.62	1.13
2:B:46:TYR:CE2	8:B:2032:HOH:O	2.01	1.13
1:E:763:ARG:HG2	8:E:2442:HOH:O	1.48	1.12
1:A:42:GLN:O	1:A:53:ILE:CG1	1.97	1.11
2:F:57:GLN:HE22	2:F:140:ARG:NH2	1.46	1.11
1:A:97:ARG:NH2	1:A:763:ARG:HH22	1.46	1.11
1:A:43:ILE:HG13	1:A:505:ARG:HB3	1.14	1.10
3:C:171:TRP:O	3:C:171:TRP:CD2	2.04	1.10
1:E:230:ALA:O	8:E:2136:HOH:O	1.66	1.10
1:A:397:GLU:HB3	1:A:398:PRO:HD3	1.11	1.10
1:E:413:ARG:HD3	8:E:2247:HOH:O	1.52	1.09
3:G:63:LEU:HD13	7:G:1251:MQ7:C2M	1.82	1.09
1:A:608:PHE:CD1	1:A:608:PHE:O	2.06	1.09
1:E:598:LYS:HD2	8:E:2329:HOH:O	1.52	1.09
1:A:583:PHE:HE2	1:A:588:GLY:N	1.39	1.08
1:A:604:PRO:C	1:A:606:PRO:HD3	1.77	1.08
1:A:165:ALA:O	1:A:415:THR:HG21	1.51	1.08
1:E:339:ASP:HB2	1:E:607:VAL:HG11	1.32	1.08
3:G:154:THR:CG2	3:G:238:ARG:HE	1.66	1.08
1:A:170:VAL:O	1:A:175:ALA:HB2	1.49	1.08
1:A:592:LEU:O	1:A:593:TYR:HB2	1.46	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HG13	1:A:283:THR:HG21	1.30	1.08
3:C:17:THR:CG2	3:C:67:GLU:HG3	1.83	1.07
1:E:511:PRO:HB3	1:E:515:THR:HG22	1.37	1.07
1:A:604:PRO:C	1:A:606:PRO:CD	2.28	1.07
2:B:134:THR:O	2:B:134:THR:HG23	1.25	1.07
1:A:172:LEU:HD13	1:A:445:SER:O	1.54	1.06
1:A:428:GLU:HB3	1:A:429:PRO:HD2	1.33	1.06
1:A:763:ARG:HG2	8:A:2378:HOH:O	1.54	1.06
1:A:186:GLY:HA3	1:A:583:PHE:O	1.53	1.06
1:E:224:LEU:HD12	8:E:2130:HOH:O	1.54	1.06
1:E:112:TYR:OH	1:E:474:MET:O	1.74	1.05
1:A:599:GLU:O	8:A:2281:HOH:O	1.73	1.05
1:A:685:THR:HB	2:B:42:GLU:OE2	1.57	1.05
2:B:41:ARG:HD2	2:B:187:THR:CG2	1.85	1.05
2:B:41:ARG:HH11	2:B:187:THR:HG22	1.19	1.05
1:E:607:VAL:O	1:E:607:VAL:HG12	1.32	1.05
3:G:38:HIS:HD2	3:G:45:ALA:HB1	1.19	1.05
1:A:591:GLU:CD	1:A:604:PRO:HG3	1.81	1.05
1:E:605:LEU:N	1:E:605:LEU:HD22	1.67	1.05
1:E:764:ARG:N	8:E:2446:HOH:O	1.89	1.05
1:E:429:PRO:HD2	8:E:2256:HOH:O	1.57	1.04
3:C:155:THR:HG22	3:C:239:ARG:HE	1.21	1.04
2:B:41:ARG:HD2	2:B:187:THR:HG21	1.35	1.04
1:E:116:THR:CG2	1:E:119:GLU:H	1.70	1.04
1:E:605:LEU:N	1:E:605:LEU:HD23	1.27	1.04
1:E:635:GLN:O	1:E:641:MET:CG	2.05	1.04
2:F:57:GLN:NE2	2:F:140:ARG:NH2	2.05	1.04
1:E:95:LEU:CD1	1:E:466:ASP:O	2.06	1.03
1:A:360:PRO:HD3	1:A:571:TRP:CE3	1.94	1.03
1:E:653:LYS:HD2	1:E:686:ALA:HB2	1.39	1.03
3:G:206:GLY:O	3:G:209:TYR:N	1.91	1.03
1:A:603:GLN:HB3	1:A:604:PRO:HD3	1.34	1.02
2:B:192:VAL:HG21	8:B:2019:HOH:O	1.60	1.02
1:E:47:CYS:HB2	8:E:2452:HOH:O	1.57	1.02
1:E:323:LYS:CD	1:E:354:LEU:HA	1.89	1.02
1:E:478:VAL:HG23	8:E:2280:HOH:O	1.58	1.02
1:A:651:ILE:HD11	1:A:682:VAL:HG13	1.39	1.02
1:A:349:TYR:OH	1:A:591:GLU:O	1.78	1.02
1:A:585:THR:O	1:A:586:ALA:HB3	1.59	1.02
1:E:342:TYR:CD1	1:E:607:VAL:HB	1.93	1.02
1:A:531:LEU:O	1:A:534:TYR:O	1.76	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:ARG:CB	1:A:580:ARG:HH11	1.74	1.01
1:E:428:GLU:O	1:E:430:TYR:N	1.92	1.01
3:G:207:PHE:HE2	3:G:211:LEU:HD13	0.99	1.01
1:E:551:LEU:O	1:E:553:LEU:N	1.93	1.01
3:G:221:TRP:HE3	3:G:225:LEU:HD22	1.20	1.01
1:A:116:THR:HG22	1:A:119:GLU:H	1.17	1.00
1:E:635:GLN:O	1:E:641:MET:HG3	1.61	1.00
3:G:111:SER:HB3	8:G:2033:HOH:O	1.60	1.00
1:E:424:MET:HE2	1:E:455:ALA:HB1	1.44	1.00
1:A:335:VAL:CG1	1:A:732:ALA:O	2.10	1.00
3:C:207:GLY:O	3:C:210:TYR:N	1.94	1.00
2:F:46:TYR:HB3	8:F:2035:HOH:O	1.60	1.00
2:B:25:MET:HE2	2:B:25:MET:HA	1.43	1.00
1:E:569:LYS:HD2	8:E:2320:HOH:O	1.60	0.99
1:E:349:TYR:OH	1:E:591:GLU:HA	1.63	0.99
1:A:345:MET:HE2	1:A:605:LEU:HD22	1.42	0.98
1:A:400:GLY:HA3	8:A:2193:HOH:O	1.64	0.98
1:A:729:SER:O	1:A:731:GLY:N	1.97	0.97
1:A:591:GLU:HB3	1:A:603:GLN:NE2	1.79	0.97
2:B:146:GLU:HG2	8:B:2109:HOH:O	1.64	0.97
2:B:160:GLU:H	2:B:179:ASN:HD21	1.10	0.97
1:E:533:GLN:HE21	1:E:533:GLN:H	1.12	0.97
1:A:116:THR:CG2	1:A:119:GLU:H	1.76	0.97
1:A:680:VAL:HG11	8:A:2310:HOH:O	1.63	0.97
1:A:763:ARG:HB2	8:A:2380:HOH:O	1.64	0.97
1:E:606:PRO:O	1:E:608:PHE:N	1.97	0.97
1:E:36:GLU:O	1:E:58:VAL:HG22	0.79	0.97
2:F:41:ARG:HD2	2:F:187:THR:HG23	1.43	0.97
2:F:41:ARG:HD2	2:F:187:THR:CG2	1.95	0.96
3:G:221:TRP:CE3	3:G:225:LEU:HD22	2.00	0.96
1:A:397:GLU:HB3	1:A:398:PRO:CD	1.95	0.96
1:E:428:GLU:O	1:E:429:PRO:C	2.05	0.96
1:A:434:GLY:HA2	1:A:461:LEU:O	1.65	0.96
1:E:209:HIS:HE1	1:E:625:ARG:H	1.11	0.96
1:E:297:THR:HG22	1:E:300:TRP:H	1.30	0.96
1:E:608:PHE:O	1:E:608:PHE:CD1	2.18	0.96
1:A:276:LYS:HA	8:A:2148:HOH:O	1.65	0.96
2:B:72:THR:HG22	2:B:74:ALA:H	1.28	0.95
3:C:17:THR:HG21	3:C:67:GLU:HG3	1.47	0.95
1:A:184:VAL:CG2	1:A:592:LEU:CD2	2.37	0.95
1:A:653:LYS:HG3	1:A:684:PRO:O	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:HIS:ND1	1:A:634:THR:HG23	1.80	0.95
1:E:604:PRO:O	1:E:606:PRO:HD3	1.65	0.95
1:E:92:PRO:O	1:E:94:ARG:N	1.99	0.94
2:F:41:ARG:HH11	2:F:187:THR:CG2	1.80	0.94
3:G:38:HIS:CD2	3:G:45:ALA:HB1	2.01	0.94
3:C:168:LYS:HE2	8:C:2064:HOH:O	1.66	0.94
3:G:206:GLY:O	3:G:210:GLY:N	1.99	0.94
1:A:395:ASP:O	1:A:399:GLU:CB	2.16	0.94
1:E:477:ASP:C	1:E:478:VAL:HG23	1.93	0.94
1:E:592:LEU:HD23	1:E:603:GLN:HE22	1.30	0.94
1:E:608:PHE:CD1	1:E:608:PHE:C	2.39	0.94
2:F:160:GLU:H	2:F:179:ASN:HD21	1.12	0.94
1:A:42:GLN:NE2	1:A:505:ARG:HD3	1.82	0.94
1:A:519:TRP:CE2	1:A:540:ILE:HG12	2.03	0.94
2:B:25:MET:HA	2:B:25:MET:CE	1.98	0.94
3:C:108:LEU:O	3:C:110:LYS:HG2	1.66	0.94
2:B:159:ALA:O	2:F:183:LYS:HE2	1.68	0.93
1:A:77:ARG:NH1	2:B:138:TYR:CE2	2.28	0.93
1:A:335:VAL:HG11	1:A:732:ALA:O	1.66	0.93
1:E:493:VAL:HG13	8:E:2013:HOH:O	1.68	0.93
1:A:607:VAL:HG12	1:A:607:VAL:O	1.69	0.93
2:B:41:ARG:NH1	2:B:187:THR:CG2	2.32	0.93
3:C:140:ASN:HD22	3:C:140:ASN:H	1.16	0.93
1:E:388:CYS:SG	1:E:413:ARG:NE	2.42	0.93
2:F:65:PRO:HD2	4:F:1196:SF4:S4	2.08	0.93
3:C:128:LEU:HB3	8:C:2062:HOH:O	1.66	0.93
1:A:314:GLU:O	1:A:318:GLU:HG3	1.68	0.92
1:A:602:HIS:ND1	1:A:606:PRO:HG3	1.82	0.92
1:A:335:VAL:O	1:A:733:GLY:HA2	1.67	0.92
1:E:397:GLU:HB3	1:E:398:PRO:HD3	1.51	0.92
2:B:46:TYR:HD1	8:B:2028:HOH:O	1.34	0.92
3:G:63:LEU:HD13	7:G:1251:MQ7:H2M3	1.51	0.92
2:B:46:TYR:HE2	8:B:2032:HOH:O	1.43	0.92
1:E:323:LYS:HD3	1:E:354:LEU:HA	0.93	0.92
3:G:196:GLU:HG2	8:G:2057:HOH:O	1.68	0.92
2:F:2:PRO:HD2	2:F:80:ASP:OD2	1.71	0.91
1:A:93:ASP:OD1	1:A:758:ARG:NH2	2.02	0.91
1:E:388:CYS:CB	1:E:593:TYR:OH	2.17	0.91
1:E:301:ALA:O	1:E:305:THR:HB	1.71	0.91
2:F:47:PRO:HD2	8:F:2035:HOH:O	1.70	0.91
1:A:602:HIS:ND1	1:A:606:PRO:CG	2.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:GLY:O	5:A:1766:MGD:O5'	1.89	0.91
1:A:42:GLN:NE2	1:A:485:TYR:O	2.04	0.91
3:G:139:ASN:H	3:G:139:ASN:HD22	1.18	0.91
1:A:429:PRO:O	1:A:430:TYR:CD2	2.23	0.91
1:E:116:THR:HG23	1:E:119:GLU:H	1.34	0.90
1:A:397:GLU:CB	1:A:398:PRO:HD3	2.01	0.90
1:A:647:ASN:C	1:A:648:GLU:HG3	1.95	0.90
1:E:81:ARG:HG2	1:E:628:VAL:O	1.71	0.90
3:C:53:ALA:O	3:C:57:ILE:HG13	1.71	0.89
2:F:146:GLU:HG2	8:F:2004:HOH:O	1.71	0.89
3:G:154:THR:HG22	3:G:238:ARG:HE	1.34	0.89
1:A:97:ARG:NH2	1:A:763:ARG:NH2	2.09	0.89
3:C:172:ALA:HA	3:C:175:PRO:HG2	1.53	0.89
1:E:590:ILE:CG1	8:E:2177:HOH:O	2.06	0.89
1:A:70:ALA:O	8:A:2036:HOH:O	1.88	0.89
1:E:614:PRO:HG2	8:E:2341:HOH:O	1.71	0.89
1:A:632:ALA:O	1:A:635:GLN:HG3	1.73	0.88
3:C:155:THR:HG21	3:C:239:ARG:HG2	1.55	0.88
1:A:183:TRP:CH2	1:A:596:ARG:HD3	2.06	0.88
1:E:498:LYS:HE2	8:E:2294:HOH:O	1.73	0.88
1:A:256:THR:HG21	1:A:305:THR:HA	1.56	0.88
3:G:63:LEU:CD1	7:G:1251:MQ7:C2M	2.51	0.88
1:A:686:ALA:HB3	8:A:2330:HOH:O	1.72	0.88
2:B:117:THR:HG21	8:B:2094:HOH:O	1.74	0.88
1:E:305:THR:HG22	1:E:307:ILE:H	1.38	0.88
1:A:183:TRP:HE1	1:A:413:ARG:HH22	1.22	0.88
1:A:97:ARG:HH21	1:A:763:ARG:HH22	0.93	0.88
2:B:16:CYS:O	2:B:16:CYS:SG	2.32	0.88
1:E:116:THR:CG2	1:E:119:GLU:HB3	2.04	0.88
1:A:284:VAL:HG23	1:A:587:SER:HB3	1.56	0.87
1:A:740:ARG:NH1	8:A:2360:HOH:O	2.05	0.87
1:E:342:TYR:HD1	1:E:607:VAL:HB	1.36	0.87
3:C:155:THR:CG2	3:C:239:ARG:HE	1.87	0.87
1:E:324:PRO:HD3	8:E:2166:HOH:O	1.73	0.87
1:A:580:ARG:HH11	1:A:580:ARG:HB3	1.36	0.87
1:E:283:THR:HG22	8:E:2178:HOH:O	1.72	0.87
1:A:608:PHE:CD1	1:A:608:PHE:C	2.47	0.87
1:E:510:GLU:HG3	8:E:2299:HOH:O	1.73	0.87
1:E:109:GLU:HG3	8:E:2065:HOH:O	1.73	0.87
1:A:48:PHE:CE1	1:A:145:HIS:CE1	2.63	0.87
1:A:585:THR:O	1:A:586:ALA:CB	2.21	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:VAL:HG13	1:A:283:THR:CG2	2.04	0.86
1:A:629:HIS:HA	1:A:634:THR:HG21	1.56	0.86
8:B:2144:HOH:O	3:C:251:LEU:HD11	1.74	0.86
1:A:75:ARG:HD2	1:A:220:GLN:HE22	1.38	0.86
1:E:116:THR:HG22	1:E:119:GLU:CB	2.04	0.86
2:F:72:THR:HG22	2:F:74:ALA:H	1.38	0.86
1:A:183:TRP:HH2	1:A:596:ARG:HD3	1.40	0.86
1:A:591:GLU:O	1:A:592:LEU:HD12	1.75	0.86
2:B:41:ARG:NH1	2:B:187:THR:HG22	1.90	0.86
1:E:305:THR:CG2	1:E:307:ILE:H	1.88	0.86
1:E:421:ILE:CG2	1:E:421:ILE:O	2.22	0.86
3:G:63:LEU:HD13	7:G:1251:MQ7:C2	2.05	0.86
3:C:207:GLY:O	3:C:209:TRP:N	2.09	0.86
1:E:629:HIS:ND1	1:E:634:THR:HG23	1.91	0.86
3:C:155:THR:HG21	3:C:239:ARG:CG	2.06	0.86
1:E:494:LEU:HD22	1:E:502:ILE:HG12	1.58	0.86
1:A:395:ASP:C	1:A:399:GLU:HB2	2.00	0.85
1:E:453:LYS:HG2	1:E:475:TRP:CH2	2.11	0.85
1:E:488:ARG:HD3	1:E:490:ASP:OD2	1.76	0.85
1:A:591:GLU:HB3	1:A:603:GLN:HE22	1.39	0.85
1:E:109:GLU:CG	8:E:2065:HOH:O	2.23	0.85
1:E:648:GLU:HG2	1:E:681:ARG:HH12	1.39	0.85
1:A:75:ARG:HH11	1:A:220:GLN:NE2	1.74	0.85
1:A:393:GLY:HA3	1:A:407:LYS:CE	2.07	0.84
1:E:95:LEU:HD21	8:E:2275:HOH:O	1.77	0.84
1:A:138:GLU:OE2	1:A:402:LYS:HB2	1.77	0.84
1:A:413:ARG:CD	1:A:413:ARG:H	1.90	0.84
2:B:57:GLN:HE22	2:B:140:ARG:HH22	1.21	0.84
1:A:336:TRP:CD1	1:A:336:TRP:H	1.92	0.84
1:E:685:THR:HG22	2:F:42:GLU:CD	2.02	0.84
1:E:89:THR:OG1	1:E:484:THR:HG21	1.77	0.84
1:A:583:PHE:HE2	1:A:588:GLY:H	1.04	0.84
1:A:170:VAL:O	1:A:175:ALA:CB	2.26	0.84
1:A:232:VAL:H	1:A:247:HIS:HD2	1.20	0.84
3:G:111:SER:O	3:G:115:LEU:HD12	1.77	0.84
1:E:256:THR:HG21	1:E:305:THR:HA	1.59	0.84
3:G:207:PHE:HE2	3:G:211:LEU:CD1	1.89	0.84
1:A:184:VAL:HG22	1:A:592:LEU:HD23	1.60	0.84
3:G:206:GLY:HA2	3:G:209:TYR:HB3	1.58	0.84
1:A:153:VAL:HG11	1:A:167:LYS:HE2	1.60	0.84
1:A:428:GLU:HB3	1:A:429:PRO:CD	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:GLU:O	1:E:281:LYS:HG2	1.77	0.84
1:A:607:VAL:HG13	1:A:609:THR:OG1	1.78	0.83
1:A:651:ILE:HD11	1:A:682:VAL:CG1	2.08	0.83
1:E:592:LEU:HA	1:E:603:GLN:HE22	1.39	0.83
2:F:1:MET:HA	8:F:2001:HOH:O	1.79	0.83
1:A:345:MET:HE3	1:A:592:LEU:HD11	1.60	0.83
1:A:393:GLY:HA3	1:A:407:LYS:HE3	1.59	0.83
3:C:241:LEU:C	3:C:241:LEU:HD12	2.02	0.83
1:E:469:PRO:O	1:E:706:MET:HG3	1.78	0.83
1:E:438:TYR:HD2	8:E:2091:HOH:O	1.61	0.83
1:A:284:VAL:O	1:A:590:ILE:CG2	2.24	0.83
1:A:583:PHE:CA	1:A:584:GLY:N	2.42	0.83
1:A:677:GLU:O	1:A:678:GLY:O	1.97	0.83
1:A:209:HIS:HE1	1:A:625:ARG:H	1.28	0.82
1:E:339:ASP:CB	1:E:607:VAL:HG11	2.09	0.82
1:A:633:ARG:HD2	5:A:1765:MGD:O2B	1.78	0.82
1:A:320:ALA:O	1:A:323:LYS:HG2	1.80	0.82
1:A:595:GLN:O	1:A:595:GLN:CG	2.27	0.82
1:A:42:GLN:HE22	1:A:505:ARG:HD3	1.42	0.82
1:E:100:ILE:HG23	1:E:478:VAL:HG22	1.61	0.82
1:E:602:HIS:HE1	1:E:606:PRO:HG3	0.72	0.82
1:E:539:THR:HG22	1:E:542:GLU:CB	2.10	0.82
2:B:46:TYR:CE2	8:B:2033:HOH:O	2.33	0.82
3:C:140:ASN:H	3:C:140:ASN:ND2	1.73	0.82
3:C:173:LEU:HG	3:C:173:LEU:O	1.79	0.82
1:E:75:ARG:HH11	1:E:220:GLN:HE21	1.26	0.82
1:A:721:THR:HG22	1:A:722:ARG:HG3	1.61	0.81
1:A:116:THR:HG22	1:A:119:GLU:HB3	1.59	0.81
1:A:231:LYS:HA	1:A:247:HIS:CD2	2.15	0.81
3:C:235:ALA:O	3:C:239:ARG:HG3	1.80	0.81
1:E:75:ARG:HH11	1:E:220:GLN:NE2	1.77	0.81
2:F:57:GLN:HE22	2:F:140:ARG:HH22	1.06	0.81
3:G:21:PHE:O	3:G:238:ARG:NH1	2.14	0.81
3:G:234:ALA:O	3:G:238:ARG:HG3	1.78	0.81
1:A:629:HIS:CA	1:A:634:THR:HG21	2.10	0.81
1:E:209:HIS:HE1	1:E:625:ARG:N	1.78	0.81
1:E:604:PRO:O	1:E:606:PRO:CD	2.28	0.81
1:A:285:GLY:O	1:A:590:ILE:HG23	1.81	0.81
2:B:46:TYR:CB	8:B:2028:HOH:O	1.69	0.81
1:A:672:GLN:NE2	1:A:738:PHE:H	1.79	0.81
1:E:608:PHE:C	8:E:2335:HOH:O	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:671:ASN:C	1:E:671:ASN:HD22	1.88	0.81
3:G:206:GLY:HA2	3:G:209:TYR:CB	2.11	0.81
2:B:41:ARG:HH11	2:B:187:THR:HG23	1.45	0.81
1:E:311:VAL:HB	8:E:2195:HOH:O	1.79	0.81
2:B:134:THR:O	2:B:134:THR:HG22	1.76	0.80
2:B:160:GLU:H	2:B:179:ASN:ND2	1.77	0.80
1:A:595:GLN:O	1:A:595:GLN:HG3	1.80	0.80
1:E:69:GLU:O	1:E:70:ALA:HB3	1.79	0.80
1:A:592:LEU:O	1:A:593:TYR:CB	2.27	0.80
1:E:539:THR:HG23	1:E:542:GLU:H	1.45	0.80
1:E:602:HIS:CD2	1:E:604:PRO:CD	2.64	0.80
1:A:377:PRO:HG2	1:A:533:GLN:HG3	1.64	0.80
1:A:604:PRO:O	1:A:606:PRO:HD3	1.70	0.80
2:B:16:CYS:O	2:B:18:ALA:N	2.14	0.80
1:E:38:LYS:HG3	8:E:2020:HOH:O	1.82	0.80
1:A:152:PHE:O	1:A:157:PRO:HD3	1.81	0.80
3:C:108:LEU:O	3:C:110:LYS:CG	2.30	0.80
1:E:388:CYS:HB2	1:E:593:TYR:HH	1.47	0.80
3:G:222:GLN:OE1	3:G:222:GLN:HA	1.82	0.80
1:A:605:LEU:H	1:A:605:LEU:CD2	1.95	0.80
1:E:297:THR:CG2	1:E:299:GLU:H	1.94	0.80
1:E:297:THR:HG23	1:E:299:GLU:H	1.44	0.80
1:A:427:GLY:O	1:A:428:GLU:O	1.99	0.79
1:A:519:TRP:NE1	1:A:540:ILE:HG12	1.95	0.79
1:E:592:LEU:CD2	1:E:603:GLN:HE22	1.95	0.79
1:E:88:THR:HG23	1:E:468:LEU:HD21	1.63	0.79
3:G:139:ASN:H	3:G:139:ASN:ND2	1.81	0.79
1:A:605:LEU:H	1:A:605:LEU:HD23	1.46	0.79
2:B:47:PRO:O	2:B:48:ASN:OD1	2.01	0.79
1:A:232:VAL:H	1:A:247:HIS:CD2	1.99	0.79
1:A:358:GLY:O	1:A:571:TRP:HA	1.81	0.79
1:A:393:GLY:HA3	1:A:407:LYS:NZ	1.96	0.79
2:F:117:THR:HG23	2:F:120:ALA:H	1.47	0.79
1:A:395:ASP:HA	1:A:399:GLU:HG3	0.85	0.79
1:A:345:MET:HE2	1:A:605:LEU:CD2	2.13	0.79
1:E:308:PRO:HB2	8:E:2195:HOH:O	1.83	0.79
1:A:209:HIS:O	1:A:213:ASP:HB3	1.82	0.79
1:E:36:GLU:C	1:E:58:VAL:HG22	2.00	0.79
1:E:511:PRO:HB3	1:E:515:THR:CG2	2.12	0.79
1:E:717:ASN:HD22	5:E:1765:MGD:H192	1.30	0.79
2:F:72:THR:HG23	2:F:89:LYS:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:ILE:HG23	1:E:478:VAL:CG2	2.13	0.78
2:F:67:VAL:HB	2:F:68:PRO:HD3	1.63	0.78
1:E:591:GLU:CD	1:E:604:PRO:CB	2.45	0.78
1:A:390:GLY:H	1:A:595:GLN:HE22	1.31	0.78
1:A:651:ILE:HD13	1:A:656:ALA:HB2	1.62	0.78
1:A:653:LYS:HD2	1:A:686:ALA:H	1.47	0.78
1:E:113:ARG:NH1	1:E:114:VAL:HG13	1.97	0.78
3:C:171:TRP:O	3:C:171:TRP:HE3	1.66	0.78
1:E:431:PRO:HD2	8:E:2259:HOH:O	1.84	0.78
1:A:400:GLY:CA	8:A:2193:HOH:O	2.24	0.78
2:B:47:PRO:HD3	8:B:2031:HOH:O	1.84	0.78
1:E:397:GLU:HB3	1:E:398:PRO:CD	2.14	0.78
1:A:186:GLY:HA3	1:A:584:GLY:N	1.99	0.78
1:A:467:VAL:HG13	8:A:2049:HOH:O	1.84	0.78
2:F:41:ARG:HH11	2:F:187:THR:HG23	1.48	0.78
1:A:390:GLY:N	1:A:595:GLN:HE22	1.82	0.77
3:C:21:HIS:HE1	3:C:64:LEU:HD11	1.49	0.77
1:A:152:PHE:O	1:A:157:PRO:CD	2.33	0.77
3:C:101:LEU:O	3:C:105:LEU:HD12	1.84	0.77
3:C:21:HIS:CE1	3:C:64:LEU:HD21	2.20	0.77
2:F:40:GLU:HB2	8:F:2021:HOH:O	1.85	0.77
1:A:429:PRO:O	1:A:430:TYR:CG	2.37	0.77
1:A:642:GLU:HG2	2:B:34:PHE:HZ	1.50	0.77
2:B:190:SER:HB3	3:C:252:GLY:N	1.98	0.77
1:E:635:GLN:NE2	1:E:635:GLN:H	1.83	0.77
1:A:360:PRO:HD3	1:A:571:TRP:CZ3	2.20	0.77
1:E:589:LYS:HB3	1:E:592:LEU:HB2	1.65	0.77
1:E:589:LYS:HG2	1:E:592:LEU:HD12	1.67	0.77
1:A:583:PHE:CE2	1:A:587:SER:C	2.63	0.77
1:A:729:SER:O	1:A:729:SER:OG	1.93	0.77
1:E:116:THR:HG21	8:E:2071:HOH:O	1.84	0.77
3:G:107:LEU:O	3:G:109:LYS:N	2.17	0.77
1:A:625:ARG:HH22	5:A:1765:MGD:H15	1.33	0.76
1:E:397:GLU:CB	1:E:398:PRO:HD3	2.15	0.76
1:A:116:THR:HG22	1:A:119:GLU:N	1.98	0.76
1:A:186:GLY:CA	1:A:583:PHE:O	2.22	0.76
1:A:301:ALA:O	1:A:305:THR:HB	1.86	0.76
1:A:388:CYS:HA	1:A:593:TYR:OH	1.84	0.76
1:A:413:ARG:H	1:A:413:ARG:HD2	1.50	0.76
3:G:206:GLY:O	3:G:207:PHE:C	2.28	0.76
2:F:169:GLN:NE2	8:F:2106:HOH:O	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:145:ASN:C	3:C:145:ASN:HD22	1.89	0.76
1:E:551:LEU:O	1:E:553:LEU:HB2	1.86	0.76
1:E:648:GLU:HG2	1:E:681:ARG:NH1	2.00	0.76
1:A:673:ASP:OD2	1:A:721:THR:HG21	1.85	0.76
1:E:297:THR:CG2	1:E:299:GLU:HG2	2.16	0.76
1:E:490:ASP:O	8:E:2288:HOH:O	2.03	0.76
2:F:3:ARG:HG2	8:F:2003:HOH:O	1.85	0.76
3:G:76:ILE:O	3:G:80:LEU:HG	1.86	0.76
3:C:197:GLU:HG2	8:C:2074:HOH:O	1.84	0.76
1:E:421:ILE:O	1:E:421:ILE:HG22	1.86	0.76
2:F:47:PRO:CD	8:F:2035:HOH:O	2.29	0.76
1:A:73:LYS:NZ	1:A:192:HIS:HD2	1.83	0.76
1:A:95:LEU:HD12	1:A:467:VAL:C	2.10	0.76
1:A:174:THR:HG23	1:A:178:GLU:HG2	1.68	0.76
1:E:483:ALA:N	1:E:516:LYS:O	2.17	0.76
1:A:349:TYR:CE2	1:A:590:ILE:O	2.39	0.76
3:C:171:TRP:O	3:C:172:ALA:HB2	1.87	0.75
1:E:71:ASN:HD22	1:E:74:SER:H	1.31	0.75
1:A:510:GLU:HG3	8:A:2023:HOH:O	1.87	0.75
1:A:342:TYR:CD1	1:A:607:VAL:HB	2.22	0.75
1:A:346:ALA:HB2	1:A:605:LEU:CD1	2.15	0.75
1:E:118:GLU:HG3	8:E:2305:HOH:O	1.86	0.75
1:E:139:ALA:O	1:E:433:LYS:O	2.04	0.75
1:E:424:MET:HG2	1:E:459:LEU:HD21	1.68	0.75
1:A:95:LEU:HD11	1:A:468:LEU:O	1.85	0.75
1:A:457:LYS:HA	8:A:2219:HOH:O	1.85	0.75
3:C:21:HIS:ND1	3:C:64:LEU:HG	2.00	0.75
1:E:232:VAL:H	1:E:247:HIS:CD2	2.04	0.75
1:E:465:ILE:O	1:E:466:ASP:HB3	1.86	0.75
1:A:166:ALA:HB2	1:A:415:THR:HG23	1.67	0.75
1:A:561:MET:O	1:A:563:THR:N	2.19	0.75
3:C:64:LEU:HD22	7:C:1252:MQ7:C2	2.15	0.75
1:E:591:GLU:HG3	1:E:591:GLU:O	1.85	0.75
1:E:632:ALA:O	1:E:635:GLN:NE2	2.19	0.75
1:A:606:PRO:O	1:A:608:PHE:N	2.19	0.75
1:E:473:VAL:HG11	8:E:2275:HOH:O	1.86	0.75
1:A:388:CYS:HA	1:A:593:TYR:CE1	2.21	0.75
3:G:150:LEU:O	3:G:154:THR:HB	1.87	0.75
1:A:382:GLU:HA	8:A:2184:HOH:O	1.86	0.75
2:B:41:ARG:HD2	2:B:187:THR:HG23	1.68	0.75
1:E:69:GLU:O	1:E:70:ALA:CB	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:438:TYR:CD2	8:E:2091:HOH:O	2.38	0.75
1:A:89:THR:OG1	1:A:484:THR:HG21	1.87	0.74
1:A:184:VAL:HG23	1:A:592:LEU:HD23	0.77	0.74
1:A:335:VAL:HG13	1:A:732:ALA:C	2.12	0.74
1:E:153:VAL:HG11	1:E:167:LYS:HE2	1.69	0.74
1:E:577:LYS:HE2	8:E:2321:HOH:O	1.87	0.74
1:E:607:VAL:O	1:E:607:VAL:HG13	1.83	0.74
1:E:686:ALA:HB1	8:E:2385:HOH:O	1.86	0.74
1:E:762:GLU:HB2	8:E:2445:HOH:O	1.85	0.74
2:B:44:GLY:O	2:B:49:LEU:HD13	1.87	0.74
1:E:95:LEU:HD11	8:E:2275:HOH:O	1.85	0.74
1:E:642:GLU:OE2	2:F:32:GLY:N	2.16	0.74
2:F:57:GLN:HE21	2:F:140:ARG:HH22	1.36	0.74
2:B:44:GLY:O	2:B:49:LEU:CD1	2.35	0.74
1:E:592:LEU:HD23	1:E:603:GLN:NE2	2.02	0.74
1:E:673:ASP:OD2	1:E:721:THR:CG2	2.36	0.74
1:E:209:HIS:CE1	1:E:625:ARG:H	2.02	0.74
3:G:63:LEU:HB3	7:G:1251:MQ7:C12	2.18	0.74
1:E:488:ARG:HB2	1:E:517:PRO:HB3	1.68	0.74
1:E:183:TRP:HH2	1:E:596:ARG:HD3	1.51	0.74
2:F:3:ARG:HD2	2:F:62:GLU:OE2	1.87	0.74
2:F:55:PRO:HG2	4:F:1194:SF4:S2	2.27	0.74
1:A:428:GLU:O	1:A:429:PRO:C	2.27	0.74
1:A:519:TRP:CE2	1:A:540:ILE:CG1	2.70	0.74
3:C:18:ASN:OD1	3:C:67:GLU:OE2	2.05	0.74
1:E:586:ALA:HB3	8:E:2324:HOH:O	1.87	0.74
1:E:708:LEU:HA	8:E:2407:HOH:O	1.87	0.74
1:A:578:GLU:HB3	1:A:580:ARG:HD3	1.70	0.74
1:A:653:LYS:CG	1:A:684:PRO:O	2.35	0.74
1:E:186:GLY:H	1:E:583:PHE:HA	1.51	0.74
1:E:386:GLY:O	1:E:388:CYS:SG	2.42	0.74
3:G:154:THR:CG2	3:G:238:ARG:NE	2.47	0.74
1:A:186:GLY:H	1:A:583:PHE:HA	1.53	0.74
1:E:97:ARG:NH2	1:E:763:ARG:HD2	2.02	0.74
1:A:710:HIS:O	8:A:2344:HOH:O	2.06	0.73
3:C:222:TRP:CG	3:C:223:GLN:N	2.52	0.73
1:E:346:ALA:N	1:E:605:LEU:HD12	2.03	0.73
1:A:483:ALA:HA	1:A:515:THR:CG2	2.17	0.73
1:E:183:TRP:CH2	1:E:596:ARG:HD3	2.23	0.73
1:A:367:GLN:HG3	8:A:2268:HOH:O	1.88	0.73
1:E:734:LEU:HD22	8:E:2419:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:154:THR:HG21	3:G:238:ARG:HG2	1.70	0.73
1:A:183:TRP:CB	1:A:592:LEU:HD22	2.19	0.73
1:A:286:PHE:HA	1:A:590:ILE:HG21	1.70	0.73
1:A:488:ARG:NH2	5:A:1765:MGD:O6	2.21	0.73
1:A:42:GLN:O	1:A:53:ILE:HG12	1.88	0.73
2:F:43:VAL:HG23	8:F:2121:HOH:O	1.89	0.73
1:A:581:LEU:CD1	8:A:2271:HOH:O	2.36	0.73
1:A:611:PRO:HB3	8:A:2136:HOH:O	1.86	0.73
2:B:6:MET:HE3	8:B:2044:HOH:O	1.87	0.73
1:E:589:LYS:HG2	1:E:592:LEU:CD1	2.19	0.73
1:E:591:GLU:OE2	1:E:604:PRO:HG3	1.88	0.73
2:F:160:GLU:H	2:F:179:ASN:ND2	1.86	0.73
1:A:580:ARG:CB	1:A:580:ARG:NH1	2.49	0.73
2:F:117:THR:HG22	2:F:119:CYS:H	1.53	0.73
1:A:422:GLU:HB3	1:A:423:PRO:HD3	1.70	0.73
1:A:582:PRO:C	8:A:2274:HOH:O	2.31	0.73
1:A:685:THR:HB	2:B:42:GLU:CD	2.14	0.73
1:E:639:VAL:HG11	2:F:25:MET:HE3	1.71	0.73
3:G:12:PHE:CZ	3:G:246:GLN:HG2	2.23	0.73
1:A:71:ASN:HD22	1:A:74:SER:H	1.33	0.73
1:A:134:LYS:HE2	8:A:2077:HOH:O	1.87	0.73
1:E:591:GLU:OE1	1:E:604:PRO:CA	2.37	0.73
3:G:51:TYR:N	8:G:2015:HOH:O	2.22	0.73
1:A:73:LYS:HZ1	1:A:192:HIS:HD2	1.37	0.72
1:A:581:LEU:HD11	8:A:2271:HOH:O	1.89	0.72
1:A:672:GLN:HE22	1:A:738:PHE:H	1.34	0.72
1:E:635:GLN:O	1:E:641:MET:HG2	1.89	0.72
1:E:232:VAL:H	1:E:247:HIS:HD2	1.36	0.72
1:E:470:GLN:HG2	1:E:706:MET:SD	2.29	0.72
2:F:117:THR:HG21	8:F:2076:HOH:O	1.88	0.72
3:G:115:LEU:HD13	8:G:2031:HOH:O	1.89	0.72
3:G:206:GLY:O	3:G:209:TYR:CA	2.36	0.72
1:A:153:VAL:CG1	1:A:167:LYS:HE2	2.20	0.72
1:A:339:ASP:HB3	1:A:607:VAL:HG11	1.70	0.72
1:E:575:TRP:O	1:E:578:GLU:HB2	1.87	0.72
1:A:36:GLU:O	1:A:58:VAL:HG22	1.90	0.72
1:A:484:THR:HG22	1:A:487:GLU:HG3	1.72	0.72
1:E:259:ALA:HB3	8:E:2193:HOH:O	1.89	0.72
1:E:315:VAL:HG12	1:E:319:MET:HE3	1.70	0.72
1:E:569:LYS:CD	8:E:2320:HOH:O	2.26	0.72
1:A:387:GLY:O	1:A:593:TYR:CE1	2.43	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ARG:HD2	1:E:220:GLN:HE22	1.55	0.72
1:A:195:ILE:HA	1:A:362:GLY:O	1.89	0.72
1:A:330:PRO:HD2	8:A:2164:HOH:O	1.89	0.72
1:A:338:GLY:O	1:A:726:ASP:HA	1.90	0.72
1:A:642:GLU:HG2	2:B:34:PHE:CZ	2.24	0.72
1:E:539:THR:CG2	1:E:542:GLU:H	2.03	0.72
2:B:46:TYR:O	8:B:2029:HOH:O	2.08	0.72
2:B:117:THR:HG22	2:B:119:CYS:N	2.04	0.72
3:C:64:LEU:HD22	7:C:1252:MQ7:C3	2.20	0.72
1:E:239:PHE:HB3	1:E:687:ARG:HB3	1.71	0.72
1:A:75:ARG:HH11	1:A:220:GLN:HE21	1.36	0.71
1:E:116:THR:CG2	1:E:119:GLU:N	2.51	0.71
1:E:311:VAL:CB	8:E:2195:HOH:O	2.37	0.71
1:E:434:GLY:HA2	1:E:461:LEU:O	1.89	0.71
1:E:477:ASP:O	1:E:478:VAL:HG22	1.88	0.71
1:A:139:ALA:O	1:A:433:LYS:O	2.08	0.71
1:A:364:TYR:HB2	1:A:570:PRO:HB3	1.72	0.71
7:C:1252:MQ7:O1	8:C:2090:HOH:O	2.08	0.71
1:E:253:LYS:O	1:E:256:THR:HB	1.90	0.71
1:A:335:VAL:HG13	1:A:732:ALA:O	1.89	0.71
2:B:47:PRO:CD	8:B:2031:HOH:O	2.37	0.71
1:E:30:ALA:HB3	8:E:2002:HOH:O	1.88	0.71
1:A:305:THR:O	1:A:306:GLU:HB2	1.89	0.71
1:A:305:THR:HG22	1:A:307:ILE:H	1.56	0.71
1:A:631:PHE:O	1:A:698:GLY:HA3	1.89	0.71
1:A:238:ARG:HG3	1:A:688:ILE:HD12	1.70	0.71
1:E:81:ARG:NH1	1:E:630:THR:OG1	2.23	0.71
1:E:495:VAL:CG2	8:E:2296:HOH:O	2.39	0.71
1:E:282:TYR:O	1:E:587:SER:HB3	1.91	0.71
1:E:424:MET:HE2	1:E:455:ALA:CB	2.19	0.71
1:E:589:LYS:NZ	8:E:2324:HOH:O	2.22	0.71
1:A:231:LYS:HA	1:A:247:HIS:NE2	2.05	0.71
1:A:349:TYR:HE1	1:A:605:LEU:HD21	1.56	0.71
1:E:465:ILE:O	1:E:466:ASP:CB	2.39	0.71
1:E:673:ASP:OD2	1:E:721:THR:HG21	1.91	0.71
1:A:396:HIS:HB3	1:A:403:PRO:HB3	1.71	0.71
1:E:91:ASP:O	1:E:92:PRO:O	2.09	0.71
1:E:320:ALA:O	1:E:323:LYS:HB2	1.91	0.71
1:A:37:VAL:HG12	1:A:38:LYS:N	2.06	0.70
1:E:391:PRO:O	1:E:413:ARG:HG2	1.90	0.70
2:B:192:VAL:HG12	2:B:193:HIS:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:TRP:HB2	1:A:592:LEU:HD22	1.74	0.70
1:A:604:PRO:C	1:A:606:PRO:HD2	2.01	0.70
1:A:292:HIS:NE2	1:A:604:PRO:HB2	2.07	0.70
1:A:603:GLN:HB3	1:A:604:PRO:CD	2.17	0.70
1:E:720:GLN:HB3	8:E:2419:HOH:O	1.92	0.70
1:A:605:LEU:HD23	1:A:605:LEU:N	2.06	0.70
3:C:241:LEU:C	3:C:241:LEU:CD1	2.63	0.70
1:E:604:PRO:C	1:E:605:LEU:CD2	2.62	0.70
1:A:336:TRP:H	1:A:336:TRP:HD1	1.35	0.70
1:A:583:PHE:HE2	1:A:588:GLY:CA	2.04	0.70
1:E:651:ILE:HD11	1:E:682:VAL:CG1	2.22	0.70
3:G:221:TRP:HZ3	3:G:225:LEU:HD13	1.55	0.70
1:A:511:PRO:HB3	1:A:515:THR:HG22	1.72	0.70
2:F:72:THR:HG21	2:F:89:LYS:O	1.90	0.70
1:A:43:ILE:CG1	1:A:505:ARG:HB3	2.08	0.70
1:A:342:TYR:HD1	1:A:607:VAL:HB	1.56	0.70
1:A:391:PRO:O	1:A:413:ARG:HB3	1.92	0.70
1:A:687:ARG:NH2	2:B:40:GLU:OE2	2.24	0.70
1:E:97:ARG:HH21	1:E:763:ARG:NH1	1.88	0.70
2:B:2:PRO:HB3	2:B:144:ASP:CG	2.16	0.70
1:E:670:VAL:HG22	1:E:676:LYS:HG3	1.73	0.69
2:F:78:THR:HG22	2:F:80:ASP:H	1.55	0.69
3:G:129:TYR:CD2	3:G:130:PRO:HD3	2.26	0.69
1:A:239:PHE:HB3	1:A:687:ARG:HB3	1.75	0.69
1:E:708:LEU:O	1:E:712:ARG:HD2	1.93	0.69
1:A:428:GLU:O	1:A:430:TYR:O	2.11	0.69
8:A:2014:HOH:O	2:B:25:MET:HE1	1.91	0.69
2:F:45:GLU:HB2	8:F:2028:HOH:O	1.91	0.69
1:A:293:VAL:HG13	1:A:293:VAL:O	1.92	0.69
1:E:267:VAL:HG22	8:E:2197:HOH:O	1.91	0.69
1:E:622:LEU:HD22	5:E:1766:MGD:H8	1.73	0.69
3:G:63:LEU:CD1	7:G:1251:MQ7:H2M1	2.23	0.69
1:A:99:LEU:O	1:A:478:VAL:HA	1.93	0.69
1:A:166:ALA:HB2	1:A:415:THR:CG2	2.21	0.69
2:B:72:THR:HG21	2:B:89:LYS:O	1.92	0.69
1:E:474:MET:HE3	8:E:2068:HOH:O	1.92	0.69
1:A:127:LYS:HE2	8:A:2223:HOH:O	1.93	0.69
1:A:635:GLN:O	1:A:709:ALA:HB2	1.92	0.69
2:B:17:ALA:HB1	2:B:20:ALA:HB3	1.75	0.69
2:F:78:THR:HG21	8:F:2058:HOH:O	1.93	0.69
3:G:196:GLU:CD	3:G:196:GLU:H	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:THR:HG23	1:E:299:GLU:HG2	1.75	0.69
1:A:53:ILE:HD12	1:A:65:VAL:HG22	1.75	0.69
1:A:427:GLY:O	1:A:430:TYR:O	2.10	0.69
1:A:539:THR:CG2	1:A:541:GLU:HG2	2.23	0.69
1:E:174:THR:HG23	1:E:178:GLU:HG2	1.74	0.69
1:E:511:PRO:CB	1:E:515:THR:HG22	2.19	0.69
1:E:539:THR:HG22	1:E:542:GLU:HB3	1.73	0.69
1:A:755:LEU:O	1:A:758:ARG:HD3	1.93	0.69
1:E:746:ARG:HH11	1:E:746:ARG:HG3	1.58	0.69
2:B:121:HIS:O	2:B:125:LYS:HE2	1.93	0.68
3:C:222:TRP:CG	3:C:223:GLN:H	2.09	0.68
1:E:305:THR:HG23	1:E:307:ILE:HG12	1.75	0.68
1:E:553:LEU:HD21	1:E:557:THR:HG21	1.75	0.68
1:E:585:THR:OG1	1:E:589:LYS:HE3	1.92	0.68
3:G:225:LEU:HB3	8:G:2069:HOH:O	1.92	0.68
1:E:418:GLN:NE2	1:E:418:GLN:H	1.91	0.68
1:A:79:CYS:HB2	1:A:80:PRO:HD2	1.74	0.68
1:A:561:MET:HE1	1:A:564:LEU:HD12	1.75	0.68
1:A:646:GLU:O	1:A:648:GLU:OE2	2.12	0.68
3:C:47:ARG:NH1	3:C:107:TYR:O	2.26	0.68
2:F:88:LYS:O	3:G:74:THR:HG22	1.93	0.68
2:B:142:PHE:C	2:B:152:VAL:HG22	2.18	0.68
3:C:155:THR:HG22	3:C:239:ARG:NE	2.04	0.68
3:C:155:THR:CG2	3:C:239:ARG:NE	2.56	0.68
1:E:297:THR:HG21	8:E:2188:HOH:O	1.93	0.68
1:E:740:ARG:NH1	8:E:2427:HOH:O	2.26	0.68
2:B:57:GLN:O	2:B:58:CYS:C	2.36	0.68
3:C:64:LEU:CD2	7:C:1252:MQ7:C5	2.72	0.68
3:C:130:TYR:CD2	3:C:131:PRO:HD3	2.29	0.68
2:F:43:VAL:CG2	8:F:2121:HOH:O	2.42	0.68
1:E:672:GLN:NE2	1:E:738:PHE:H	1.91	0.68
1:A:256:THR:CG2	1:A:305:THR:HA	2.23	0.67
1:A:642:GLU:OE2	2:B:31:PRO:O	2.12	0.67
1:A:121:LEU:HD13	1:A:524:GLU:HB3	1.76	0.67
1:A:580:ARG:HH11	1:A:580:ARG:HB2	1.56	0.67
2:B:78:THR:HG21	8:B:2068:HOH:O	1.94	0.67
1:E:632:ALA:C	1:E:635:GLN:NE2	2.51	0.67
2:F:41:ARG:HH11	2:F:187:THR:HG22	1.59	0.67
3:G:206:GLY:C	3:G:209:TYR:H	2.01	0.67
1:A:293:VAL:O	1:A:293:VAL:CG1	2.41	0.67
3:C:64:LEU:HD22	7:C:1252:MQ7:C1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:633:ARG:HD2	5:E:1765:MGD:O2B	1.94	0.67
3:G:38:HIS:CE1	8:G:2011:HOH:O	2.46	0.67
1:A:349:TYR:CE1	1:A:605:LEU:HD21	2.30	0.67
1:A:495:VAL:HG13	8:A:2019:HOH:O	1.94	0.67
2:B:166:ARG:HH22	3:C:249:GLN:NE2	1.92	0.67
1:A:721:THR:OG1	8:A:2351:HOH:O	2.12	0.67
2:B:72:THR:HG23	2:B:89:LYS:HB3	1.76	0.67
1:E:345:MET:HB2	1:E:605:LEU:HD13	1.76	0.67
1:E:606:PRO:CD	1:E:607:VAL:H	2.07	0.67
8:E:2385:HOH:O	2:F:49:LEU:HD11	1.95	0.67
2:F:194:HIS:N	8:F:2128:HOH:O	2.26	0.67
1:A:277:GLU:HB3	1:A:281:LYS:HZ3	1.60	0.67
1:A:314:GLU:HG2	8:A:2161:HOH:O	1.95	0.67
3:G:63:LEU:CD1	7:G:1251:MQ7:C2	2.73	0.67
1:A:609:THR:O	1:A:610:PRO:C	2.38	0.67
1:E:318:GLU:O	1:E:322:HIS:HD2	1.79	0.67
1:E:539:THR:HG22	1:E:542:GLU:HB2	1.77	0.67
1:A:75:ARG:NH1	1:A:220:GLN:NE2	2.42	0.66
1:A:647:ASN:HD22	1:A:647:ASN:H	1.42	0.66
1:E:90:TYR:OH	1:E:509:HIS:HE1	1.78	0.66
1:E:116:THR:HG22	1:E:119:GLU:H	1.50	0.66
2:B:166:ARG:NH2	3:C:249:GLN:NE2	2.43	0.66
1:A:186:GLY:C	1:A:583:PHE:O	2.38	0.66
3:C:17:THR:CG2	3:C:67:GLU:CG	2.68	0.66
1:A:346:ALA:HB2	1:A:605:LEU:HD13	1.75	0.66
1:A:471:GLU:O	1:A:471:GLU:HG2	1.96	0.66
3:C:171:TRP:O	3:C:171:TRP:CG	2.47	0.66
3:C:197:GLU:CD	3:C:197:GLU:H	2.03	0.66
3:G:208:TRP:HA	3:G:208:TRP:CE3	2.31	0.66
1:A:204:VAL:HB	1:A:328:LEU:HG	1.78	0.66
1:A:603:GLN:CB	1:A:604:PRO:HD3	2.19	0.66
1:A:607:VAL:O	1:A:607:VAL:CG1	2.41	0.66
1:E:679:PRO:HG2	1:E:747:PRO:HB3	1.78	0.66
1:A:708:LEU:HD22	1:A:755:LEU:HB3	1.77	0.66
8:B:2027:HOH:O	3:C:2:ALA:HB1	1.95	0.66
1:A:630:THR:H	1:A:634:THR:HG21	1.60	0.66
2:F:193:HIS:HB2	8:F:2129:HOH:O	1.95	0.66
3:G:207:PHE:C	3:G:207:PHE:CD2	2.73	0.66
2:B:57:GLN:HE22	2:B:140:ARG:NH2	1.92	0.65
1:A:413:ARG:H	1:A:413:ARG:NE	1.93	0.65
1:E:642:GLU:HG3	8:E:2436:HOH:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:105:LEU:HB3	8:G:2011:HOH:O	1.96	0.65
1:A:594:CYS:O	1:A:598:LYS:HG3	1.95	0.65
2:B:3:ARG:HG2	8:B:2001:HOH:O	1.96	0.65
3:C:59:LEU:O	3:C:63:ILE:HG23	1.96	0.65
1:E:479:ILE:O	1:E:480:LEU:HD23	1.97	0.65
1:A:37:VAL:HG13	1:A:57:ALA:O	1.97	0.65
1:A:558:MET:HE2	1:A:558:MET:HA	1.78	0.65
1:E:588:GLY:HA3	8:E:2173:HOH:O	1.96	0.65
1:A:345:MET:HG2	1:A:592:LEU:HD21	1.79	0.65
1:A:602:HIS:HE1	1:A:606:PRO:HG3	0.87	0.65
3:G:39:LEU:HD13	3:G:116:ALA:HB3	1.79	0.65
1:A:107:ARG:HG2	1:A:475:TRP:O	1.96	0.65
1:A:467:VAL:CG2	8:A:2226:HOH:O	2.44	0.65
1:E:669:LEU:CD2	1:E:741:LEU:HD22	2.26	0.65
3:G:105:LEU:HG	8:G:2031:HOH:O	1.94	0.65
1:A:689:ARG:NH2	1:A:691:ASP:OD2	2.30	0.65
2:B:88:LYS:O	3:C:75:THR:HG22	1.95	0.65
1:E:310:GLN:NE2	1:E:314:GLU:OE2	2.30	0.65
2:F:164:VAL:HG22	2:F:173:PRO:HB2	1.79	0.65
1:A:39:SER:HB2	8:A:2005:HOH:O	1.97	0.65
1:A:658:ARG:C	1:A:659:LEU:O	2.33	0.65
3:G:189:TYR:O	3:G:192:THR:HB	1.97	0.65
1:A:252:ILE:CD1	1:A:256:THR:HG22	2.26	0.65
2:B:27:ASN:HD21	2:B:121:HIS:CE1	2.15	0.65
3:C:207:GLY:C	3:C:209:TRP:N	2.54	0.65
1:E:639:VAL:HG21	2:F:25:MET:HE1	1.78	0.65
1:A:540:ILE:O	1:A:544:LEU:HG	1.97	0.64
1:A:42:GLN:CD	1:A:505:ARG:HB2	2.22	0.64
1:A:319:MET:CE	1:A:328:LEU:HD11	2.26	0.64
1:E:647:ASN:HD21	1:E:714:ALA:H	1.45	0.64
1:A:120:ALA:HB3	8:A:2067:HOH:O	1.97	0.64
1:A:427:GLY:C	1:A:428:GLU:O	2.41	0.64
1:A:428:GLU:O	1:A:430:TYR:N	2.31	0.64
2:B:117:THR:CG2	2:B:120:ALA:H	2.10	0.64
2:B:117:THR:HB	8:B:2010:HOH:O	1.96	0.64
3:G:115:LEU:HB3	8:G:2031:HOH:O	1.97	0.64
1:A:345:MET:HE3	1:A:592:LEU:CD1	2.27	0.64
1:A:382:GLU:HB3	8:A:2185:HOH:O	1.97	0.64
1:A:602:HIS:HE1	1:A:606:PRO:CG	1.81	0.64
2:B:57:GLN:NE2	2:B:140:ARG:HH22	1.92	0.64
1:E:345:MET:CB	1:E:605:LEU:HD13	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HZ1	1:A:192:HIS:CD2	2.15	0.64
1:A:81:ARG:HH21	1:A:214:THR:HG22	1.61	0.64
1:A:109:GLU:OE2	1:A:111:LYS:HE2	1.97	0.64
1:A:519:TRP:CZ2	1:A:540:ILE:HG13	2.32	0.64
1:A:558:MET:CE	1:A:561:MET:SD	2.86	0.64
1:E:649:VAL:HG13	1:E:695:ILE:CG2	2.27	0.64
1:A:39:SER:OG	8:A:2004:HOH:O	2.15	0.64
1:A:152:PHE:O	1:A:157:PRO:CG	2.45	0.64
1:E:100:ILE:HG12	1:E:478:VAL:HG22	1.78	0.64
1:A:285:GLY:C	1:A:590:ILE:HG23	2.23	0.64
1:A:580:ARG:NH1	1:A:580:ARG:HB2	2.12	0.64
1:A:635:GLN:HG3	1:A:701:HIS:NE2	2.13	0.64
7:C:1252:MQ7:C12	7:C:1252:MQ7:H2M2	2.27	0.64
1:E:551:LEU:O	1:E:552:GLY:C	2.41	0.64
2:B:36:LEU:HD11	8:B:2103:HOH:O	1.98	0.64
1:E:591:GLU:O	1:E:603:GLN:NE2	2.31	0.64
1:E:632:ALA:C	1:E:635:GLN:HE22	2.06	0.64
3:G:63:LEU:CD2	7:G:1251:MQ7:C1	2.76	0.64
1:A:53:ILE:HD12	1:A:65:VAL:CG2	2.28	0.64
3:C:207:GLY:HA2	3:C:210:TYR:HB3	1.80	0.64
1:E:204:VAL:HG21	1:E:319:MET:HE2	1.79	0.64
1:E:204:VAL:HB	1:E:328:LEU:HG	1.79	0.64
2:F:166:ARG:HH22	3:G:248:GLN:HE21	1.46	0.64
1:E:391:PRO:HG3	1:E:411:PHE:CZ	2.33	0.64
1:E:77:ARG:NE	8:E:2044:HOH:O	2.31	0.63
1:E:418:GLN:H	1:E:418:GLN:HE21	1.44	0.63
1:E:671:ASN:ND2	1:E:673:ASP:H	1.96	0.63
2:F:2:PRO:HB3	2:F:144:ASP:CG	2.22	0.63
3:G:206:GLY:CA	3:G:209:TYR:CB	2.76	0.63
1:A:122:ASP:OD1	1:A:528:ARG:NH1	2.31	0.63
1:A:583:PHE:CE2	1:A:588:GLY:CA	2.79	0.63
2:B:192:VAL:HG12	2:B:193:HIS:H	1.62	0.63
1:E:687:ARG:NH2	2:F:40:GLU:OE2	2.31	0.63
1:A:336:TRP:O	1:A:735:ARG:HB2	1.97	0.63
3:C:64:LEU:HD21	7:C:1252:MQ7:C5	2.28	0.63
1:E:279:VAL:O	1:E:283:THR:HB	1.97	0.63
1:E:311:VAL:CG2	8:E:2195:HOH:O	2.46	0.63
2:B:114:SER:O	2:B:115:LYS:HB3	1.98	0.63
1:E:339:ASP:HB2	1:E:607:VAL:CG1	2.19	0.63
1:E:108:GLY:HA3	8:E:2063:HOH:O	1.98	0.63
1:A:384:ALA:N	8:A:2186:HOH:O	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:ASN:HD22	3:C:140:ASN:N	1.93	0.63
1:E:323:LYS:CD	1:E:354:LEU:CA	2.64	0.63
1:E:428:GLU:OE1	1:E:428:GLU:HA	1.97	0.63
3:G:207:PHE:O	3:G:211:LEU:N	2.32	0.63
3:C:128:LEU:HD22	8:C:2062:HOH:O	1.99	0.63
1:A:633:ARG:CD	5:A:1765:MGD:O2B	2.47	0.62
3:C:207:GLY:O	3:C:208:PHE:C	2.39	0.62
3:C:239:ARG:NH2	8:C:2083:HOH:O	2.29	0.62
1:A:81:ARG:HE	1:A:214:THR:HG22	1.64	0.62
2:B:117:THR:HG22	2:B:119:CYS:H	1.64	0.62
1:E:297:THR:HG22	1:E:300:TRP:N	2.10	0.62
1:E:539:THR:HG23	1:E:541:GLU:HG2	1.81	0.62
1:E:684:PRO:O	1:E:685:THR:C	2.41	0.62
1:A:519:TRP:CD1	1:A:540:ILE:HG21	2.34	0.62
1:E:605:LEU:H	1:E:605:LEU:HD23	0.45	0.62
1:A:286:PHE:CA	1:A:590:ILE:HG21	2.29	0.62
1:E:256:THR:CG2	1:E:305:THR:HA	2.30	0.62
1:A:426:THR:HG23	8:A:2051:HOH:O	1.98	0.62
1:E:553:LEU:CD2	1:E:557:THR:HG21	2.29	0.62
1:E:590:ILE:O	1:E:592:LEU:HG	2.00	0.62
1:E:591:GLU:OE2	1:E:604:PRO:HB3	1.99	0.62
1:A:319:MET:HE1	1:A:328:LEU:HD11	1.79	0.62
1:A:483:ALA:CA	1:A:515:THR:HG23	2.30	0.62
1:E:549:GLN:HG3	8:E:2311:HOH:O	2.00	0.62
3:G:63:LEU:HD22	7:G:1251:MQ7:C4	2.30	0.62
1:E:477:ASP:C	1:E:478:VAL:CG2	2.60	0.62
3:C:172:ALA:CA	3:C:175:PRO:HG2	2.29	0.62
1:E:116:THR:HG23	1:E:119:GLU:N	2.12	0.62
1:E:421:ILE:O	1:E:421:ILE:HG23	2.00	0.62
1:A:630:THR:N	1:A:634:THR:HG21	2.15	0.61
1:E:396:HIS:CE1	1:E:404:ARG:H	2.18	0.61
1:E:598:LYS:HB3	1:E:599:GLU:OE1	2.00	0.61
2:F:41:ARG:HD2	2:F:187:THR:HG21	1.78	0.61
1:E:470:GLN:NE2	8:E:2276:HOH:O	2.33	0.61
3:G:63:LEU:HD22	7:G:1251:MQ7:C5	2.30	0.61
1:E:651:ILE:HD13	1:E:656:ALA:HB2	1.81	0.61
1:A:151:TRP:O	1:A:156:LEU:HB2	1.99	0.61
2:B:46:TYR:CD2	8:B:2033:HOH:O	2.52	0.61
1:E:208:HIS:HE1	1:E:218:GLN:NE2	1.98	0.61
1:A:93:ASP:CG	1:A:758:ARG:HH22	2.08	0.61
1:A:299:GLU:OE2	1:A:313:ARG:NH2	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:PRO:HD3	1:A:534:TYR:OH	2.00	0.61
1:A:388:CYS:HA	1:A:593:TYR:CZ	2.35	0.61
1:A:534:TYR:O	1:A:535:PHE:HB2	1.99	0.61
2:F:72:THR:HG22	2:F:74:ALA:N	2.11	0.61
1:A:81:ARG:HE	1:A:214:THR:CG2	2.14	0.61
1:E:81:ARG:HE	1:E:214:THR:HG22	1.65	0.61
1:E:724:LYS:HG2	8:E:2424:HOH:O	1.99	0.61
1:A:483:ALA:HA	1:A:515:THR:HG21	1.82	0.61
1:E:194:PRO:O	1:E:363:PHE:HA	2.00	0.61
1:E:604:PRO:C	1:E:606:PRO:HD3	2.26	0.61
1:E:647:ASN:H	1:E:647:ASN:HD22	1.46	0.61
1:E:658:ARG:C	1:E:659:LEU:O	2.33	0.61
2:B:2:PRO:HB3	2:B:144:ASP:HB2	1.83	0.61
1:E:345:MET:HB3	1:E:605:LEU:CD1	2.31	0.61
1:E:346:ALA:H	1:E:605:LEU:HD12	1.64	0.61
3:G:220:PHE:HD1	8:G:2065:HOH:O	1.84	0.61
1:A:285:GLY:C	1:A:590:ILE:CG2	2.74	0.61
1:A:421:ILE:HG22	1:A:421:ILE:O	2.00	0.61
1:A:429:PRO:C	1:A:430:TYR:CD2	2.78	0.61
1:E:79:CYS:HB2	1:E:80:PRO:HD2	1.83	0.61
1:E:109:GLU:HG2	8:E:2065:HOH:O	1.94	0.61
1:E:396:HIS:HB3	1:E:407:LYS:HE3	1.83	0.61
1:E:671:ASN:C	1:E:671:ASN:ND2	2.58	0.61
3:G:221:TRP:HD1	8:G:2032:HOH:O	1.84	0.61
1:A:647:ASN:C	1:A:648:GLU:CG	2.73	0.61
1:E:93:ASP:OD1	1:E:758:ARG:NH2	2.34	0.61
1:E:129:LEU:O	1:E:133:GLU:HG2	2.00	0.61
1:E:299:GLU:OE2	1:E:313:ARG:NH2	2.22	0.61
1:E:519:TRP:CE2	1:E:540:ILE:CG1	2.84	0.61
1:A:36:GLU:O	1:A:36:GLU:HG2	2.01	0.60
1:A:79:CYS:CB	1:A:80:PRO:HD2	2.31	0.60
1:A:187:ARG:NH2	1:A:367:GLN:NE2	2.49	0.60
1:A:336:TRP:CD1	1:A:336:TRP:N	2.60	0.60
2:B:57:GLN:NE2	8:B:2044:HOH:O	2.33	0.60
3:G:63:LEU:HD11	7:G:1251:MQ7:H2M1	1.81	0.60
3:G:156:LEU:HD12	3:G:178:LEU:HD13	1.83	0.60
1:A:558:MET:HE2	1:A:561:MET:SD	2.41	0.60
1:E:474:MET:HE2	1:E:705:LEU:CD1	2.31	0.60
1:E:497:HIS:O	1:E:498:LYS:C	2.43	0.60
1:A:232:VAL:N	1:A:247:HIS:HD2	1.95	0.60
1:A:523:ARG:HG3	1:A:535:PHE:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:622:LEU:HD22	8:E:2426:HOH:O	2.00	0.60
1:A:193:GLU:HG2	8:A:2118:HOH:O	2.02	0.60
1:A:636:ASN:HB2	1:A:706:MET:HE2	1.84	0.60
3:C:67:GLU:HG2	3:C:67:GLU:O	2.01	0.60
1:E:88:THR:HG21	1:E:467:VAL:HG11	1.81	0.60
1:A:422:GLU:HB2	8:A:2201:HOH:O	2.00	0.60
1:A:519:TRP:CZ2	1:A:540:ILE:CG1	2.85	0.60
2:B:32:GLY:N	8:B:2011:HOH:O	2.33	0.60
1:A:134:LYS:CE	8:A:2077:HOH:O	2.46	0.60
1:A:295:ASP:HB2	8:A:2156:HOH:O	2.01	0.60
1:A:364:TYR:HB2	1:A:570:PRO:CB	2.32	0.60
1:A:678:GLY:HA3	8:A:2328:HOH:O	2.01	0.60
2:B:25:MET:HE2	2:B:25:MET:CA	2.26	0.60
3:G:206:GLY:CA	3:G:209:TYR:HB3	2.31	0.60
3:G:240:LEU:C	3:G:240:LEU:HD12	2.26	0.60
1:A:320:ALA:O	1:A:323:LYS:CG	2.49	0.60
1:A:671:ASN:HD21	1:A:675:VAL:H	1.50	0.60
2:B:140:ARG:NH2	8:B:2044:HOH:O	2.34	0.60
1:E:568:GLY:O	1:E:570:PRO:HD3	2.01	0.60
3:C:21:HIS:CE1	3:C:64:LEU:HD11	2.36	0.60
3:G:30:VAL:HG12	3:G:52:ALA:HB2	1.84	0.60
1:E:512:LEU:O	1:E:515:THR:HB	2.02	0.59
1:A:239:PHE:O	1:A:687:ARG:HD2	2.02	0.59
1:A:415:THR:HG22	8:A:2200:HOH:O	2.03	0.59
1:A:602:HIS:ND1	1:A:606:PRO:HG2	2.15	0.59
1:E:239:PHE:CB	1:E:687:ARG:HB3	2.32	0.59
1:E:604:PRO:C	1:E:605:LEU:HD23	2.18	0.59
1:E:635:GLN:NE2	1:E:635:GLN:N	2.48	0.59
1:A:629:HIS:NE2	1:A:644:ASP:O	2.29	0.59
1:E:608:PHE:O	1:E:608:PHE:HD1	1.81	0.59
1:E:689:ARG:NH2	1:E:691:ASP:OD2	2.23	0.59
2:B:121:HIS:O	2:B:125:LYS:CE	2.50	0.59
8:B:2074:HOH:O	3:C:82:SER:HB3	2.02	0.59
3:C:151:LEU:O	3:C:155:THR:HB	2.03	0.59
1:E:281:LYS:HG3	1:E:282:TYR:CE1	2.38	0.59
1:A:536:PRO:HG2	1:A:537:TRP:H	1.68	0.59
1:A:379:LEU:O	1:A:380:PRO:C	2.46	0.59
1:E:359:ARG:HD3	8:E:2220:HOH:O	2.02	0.59
1:E:391:PRO:HG2	1:E:392:SER:H	1.66	0.59
1:E:467:VAL:HG12	1:E:468:LEU:HG	1.83	0.59
2:F:41:ARG:CD	2:F:187:THR:HG23	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ALA:HB2	1:A:605:LEU:HD12	1.85	0.59
1:A:608:PHE:O	1:A:608:PHE:HD1	1.82	0.59
1:A:635:GLN:C	1:A:709:ALA:HB2	2.27	0.59
2:B:2:PRO:HB3	2:B:144:ASP:CB	2.32	0.59
2:B:72:THR:CG2	2:B:74:ALA:H	2.09	0.59
1:E:342:TYR:HD1	1:E:607:VAL:CB	2.11	0.59
2:F:166:ARG:HH22	3:G:248:GLN:NE2	2.00	0.59
3:C:145:ASN:C	3:C:145:ASN:ND2	2.57	0.59
1:E:81:ARG:HE	1:E:214:THR:CG2	2.16	0.59
1:E:112:TYR:CZ	1:E:474:MET:O	2.55	0.59
1:A:73:LYS:NZ	1:A:192:HIS:CD2	2.68	0.59
3:C:171:TRP:O	3:C:172:ALA:CB	2.49	0.59
1:E:81:ARG:HD2	1:E:630:THR:OG1	2.03	0.59
3:G:226:ALA:HB3	3:G:227:PRO:HD3	1.85	0.59
2:B:86:ASP:OD1	2:B:88:LYS:HB2	2.03	0.59
3:C:64:LEU:HD22	7:C:1252:MQ7:C4	2.33	0.59
1:E:273:LEU:O	1:E:323:LYS:NZ	2.26	0.59
3:G:132:LEU:O	3:G:136:VAL:HB	2.03	0.59
1:A:357:TYR:HA	1:A:363:PHE:HB2	1.85	0.58
1:E:397:GLU:CG	1:E:398:PRO:HD3	2.33	0.58
3:G:66:GLU:O	3:G:66:GLU:HG2	2.03	0.58
1:A:335:VAL:HG13	1:A:733:GLY:HA2	1.84	0.58
1:A:367:GLN:O	1:A:500:PRO:HG3	2.02	0.58
1:A:519:TRP:CG	1:A:540:ILE:HG21	2.37	0.58
3:C:155:THR:CG2	3:C:239:ARG:CG	2.79	0.58
3:G:46:ARG:HG3	8:G:2014:HOH:O	2.02	0.58
1:A:48:PHE:HE1	1:A:145:HIS:CE1	2.21	0.58
3:C:64:LEU:CD2	7:C:1252:MQ7:C4	2.80	0.58
1:E:81:ARG:NE	1:E:214:THR:HG22	2.18	0.58
3:G:144:ASN:OD1	3:G:192:THR:CG2	2.52	0.58
1:A:457:LYS:HD3	8:A:2221:HOH:O	2.03	0.58
3:C:112:SER:O	3:C:113:GLN:HG2	2.03	0.58
1:E:345:MET:CB	1:E:605:LEU:CD1	2.82	0.58
1:E:421:ILE:HA	1:E:424:MET:SD	2.44	0.58
1:E:474:MET:HE2	1:E:705:LEU:HD11	1.85	0.58
3:C:68:SER:O	3:C:71:ARG:HB3	2.04	0.58
1:E:209:HIS:CG	5:E:1766:MGD:H5'1	2.39	0.58
1:A:483:ALA:HA	1:A:515:THR:HG23	1.84	0.58
1:A:591:GLU:CB	1:A:603:GLN:HE22	2.13	0.58
3:C:248:TRP:CE2	3:C:250:GLY:HA3	2.38	0.58
1:E:153:VAL:CG1	1:E:167:LYS:HE2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:604:PRO:C	1:E:605:LEU:HD22	2.25	0.58
1:A:605:LEU:N	1:A:606:PRO:CD	2.62	0.58
1:A:708:LEU:N	1:A:708:LEU:HD23	2.19	0.58
3:C:208:PHE:C	3:C:208:PHE:CD2	2.80	0.58
1:A:512:LEU:O	1:A:515:THR:HB	2.04	0.58
1:A:525:LEU:O	1:A:529:LEU:HG	2.04	0.58
1:A:592:LEU:C	1:A:592:LEU:HD13	2.28	0.58
2:B:122:ARG:HB3	2:B:127:LYS:HB2	1.84	0.58
3:C:140:ASN:ND2	3:C:140:ASN:N	2.48	0.58
1:E:454:GLU:HG2	8:E:2271:HOH:O	2.04	0.58
3:G:49:THR:HG21	8:G:2011:HOH:O	2.03	0.58
1:A:80:PRO:HD3	2:B:18:ALA:HB2	1.85	0.57
1:A:583:PHE:CZ	1:A:587:SER:HA	2.39	0.57
3:C:89:ILE:HD12	7:C:1252:MQ7:C6	2.34	0.57
3:G:63:LEU:HD22	7:G:1251:MQ7:C10	2.34	0.57
1:A:75:ARG:HD2	1:A:220:GLN:NE2	2.13	0.57
1:A:96:LYS:HB3	1:A:513:PHE:HB3	1.86	0.57
1:A:388:CYS:O	1:A:391:PRO:HD3	2.04	0.57
1:A:583:PHE:HB2	1:A:584:GLY:N	2.13	0.57
2:B:160:GLU:N	2:B:179:ASN:HD21	1.92	0.57
1:A:519:TRP:CD2	1:A:540:ILE:HG23	2.38	0.57
1:E:95:LEU:CD2	8:E:2275:HOH:O	2.45	0.57
3:G:76:ILE:HG12	3:G:80:LEU:HD11	1.86	0.57
1:A:118:GLU:H	1:A:118:GLU:CD	2.11	0.57
1:A:388:CYS:HA	1:A:593:TYR:HE1	1.65	0.57
1:A:607:VAL:HG13	1:A:609:THR:CB	2.33	0.57
1:E:519:TRP:NE1	1:E:540:ILE:HG12	2.19	0.57
2:F:46:TYR:C	2:F:46:TYR:CD1	2.81	0.57
2:F:67:VAL:CB	2:F:68:PRO:HD3	2.34	0.57
2:F:115:LYS:HG3	2:F:116:CYS:O	2.05	0.57
3:G:222:GLN:C	8:G:2069:HOH:O	2.47	0.57
1:A:449:VAL:O	1:A:453:LYS:HG3	2.04	0.57
1:A:454:GLU:HG2	8:A:2099:HOH:O	2.04	0.57
2:B:57:GLN:CD	8:B:2044:HOH:O	2.47	0.57
1:E:93:ASP:O	1:E:469:PRO:HD3	2.04	0.57
1:E:601:GLY:HA2	8:E:2332:HOH:O	2.04	0.57
2:F:39:ARG:HD2	2:F:56:GLU:OE2	2.03	0.57
2:F:117:THR:HG22	2:F:119:CYS:N	2.19	0.57
1:A:558:MET:HE1	1:A:561:MET:SD	2.45	0.57
2:B:47:PRO:CG	8:B:2031:HOH:O	2.53	0.57
1:A:595:GLN:HA	1:A:598:LYS:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:140:ASN:O	3:C:142:PRO:HD3	2.04	0.57
1:E:285:GLY:HA3	1:E:592:LEU:HD11	1.85	0.57
1:E:519:TRP:CE2	1:E:540:ILE:HG13	2.39	0.57
3:G:172:LEU:O	3:G:176:ARG:HG3	2.05	0.57
1:A:183:TRP:HB3	1:A:592:LEU:O	2.05	0.57
1:E:91:ASP:C	1:E:92:PRO:O	2.48	0.57
1:E:342:TYR:CE1	1:E:607:VAL:HB	2.38	0.57
1:E:533:GLN:HE21	1:E:533:GLN:N	1.93	0.57
1:A:113:ARG:NH2	8:A:2065:HOH:O	2.37	0.57
3:C:17:THR:HG22	3:C:18:ASN:N	2.20	0.57
1:E:686:ALA:CB	8:E:2385:HOH:O	2.47	0.57
1:A:548:LEU:HD13	1:A:558:MET:HB2	1.87	0.57
1:A:627:PRO:HB2	2:B:16:CYS:HA	1.87	0.57
3:C:21:HIS:CE1	3:C:64:LEU:CD2	2.88	0.56
1:E:41:TYR:HE1	1:E:560:GLY:O	1.88	0.56
1:E:323:LYS:HD3	1:E:354:LEU:C	2.30	0.56
1:E:466:ASP:HA	5:E:1765:MGD:N2	2.20	0.56
1:E:630:THR:HG23	8:E:2452:HOH:O	2.04	0.56
1:E:519:TRP:CE2	1:E:540:ILE:HG12	2.39	0.56
1:A:103:GLU:OE1	1:A:103:GLU:HA	2.05	0.56
1:A:483:ALA:CA	1:A:515:THR:CG2	2.83	0.56
2:B:2:PRO:HD2	2:B:80:ASP:OD2	2.05	0.56
8:B:2079:HOH:O	3:C:251:LEU:HD11	2.04	0.56
1:E:607:VAL:HG23	8:E:2144:HOH:O	2.05	0.56
1:E:620:ARG:HB3	8:E:2391:HOH:O	2.04	0.56
1:E:623:TYR:HA	1:E:695:ILE:O	2.05	0.56
1:E:755:LEU:O	1:E:758:ARG:HD3	2.05	0.56
3:G:139:ASN:HD22	3:G:139:ASN:N	1.97	0.56
1:A:64:LYS:CE	2:B:26:GLU:HB2	2.35	0.56
1:A:183:TRP:HB3	1:A:592:LEU:HD22	1.86	0.56
1:A:209:HIS:CE1	1:A:625:ARG:H	2.16	0.56
1:A:64:LYS:HE2	2:B:26:GLU:HB2	1.87	0.56
1:A:673:ASP:OD2	1:A:721:THR:CG2	2.52	0.56
3:C:64:LEU:CD2	7:C:1252:MQ7:C10	2.83	0.56
3:G:70:ARG:HG2	3:G:71:PHE:H	1.70	0.56
1:A:276:LYS:CA	8:A:2148:HOH:O	2.39	0.56
1:E:214:THR:HG21	1:E:627:PRO:O	2.05	0.56
1:E:231:LYS:HA	1:E:247:HIS:CD2	2.41	0.56
3:G:63:LEU:HD21	7:G:1251:MQ7:C1	2.36	0.56
1:A:132:ARG:CD	8:A:2075:HOH:O	2.52	0.56
1:A:183:TRP:HE1	1:A:413:ARG:NH2	1.98	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ILE:HG12	1:A:329:PRO:HB3	1.88	0.56
2:B:183:LYS:HE3	8:B:2141:HOH:O	2.06	0.56
1:E:116:THR:HG22	1:E:119:GLU:N	2.20	0.56
3:G:227:PRO:O	3:G:231:LEU:HB2	2.05	0.56
1:A:75:ARG:NH1	1:A:220:GLN:HE21	1.99	0.56
1:A:231:LYS:CA	1:A:247:HIS:CD2	2.88	0.56
1:A:231:LYS:HB2	1:A:247:HIS:CD2	2.41	0.56
1:A:305:THR:CG2	1:A:307:ILE:H	2.19	0.56
1:A:404:ARG:HG3	1:A:406:ASP:OD2	2.06	0.56
1:A:519:TRP:CG	1:A:540:ILE:CG2	2.88	0.56
1:E:265:ILE:HD11	1:E:349:TYR:HB2	1.88	0.56
1:E:397:GLU:HB3	8:E:2239:HOH:O	2.05	0.56
3:G:206:GLY:HA2	3:G:209:TYR:HB2	1.87	0.56
3:C:89:ILE:CD1	7:C:1252:MQ7:C6	2.84	0.56
1:E:620:ARG:CG	1:E:620:ARG:O	2.53	0.56
3:G:225:LEU:CB	8:G:2069:HOH:O	2.52	0.56
1:A:71:ASN:HD21	1:A:73:LYS:HB2	1.70	0.56
1:A:284:VAL:CG2	1:A:587:SER:HB3	2.30	0.56
3:C:174:PHE:H	3:C:175:PRO:HD2	1.71	0.56
1:E:45:GLU:HG3	8:E:2011:HOH:O	2.05	0.56
1:E:371:LEU:HD13	1:E:547:ARG:CZ	2.35	0.56
1:E:621:LEU:HD22	1:E:622:LEU:O	2.06	0.56
3:G:38:HIS:CE1	3:G:105:LEU:HD22	2.40	0.56
1:A:85:ALA:HA	8:A:2042:HOH:O	2.05	0.55
1:A:184:VAL:HG22	1:A:592:LEU:CB	2.36	0.55
1:A:422:GLU:HB3	1:A:423:PRO:CD	2.36	0.55
1:A:602:HIS:CD2	1:A:604:PRO:HD2	2.42	0.55
3:C:21:HIS:CE1	3:C:64:LEU:CG	2.89	0.55
1:E:160:TRP:CG	1:E:160:TRP:O	2.59	0.55
1:E:286:PHE:C	1:E:288:GLU:H	2.12	0.55
2:F:190:SER:O	2:F:194:HIS:N	2.38	0.55
1:A:591:GLU:OE2	1:A:604:PRO:HG2	1.98	0.55
2:B:36:LEU:CD1	8:B:2103:HOH:O	2.54	0.55
2:B:117:THR:HG23	2:B:117:THR:O	2.06	0.55
1:A:81:ARG:NH2	1:A:214:THR:HG22	2.20	0.55
1:A:548:LEU:C	1:A:553:LEU:O	2.50	0.55
3:C:20:LEU:HD13	3:C:63:ILE:HD13	1.88	0.55
1:E:201:ARG:HD3	8:E:2121:HOH:O	2.05	0.55
1:E:311:VAL:HG23	8:E:2195:HOH:O	2.05	0.55
1:A:187:ARG:HH22	1:A:367:GLN:NE2	2.04	0.55
1:A:647:ASN:HD21	1:A:714:ALA:H	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:GLU:HB3	8:E:2005:HOH:O	2.06	0.55
1:E:119:GLU:HG2	8:E:2075:HOH:O	2.07	0.55
8:A:2040:HOH:O	2:B:133:GLU:HG3	2.07	0.55
1:E:75:ARG:NH1	1:E:220:GLN:HE21	1.99	0.55
1:E:97:ARG:HH22	1:E:763:ARG:HD2	1.70	0.55
1:A:342:TYR:CD2	1:A:605:LEU:HA	2.42	0.55
1:A:413:ARG:HD2	1:A:413:ARG:N	2.14	0.55
1:A:555:LEU:O	1:A:559:LYS:HG3	2.05	0.55
1:E:495:VAL:HG21	8:E:2296:HOH:O	2.05	0.55
1:E:724:LYS:CG	8:E:2424:HOH:O	2.54	0.55
1:A:468:LEU:HD13	1:A:706:MET:HE3	1.88	0.55
1:A:483:ALA:HB2	1:A:515:THR:CG2	2.37	0.55
1:A:533:GLN:HG2	1:A:534:TYR:N	2.20	0.55
1:A:575:TRP:O	1:A:580:ARG:HG2	2.07	0.55
3:G:63:LEU:CD2	7:G:1251:MQ7:C10	2.84	0.55
1:A:345:MET:CE	1:A:592:LEU:HD11	2.34	0.55
1:E:397:GLU:CB	1:E:398:PRO:CD	2.82	0.55
2:F:88:LYS:O	3:G:74:THR:CG2	2.54	0.55
1:A:81:ARG:HH21	1:A:214:THR:CG2	2.20	0.55
1:E:469:PRO:O	1:E:706:MET:CG	2.51	0.55
1:E:622:LEU:HB2	1:E:693:VAL:O	2.07	0.55
1:E:647:ASN:C	1:E:648:GLU:HG3	2.33	0.55
1:A:194:PRO:O	1:A:363:PHE:HA	2.07	0.54
1:A:396:HIS:CB	1:A:403:PRO:HB3	2.35	0.54
2:B:139:CYS:SG	4:B:1194:SF4:S3	3.04	0.54
1:E:100:ILE:CG2	1:E:478:VAL:HG22	2.36	0.54
1:E:635:GLN:H	1:E:635:GLN:HE21	1.54	0.54
2:F:35:ASN:ND2	2:F:106:TYR:HE2	2.06	0.54
1:A:255:GLY:HA2	1:A:337:TYR:CE1	2.42	0.54
1:A:599:GLU:HB2	8:A:2279:HOH:O	2.07	0.54
1:A:655:GLU:CD	1:A:658:ARG:HH22	2.14	0.54
1:A:183:TRP:HH2	1:A:596:ARG:CD	2.18	0.54
1:A:289:LEU:HD12	1:A:590:ILE:HD11	1.90	0.54
1:A:310:GLN:HG3	8:A:2160:HOH:O	2.07	0.54
1:A:395:ASP:CA	1:A:399:GLU:CG	2.54	0.54
3:C:222:TRP:C	3:C:222:TRP:CD1	2.85	0.54
1:E:433:LYS:HB3	1:E:460:ASP:HB2	1.88	0.54
1:E:590:ILE:HB	8:E:2177:HOH:O	2.05	0.54
2:F:44:GLY:O	2:F:45:GLU:HB2	2.07	0.54
3:G:100:LEU:HB3	8:G:2030:HOH:O	2.07	0.54
3:G:206:GLY:CA	3:G:209:TYR:HB2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:247:HIS:CE1	8:E:2145:HOH:O	2.60	0.54
1:E:380:PRO:HD3	1:E:534:TYR:OH	2.07	0.54
1:E:453:LYS:HG2	1:E:475:TRP:CZ2	2.42	0.54
1:E:536:PRO:O	8:E:2308:HOH:O	2.17	0.54
1:E:701:HIS:O	1:E:710:HIS:O	2.24	0.54
2:F:35:ASN:HD22	2:F:106:TYR:HE2	1.55	0.54
3:G:144:ASN:C	3:G:144:ASN:HD22	2.14	0.54
1:A:37:VAL:CG1	1:A:38:LYS:N	2.69	0.54
1:A:184:VAL:HG22	1:A:592:LEU:CG	2.37	0.54
1:A:589:LYS:O	1:A:592:LEU:CA	2.55	0.54
1:E:142:PHE:CG	1:E:157:PRO:HG3	2.42	0.54
1:E:149:ASP:CB	8:E:2091:HOH:O	2.54	0.54
1:E:209:HIS:CD2	5:E:1766:MGD:H5'1	2.43	0.54
1:E:412:ALA:HB1	1:E:413:ARG:NH1	2.22	0.54
1:E:428:GLU:O	1:E:430:TYR:CA	2.55	0.54
1:A:214:THR:HG23	1:A:214:THR:O	2.07	0.54
1:A:391:PRO:O	1:A:413:ARG:CB	2.55	0.54
2:F:78:THR:CG2	2:F:79:LYS:N	2.71	0.54
3:G:52:ALA:O	3:G:56:ILE:HG13	2.08	0.54
2:B:27:ASN:HD21	2:B:121:HIS:HE1	1.54	0.54
3:C:50:THR:O	3:C:54:LEU:HG	2.08	0.54
1:E:169:SER:O	1:E:174:THR:HB	2.08	0.54
1:E:336:TRP:O	1:E:340:ASP:OD1	2.26	0.54
3:G:63:LEU:HD22	7:G:1251:MQ7:C1	2.38	0.54
1:A:116:THR:HG23	1:A:118:GLU:N	2.23	0.54
1:A:462:TYR:OH	1:A:472:HIS:O	2.21	0.54
1:A:554:ASP:OD2	1:A:554:ASP:N	2.41	0.54
1:E:553:LEU:HD21	1:E:557:THR:CG2	2.38	0.54
1:E:591:GLU:OE2	1:E:604:PRO:CG	2.55	0.54
3:G:63:LEU:HD22	7:G:1251:MQ7:C3	2.37	0.54
3:C:21:HIS:C	3:C:21:HIS:CD2	2.86	0.54
1:E:412:ALA:HB1	1:E:413:ARG:HH12	1.72	0.54
1:A:124:ILE:HD11	1:A:478:VAL:HG11	1.90	0.54
3:C:108:LEU:HB3	3:C:110:LYS:HG3	1.90	0.54
1:E:97:ARG:NH2	1:E:763:ARG:NH1	2.56	0.54
1:E:197:TRP:CG	1:E:221:ASP:HB3	2.43	0.54
1:E:302:GLU:O	1:E:302:GLU:HG2	2.08	0.54
3:G:17:ASN:O	3:G:21:PHE:HD1	1.91	0.54
2:B:117:THR:CG2	2:B:117:THR:O	2.53	0.53
3:C:77:ILE:HG12	3:C:81:LEU:HD11	1.90	0.53
1:E:37:VAL:HA	1:E:57:ALA:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:GLY:HA3	1:E:584:GLY:N	2.23	0.53
1:E:305:THR:HG23	1:E:307:ILE:H	1.70	0.53
1:E:627:PRO:HB2	2:F:16:CYS:HA	1.90	0.53
1:E:651:ILE:HD11	1:E:682:VAL:HG12	1.90	0.53
8:E:2164:HOH:O	2:F:46:TYR:HB2	2.07	0.53
1:A:305:THR:HG23	1:A:307:ILE:HD12	1.90	0.53
1:A:490:ASP:OD2	1:A:505:ARG:NH1	2.40	0.53
1:A:671:ASN:ND2	1:A:675:VAL:H	2.05	0.53
1:E:609:THR:HG23	8:E:2336:HOH:O	2.08	0.53
1:E:638:TRP:O	1:E:642:GLU:HB2	2.08	0.53
1:E:683:LYS:HE2	1:E:685:THR:HB	1.88	0.53
1:E:97:ARG:HH21	1:E:763:ARG:CZ	2.22	0.53
1:E:100:ILE:HG12	1:E:478:VAL:CG2	2.38	0.53
2:B:55:PRO:HB2	8:B:2103:HOH:O	2.07	0.53
1:E:252:ILE:HG12	1:E:256:THR:HG22	1.90	0.53
1:E:346:ALA:N	1:E:605:LEU:CD1	2.70	0.53
1:E:717:ASN:ND2	5:E:1765:MGD:H192	2.02	0.53
1:A:124:ILE:O	1:A:128:MET:HG3	2.08	0.53
1:A:341:THR:OG1	1:A:729:SER:HB3	2.08	0.53
1:A:535:PHE:N	1:A:536:PRO:CD	2.71	0.53
1:A:654:GLU:HG3	8:A:2315:HOH:O	2.08	0.53
1:A:279:VAL:HA	1:A:283:THR:HB	1.91	0.53
1:E:336:TRP:O	1:E:338:GLY:N	2.42	0.53
1:E:519:TRP:CZ2	1:E:540:ILE:HG13	2.44	0.53
2:F:63:ASN:HB2	8:F:2109:HOH:O	2.07	0.53
3:G:40:LYS:HG3	3:G:40:LYS:O	2.08	0.53
1:A:284:VAL:HG12	1:A:285:GLY:N	2.23	0.53
1:A:572:LEU:HD22	8:A:2271:HOH:O	2.08	0.53
2:B:155:ALA:HB1	8:B:2113:HOH:O	2.09	0.53
1:E:591:GLU:O	1:E:591:GLU:CG	2.55	0.53
1:A:488:ARG:HD3	1:A:490:ASP:OD2	2.09	0.53
1:A:583:PHE:C	1:A:584:GLY:CA	2.77	0.53
1:A:623:TYR:HA	1:A:695:ILE:O	2.09	0.53
3:C:143:LEU:CD2	3:C:198:ALA:HB1	2.39	0.53
1:A:428:GLU:CB	1:A:429:PRO:CD	2.85	0.53
1:A:585:THR:O	1:A:585:THR:HG22	2.08	0.53
1:A:761:ASP:C	1:A:763:ARG:H	2.16	0.53
3:C:229:TRP:O	3:C:233:LEU:HG	2.08	0.53
1:E:447:PRO:HB3	8:E:2419:HOH:O	2.08	0.53
3:G:205:ALA:HB1	3:G:240:LEU:CD2	2.39	0.53
3:G:46:ARG:CG	8:G:2014:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:HB2	8:A:2069:HOH:O	2.08	0.52
1:A:284:VAL:HG23	1:A:587:SER:CB	2.35	0.52
1:A:369:PRO:HG2	1:A:494:LEU:HB3	1.91	0.52
1:A:231:LYS:HB2	1:A:247:HIS:CG	2.44	0.52
1:A:72:PRO:HG2	1:A:501:PHE:CD2	2.44	0.52
1:A:295:ASP:O	1:A:297:THR:HG22	2.10	0.52
1:A:651:ILE:HG23	1:A:693:VAL:HG23	1.90	0.52
1:A:676:LYS:NZ	1:A:742:GLU:OE1	2.41	0.52
3:C:57:ILE:HG21	3:C:100:PHE:HB2	1.91	0.52
1:E:81:ARG:HB2	4:E:1764:SF4:S3	2.49	0.52
1:E:99:LEU:O	1:E:478:VAL:HA	2.09	0.52
1:E:576:GLU:C	1:E:578:GLU:H	2.17	0.52
1:E:606:PRO:CG	1:E:607:VAL:N	2.72	0.52
1:E:672:GLN:NE2	1:E:672:GLN:H	2.07	0.52
1:A:207:GLY:O	5:A:1766:MGD:PB	2.68	0.52
1:A:286:PHE:HA	1:A:590:ILE:CG2	2.37	0.52
3:C:155:THR:CG2	3:C:239:ARG:CD	2.87	0.52
1:E:286:PHE:CB	8:E:2177:HOH:O	2.57	0.52
2:F:57:GLN:HE22	2:F:140:ARG:HH21	1.50	0.52
1:A:115:ALA:HB1	1:A:119:GLU:HG2	1.91	0.52
1:A:548:LEU:O	1:A:553:LEU:O	2.28	0.52
1:E:69:GLU:HA	8:E:2037:HOH:O	2.08	0.52
3:G:70:ARG:CG	3:G:71:PHE:N	2.72	0.52
1:A:335:VAL:HG13	1:A:733:GLY:CA	2.39	0.52
1:A:680:VAL:HG22	1:A:714:ALA:HB2	1.92	0.52
1:A:686:ALA:CB	8:A:2330:HOH:O	2.44	0.52
2:B:78:THR:HG22	2:B:80:ASP:H	1.75	0.52
2:B:129:PRO:HB3	4:B:1195:SF4:S3	2.50	0.52
1:E:39:SER:OG	1:E:56:HIS:ND1	2.31	0.52
1:E:397:GLU:CB	8:E:2239:HOH:O	2.57	0.52
1:E:421:ILE:HD11	1:E:452:THR:HG23	1.92	0.52
2:F:44:GLY:HA3	8:F:2025:HOH:O	2.08	0.52
3:G:189:TYR:HB3	3:G:190:PRO:HD3	1.92	0.52
1:A:101:ARG:HB2	1:A:477:ASP:HA	1.92	0.52
1:A:483:ALA:CB	1:A:515:THR:CG2	2.88	0.52
1:A:592:LEU:O	1:A:592:LEU:HD13	2.09	0.52
2:B:91:ILE:HD12	7:C:1252:MQ7:H2M1	1.92	0.52
3:C:222:TRP:CD1	3:C:223:GLN:N	2.78	0.52
1:E:583:PHE:N	1:E:583:PHE:CD2	2.68	0.52
1:A:107:ARG:HB2	8:A:2219:HOH:O	2.09	0.52
1:A:499:THR:HB	1:A:565:VAL:CG1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:TYR:HB3	3:C:73:ARG:NH2	2.24	0.52
3:C:108:LEU:O	3:C:109:GLY:C	2.53	0.52
1:E:761:ASP:C	1:E:763:ARG:H	2.17	0.52
3:G:160:LEU:HB3	3:G:175:LEU:HB2	1.91	0.52
1:A:212:GLU:OE1	1:A:240:SER:HB2	2.10	0.52
1:E:313:ARG:HD3	1:E:317:ARG:NH2	2.25	0.52
1:E:591:GLU:OE2	1:E:604:PRO:CB	2.57	0.52
1:A:254:PRO:HG2	1:A:692:CYS:SG	2.50	0.51
1:E:48:PHE:CZ	1:E:145:HIS:CE1	2.98	0.51
1:E:107:ARG:O	1:E:108:GLY:C	2.50	0.51
1:A:583:PHE:CZ	1:A:587:SER:CA	2.93	0.51
3:C:185:LEU:O	3:C:189:LEU:HG	2.09	0.51
1:E:492:PHE:HZ	1:E:548:LEU:HG	1.74	0.51
1:A:81:ARG:NE	1:A:214:THR:HG22	2.24	0.51
1:A:156:LEU:HB3	1:A:157:PRO:HD3	1.93	0.51
1:A:209:HIS:HD2	5:A:1766:MGD:O2A	1.93	0.51
3:C:64:LEU:HD22	7:C:1252:MQ7:C10	2.40	0.51
3:C:145:ASN:OD1	3:C:193:THR:CG2	2.57	0.51
1:E:248:ARG:NH1	1:E:318:GLU:OE2	2.44	0.51
1:E:574:ASP:HA	1:E:577:LYS:HD3	1.91	0.51
1:E:604:PRO:CA	1:E:605:LEU:CD2	2.87	0.51
1:E:606:PRO:CD	1:E:607:VAL:N	2.73	0.51
1:E:647:ASN:HD22	1:E:647:ASN:N	2.03	0.51
1:E:685:THR:HG22	2:F:42:GLU:OE2	2.10	0.51
3:G:16:THR:HG21	3:G:66:GLU:HB2	1.93	0.51
1:A:158:ALA:HB1	1:A:381:LEU:O	2.10	0.51
1:A:591:GLU:O	1:A:592:LEU:CD1	2.53	0.51
2:B:46:TYR:HE2	8:B:2033:HOH:O	1.82	0.51
1:E:142:PHE:CD1	1:E:157:PRO:HB3	2.45	0.51
1:E:272:ASP:OD2	1:E:276:LYS:NZ	2.25	0.51
1:A:159:ALA:HA	1:A:380:PRO:HD2	1.92	0.51
2:B:5:ALA:HB3	2:B:145:LEU:HD13	1.93	0.51
2:B:25:MET:HA	2:B:25:MET:HE3	1.91	0.51
2:B:88:LYS:O	3:C:75:THR:CG2	2.58	0.51
1:E:100:ILE:HA	1:E:478:VAL:HG22	1.92	0.51
1:E:391:PRO:HD3	1:E:595:GLN:CD	2.35	0.51
1:A:42:GLN:OE1	1:A:506:THR:N	2.43	0.51
1:A:288:GLU:HB3	1:A:591:GLU:CG	2.22	0.51
2:B:192:VAL:CG1	2:B:193:HIS:H	2.23	0.51
1:E:553:LEU:CD2	1:E:557:THR:CG2	2.88	0.51
3:G:139:ASN:ND2	8:G:2040:HOH:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:206:GLY:O	3:G:209:TYR:C	2.54	0.51
1:A:138:GLU:CD	1:A:402:LYS:HB2	2.35	0.51
2:B:132:VAL:HA	2:B:140:ARG:HG3	1.93	0.51
1:E:158:ALA:HB1	1:E:381:LEU:O	2.10	0.51
1:E:275:ASP:N	1:E:323:LYS:HE3	2.25	0.51
3:G:63:LEU:HD22	7:G:1251:MQ7:C2	2.40	0.51
1:A:166:ALA:CB	1:A:415:THR:CG2	2.88	0.51
1:A:170:VAL:HG12	1:A:171:SER:N	2.25	0.51
1:A:305:THR:CG2	1:A:307:ILE:HB	2.41	0.51
2:B:61:CYS:HB2	4:B:1196:SF4:S3	2.51	0.51
1:E:166:ALA:HB2	1:E:415:THR:CG2	2.40	0.51
1:E:499:THR:HA	1:E:567:ARG:O	2.11	0.51
3:G:205:ALA:HB1	3:G:240:LEU:HD22	1.92	0.51
3:G:249:GLY:HA2	8:G:2078:HOH:O	2.11	0.51
1:A:43:ILE:HB	1:A:505:ARG:HH21	1.76	0.51
1:A:534:TYR:O	1:A:535:PHE:CB	2.59	0.51
1:A:589:LYS:O	1:A:592:LEU:HA	2.11	0.51
2:B:25:MET:CE	2:B:25:MET:CA	2.80	0.51
2:B:64:PRO:HB3	4:B:1196:SF4:S3	2.51	0.51
1:E:138:GLU:CD	1:E:402:LYS:HB2	2.36	0.51
1:E:484:THR:HB	1:E:487:GLU:OE1	2.10	0.51
2:F:67:VAL:HB	2:F:68:PRO:CD	2.39	0.51
3:G:39:LEU:HD13	3:G:116:ALA:CB	2.41	0.51
3:G:42:ASP:OD1	3:G:44:GLU:HG3	2.11	0.51
1:A:90:TYR:OH	1:A:509:HIS:HE1	1.93	0.51
1:A:195:ILE:HD12	1:A:195:ILE:N	2.25	0.51
1:A:596:ARG:NH1	1:A:600:ALA:CB	2.73	0.51
2:B:191:GLU:HG3	8:B:2143:HOH:O	2.10	0.51
1:E:48:PHE:CE1	1:E:145:HIS:CE1	2.99	0.51
1:E:149:ASP:HA	8:E:2091:HOH:O	2.11	0.51
1:E:651:ILE:HD11	1:E:682:VAL:HG13	1.92	0.51
1:E:708:LEU:HD22	1:E:755:LEU:HB3	1.93	0.51
8:F:2029:HOH:O	3:G:250:LEU:HD12	2.09	0.51
3:G:70:ARG:HG2	3:G:71:PHE:N	2.25	0.51
1:A:65:VAL:HG13	1:A:78:LEU:HD21	1.93	0.50
3:C:133:LEU:O	3:C:137:VAL:HG22	2.11	0.50
2:F:172:ARG:N	2:F:173:PRO:HD3	2.26	0.50
3:G:44:GLU:OE1	3:G:47:ARG:NH1	2.43	0.50
1:A:390:GLY:H	1:A:595:GLN:NE2	2.05	0.50
1:A:587:SER:O	1:A:589:LYS:HE2	2.11	0.50
1:A:647:ASN:HD22	1:A:647:ASN:N	2.03	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ARG:NH2	8:A:2346:HOH:O	2.43	0.50
3:C:173:LEU:O	3:C:173:LEU:CG	2.55	0.50
1:E:100:ILE:HG12	1:E:478:VAL:HG13	1.93	0.50
1:E:101:ARG:HB2	1:E:477:ASP:HA	1.93	0.50
1:E:595:GLN:HA	1:E:598:LYS:HB2	1.93	0.50
1:A:252:ILE:HG13	1:A:307:ILE:HD11	1.92	0.50
1:A:488:ARG:CD	1:A:490:ASP:OD2	2.59	0.50
1:A:501:PHE:HA	1:A:564:LEU:O	2.11	0.50
1:E:88:THR:CG2	1:E:467:VAL:HG11	2.41	0.50
1:E:201:ARG:CD	8:E:2121:HOH:O	2.58	0.50
1:E:708:LEU:HD22	8:E:2407:HOH:O	2.11	0.50
1:A:42:GLN:NE2	1:A:505:ARG:CD	2.66	0.50
3:C:190:TYR:HB3	3:C:191:PRO:HD3	1.93	0.50
1:E:335:VAL:HG13	1:E:732:ALA:O	2.12	0.50
1:E:630:THR:HA	5:E:1766:MGD:N18	2.26	0.50
2:F:55:PRO:CG	4:F:1194:SF4:S2	2.98	0.50
2:F:147:ASP:O	2:F:150:SER:HB2	2.10	0.50
1:A:422:GLU:N	1:A:423:PRO:HD2	2.26	0.50
1:A:628:VAL:HG13	1:A:640:LEU:HD22	1.93	0.50
1:E:575:TRP:HB3	1:E:580:ARG:O	2.11	0.50
2:F:16:CYS:SG	2:F:16:CYS:O	2.69	0.50
2:F:166:ARG:HD2	8:F:2104:HOH:O	2.11	0.50
3:G:148:ALA:HA	8:G:2047:HOH:O	2.12	0.50
1:A:193:GLU:CG	8:A:2118:HOH:O	2.57	0.50
2:B:160:GLU:N	2:B:179:ASN:ND2	2.55	0.50
1:E:263:ALA:HB2	1:E:301:ALA:HB2	1.94	0.50
1:E:426:THR:C	1:E:428:GLU:N	2.70	0.50
2:F:35:ASN:ND2	2:F:106:TYR:CE2	2.78	0.50
1:A:702:LYS:HG3	8:A:2231:HOH:O	2.11	0.50
2:B:190:SER:CB	3:C:252:GLY:N	2.71	0.50
1:E:93:ASP:CG	1:E:758:ARG:HH22	2.19	0.50
1:E:95:LEU:HD11	1:E:466:ASP:O	2.04	0.50
1:E:297:THR:HG22	1:E:299:GLU:H	1.75	0.50
1:E:488:ARG:HG3	8:E:2287:HOH:O	2.11	0.50
1:E:651:ILE:HD12	1:E:684:PRO:HA	1.93	0.50
1:E:669:LEU:HD23	1:E:741:LEU:HD22	1.92	0.50
8:E:2130:HOH:O	2:F:138:TYR:CD1	2.55	0.50
3:C:228:PRO:O	3:C:232:LEU:HD12	2.12	0.50
1:E:369:PRO:HG2	1:E:494:LEU:HB3	1.94	0.50
1:E:423:PRO:HB2	1:E:432:ILE:HG13	1.93	0.50
1:E:630:THR:HA	5:E:1766:MGD:C17	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:734:LEU:CD2	8:E:2419:HOH:O	2.54	0.50
3:G:91:GLY:O	3:G:95:LEU:HD12	2.11	0.50
2:B:52:GLU:OE2	2:B:187:THR:HB	2.12	0.50
8:E:2130:HOH:O	2:F:138:TYR:CE1	2.65	0.50
2:F:117:THR:HB	8:F:2012:HOH:O	2.10	0.50
1:A:232:VAL:N	1:A:247:HIS:CD2	2.74	0.49
1:A:629:HIS:ND1	1:A:634:THR:CG2	2.65	0.49
2:F:125:LYS:HE2	8:F:2077:HOH:O	2.12	0.49
3:G:65:ALA:O	3:G:70:ARG:NH1	2.45	0.49
3:G:129:TYR:OH	7:G:1251:MQ7:O1	2.22	0.49
3:G:206:GLY:O	3:G:209:TYR:CB	2.60	0.49
3:G:240:LEU:C	3:G:240:LEU:CD1	2.84	0.49
1:A:284:VAL:N	1:A:588:GLY:O	2.28	0.49
1:A:405:ALA:HB2	1:A:430:TYR:CZ	2.48	0.49
1:A:677:GLU:C	1:A:678:GLY:O	2.55	0.49
1:E:287:GLU:N	1:E:287:GLU:OE1	2.45	0.49
1:E:345:MET:HB3	1:E:605:LEU:HD11	1.94	0.49
1:E:524:GLU:OE1	1:E:528:ARG:NH2	2.45	0.49
2:F:129:PRO:HB3	4:F:1195:SF4:S2	2.52	0.49
1:A:116:THR:HG23	1:A:118:GLU:H	1.76	0.49
1:A:193:GLU:HB2	1:A:195:ILE:CD1	2.42	0.49
2:B:106:TYR:CE1	2:B:114:SER:HB3	2.46	0.49
1:A:77:ARG:NH2	8:A:2040:HOH:O	2.34	0.49
1:A:184:VAL:HG22	1:A:592:LEU:CD2	2.28	0.49
1:A:530:GLY:HA2	1:A:532:GLU:OE2	2.12	0.49
1:A:666:TYR:CZ	1:A:681:ARG:HG3	2.47	0.49
8:B:2079:HOH:O	3:C:251:LEU:CD1	2.59	0.49
3:C:143:LEU:HD23	3:C:198:ALA:HB1	1.95	0.49
1:E:371:LEU:HD12	1:E:494:LEU:HD21	1.95	0.49
1:E:548:LEU:CD1	1:E:555:LEU:HA	2.42	0.49
2:F:107:LEU:HD21	3:G:68:PRO:HG2	1.94	0.49
2:F:117:THR:CG2	2:F:119:CYS:N	2.74	0.49
1:A:65:VAL:CG1	1:A:78:LEU:HD21	2.42	0.49
1:A:682:VAL:HG12	1:A:684:PRO:HD3	1.95	0.49
2:B:192:VAL:CG1	2:B:193:HIS:N	2.73	0.49
3:C:161:LEU:CD1	3:C:179:LEU:HD12	2.43	0.49
1:E:95:LEU:CD1	8:E:2275:HOH:O	2.54	0.49
1:E:204:VAL:HG21	1:E:319:MET:CE	2.42	0.49
1:E:504:LEU:HD22	1:E:505:ARG:N	2.28	0.49
1:E:627:PRO:CB	2:F:16:CYS:HA	2.42	0.49
1:E:647:ASN:H	1:E:647:ASN:ND2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:TYR:CD1	1:A:540:ILE:HD13	2.48	0.49
1:A:506:THR:CG2	8:A:2244:HOH:O	2.60	0.49
1:A:689:ARG:NE	1:A:691:ASP:OD2	2.43	0.49
2:B:22:ALA:HB2	2:B:134:THR:HG21	1.95	0.49
2:B:41:ARG:CD	2:B:187:THR:HG23	2.41	0.49
1:E:53:ILE:HG22	1:E:78:LEU:HD11	1.95	0.49
1:E:591:GLU:O	1:E:603:GLN:CD	2.55	0.49
1:A:42:GLN:OE1	1:A:506:THR:O	2.31	0.49
1:A:96:LYS:HB3	1:A:513:PHE:CB	2.42	0.49
1:A:186:GLY:N	1:A:583:PHE:HA	2.22	0.49
1:A:586:ALA:O	1:A:587:SER:CB	2.60	0.49
1:E:384:ALA:HB1	8:E:2237:HOH:O	2.13	0.49
2:F:190:SER:N	3:G:251:GLY:N	2.61	0.49
1:A:393:GLY:HA3	1:A:407:LYS:HZ1	1.72	0.49
3:C:76:HIS:O	3:C:79:LEU:HB2	2.13	0.49
1:E:113:ARG:HB3	8:E:2042:HOH:O	2.13	0.49
1:E:225:ALA:O	1:E:230:ALA:HB3	2.13	0.49
1:E:606:PRO:CG	1:E:607:VAL:H	2.26	0.49
3:G:86:SER:O	3:G:87:PRO:C	2.53	0.49
1:A:116:THR:HG22	1:A:119:GLU:CB	2.37	0.49
1:A:122:ASP:CB	8:A:2069:HOH:O	2.60	0.49
1:A:256:THR:HG23	1:A:256:THR:O	2.11	0.49
1:A:394:GLY:CA	8:A:2189:HOH:O	2.61	0.49
1:A:482:GLU:HG2	1:A:483:ALA:H	1.78	0.49
1:E:539:THR:CG2	1:E:541:GLU:HG2	2.42	0.49
2:B:164:VAL:HG22	2:B:173:PRO:HB2	1.94	0.49
1:E:540:ILE:O	1:E:544:LEU:HG	2.13	0.49
1:A:113:ARG:NE	8:A:2065:HOH:O	2.46	0.48
2:B:166:ARG:HH22	3:C:249:GLN:HE21	1.59	0.48
1:E:315:VAL:HG12	1:E:319:MET:CE	2.39	0.48
2:F:27:ASN:O	2:F:28:GLU:C	2.56	0.48
2:F:160:GLU:N	2:F:179:ASN:HD21	1.96	0.48
1:A:561:MET:O	1:A:563:THR:O	2.31	0.48
1:E:227:LYS:HE2	2:F:12:LEU:HD11	1.94	0.48
1:E:677:GLU:O	1:E:678:GLY:O	2.30	0.48
2:F:9:ASP:HA	2:F:178:LEU:HB2	1.94	0.48
1:A:43:ILE:HB	1:A:505:ARG:NH2	2.28	0.48
1:A:175:ALA:HB3	1:A:176:PRO:HD3	1.95	0.48
1:A:647:ASN:ND2	1:A:713:GLY:HA3	2.27	0.48
2:B:71:PRO:HB2	3:C:79:LEU:CD1	2.43	0.48
3:C:21:HIS:ND1	3:C:64:LEU:CG	2.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:650:TRP:HB2	1:E:694:TYR:HB3	1.95	0.48
2:F:117:THR:HG23	2:F:117:THR:O	2.12	0.48
2:B:159:ALA:O	2:F:183:LYS:CE	2.53	0.48
1:E:233:VAL:HG13	1:E:248:ARG:HB2	1.95	0.48
1:E:647:ASN:C	1:E:648:GLU:CG	2.87	0.48
2:F:122:ARG:HG2	2:F:127:LYS:HE3	1.95	0.48
3:G:47:ARG:O	3:G:50:LEU:O	2.31	0.48
1:A:371:LEU:HD23	1:A:551:LEU:CD1	2.44	0.48
1:E:50:ARG:HD2	8:E:2013:HOH:O	2.12	0.48
1:E:325:ARG:NH1	8:E:2211:HOH:O	2.26	0.48
1:E:730:GLY:HA3	8:E:2250:HOH:O	2.13	0.48
1:A:628:VAL:HG11	1:A:643:MET:HB2	1.95	0.48
3:C:64:LEU:HD21	7:C:1252:MQ7:C4	2.43	0.48
1:E:112:TYR:OH	1:E:476:ALA:O	2.32	0.48
1:E:250:LEU:HD13	1:E:307:ILE:HG21	1.95	0.48
1:E:588:GLY:HA3	8:E:2106:HOH:O	2.13	0.48
1:E:670:VAL:HB	1:E:740:ARG:HG3	1.94	0.48
2:F:72:THR:HG21	2:F:89:LYS:C	2.38	0.48
3:G:112:GLN:N	8:G:2033:HOH:O	2.45	0.48
1:A:435:LEU:O	1:A:462:TYR:HA	2.13	0.48
3:C:207:GLY:C	3:C:209:TRP:H	2.21	0.48
1:E:297:THR:HG21	1:E:299:GLU:HG2	1.94	0.48
1:A:349:TYR:OH	1:A:592:LEU:HG	2.13	0.48
1:A:753:THR:CG2	1:A:757:LYS:HE2	2.44	0.48
1:E:79:CYS:CB	1:E:80:PRO:HD2	2.43	0.48
1:E:247:HIS:CD2	1:E:247:HIS:N	2.80	0.48
1:E:256:THR:HG23	8:E:2193:HOH:O	2.13	0.48
1:E:282:TYR:C	1:E:587:SER:HB3	2.38	0.48
2:F:27:ASN:HD21	2:F:121:HIS:HE1	1.62	0.48
3:G:223:GLU:C	3:G:225:LEU:H	2.21	0.48
1:A:596:ARG:CZ	1:A:600:ALA:HB1	2.44	0.48
1:A:722:ARG:NE	8:A:2353:HOH:O	2.47	0.48
2:B:57:GLN:O	2:B:59:LEU:HD23	2.14	0.48
2:B:117:THR:HG23	2:B:120:ALA:H	1.78	0.48
1:E:123:HIS:CE1	8:E:2079:HOH:O	2.67	0.48
1:A:477:ASP:C	1:A:478:VAL:HG23	2.39	0.47
1:A:509:HIS:HD2	1:A:510:GLU:O	1.97	0.47
1:A:541:GLU:HB2	1:A:555:LEU:HD12	1.95	0.47
1:E:491:ASP:OD1	1:E:492:PHE:N	2.47	0.47
2:F:135:CYS:HA	2:F:136:PRO:HD3	1.73	0.47
1:A:743:LYS:HG3	8:A:2364:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:LYS:HD3	8:F:2039:HOH:O	2.14	0.47
1:E:53:ILE:HD12	1:E:65:VAL:HG22	1.96	0.47
2:F:164:VAL:CG2	2:F:173:PRO:HB2	2.43	0.47
3:G:195:PRO:HD2	3:G:196:GLU:OE2	2.14	0.47
1:A:87:GLN:HG3	1:A:637:ASN:CG	2.39	0.47
1:A:253:LYS:O	1:A:256:THR:HB	2.14	0.47
1:E:292:HIS:HD2	8:E:2083:HOH:O	1.96	0.47
1:E:370:TYR:OH	1:E:372:GLU:HG3	2.14	0.47
1:E:590:ILE:HG22	1:E:591:GLU:N	2.28	0.47
1:A:193:GLU:OE2	1:A:332:ARG:NH1	2.47	0.47
1:A:252:ILE:HD11	1:A:256:THR:HG22	1.95	0.47
1:A:319:MET:CE	1:A:328:LEU:CD1	2.93	0.47
3:C:215:LEU:O	3:C:216:LEU:C	2.57	0.47
1:E:308:PRO:CB	8:E:2195:HOH:O	2.51	0.47
1:E:346:ALA:HB2	1:E:605:LEU:HD12	1.96	0.47
1:E:602:HIS:CE1	1:E:606:PRO:CG	2.53	0.47
1:A:66:GLU:HG3	8:A:2039:HOH:O	2.15	0.47
1:A:277:GLU:HB3	1:A:281:LYS:NZ	2.29	0.47
1:A:393:GLY:CA	1:A:407:LYS:HE3	2.39	0.47
1:E:289:LEU:HD12	1:E:590:ILE:HG21	1.96	0.47
1:E:314:GLU:HG3	8:E:2199:HOH:O	2.13	0.47
1:E:589:LYS:CB	1:E:592:LEU:HB2	2.42	0.47
2:F:99:ALA:HB2	3:G:137:ASN:ND2	2.29	0.47
1:A:209:HIS:CD2	1:A:209:HIS:H	2.32	0.47
1:A:536:PRO:O	8:A:2256:HOH:O	2.20	0.47
1:A:596:ARG:O	1:A:600:ALA:N	2.34	0.47
1:E:324:PRO:HD2	8:E:2210:HOH:O	2.08	0.47
1:E:492:PHE:CZ	1:E:548:LEU:HG	2.50	0.47
1:E:537:TRP:CD1	1:E:537:TRP:H	2.32	0.47
1:E:606:PRO:HG2	1:E:607:VAL:N	2.30	0.47
3:G:208:TRP:HA	3:G:208:TRP:HE3	1.76	0.47
1:A:284:VAL:HB	1:A:589:LYS:HA	1.96	0.47
1:A:615:PRO:O	1:A:618:PHE:HB2	2.15	0.47
1:A:671:ASN:C	1:A:671:ASN:HD22	2.22	0.47
2:B:41:ARG:NH1	2:B:187:THR:HG23	2.15	0.47
1:E:47:CYS:HB3	1:E:81:ARG:HH12	1.79	0.47
1:E:51:CYS:SG	1:E:216:ASN:HB3	2.55	0.47
1:E:197:TRP:CB	1:E:221:ASP:HB3	2.44	0.47
1:E:422:GLU:HG3	8:E:2103:HOH:O	2.13	0.47
2:F:23:CYS:SG	2:F:35:ASN:HB2	2.53	0.47
2:F:166:ARG:NH2	3:G:248:GLN:NE2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:17:ASN:HB2	8:G:2010:HOH:O	2.14	0.47
1:A:390:GLY:N	1:A:391:PRO:HD3	2.30	0.47
1:E:500:PRO:CD	1:E:567:ARG:O	2.63	0.47
3:G:19:LEU:HD23	3:G:19:LEU:O	2.14	0.47
1:A:113:ARG:CZ	8:A:2065:HOH:O	2.63	0.47
1:A:433:LYS:HD3	1:A:460:ASP:OD2	2.15	0.47
1:A:434:GLY:CA	1:A:461:LEU:O	2.52	0.47
1:A:651:ILE:HG23	1:A:693:VAL:CG2	2.45	0.47
1:E:177:ARG:HA	1:E:344:VAL:HG11	1.96	0.47
1:A:118:GLU:HG3	8:A:2252:HOH:O	2.14	0.47
1:A:231:LYS:HB3	1:A:231:LYS:HE3	1.55	0.47
1:A:266:HIS:HB2	1:A:293:VAL:HG13	1.95	0.47
1:A:494:LEU:HD22	1:A:502:ILE:HG12	1.96	0.47
1:E:166:ALA:HB2	1:E:415:THR:HG21	1.97	0.47
3:G:26:LEU:HG	3:G:158:LEU:HB3	1.97	0.47
1:A:263:ALA:O	1:A:267:VAL:HG23	2.15	0.46
1:A:370:TYR:CD2	1:A:551:LEU:HD21	2.50	0.46
1:E:53:ILE:HD12	1:E:65:VAL:CG2	2.45	0.46
1:E:239:PHE:O	1:E:687:ARG:HD2	2.15	0.46
1:E:391:PRO:C	1:E:413:ARG:CG	2.88	0.46
1:E:753:THR:HG22	1:E:757:LYS:HE3	1.96	0.46
1:A:186:GLY:N	1:A:583:PHE:C	2.68	0.46
1:A:339:ASP:HB3	1:A:607:VAL:CG1	2.42	0.46
1:A:541:GLU:O	1:A:545:GLU:HG2	2.14	0.46
2:B:3:ARG:HD2	2:B:62:GLU:OE2	2.15	0.46
2:B:118:PHE:HD1	2:B:118:PHE:HA	1.65	0.46
2:B:190:SER:CA	3:C:252:GLY:N	2.78	0.46
3:C:109:GLY:C	3:C:110:LYS:HG2	2.39	0.46
1:E:95:LEU:HG	1:E:468:LEU:O	2.15	0.46
1:E:201:ARG:NH2	1:E:228:ASN:O	2.37	0.46
1:E:523:ARG:HG2	1:E:523:ARG:HH11	1.81	0.46
1:E:621:LEU:HD22	1:E:622:LEU:N	2.30	0.46
1:E:636:ASN:HA	1:E:708:LEU:HB2	1.96	0.46
2:F:16:CYS:O	4:F:1194:SF4:S3	2.74	0.46
1:A:41:TYR:HD1	1:A:559:LYS:O	1.97	0.46
1:A:174:THR:HG23	1:A:178:GLU:CG	2.42	0.46
1:A:248:ARG:HB3	8:A:2133:HOH:O	2.14	0.46
1:A:583:PHE:N	8:A:2274:HOH:O	2.46	0.46
1:A:683:LYS:HA	1:A:684:PRO:HD2	1.58	0.46
2:B:117:THR:HG22	2:B:119:CYS:CA	2.45	0.46
3:C:207:GLY:HA2	3:C:210:TYR:CB	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:241:LEU:CD1	3:C:241:LEU:O	2.63	0.46
1:E:209:HIS:CE1	1:E:625:ARG:N	2.70	0.46
1:E:339:ASP:CB	1:E:607:VAL:CG1	2.87	0.46
1:E:606:PRO:HD2	1:E:607:VAL:H	1.79	0.46
1:E:620:ARG:HA	1:E:738:PHE:HD2	1.80	0.46
1:E:634:THR:H	1:E:635:GLN:NE2	2.13	0.46
3:G:165:LEU:C	3:G:167:LYS:H	2.22	0.46
3:G:249:GLY:O	8:G:2076:HOH:O	2.21	0.46
1:A:65:VAL:CG1	1:A:78:LEU:CD2	2.92	0.46
1:A:581:LEU:HD23	1:A:583:PHE:HE1	1.81	0.46
1:A:686:ALA:O	1:A:687:ARG:HG2	2.15	0.46
2:B:161:ARG:HG2	2:B:179:ASN:HA	1.95	0.46
3:C:17:THR:HG21	8:C:2015:HOH:O	2.14	0.46
1:E:342:TYR:CD1	1:E:607:VAL:CB	2.83	0.46
1:E:468:LEU:HB3	1:E:469:PRO:HD2	1.97	0.46
1:E:597:PHE:HB3	8:E:2325:HOH:O	2.16	0.46
8:F:2074:HOH:O	3:G:72:ARG:HD3	2.15	0.46
1:A:647:ASN:H	1:A:647:ASN:ND2	2.09	0.46
2:B:47:PRO:C	2:B:48:ASN:OD1	2.57	0.46
2:B:57:GLN:OE1	8:B:2044:HOH:O	2.20	0.46
1:E:60:ASN:ND2	8:E:2021:HOH:O	2.47	0.46
1:E:591:GLU:O	1:E:603:GLN:HG2	2.14	0.46
2:F:79:LYS:HD2	2:F:79:LYS:HA	1.77	0.46
8:F:2031:HOH:O	3:G:1:ALA:CB	2.63	0.46
1:A:253:LYS:NZ	1:A:613:GLU:OE2	2.36	0.46
1:A:483:ALA:HB2	1:A:515:THR:HG22	1.97	0.46
1:E:45:GLU:HB2	1:E:485:TYR:HB3	1.96	0.46
1:E:106:GLN:NE2	8:E:2061:HOH:O	2.49	0.46
2:F:175:LEU:HD12	2:F:175:LEU:C	2.40	0.46
1:A:267:VAL:O	1:A:271:GLU:HB2	2.15	0.46
1:A:371:LEU:HG	1:A:502:ILE:HD13	1.97	0.46
3:C:174:PHE:N	3:C:175:PRO:HD2	2.31	0.46
1:E:187:ARG:HB3	1:E:188:PRO:HD2	1.97	0.46
1:E:288:GLU:HG3	8:E:2182:HOH:O	2.15	0.46
1:E:470:GLN:O	1:E:471:GLU:C	2.57	0.46
2:F:36:LEU:HD22	4:F:1195:SF4:S4	2.56	0.46
3:G:214:LEU:O	3:G:217:LEU:HB2	2.16	0.46
1:A:129:LEU:O	1:A:133:GLU:HG2	2.16	0.46
1:A:538:LYS:HE2	1:A:538:LYS:N	2.30	0.46
3:C:166:LEU:HD21	3:C:228:PRO:HB2	1.97	0.46
1:E:625:ARG:HD2	5:E:1766:MGD:C17	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:672:GLN:HE22	1:E:738:PHE:H	1.64	0.46
3:G:20:HIS:CE1	3:G:63:LEU:HD21	2.51	0.46
1:A:121:LEU:HD22	1:A:525:LEU:HG	1.97	0.46
1:A:349:TYR:CZ	1:A:590:ILE:O	2.68	0.46
1:A:589:LYS:H	1:A:589:LYS:HG2	1.54	0.46
1:E:30:ALA:N	1:E:31:PRO:CD	2.79	0.46
1:E:630:THR:HA	5:E:1766:MGD:H18	1.81	0.46
1:E:664:GLY:N	8:E:2374:HOH:O	2.45	0.46
1:A:220:GLN:HG2	2:B:136:PRO:O	2.15	0.46
1:A:225:ALA:C	1:A:230:ALA:HB3	2.41	0.46
1:A:447:PRO:HD3	8:A:2212:HOH:O	2.16	0.46
1:A:618:PHE:CZ	1:A:740:ARG:HD3	2.51	0.46
2:B:169:GLN:NE2	8:B:2127:HOH:O	2.32	0.46
1:E:249:TRP:CZ2	1:E:251:PRO:HB3	2.50	0.46
1:E:501:PHE:HB3	1:E:565:VAL:HG13	1.97	0.46
5:E:1766:MGD:H8	8:E:2426:HOH:O	2.16	0.46
2:F:59:LEU:O	2:F:60:HIS:C	2.59	0.46
1:A:186:GLY:CA	1:A:584:GLY:N	2.75	0.45
1:A:241:THR:HG21	2:B:14:VAL:HB	1.98	0.45
1:A:266:HIS:C	1:A:266:HIS:CD2	2.94	0.45
2:B:35:ASN:HB3	2:B:116:CYS:HB2	1.99	0.45
3:C:145:ASN:OD1	3:C:193:THR:HG23	2.16	0.45
1:E:117:TRP:CE2	1:E:516:LYS:HG3	2.51	0.45
1:E:275:ASP:C	1:E:275:ASP:OD1	2.55	0.45
1:E:494:LEU:HD23	1:E:502:ILE:HG23	1.98	0.45
1:E:648:GLU:CG	1:E:681:ARG:NH1	2.76	0.45
3:G:208:TRP:O	3:G:212:PHE:CD2	2.69	0.45
1:E:75:ARG:NH1	1:E:220:GLN:NE2	2.55	0.45
1:E:160:TRP:O	1:E:160:TRP:CD1	2.70	0.45
1:E:369:PRO:CG	1:E:494:LEU:HB3	2.46	0.45
1:E:413:ARG:NH1	1:E:413:ARG:H	2.14	0.45
1:E:435:LEU:HB3	1:E:459:LEU:CD1	2.46	0.45
1:E:462:TYR:CE1	1:E:463:VAL:O	2.69	0.45
2:F:19:CYS:HB2	2:F:131:CYS:HB2	1.98	0.45
3:G:60:LEU:HD23	3:G:63:LEU:HD12	1.96	0.45
1:A:430:TYR:HB2	1:A:431:PRO:CD	2.46	0.45
1:A:449:VAL:CG1	1:A:453:LYS:HE3	2.47	0.45
1:A:743:LYS:CG	8:A:2364:HOH:O	2.65	0.45
1:E:457:LYS:HD3	8:E:2064:HOH:O	2.15	0.45
1:E:614:PRO:HB3	1:E:738:PHE:CD2	2.52	0.45
1:A:389:SER:CA	1:A:595:GLN:HE22	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLU:N	1:A:423:PRO:CD	2.79	0.45
2:B:50:VAL:HG13	2:B:181:PRO:HB2	1.98	0.45
3:C:64:LEU:HD22	7:C:1252:MQ7:C5	2.45	0.45
1:E:427:GLY:O	1:E:428:GLU:O	2.35	0.45
1:E:500:PRO:HD3	1:E:567:ARG:O	2.15	0.45
1:E:537:TRP:O	1:E:537:TRP:CE3	2.69	0.45
1:A:70:ALA:C	8:A:2036:HOH:O	2.49	0.45
1:A:319:MET:HE1	1:A:328:LEU:CD1	2.44	0.45
1:E:127:LYS:HD3	8:E:2082:HOH:O	2.16	0.45
1:E:625:ARG:HH22	5:E:1765:MGD:H15	1.63	0.45
2:F:46:TYR:HB2	8:F:2034:HOH:O	2.15	0.45
2:F:184:LYS:HE2	8:F:2120:HOH:O	2.17	0.45
3:G:170:TRP:CE3	3:G:171:ALA:N	2.85	0.45
1:A:630:THR:H	1:A:634:THR:CG2	2.27	0.45
1:E:457:LYS:CD	8:E:2064:HOH:O	2.64	0.45
2:F:78:THR:HG23	2:F:79:LYS:N	2.31	0.45
3:G:73:PHE:HA	8:G:2021:HOH:O	2.17	0.45
1:A:430:TYR:HB2	1:A:431:PRO:HD3	1.98	0.45
1:A:471:GLU:HB2	1:A:702:LYS:O	2.16	0.45
1:A:523:ARG:HG2	1:A:523:ARG:HH11	1.81	0.45
2:B:166:ARG:HD2	8:B:2124:HOH:O	2.16	0.45
3:C:153:PRO:HB3	8:C:2062:HOH:O	2.15	0.45
3:C:193:THR:HG23	3:C:193:THR:O	2.17	0.45
1:E:462:TYR:CD2	1:E:476:ALA:HA	2.51	0.45
1:E:497:HIS:HB3	1:E:499:THR:O	2.17	0.45
1:A:213:ASP:OD1	1:A:213:ASP:C	2.59	0.45
1:A:302:GLU:O	1:A:302:GLU:HG3	2.15	0.45
1:A:423:PRO:HB2	1:A:432:ILE:HD12	1.97	0.45
1:A:588:GLY:HA3	8:A:2152:HOH:O	2.17	0.45
3:C:25:VAL:HB	3:C:60:ASP:OD2	2.17	0.45
1:E:113:ARG:CB	8:E:2042:HOH:O	2.64	0.45
1:E:557:THR:O	1:E:561:MET:HG3	2.17	0.45
1:E:717:ASN:ND2	8:E:2415:HOH:O	2.49	0.45
2:B:150:SER:O	2:B:154:LYS:HG2	2.17	0.45
2:B:166:ARG:HG2	8:B:2144:HOH:O	2.17	0.45
1:E:283:THR:HG23	1:E:590:ILE:HG13	1.99	0.45
1:E:604:PRO:CA	1:E:605:LEU:HD23	2.47	0.45
2:F:54:ARG:NH1	2:F:56:GLU:OE2	2.42	0.45
2:F:146:GLU:O	2:F:148:PRO:HD3	2.17	0.45
1:A:418:GLN:NE2	1:A:730:GLY:O	2.50	0.45
1:A:429:PRO:HD2	8:A:2202:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:ALA:HB3	4:B:1195:SF4:S2	2.57	0.45
3:C:40:LEU:HD13	3:C:117:ALA:CB	2.47	0.45
1:E:75:ARG:HD2	1:E:220:GLN:NE2	2.26	0.45
1:E:195:ILE:CD1	1:E:363:PHE:CE2	3.00	0.45
1:E:255:GLY:HA2	1:E:337:TYR:CE1	2.52	0.45
1:E:335:VAL:O	1:E:335:VAL:CG1	2.65	0.45
1:E:391:PRO:HD2	1:E:595:GLN:OE1	2.17	0.45
3:G:134:LEU:N	8:G:2035:HOH:O	2.49	0.45
1:A:39:SER:C	8:A:2005:HOH:O	2.60	0.44
1:A:60:ASN:HB2	8:A:2022:HOH:O	2.16	0.44
1:A:66:GLU:HB3	8:A:2017:HOH:O	2.17	0.44
1:A:275:ASP:C	1:A:275:ASP:OD1	2.60	0.44
1:A:403:PRO:O	1:A:404:ARG:C	2.59	0.44
1:A:504:LEU:HD22	1:A:505:ARG:N	2.31	0.44
1:A:573:GLU:O	1:A:577:LYS:HG3	2.16	0.44
1:A:653:LYS:HD3	8:B:2025:HOH:O	2.17	0.44
1:A:727:PRO:HA	8:A:2197:HOH:O	2.16	0.44
3:C:25:VAL:HG23	3:C:96:LEU:HD21	2.00	0.44
1:E:114:VAL:HG21	8:E:2038:HOH:O	2.17	0.44
1:E:284:VAL:HG12	1:E:592:LEU:CD1	2.47	0.44
1:E:297:THR:CG2	1:E:299:GLU:N	2.73	0.44
1:E:388:CYS:O	1:E:389:SER:C	2.59	0.44
2:F:82:LEU:HD12	2:F:84:LEU:HD11	1.98	0.44
1:A:644:ASP:HA	1:A:645:PRO:HD3	1.72	0.44
2:B:35:ASN:ND2	2:B:106:TYR:OH	2.50	0.44
3:C:13:PHE:CZ	3:C:247:GLN:HG2	2.52	0.44
1:E:597:PHE:O	1:E:597:PHE:CD1	2.70	0.44
1:A:98:PRO:HD3	1:A:481:PRO:HD2	1.99	0.44
1:A:183:TRP:NE1	1:A:413:ARG:HH22	2.03	0.44
1:A:602:HIS:CE1	1:A:606:PRO:CD	2.94	0.44
2:B:143:GLY:N	2:B:152:VAL:CG2	2.80	0.44
3:C:89:ILE:HD12	7:C:1252:MQ7:C5	2.46	0.44
3:C:128:LEU:HA	8:C:2050:HOH:O	2.16	0.44
1:E:71:ASN:HD21	1:E:73:LYS:HB2	1.83	0.44
1:E:196:ASP:OD1	1:E:360:PRO:HA	2.17	0.44
1:E:502:ILE:O	1:E:563:THR:HA	2.16	0.44
1:E:633:ARG:HB2	5:E:1765:MGD:H2'	2.00	0.44
1:E:708:LEU:O	1:E:712:ARG:CD	2.64	0.44
3:G:206:GLY:H	3:G:209:TYR:HB2	1.83	0.44
1:A:335:VAL:HG13	1:A:733:GLY:N	2.32	0.44
1:A:457:LYS:HD2	8:A:2219:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:SER:HB2	1:A:696:VAL:HG11	2.00	0.44
3:C:71:ARG:HG2	3:C:72:PHE:N	2.33	0.44
3:C:220:THR:HA	3:C:227:ALA:HA	1.98	0.44
1:E:630:THR:H	1:E:634:THR:HG21	1.81	0.44
1:E:636:ASN:HB2	1:E:706:MET:HE2	1.99	0.44
1:A:95:LEU:N	1:A:467:VAL:O	2.41	0.44
1:A:336:TRP:HA	1:A:735:ARG:HG3	1.98	0.44
1:A:552:GLY:O	8:A:2261:HOH:O	2.21	0.44
1:A:647:ASN:HD21	1:A:713:GLY:CA	2.30	0.44
3:C:17:THR:HG22	3:C:67:GLU:HG3	1.89	0.44
3:C:63:ILE:O	3:C:67:GLU:HB3	2.16	0.44
3:C:172:ALA:HA	3:C:175:PRO:CG	2.35	0.44
3:C:186:LEU:HD22	3:G:149:GLY:HA2	2.00	0.44
1:E:45:GLU:HB2	1:E:485:TYR:CB	2.48	0.44
1:A:132:ARG:HD3	8:A:2075:HOH:O	2.14	0.44
1:A:558:MET:HA	1:A:558:MET:CE	2.41	0.44
1:A:587:SER:O	1:A:589:LYS:CE	2.65	0.44
3:C:31:VAL:HG12	3:C:53:ALA:HB2	1.99	0.44
3:C:227:ALA:HB3	3:C:228:PRO:HD3	2.00	0.44
1:E:187:ARG:HB3	1:E:188:PRO:CD	2.47	0.44
1:E:208:HIS:HE1	1:E:218:GLN:HE22	1.65	0.44
1:E:297:THR:HG22	1:E:299:GLU:N	2.32	0.44
1:E:607:VAL:CG2	8:E:2144:HOH:O	2.63	0.44
1:A:65:VAL:HG13	1:A:78:LEU:CD2	2.48	0.44
1:A:249:TRP:O	1:A:251:PRO:HD3	2.18	0.44
1:A:498:LYS:HE3	8:A:2107:HOH:O	2.15	0.44
1:A:605:LEU:N	1:A:606:PRO:HD3	2.28	0.44
1:A:647:ASN:HD21	1:A:713:GLY:HA3	1.83	0.44
1:E:278:TYR:O	1:E:279:VAL:C	2.61	0.44
1:A:358:GLY:N	1:A:363:PHE:O	2.48	0.44
1:A:523:ARG:HG2	1:A:523:ARG:NH1	2.32	0.44
1:A:712:ARG:NH1	8:A:2345:HOH:O	2.49	0.44
1:E:257:ASP:OD2	5:E:1766:MGD:N1	2.43	0.44
2:F:86:ASP:OD1	2:F:88:LYS:HB2	2.18	0.44
3:G:216:GLY:C	3:G:218:GLY:H	2.26	0.44
1:A:428:GLU:OE2	1:A:428:GLU:HA	1.96	0.44
1:A:488:ARG:HG2	1:A:489:TYR:O	2.18	0.44
1:A:596:ARG:CZ	1:A:600:ALA:CB	2.96	0.44
1:A:642:GLU:OE2	2:B:31:PRO:C	2.61	0.44
2:B:39:ARG:HD2	2:B:56:GLU:OE2	2.18	0.44
3:C:161:LEU:HD12	3:C:179:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:SER:HB2	1:E:77:ARG:O	2.18	0.44
1:E:187:ARG:NH1	8:E:2107:HOH:O	2.47	0.44
1:E:466:ASP:OD1	1:E:473:VAL:HG21	2.18	0.44
1:E:604:PRO:O	1:E:606:PRO:HD2	2.15	0.44
1:E:730:GLY:N	8:E:2249:HOH:O	2.42	0.44
2:F:6:MET:HG2	2:F:175:LEU:HD22	2.00	0.44
1:A:88:THR:HG23	1:A:468:LEU:HD21	1.99	0.43
1:A:666:TYR:CE1	1:A:681:ARG:HG3	2.53	0.43
3:C:111:GLY:O	3:C:116:LEU:HD11	2.18	0.43
1:E:77:ARG:NH1	2:F:135:CYS:O	2.51	0.43
1:E:292:HIS:HE1	1:E:605:LEU:O	2.01	0.43
2:F:101:PRO:HD2	2:F:102:TYR:CD1	2.53	0.43
1:A:38:LYS:HG2	8:A:2021:HOH:O	2.18	0.43
1:A:257:ASP:OD2	8:A:2138:HOH:O	2.21	0.43
1:A:425:ILE:HD11	1:A:451:ARG:HG2	2.00	0.43
2:B:38:ILE:HD12	4:B:1194:SF4:S1	2.58	0.43
1:E:302:GLU:HG3	1:E:307:ILE:O	2.18	0.43
1:E:391:PRO:C	1:E:413:ARG:HG3	2.43	0.43
1:E:622:LEU:O	1:E:623:TYR:HB3	2.18	0.43
1:E:622:LEU:HD23	1:E:622:LEU:HA	1.87	0.43
1:E:708:LEU:CA	8:E:2407:HOH:O	2.58	0.43
1:E:745:GLU:HG3	8:E:2431:HOH:O	2.17	0.43
2:F:29:VAL:HA	2:F:30:PRO:HD3	1.63	0.43
2:F:166:ARG:NH2	3:G:248:GLN:HG3	2.33	0.43
3:G:223:GLU:N	8:G:2069:HOH:O	2.50	0.43
1:A:81:ARG:HD2	1:A:630:THR:OG1	2.18	0.43
1:A:394:GLY:N	8:A:2189:HOH:O	2.52	0.43
1:A:395:ASP:C	1:A:399:GLU:CB	2.77	0.43
1:A:539:THR:HG21	1:A:541:GLU:HG2	2.00	0.43
1:A:604:PRO:HA	1:A:605:LEU:HD23	2.00	0.43
1:E:48:PHE:CE1	1:E:631:PHE:CE1	3.06	0.43
1:E:474:MET:HE2	1:E:705:LEU:HD12	2.01	0.43
2:F:191:GLU:HB2	8:F:2122:HOH:O	2.18	0.43
1:A:252:ILE:HG13	1:A:307:ILE:CD1	2.48	0.43
1:A:418:GLN:H	1:A:418:GLN:HG3	1.39	0.43
1:E:186:GLY:HA3	1:E:584:GLY:CA	2.48	0.43
1:E:328:LEU:N	1:E:328:LEU:HD12	2.32	0.43
1:E:403:PRO:O	1:E:430:TYR:OH	2.34	0.43
1:E:423:PRO:O	1:E:427:GLY:HA2	2.19	0.43
2:F:35:ASN:ND2	2:F:106:TYR:OH	2.46	0.43
2:F:52:GLU:CD	2:F:187:THR:HB	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:106:TYR:CE1	2:F:114:SER:HB3	2.53	0.43
1:A:264:TRP:CZ2	1:A:315:VAL:HG11	2.53	0.43
1:A:753:THR:HG22	1:A:757:LYS:HE2	1.99	0.43
1:E:346:ALA:CA	1:E:605:LEU:HD12	2.49	0.43
1:E:591:GLU:CD	1:E:604:PRO:CG	2.92	0.43
1:E:596:ARG:CZ	1:E:601:GLY:HA3	2.49	0.43
1:E:602:HIS:NE2	1:E:604:PRO:CD	2.56	0.43
1:A:412:ALA:HB2	1:A:728:ILE:O	2.17	0.43
1:A:638:TRP:HB2	1:A:756:ALA:HB2	2.01	0.43
2:B:1:MET:O	2:B:146:GLU:OE1	2.36	0.43
2:B:142:PHE:C	2:B:152:VAL:CG2	2.90	0.43
2:B:168:GLU:C	2:B:169:GLN:O	2.50	0.43
3:C:21:HIS:CE1	3:C:64:LEU:CD1	3.01	0.43
1:E:239:PHE:HB3	1:E:687:ARG:CD	2.49	0.43
1:E:457:LYS:HE2	8:E:2060:HOH:O	2.18	0.43
1:E:534:TYR:C	1:E:536:PRO:HD3	2.43	0.43
2:F:71:PRO:HB2	3:G:78:LEU:HD12	2.01	0.43
3:G:38:HIS:CE1	3:G:105:LEU:HD13	2.53	0.43
3:G:222:GLN:CB	8:G:2069:HOH:O	2.67	0.43
1:A:335:VAL:O	1:A:337:TYR:N	2.52	0.43
1:A:581:LEU:HD12	1:A:581:LEU:HA	1.91	0.43
3:C:11:GLN:NE2	3:C:11:GLN:H	2.17	0.43
1:E:103:GLU:HG2	1:E:104:GLY:N	2.34	0.43
1:E:422:GLU:HB2	8:E:2252:HOH:O	2.18	0.43
3:G:247:TRP:CE2	3:G:249:GLY:HA3	2.54	0.43
1:A:47:CYS:HB3	1:A:81:ARG:HH12	1.83	0.43
2:B:183:LYS:NZ	2:F:157:LYS:O	2.52	0.43
1:E:604:PRO:HA	1:E:605:LEU:CD2	2.47	0.43
1:E:626:SER:HB3	1:E:696:VAL:HG11	2.01	0.43
1:E:630:THR:HA	5:E:1766:MGD:O17	2.17	0.43
1:E:746:ARG:HH11	1:E:746:ARG:CG	2.30	0.43
2:F:72:THR:CG2	2:F:89:LYS:HB3	2.44	0.43
1:A:519:TRP:CG	1:A:540:ILE:HG23	2.53	0.43
1:A:607:VAL:C	1:A:609:THR:N	2.74	0.43
1:A:649:VAL:HA	1:A:695:ILE:HG22	2.00	0.43
1:A:753:THR:HG22	1:A:757:LYS:CE	2.49	0.43
3:C:150:GLY:HA2	3:G:185:LEU:HD22	2.00	0.43
1:E:626:SER:O	1:E:628:VAL:N	2.52	0.43
3:G:32:LEU:HD12	3:G:120:LEU:HD12	2.01	0.43
3:G:112:GLN:O	3:G:114:ALA:N	2.52	0.43
1:A:124:ILE:HG12	1:A:463:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:C	1:A:208:HIS:H	2.25	0.43
1:A:386:GLY:HA3	1:A:391:PRO:HB2	2.00	0.43
1:A:629:HIS:CB	1:A:634:THR:HG21	2.48	0.43
1:A:657:LYS:O	1:A:659:LEU:O	2.35	0.43
1:A:717:ASN:HA	1:A:720:GLN:OE1	2.19	0.43
2:B:72:THR:CG2	2:B:73:GLY:N	2.80	0.43
2:B:165:LEU:O	2:B:166:ARG:C	2.61	0.43
3:C:40:LEU:HD12	3:C:40:LEU:HA	1.91	0.43
3:C:171:TRP:CE3	3:C:172:ALA:HB2	2.54	0.43
1:E:100:ILE:HG12	1:E:478:VAL:CG1	2.49	0.43
1:E:193:GLU:H	1:E:193:GLU:CD	2.27	0.43
1:E:407:LYS:O	1:E:407:LYS:HG3	2.18	0.43
3:G:217:LEU:CD2	8:G:2065:HOH:O	2.66	0.43
1:A:183:TRP:CH2	1:A:596:ARG:CD	2.90	0.42
1:A:192:HIS:O	1:A:193:GLU:C	2.62	0.42
1:A:338:GLY:HA3	1:A:724:LYS:HG2	2.00	0.42
1:A:482:GLU:HG2	1:A:483:ALA:N	2.34	0.42
1:A:536:PRO:HG2	1:A:537:TRP:N	2.32	0.42
1:A:625:ARG:HD2	5:A:1766:MGD:C17	2.49	0.42
1:E:30:ALA:C	8:E:2002:HOH:O	2.61	0.42
1:E:469:PRO:O	1:E:706:MET:SD	2.77	0.42
3:G:58:LEU:HD12	3:G:58:LEU:O	2.19	0.42
3:G:144:ASN:C	3:G:144:ASN:ND2	2.76	0.42
1:A:73:LYS:HG3	1:A:501:PHE:HZ	1.83	0.42
1:A:189:ILE:O	1:A:194:PRO:HD3	2.19	0.42
1:A:498:LYS:HD2	8:A:2241:HOH:O	2.17	0.42
2:B:36:LEU:HD12	2:B:37:TRP:N	2.34	0.42
3:C:21:HIS:CE1	3:C:64:LEU:HG	2.50	0.42
3:C:166:LEU:C	3:C:168:LYS:H	2.27	0.42
1:E:186:GLY:N	1:E:583:PHE:HA	2.28	0.42
1:E:281:LYS:HG3	1:E:282:TYR:CD1	2.54	0.42
2:F:164:VAL:HG12	2:F:167:PRO:HB3	2.00	0.42
1:A:572:LEU:O	1:A:576:GLU:HB2	2.18	0.42
1:E:172:LEU:HB3	5:E:1765:MGD:H23	2.01	0.42
1:E:349:TYR:CE1	1:E:605:LEU:HD11	2.53	0.42
1:E:574:ASP:O	1:E:578:GLU:HG3	2.19	0.42
1:E:702:LYS:HE3	1:E:718:TYR:CE2	2.54	0.42
1:E:707:ARG:NE	8:E:2404:HOH:O	2.50	0.42
8:F:2052:HOH:O	3:G:88:ILE:HG13	2.18	0.42
3:G:117:TRP:CB	8:G:2034:HOH:O	2.67	0.42
1:A:77:ARG:HD2	2:B:138:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:GLU:OE2	1:A:718:TYR:OH	2.32	0.42
3:C:241:LEU:HD12	3:C:242:LEU:N	2.34	0.42
1:E:151:TRP:O	1:E:156:LEU:HB3	2.19	0.42
1:E:239:PHE:HB3	1:E:687:ARG:HD2	2.00	0.42
1:E:576:GLU:C	1:E:578:GLU:N	2.75	0.42
1:E:650:TRP:O	1:E:693:VAL:HG22	2.19	0.42
1:E:669:LEU:CD2	1:E:741:LEU:CD2	2.96	0.42
2:F:10:LEU:HD22	2:F:53:PHE:O	2.19	0.42
2:F:132:VAL:HA	2:F:140:ARG:HG3	2.01	0.42
1:A:95:LEU:HG	1:A:467:VAL:O	2.19	0.42
1:A:336:TRP:HB3	1:A:337:TYR:CD1	2.53	0.42
1:A:453:LYS:HB3	1:A:475:TRP:CH2	2.54	0.42
2:B:172:ARG:HD3	8:F:2126:HOH:O	2.20	0.42
1:E:183:TRP:CG	1:E:593:TYR:CD1	3.07	0.42
1:E:278:TYR:OH	1:E:357:TYR:HB3	2.19	0.42
1:E:634:THR:H	1:E:635:GLN:HE22	1.66	0.42
3:G:23:LEU:HD22	3:G:62:ILE:HD12	2.01	0.42
3:G:70:ARG:HG3	3:G:71:PHE:CD2	2.54	0.42
1:A:355:GLY:O	1:A:359:ARG:HG3	2.19	0.42
1:A:655:GLU:CD	1:A:658:ARG:NH2	2.77	0.42
3:C:145:ASN:HD21	3:C:147:LEU:HB2	1.84	0.42
1:E:90:TYR:OH	1:E:509:HIS:CE1	2.65	0.42
1:E:327:VAL:HG13	1:E:362:GLY:HA2	2.01	0.42
1:E:620:ARG:O	1:E:620:ARG:HG2	2.19	0.42
1:E:648:GLU:CG	1:E:681:ARG:HH12	2.21	0.42
1:E:669:LEU:HD21	1:E:741:LEU:HD22	1.98	0.42
8:F:2029:HOH:O	3:G:250:LEU:CD1	2.65	0.42
3:G:207:PHE:CE2	3:G:211:LEU:CD1	2.61	0.42
1:A:80:PRO:HG2	1:A:627:PRO:O	2.18	0.42
1:A:421:ILE:O	1:A:421:ILE:CG2	2.65	0.42
1:A:589:LYS:O	1:A:592:LEU:CB	2.67	0.42
2:B:7:ALA:HB3	2:B:141:THR:OG1	2.20	0.42
3:C:108:LEU:HB3	3:C:110:LYS:CG	2.50	0.42
1:E:79:CYS:HB2	1:E:80:PRO:CD	2.50	0.42
1:E:128:MET:HE1	1:E:529:LEU:HD11	2.01	0.42
1:E:293:VAL:O	1:E:293:VAL:HG13	2.18	0.42
3:G:134:LEU:HG	8:G:2035:HOH:O	2.19	0.42
3:G:154:THR:HG21	3:G:238:ARG:CG	2.45	0.42
3:G:165:LEU:HG	3:G:227:PRO:HB2	2.01	0.42
1:A:117:TRP:CE2	1:A:516:LYS:HG3	2.54	0.42
1:A:265:ILE:CG2	1:A:293:VAL:HG21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.77	0.42
1:E:159:ALA:HA	1:E:380:PRO:HD2	2.02	0.42
1:E:391:PRO:C	1:E:413:ARG:HG2	2.45	0.42
1:E:613:GLU:HB3	1:E:614:PRO:HD2	2.01	0.42
1:E:649:VAL:HG13	1:E:695:ILE:HG23	1.99	0.42
1:E:683:LYS:O	1:E:683:LYS:HG2	2.18	0.42
1:E:757:LYS:O	1:E:758:ARG:C	2.63	0.42
3:G:206:GLY:N	3:G:209:TYR:HB2	2.35	0.42
1:A:37:VAL:HG12	1:A:38:LYS:H	1.82	0.42
1:A:39:SER:CB	8:A:2005:HOH:O	2.64	0.42
1:A:214:THR:HG21	1:A:627:PRO:O	2.19	0.42
1:A:396:HIS:CD2	1:A:403:PRO:CB	3.03	0.42
1:A:427:GLY:C	1:A:430:TYR:O	2.62	0.42
1:A:582:PRO:CB	8:A:2274:HOH:O	1.94	0.42
3:C:241:LEU:HD12	3:C:241:LEU:O	2.17	0.42
1:E:315:VAL:O	1:E:319:MET:HG2	2.20	0.42
1:E:525:LEU:O	1:E:529:LEU:HG	2.20	0.42
1:E:602:HIS:CE1	1:E:606:PRO:CD	3.02	0.42
1:A:64:LYS:HE3	2:B:26:GLU:HB2	2.02	0.42
1:A:186:GLY:N	1:A:583:PHE:CA	2.83	0.42
1:A:187:ARG:HB3	1:A:188:PRO:HD2	2.02	0.42
1:A:497:HIS:O	1:A:498:LYS:C	2.61	0.42
1:A:519:TRP:CD2	1:A:540:ILE:CG2	3.02	0.42
1:A:533:GLN:HE21	1:A:533:GLN:H	1.68	0.42
1:A:629:HIS:CB	1:A:634:THR:CG2	2.98	0.42
3:C:173:LEU:O	3:C:177:ARG:HG3	2.20	0.42
1:E:138:GLU:OE2	1:E:402:LYS:HB2	2.19	0.42
2:F:175:LEU:C	2:F:175:LEU:CD1	2.93	0.42
1:A:71:ASN:ND2	1:A:74:SER:H	2.08	0.41
1:A:144:GLY:HA2	1:A:438:TYR:O	2.20	0.41
1:A:310:GLN:CG	8:A:2160:HOH:O	2.67	0.41
1:A:667:VAL:HG11	1:A:741:LEU:HB3	2.01	0.41
1:E:183:TRP:CD1	1:E:593:TYR:CE1	3.08	0.41
1:E:642:GLU:OE2	2:F:31:PRO:HA	2.20	0.41
1:E:708:LEU:CB	8:E:2407:HOH:O	2.68	0.41
3:G:81:SER:HB2	3:G:83:HIS:CD2	2.55	0.41
1:A:108:GLY:C	1:A:109:GLU:O	2.60	0.41
1:A:224:LEU:HB3	8:A:2124:HOH:O	2.20	0.41
1:A:342:TYR:CG	1:A:605:LEU:HA	2.56	0.41
1:A:502:ILE:N	1:A:564:LEU:O	2.49	0.41
2:B:71:PRO:HB2	3:C:79:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:GLY:HA3	1:E:583:PHE:C	2.45	0.41
1:E:237:PRO:CB	1:E:689:ARG:HD3	2.50	0.41
1:E:252:ILE:CG1	1:E:256:THR:HG22	2.49	0.41
1:E:428:GLU:C	1:E:430:TYR:N	2.69	0.41
3:G:206:GLY:O	3:G:209:TYR:HB3	2.20	0.41
1:A:77:ARG:HH12	2:B:138:TYR:HE2	1.53	0.41
1:A:118:GLU:CD	1:A:118:GLU:N	2.77	0.41
1:A:292:HIS:CD2	1:A:604:PRO:HB2	2.55	0.41
1:A:534:TYR:O	1:A:535:PHE:CD1	2.73	0.41
8:B:2074:HOH:O	3:C:78:TRP:HE3	2.02	0.41
1:E:42:GLN:CB	1:E:53:ILE:HG13	2.51	0.41
1:E:47:CYS:CB	8:E:2452:HOH:O	2.37	0.41
1:E:64:LYS:HD2	8:E:2046:HOH:O	2.19	0.41
1:E:430:TYR:HB2	1:E:431:PRO:CD	2.50	0.41
1:E:553:LEU:HA	1:E:553:LEU:HD23	1.76	0.41
3:G:142:LEU:HD23	3:G:197:ALA:HB1	2.02	0.41
1:A:510:GLU:HG3	1:A:510:GLU:H	1.62	0.41
1:A:520:TRP:O	1:A:524:GLU:HG2	2.20	0.41
1:A:717:ASN:HD22	5:A:1765:MGD:H192	1.68	0.41
3:C:92:GLY:O	3:C:96:LEU:HD12	2.20	0.41
3:C:111:GLY:O	3:C:112:SER:HB3	2.20	0.41
3:C:180:ALA:O	3:C:184:LEU:HG	2.21	0.41
3:C:251:LEU:HD23	8:C:2087:HOH:O	2.20	0.41
1:E:112:TYR:CE1	1:E:474:MET:O	2.73	0.41
1:E:548:LEU:HA	1:E:548:LEU:HD23	1.81	0.41
1:E:595:GLN:O	1:E:595:GLN:HG3	2.15	0.41
1:E:607:VAL:HG22	1:E:609:THR:OG1	2.20	0.41
2:F:135:CYS:SG	2:F:135:CYS:CA	3.00	0.41
1:A:655:GLU:OE2	1:A:658:ARG:NH2	2.53	0.41
1:A:685:THR:CG2	8:B:2026:HOH:O	2.67	0.41
1:A:693:VAL:HG21	1:A:741:LEU:HD21	2.01	0.41
1:E:69:GLU:H	1:E:69:GLU:HG2	1.62	0.41
1:E:629:HIS:HA	1:E:634:THR:HG21	2.01	0.41
3:G:178:LEU:HD23	3:G:178:LEU:HA	1.84	0.41
1:A:394:GLY:HA2	8:A:2188:HOH:O	2.20	0.41
1:A:532:GLU:HB3	8:A:2253:HOH:O	2.20	0.41
1:A:708:LEU:HB3	1:A:752:LEU:HD23	2.01	0.41
2:B:46:TYR:HB2	2:B:47:PRO:HD3	2.03	0.41
1:E:512:LEU:O	1:E:513:PHE:HB2	2.21	0.41
1:E:667:VAL:HG11	1:E:741:LEU:HD13	2.02	0.41
2:F:7:ALA:HB1	2:F:178:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:46:TYR:N	8:F:2035:HOH:O	2.53	0.41
2:F:96:CYS:SG	2:F:113:VAL:HG11	2.61	0.41
2:F:109:PRO:HG3	8:F:2015:HOH:O	2.19	0.41
1:A:37:VAL:CG1	1:A:38:LYS:H	2.33	0.41
1:A:44:CYS:SG	1:A:46:GLY:N	2.90	0.41
1:A:318:GLU:O	1:A:322:HIS:HD2	2.03	0.41
2:B:61:CYS:HB3	2:B:171:THR:O	2.19	0.41
2:B:128:VAL:HG11	8:B:2069:HOH:O	2.19	0.41
1:E:79:CYS:CB	1:E:80:PRO:CD	2.99	0.41
1:E:510:GLU:HG3	1:E:510:GLU:H	1.47	0.41
3:G:63:LEU:CD2	7:G:1251:MQ7:C2	2.98	0.41
3:G:83:HIS:HA	3:G:84:PRO:HD2	1.85	0.41
1:A:116:THR:CG2	1:A:119:GLU:N	2.61	0.41
1:A:132:ARG:O	1:A:132:ARG:HG2	2.20	0.41
1:A:181:SER:HB2	1:A:189:ILE:HD12	2.03	0.41
1:A:596:ARG:NH1	1:A:600:ALA:HB1	2.34	0.41
1:A:650:TRP:O	1:A:693:VAL:HA	2.20	0.41
1:A:717:ASN:ND2	5:A:1765:MGD:H192	2.19	0.41
2:B:18:ALA:HB3	4:B:1194:SF4:S2	2.61	0.41
2:B:48:ASN:ND2	2:F:157:LYS:HE2	2.36	0.41
1:E:545:GLU:CD	1:E:555:LEU:HB2	2.46	0.41
1:E:680:VAL:HG22	1:E:714:ALA:HB2	2.03	0.41
2:F:71:PRO:HB2	3:G:78:LEU:CD1	2.51	0.41
2:F:174:LYS:HE2	8:F:2046:HOH:O	2.21	0.41
3:G:23:LEU:CD2	3:G:62:ILE:HD12	2.51	0.41
1:A:258:THR:HB	1:A:608:PHE:HA	2.03	0.41
1:A:263:ALA:HB2	1:A:301:ALA:HB2	2.02	0.41
1:A:289:LEU:O	1:A:293:VAL:HB	2.21	0.41
1:A:327:VAL:HG13	1:A:362:GLY:HA3	2.03	0.41
1:A:333:HIS:O	1:A:336:TRP:NE1	2.52	0.41
1:A:429:PRO:C	1:A:430:TYR:CG	2.98	0.41
2:B:8:ILE:HD13	2:B:55:PRO:HG2	2.02	0.41
3:C:157:LEU:HB3	3:C:179:LEU:HD13	2.02	0.41
3:C:201:HIS:CE1	3:C:205:GLU:HG3	2.56	0.41
1:E:64:LYS:HE3	2:F:26:GLU:HB2	2.03	0.41
1:E:174:THR:HG23	1:E:178:GLU:CG	2.48	0.41
1:E:512:LEU:HA	1:E:512:LEU:HD12	1.79	0.41
1:E:621:LEU:HD22	1:E:622:LEU:H	1.84	0.41
2:F:67:VAL:CB	2:F:68:PRO:CD	2.98	0.41
2:F:72:THR:CG2	2:F:89:LYS:O	2.64	0.41
2:F:118:PHE:HD1	2:F:118:PHE:HA	1.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:46:ARG:NH1	3:G:106:TYR:O	2.54	0.41
3:G:47:ARG:HH21	3:G:166:LEU:HB3	1.84	0.41
3:G:100:LEU:O	3:G:103:GLY:N	2.51	0.41
3:G:153:LEU:HD23	3:G:153:LEU:HA	1.93	0.41
3:G:221:TRP:CZ3	3:G:225:LEU:HD13	2.45	0.41
1:A:95:LEU:CG	1:A:467:VAL:O	2.68	0.41
1:A:207:GLY:O	5:A:1766:MGD:O2B	2.39	0.41
1:A:286:PHE:O	1:A:286:PHE:CG	2.71	0.41
1:A:539:THR:HG23	1:A:541:GLU:H	1.85	0.41
1:A:592:LEU:CD1	1:A:592:LEU:C	2.92	0.41
1:A:641:MET:CE	1:A:645:PRO:HA	2.51	0.41
2:B:78:THR:CG2	8:B:2068:HOH:O	2.61	0.41
3:C:169:SER:HA	3:C:170:PRO:HD3	1.81	0.41
1:E:115:ALA:HB1	1:E:119:GLU:CG	2.51	0.41
1:E:133:GLU:HB2	8:E:2086:HOH:O	2.20	0.41
1:E:308:PRO:HD2	8:E:2195:HOH:O	2.20	0.41
1:E:322:HIS:O	1:E:323:LYS:O	2.39	0.41
1:E:333:HIS:HB2	5:E:1766:MGD:S12	2.60	0.41
1:E:340:ASP:O	1:E:344:VAL:HG23	2.20	0.41
1:E:620:ARG:HD3	1:E:735:ARG:O	2.20	0.41
2:F:3:ARG:O	2:F:145:LEU:HB2	2.20	0.41
3:G:117:TRP:HB3	8:G:2034:HOH:O	2.21	0.41
1:A:155:PHE:O	1:A:156:LEU:C	2.64	0.40
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.94	0.40
1:A:399:GLU:OE1	1:A:399:GLU:HA	2.22	0.40
1:A:435:LEU:N	1:A:461:LEU:O	2.53	0.40
1:A:591:GLU:HB3	1:A:603:GLN:HE21	1.77	0.40
2:B:9:ASP:HA	2:B:178:LEU:HB2	2.03	0.40
3:C:12:GLU:OE1	3:C:15:HIS:ND1	2.43	0.40
1:E:551:LEU:O	1:E:553:LEU:CB	2.64	0.40
2:F:46:TYR:CD2	2:F:47:PRO:HD3	2.56	0.40
1:A:94:ARG:O	1:A:94:ARG:HG3	2.22	0.40
1:A:116:THR:HG23	1:A:118:GLU:OE1	2.21	0.40
1:A:239:PHE:HB3	1:A:687:ARG:CB	2.49	0.40
1:A:389:SER:HA	1:A:595:GLN:NE2	2.36	0.40
1:A:608:PHE:O	1:A:608:PHE:CE1	2.67	0.40
2:B:78:THR:CG2	2:B:80:ASP:H	2.33	0.40
3:C:128:LEU:HD23	3:C:156:ALA:CB	2.51	0.40
1:E:80:PRO:HD3	2:F:18:ALA:HB2	2.04	0.40
1:E:391:PRO:O	1:E:413:ARG:CG	2.66	0.40
1:E:671:ASN:ND2	1:E:673:ASP:N	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LEU:HD23	1:A:121:LEU:HA	1.97	0.40
1:A:142:PHE:O	1:A:165:ALA:HA	2.21	0.40
1:A:477:ASP:O	1:A:478:VAL:HG23	2.20	0.40
1:A:539:THR:HG22	1:A:542:GLU:H	1.86	0.40
1:A:638:TRP:HB2	1:A:756:ALA:CB	2.51	0.40
2:B:54:ARG:NH2	2:B:187:THR:O	2.51	0.40
1:E:159:ALA:O	1:E:380:PRO:HG2	2.21	0.40
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.90	0.40
1:E:494:LEU:CD2	1:E:502:ILE:HG23	2.52	0.40
2:F:19:CYS:SG	2:F:20:ALA:N	2.95	0.40
3:G:63:LEU:CD1	7:G:1251:MQ7:H2M3	2.33	0.40
3:G:217:LEU:HD22	8:G:2065:HOH:O	2.21	0.40
1:A:107:ARG:O	1:A:457:LYS:HE3	2.22	0.40
3:C:209:TRP:CD1	8:C:2081:HOH:O	2.74	0.40
1:E:413:ARG:HH11	1:E:413:ARG:HD2	1.72	0.40
1:E:484:THR:O	1:E:485:TYR:C	2.62	0.40
3:G:38:HIS:O	3:G:40:LYS:N	2.55	0.40
3:G:53:LEU:O	3:G:99:PHE:HE1	2.04	0.40
3:G:142:LEU:O	3:G:189:TYR:OH	2.37	0.40
1:A:197:TRP:HB2	1:A:221:ASP:HB3	2.02	0.40
1:A:532:GLU:H	1:A:532:GLU:HG2	1.48	0.40
3:C:51:LEU:O	3:C:54:LEU:HB2	2.22	0.40
1:E:266:HIS:HB2	1:E:293:VAL:HG13	2.04	0.40
1:E:441:ASN:CG	1:E:444:HIS:HB2	2.46	0.40
1:E:466:ASP:OD1	1:E:473:VAL:CG2	2.69	0.40
1:E:510:GLU:CG	8:E:2299:HOH:O	2.51	0.40
1:E:624:GLY:HA3	1:E:694:TYR:OH	2.22	0.40
3:G:165:LEU:HD22	3:G:224:ARG:HH11	1.85	0.40
3:G:222:GLN:HB2	8:G:2069:HOH:O	2.21	0.40
3:G:223:GLU:C	3:G:225:LEU:N	2.78	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]	1.32	0.88
1:A:399:GLU:OE2	1:E:134:LYS:N[2_674]	1.51	0.69
1:A:399:GLU:OE2	1:E:133:GLU:O[2_674]	1.91	0.29

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	733/765 (96%)	651 (89%)	46 (6%)	36 (5%)	1	11
1	E	733/765 (96%)	634 (86%)	65 (9%)	34 (5%)	2	12
2	B	192/195 (98%)	176 (92%)	12 (6%)	4 (2%)	5	25
2	F	192/195 (98%)	181 (94%)	7 (4%)	4 (2%)	5	25
3	C	249/253 (98%)	232 (93%)	12 (5%)	5 (2%)	6	25
3	G	249/253 (98%)	220 (88%)	20 (8%)	9 (4%)	2	16
All	All	2348/2426 (97%)	2094 (89%)	162 (7%)	92 (4%)	2	14

All (92) 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	430	TYR
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	592	LEU
1	A	593	TYR
1	A	605	LEU
1	A	678	GLY
1	A	687	ARG
1	A	730	GLY
2	B	193	HIS
3	C	208	PHE
3	C	250	GLY

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Mol	Chain	Res	Type
1	E	92	PRO
1	E	93	ASP
1	E	109	GLU
1	E	324	PRO
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
1	E	631	PHE
1	E	678	GLY
1	E	686	ALA
2	F	46	TYR
3	G	108	GLY
3	G	110	GLY
3	G	222	GLN
1	A	365	ILE
1	A	399	GLU
1	A	434	GLY
1	A	582	PRO
1	A	631	PHE
2	B	17	ALA
3	C	112	SER
3	C	172	ALA
1	E	337	TYR
1	E	391	PRO
1	E	570	PRO
1	E	606	PRO
1	E	685	THR
3	G	39	LEU
3	G	51	TYR
3	G	113	ARG
1	A	398	PRO
1	A	633	ARG
2	B	115	LYS
3	C	113	GLN
1	E	466	ASP
1	E	469	PRO

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Mol	Chain	Res	Type
1	E	471	GLU
1	E	513	PHE
1	E	763	ARG
2	F	45	GLU
2	F	178	LEU
2	F	179	ASN
1	A	389	SER
1	A	478	VAL
1	A	607	VAL
1	E	478	VAL
1	E	627	PRO
3	G	38	HIS
1	A	216	ASN
1	A	387	GLY
1	A	597	PHE
1	A	598	LYS
1	A	610	PRO
1	E	70	ALA
1	E	604	PRO
3	G	167	LYS
3	G	207	PHE
1	A	609	THR
1	E	468	LEU
2	B	47	PRO
1	E	610	PRO
1	A	584	GLY
1	A	684	PRO
1	E	434	GLY
1	E	609	THR
1	A	362	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	610/632 (96%)	489 (80%)	121 (20%)	1 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	610/632 (96%)	491 (80%)	119 (20%)	1	6
2	B	162/163 (99%)	139 (86%)	23 (14%)	3	14
2	F	162/163 (99%)	142 (88%)	20 (12%)	4	20
3	C	185/187 (99%)	159 (86%)	26 (14%)	3	15
3	G	185/187 (99%)	160 (86%)	25 (14%)	4	16
All	All	1914/1964 (98%)	1580 (82%)	334 (18%)	2	9

All (334) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	43	ILE
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	170	VAL
1	A	174	THR
1	A	187	ARG
1	A	189	ILE
1	A	193	GLU
1	A	213	ASP
1	A	214	THR
1	A	217	THR
1	A	231	LYS
1	A	250	LEU
1	A	252	ILE
1	A	256	THR
1	A	260	LEU
1	A	281	LYS
1	A	283	THR

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Mol	Chain	Res	Type
1	A	286	PHE
1	A	289	LEU
1	A	293	VAL
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	371	LEU
1	A	372	GLU
1	A	378	PRO
1	A	379	LEU
1	A	382	GLU
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	433	LYS
1	A	440	ILE
1	A	441	ASN
1	A	454	GLU
1	A	457	LYS
1	A	465	ILE
1	A	470	GLN
1	A	477	ASP
1	A	478	VAL
1	A	484	THR
1	A	504	LEU
1	A	510	GLU
1	A	512	LEU
1	A	515	THR
1	A	528	ARG
1	A	529	LEU
1	A	532	GLU
1	A	533	GLN
1	A	538	LYS

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Mol	Chain	Res	Type
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	581	LEU
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	603	GLN
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	648	GLU
1	A	649	VAL
1	A	651	ILE
1	A	662	LYS
1	A	663	GLU
1	A	667	VAL
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	725	LEU

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Mol	Chain	Res	Type
1	A	728	ILE
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	24	LYS
2	B	25	MET
2	B	39	ARG
2	B	41	ARG
2	B	45	GLU
2	B	54	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	134	THR
2	B	141	THR
2	B	152	VAL
2	B	164	VAL
2	B	166	ARG
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	21	HIS
3	C	40	LEU
3	C	57	ILE
3	C	63	ILE
3	C	67	GLU
3	C	71	ARG
3	C	75	THR
3	C	79	LEU

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Mol	Chain	Res	Type
3	C	105	LEU
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	197	GLU
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	102	VAL
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	189	ILE
1	E	193	GLU
1	E	208	HIS
1	E	213	ASP
1	E	214	THR
1	E	217	THR
1	E	224	LEU
1	E	240	SER
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

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Mol	Chain	Res	Type
1	E	297	THR
1	E	298	PRO
1	E	299	GLU
1	E	305	THR
1	E	310	GLN
1	E	314	GLU
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	457	LYS
1	E	466	ASP
1	E	467	VAL
1	E	470	GLN
1	E	474	MET
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
1	E	540	ILE
1	E	541	GLU
1	E	554	ASP
1	E	555	LEU

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Mol	Chain	Res	Type
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	589	LYS
1	E	590	ILE
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	612	GLU
1	E	620	ARG
1	E	621	LEU
1	E	626	SER
1	E	628	VAL
1	E	633	ARG
1	E	647	ASN
1	E	649	VAL
1	E	651	ILE
1	E	657	LYS
1	E	663	GLU
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	696	VAL
1	E	702	LYS
1	E	708	LEU
1	E	721	THR
1	E	725	LEU
1	E	736	VAL

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Mol	Chain	Res	Type
1	E	739	VAL
1	E	740	ARG
1	E	741	LEU
1	E	746	ARG
1	E	748	ARG
1	E	751	SER
1	E	752	LEU
2	F	49	LEU
2	F	68	PRO
2	F	69	VAL
2	F	72	THR
2	F	78	THR
2	F	80	ASP
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	166	ARG
2	F	171	THR
2	F	175	LEU
2	F	187	THR
2	F	191	GLU
3	G	10	GLN
3	G	17	ASN
3	G	20	HIS
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	109	LYS
3	G	113	ARG
3	G	129	TYR
3	G	136	VAL
3	G	139	ASN
3	G	144	ASN

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Mol	Chain	Res	Type
3	G	154	THR
3	G	162	LEU
3	G	167	LYS
3	G	175	LEU
3	G	192	THR
3	G	196	GLU
3	G	204	GLU
3	G	215	LEU
3	G	222	GLN
3	G	240	LEU

Sometimes 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	123	HIS
1	A	192	HIS
1	A	208	HIS
1	A	209	HIS
1	A	218	GLN
1	A	220	GLN
1	A	247	HIS
1	A	322	HIS
1	A	367	GLN
1	A	396	HIS
1	A	441	ASN
1	A	470	GLN
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

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Mol	Chain	Res	Type
2	B	77	GLN
2	B	179	ASN
3	C	11	GLN
3	C	21	HIS
3	C	76	HIS
3	C	84	HIS
3	C	140	ASN
3	C	145	ASN
3	C	249	GLN
1	E	60	ASN
1	E	71	ASN
1	E	83	GLN
1	E	192	HIS
1	E	208	HIS
1	E	209	HIS
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	470	GLN
1	E	509	HIS
1	E	533	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	169	GLN
2	F	179	ASN
3	G	10	GLN
3	G	38	HIS
3	G	83	HIS

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Mol	Chain	Res	Type
3	G	137	ASN
3	G	139	ASN
3	G	248	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	1197	2	0,12,12	-	-	-		
4	SF4	B	1194	2	0,12,12	-	-	-		
7	MQ7	C	1252	-	16,16,49	0.30	0	21,23,63	1.41	3 (14%)
4	SF4	B	1196	2	0,12,12	-	-	-		
4	SF4	F	1196	2	0,12,12	-	-	-		
4	SF4	F	1197	2	0,12,12	-	-	-		
4	SF4	A	1764	1	0,12,12	-	-	-		
4	SF4	F	1195	2	0,12,12	-	-	-		
5	MGD	A	1765	6	47,52,52	2.50	18 (38%)	58,81,81	2.96	20 (34%)
4	SF4	F	1194	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MGD	E	1765	6	47,52,52	2.54	21 (44%)	58,81,81	3.12	22 (37%)
5	MGD	A	1766	6	47,52,52	2.60	19 (40%)	58,81,81	2.94	21 (36%)
7	MQ7	G	1251	-	16,16,49	0.34	0	21,23,63	1.45	3 (14%)
4	SF4	E	1764	1	0,12,12	-	-	-	-	-
4	SF4	B	1195	2	0,12,12	-	-	-	-	-
5	MGD	E	1766	6	47,52,52	2.77	19 (40%)	58,81,81	2.57	18 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	B	1194	2	-	-	0/6/5/5
4	SF4	B	1197	2	-	-	0/6/5/5
7	MQ7	C	1252	-	-	2/2/22/61	0/2/2/2
4	SF4	B	1196	2	-	-	0/6/5/5
4	SF4	F	1196	2	-	-	0/6/5/5
4	SF4	F	1197	2	-	-	0/6/5/5
4	SF4	A	1764	1	-	-	0/6/5/5
4	SF4	F	1195	2	-	-	0/6/5/5
5	MGD	A	1765	6	-	5/22/66/66	0/6/6/6
5	MGD	E	1765	6	-	2/22/66/66	0/6/6/6
4	SF4	F	1194	2	-	-	0/6/5/5
5	MGD	A	1766	6	-	1/22/66/66	0/6/6/6
7	MQ7	G	1251	-	-	0/2/22/61	0/2/2/2
4	SF4	E	1764	1	-	-	0/6/5/5
4	SF4	B	1195	2	-	-	0/6/5/5
5	MGD	E	1766	6	-	1/22/66/66	0/6/6/6

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1765	MGD	C23-C14	-9.69	1.45	1.53
5	E	1766	MGD	C21-N22	-9.44	1.25	1.35
5	A	1766	MGD	C23-C14	-7.61	1.47	1.53
5	E	1765	MGD	C23-C14	-7.15	1.48	1.53
5	A	1766	MGD	C14-N15	-7.07	1.38	1.46
5	E	1766	MGD	C23-C14	-6.91	1.48	1.53
5	E	1766	MGD	C14-N15	-6.04	1.39	1.46
5	A	1766	MGD	C21-N22	-5.99	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1765	MGD	C5-N7	-5.37	1.28	1.39
5	E	1765	MGD	C10-C11	-5.20	1.44	1.51
5	A	1765	MGD	C21-N22	-5.12	1.30	1.35
5	E	1765	MGD	C16-C21	4.43	1.46	1.38
5	E	1766	MGD	C5-N7	-4.43	1.30	1.39
5	A	1766	MGD	C6-N1	-4.36	1.30	1.38
5	E	1765	MGD	C8-N9	-4.23	1.28	1.37
5	E	1766	MGD	C19-N18	-4.03	1.27	1.37
5	A	1765	MGD	C10-C11	-4.00	1.46	1.51
5	A	1765	MGD	C17-N18	-3.91	1.31	1.38
5	E	1766	MGD	C6-N1	-3.81	1.31	1.38
5	A	1765	MGD	C5-N7	-3.80	1.31	1.39
5	E	1766	MGD	C19-N19	-3.71	1.25	1.34
5	E	1766	MGD	C16-N15	-3.67	1.29	1.37
5	E	1766	MGD	C5-C4	3.60	1.48	1.38
5	A	1766	MGD	C10-C11	-3.55	1.46	1.51
5	E	1765	MGD	C21-N22	-3.54	1.31	1.35
5	E	1766	MGD	PB-O3B	-3.52	1.55	1.59
5	A	1765	MGD	C21-N20	-3.39	1.30	1.36
5	E	1765	MGD	C19-N18	-3.28	1.29	1.37
5	A	1765	MGD	C16-C21	3.21	1.44	1.38
5	E	1766	MGD	C16-C21	3.20	1.44	1.38
5	E	1765	MGD	C3'-C4'	-3.18	1.44	1.53
5	A	1766	MGD	C23-N22	-3.17	1.39	1.45
5	A	1765	MGD	C23-N22	-3.16	1.39	1.45
5	E	1765	MGD	C14-N15	-3.16	1.42	1.46
5	A	1765	MGD	C4-N9	-3.13	1.30	1.38
5	E	1765	MGD	C17-N18	-3.08	1.33	1.38
5	A	1766	MGD	C5-N7	-3.07	1.32	1.39
5	A	1766	MGD	PB-O2B	-3.06	1.41	1.55
5	E	1765	MGD	C6-N1	-3.06	1.33	1.38
5	A	1765	MGD	C8-N9	-3.04	1.30	1.37
5	E	1766	MGD	O4'-C4'	-3.03	1.38	1.45
5	E	1765	MGD	C4-N9	-2.95	1.30	1.38
5	A	1766	MGD	C16-C21	2.94	1.43	1.38
5	E	1765	MGD	C2-N1	-2.89	1.30	1.37
5	A	1765	MGD	C5-C4	2.85	1.46	1.38
5	A	1766	MGD	PA-O2A	-2.85	1.42	1.55
5	A	1766	MGD	C5-C4	2.80	1.46	1.38
5	E	1766	MGD	C23-N22	-2.79	1.40	1.45
5	E	1765	MGD	C5-C4	2.71	1.46	1.38
5	A	1766	MGD	PB-O3B	-2.70	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1766	MGD	C4-N9	-2.66	1.31	1.38
5	A	1765	MGD	C6-N1	-2.60	1.34	1.38
5	E	1765	MGD	O3'-C3'	-2.53	1.36	1.43
5	A	1766	MGD	PA-O1A	-2.53	1.42	1.50
5	E	1766	MGD	O11-C11	-2.53	1.38	1.43
5	A	1766	MGD	O4'-C4'	-2.51	1.39	1.45
5	A	1765	MGD	C19-N18	-2.47	1.31	1.37
5	E	1766	MGD	C17-N18	-2.42	1.34	1.38
5	E	1766	MGD	O3'-C3'	2.40	1.48	1.43
5	A	1765	MGD	O4'-C4'	-2.40	1.39	1.45
5	E	1765	MGD	C23-N22	-2.36	1.41	1.45
5	A	1765	MGD	O2'-C2'	-2.36	1.37	1.43
5	E	1766	MGD	O17-C17	-2.31	1.19	1.23
5	E	1765	MGD	O3A-C10	-2.31	1.35	1.44
5	A	1766	MGD	C19-N19	-2.28	1.28	1.34
5	A	1765	MGD	O11-C23	-2.26	1.40	1.43
5	A	1765	MGD	C3'-C4'	-2.26	1.47	1.53
5	A	1766	MGD	C17-N18	-2.25	1.34	1.38
5	E	1766	MGD	PA-O1A	-2.24	1.43	1.50
5	E	1765	MGD	C2'-C1'	-2.22	1.46	1.53
5	A	1766	MGD	O11-C23	2.19	1.46	1.43
5	E	1765	MGD	PB-O3B	2.16	1.61	1.59
5	E	1766	MGD	C4-N9	-2.13	1.32	1.38
5	A	1765	MGD	PA-O2A	-2.08	1.45	1.55
5	E	1765	MGD	O2'-C2'	-2.04	1.37	1.43
5	A	1766	MGD	PB-O5'	-2.00	1.51	1.59
5	E	1765	MGD	PA-O2A	-2.00	1.46	1.55

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1766	MGD	O11-C23-C14	13.19	117.76	108.96
5	A	1765	MGD	O11-C23-C14	11.86	116.88	108.96
5	E	1765	MGD	O11-C23-N22	-10.48	99.10	108.61
5	E	1766	MGD	O11-C23-C14	9.67	115.42	108.96
5	E	1765	MGD	C23-C14-N15	9.05	116.76	107.87
5	E	1765	MGD	O11-C23-C14	-8.05	103.60	108.96
5	A	1765	MGD	C23-C14-N15	7.74	115.47	107.87
5	A	1765	MGD	C5-C4-N3	-7.05	117.18	128.39
5	E	1766	MGD	C5-C4-N3	-6.99	117.26	128.39
5	A	1765	MGD	C2-N3-C4	6.85	124.10	112.30
5	E	1765	MGD	C5-C4-N3	-6.77	117.61	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1765	MGD	C2-N3-C4	6.20	122.97	112.30
5	A	1766	MGD	C5-C4-N3	-6.14	118.62	128.39
5	E	1765	MGD	C19-N20-C21	6.01	123.97	113.36
5	E	1766	MGD	O17-C17-C16	-5.65	113.64	127.26
5	A	1765	MGD	C19-N20-C21	5.58	123.20	113.36
5	E	1766	MGD	C23-C14-N15	5.18	112.95	107.87
5	A	1766	MGD	O4'-C1'-N9	5.16	120.05	108.36
5	E	1765	MGD	C6-C5-N7	5.02	139.42	130.29
5	A	1766	MGD	O11-C23-N22	4.98	113.12	108.61
5	A	1766	MGD	N9-C4-N3	4.93	135.81	125.95
5	A	1766	MGD	C2-N3-C4	4.92	120.77	112.30
5	A	1766	MGD	C23-C14-N15	4.88	112.66	107.87
5	E	1766	MGD	C2-N3-C4	4.42	119.91	112.30
5	A	1766	MGD	O3B-PB-O1B	-4.30	97.76	110.70
5	E	1766	MGD	N9-C4-N3	4.29	134.53	125.95
5	E	1765	MGD	C4-C5-N7	-4.29	103.88	110.67
5	A	1765	MGD	N9-C4-N3	4.16	134.27	125.95
5	E	1766	MGD	C19-N20-C21	4.09	120.58	113.36
5	A	1765	MGD	C17-C16-N15	3.96	127.07	116.27
5	E	1765	MGD	N9-C4-N3	3.75	133.46	125.95
5	A	1765	MGD	C6-C5-N7	3.72	137.06	130.29
5	A	1766	MGD	C19-N18-C17	-3.72	118.37	125.11
5	A	1765	MGD	C4-C5-N7	-3.71	104.80	110.67
5	E	1766	MGD	C16-C17-N18	3.60	122.01	112.13
5	E	1765	MGD	C17-C16-N15	3.59	126.05	116.27
7	C	1252	MQ7	C11-C3-C4	3.51	119.60	115.64
5	E	1766	MGD	O4'-C1'-N9	3.49	116.26	108.36
5	A	1765	MGD	O2B-PB-O3B	3.48	116.67	107.27
7	G	1251	MQ7	C11-C3-C4	3.46	119.53	115.64
5	A	1766	MGD	O6-C6-C5	-3.43	117.47	126.53
5	A	1765	MGD	N2-C2-N1	3.25	123.62	116.76
5	A	1766	MGD	O17-C17-C16	-3.22	119.48	127.26
5	A	1766	MGD	O2B-PB-O3B	3.22	115.98	107.27
5	A	1766	MGD	C17-C16-N15	3.22	125.04	116.27
5	E	1765	MGD	C16-C17-N18	3.18	120.85	112.13
7	C	1252	MQ7	C11-C3-C2	-3.15	119.48	124.23
7	G	1251	MQ7	C11-C3-C2	-3.11	119.54	124.23
5	A	1765	MGD	O17-C17-C16	-3.01	119.99	127.26
5	E	1766	MGD	O2A-PA-O1A	2.98	126.32	112.44
7	G	1251	MQ7	C2M-C2-C3	-2.96	119.58	124.45
7	C	1252	MQ7	C2M-C2-C3	-2.96	119.59	124.45
5	A	1765	MGD	O3B-PA-O1A	-2.82	102.21	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1765	MGD	O4'-C4'-C5'	-2.82	100.29	109.33
5	E	1765	MGD	O2A-PA-O3B	-2.80	99.71	107.27
5	A	1766	MGD	O5'-C5'-C4'	-2.78	99.52	108.99
5	E	1765	MGD	O3'-C3'-C4'	-2.75	103.18	111.08
5	A	1766	MGD	C16-C17-N18	2.70	119.54	112.13
5	A	1765	MGD	N19-C19-N18	2.67	122.40	116.76
5	E	1765	MGD	O17-C17-C16	-2.65	120.88	127.26
5	E	1766	MGD	C19-N18-C17	-2.64	120.32	125.11
5	E	1766	MGD	O3'-C3'-C4'	2.59	118.52	111.08
5	A	1765	MGD	O3B-PB-O1B	-2.58	102.95	110.70
5	A	1765	MGD	O4'-C1'-C2'	-2.57	101.12	106.62
5	E	1765	MGD	O2B-PB-O1B	2.55	124.32	112.44
5	E	1766	MGD	O11-C23-N22	-2.55	106.29	108.61
5	E	1766	MGD	C2-N1-C6	-2.54	120.51	125.11
5	E	1765	MGD	O3B-PB-O1B	-2.53	103.10	110.70
5	E	1766	MGD	O6-C6-C5	-2.47	120.02	126.53
5	E	1766	MGD	C4-C5-N7	-2.46	106.77	110.67
5	A	1766	MGD	C6-C5-N7	2.44	134.73	130.29
5	E	1765	MGD	C8-N7-C5	2.43	108.59	104.26
5	A	1766	MGD	C19-N20-C21	2.41	117.61	113.36
5	E	1765	MGD	O2A-PA-O1A	2.36	123.44	112.44
5	E	1765	MGD	O6-C6-C5	-2.27	120.55	126.53
5	A	1765	MGD	C16-C17-N18	2.22	118.24	112.13
5	E	1766	MGD	O17-C17-N18	2.22	124.29	120.11
5	A	1766	MGD	O4'-C4'-C5'	-2.22	102.22	109.33
5	E	1765	MGD	N2-C2-N1	2.18	121.37	116.76
5	A	1765	MGD	C2'-C1'-N9	2.15	119.23	113.25
5	A	1766	MGD	C5-C6-N1	2.15	118.71	113.25
5	A	1765	MGD	N2-C2-N3	-2.14	115.48	119.67
5	E	1765	MGD	C19-N18-C17	-2.10	121.31	125.11
5	E	1765	MGD	O2B-PB-O3B	-2.08	101.66	107.27
5	E	1766	MGD	C6-C5-N7	2.06	134.05	130.29
5	A	1766	MGD	C2'-C1'-N9	2.06	118.97	113.25
5	A	1766	MGD	N18-C19-N20	2.04	127.05	123.32

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1765	MGD	C5'-O5'-PB-O2B
5	A	1765	MGD	C5'-O5'-PB-O3B
7	C	1252	MQ7	C12-C11-C3-C2

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Mol	Chain	Res	Type	Atoms
7	C	1252	MQ7	C12-C11-C3-C4
5	E	1765	MGD	O4'-C4'-C5'-O5'
5	A	1765	MGD	PA-O3B-PB-O5'
5	E	1765	MGD	PA-O3B-PB-O5'
5	A	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	C5'-O5'-PB-O1B
5	E	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	PA-O3B-PB-O1B

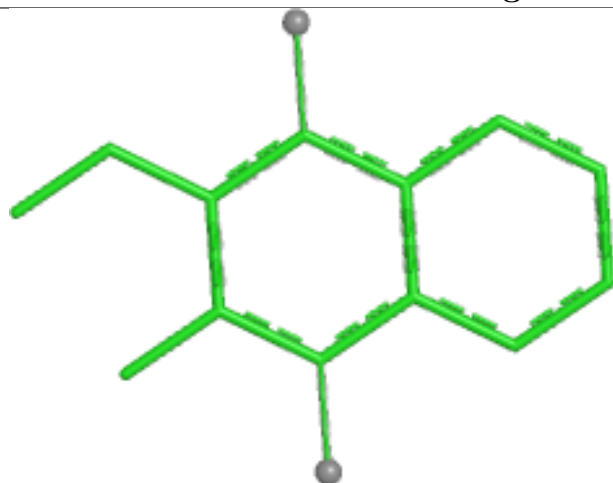
There are no ring outliers.

13 monomers are involved in 82 short contacts:

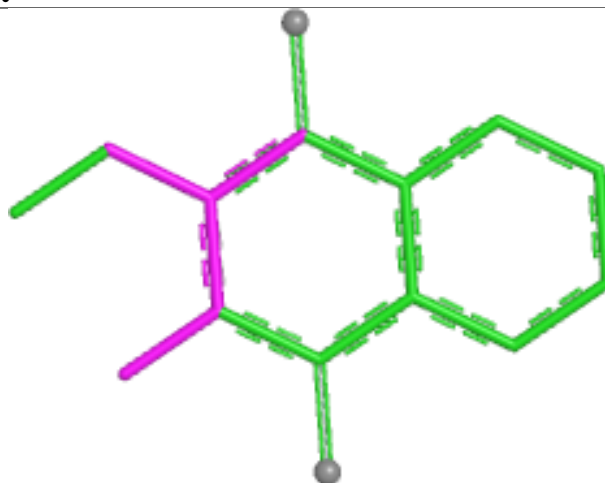
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1194	SF4	3	0
7	C	1252	MQ7	19	0
4	B	1196	SF4	2	0
4	F	1196	SF4	1	0
4	F	1195	SF4	2	0
5	A	1765	MGD	6	0
4	F	1194	SF4	3	0
5	E	1765	MGD	7	0
5	A	1766	MGD	5	0
7	G	1251	MQ7	20	0
4	E	1764	SF4	1	0
4	B	1195	SF4	2	0
5	E	1766	MGD	11	0

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

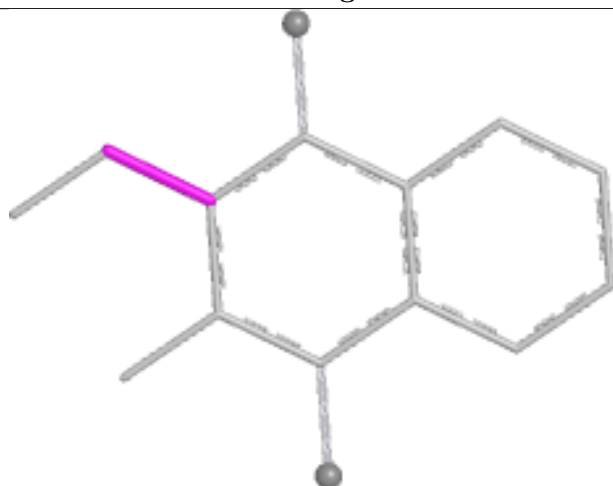
Ligand MQ7 C 1252



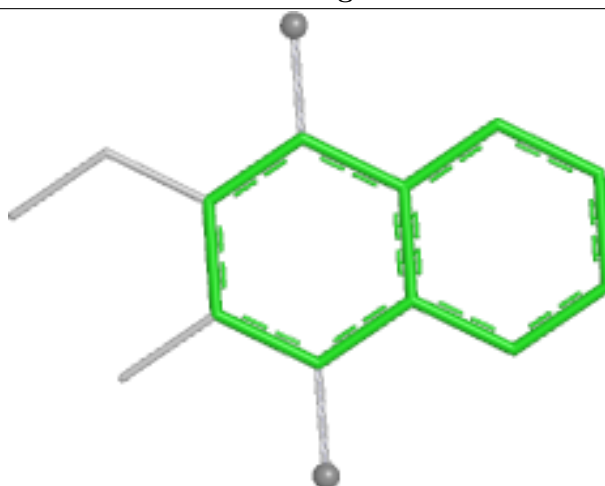
Bond lengths



Bond angles

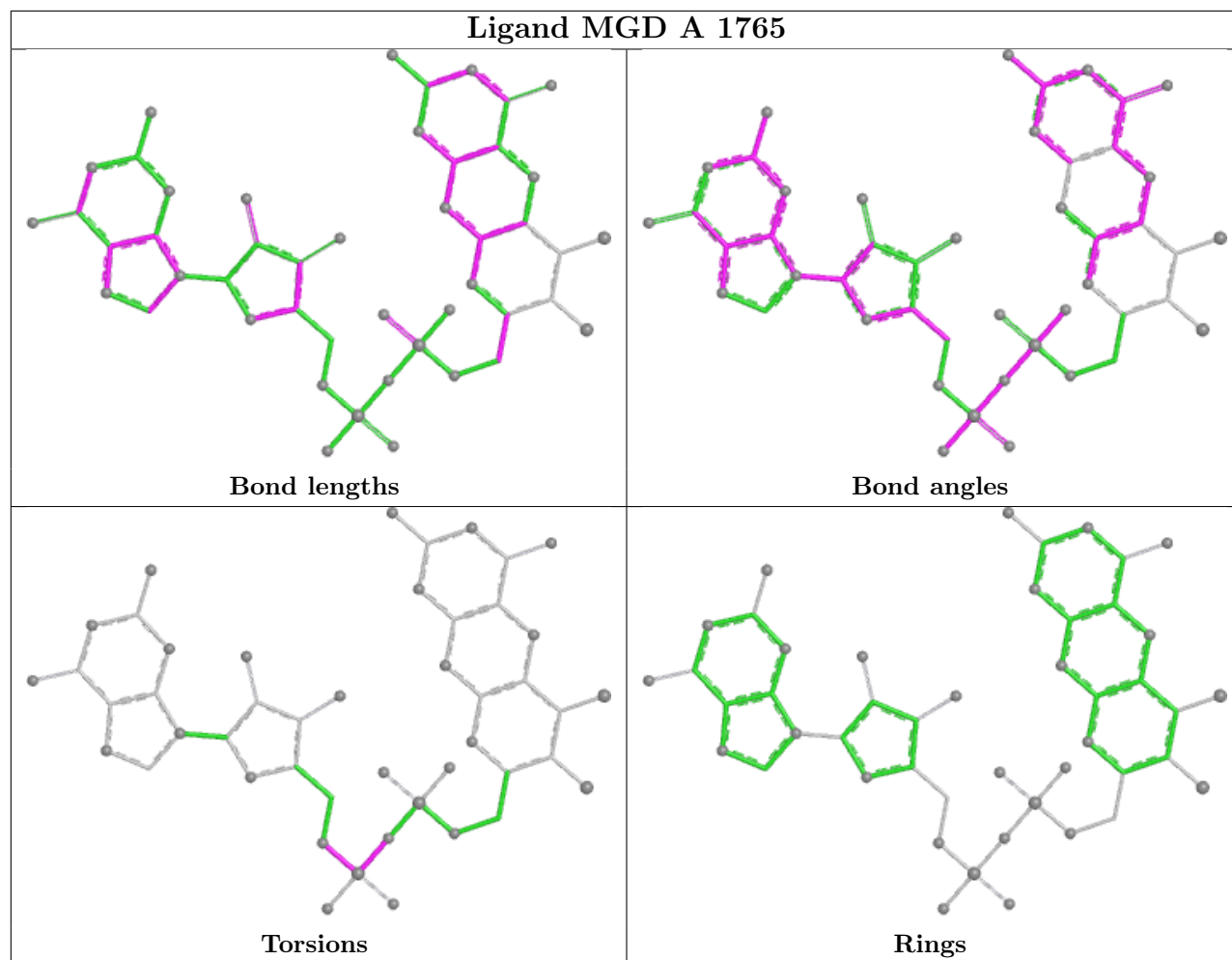


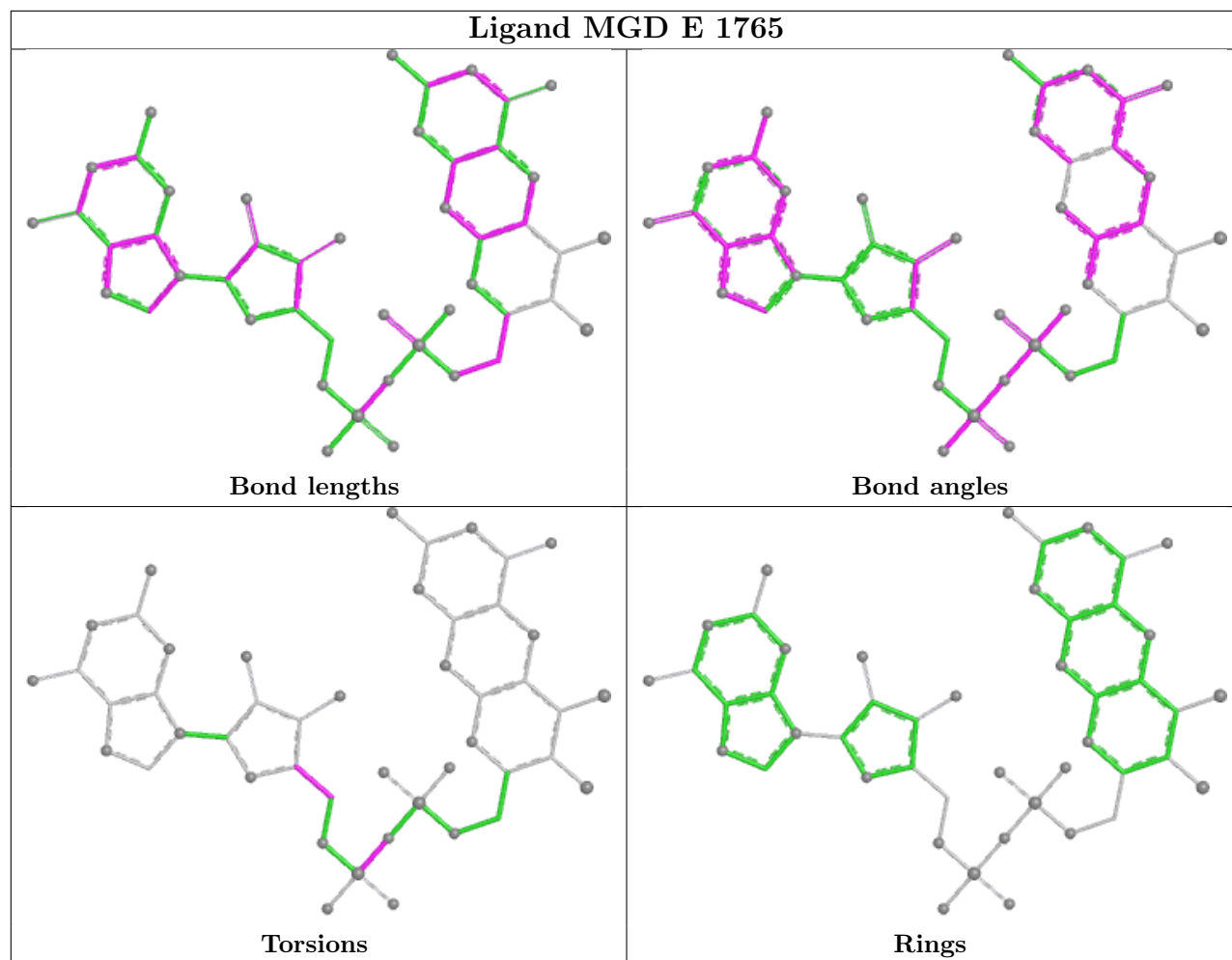
Torsions



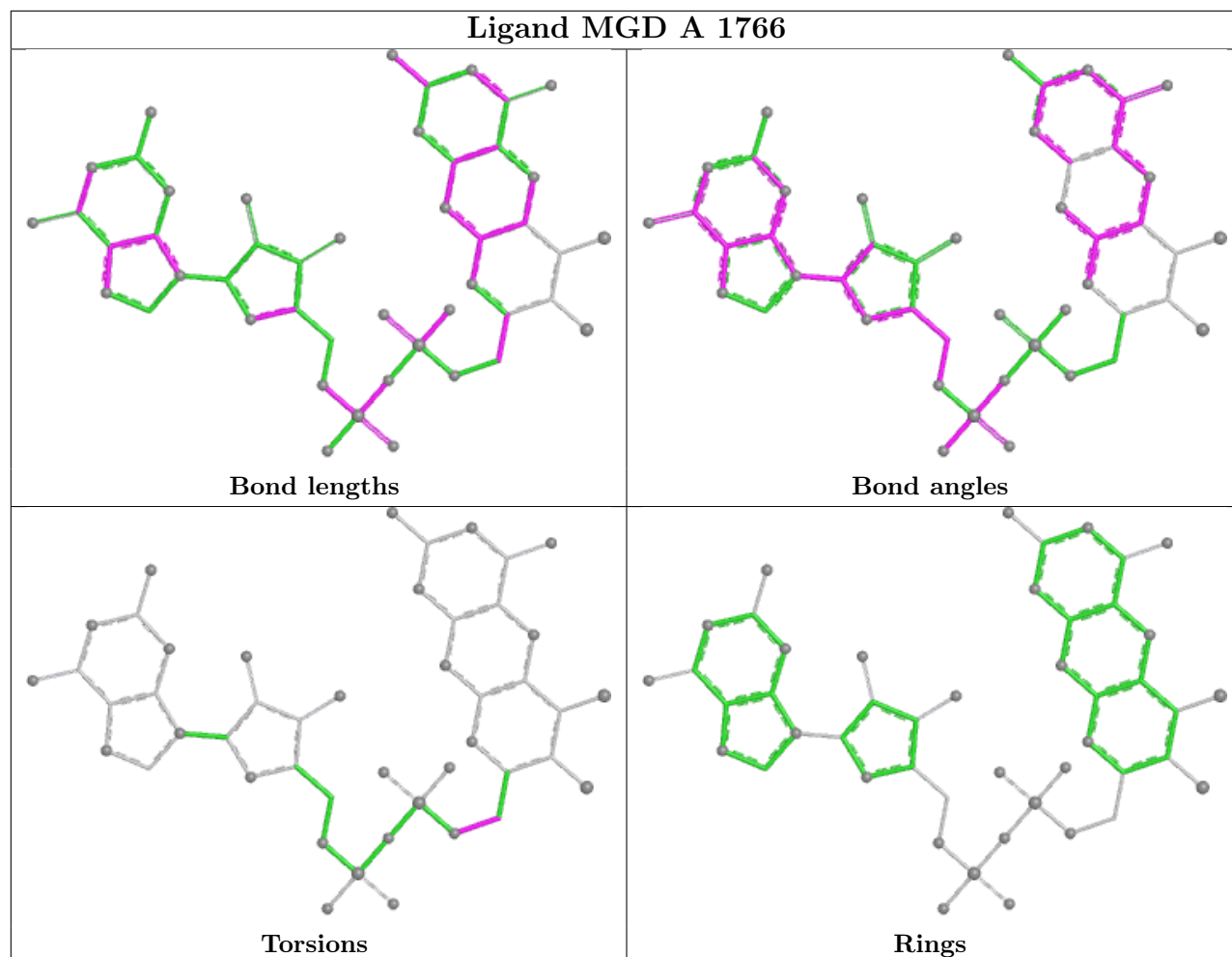
Rings

Ligand MGD A 1765

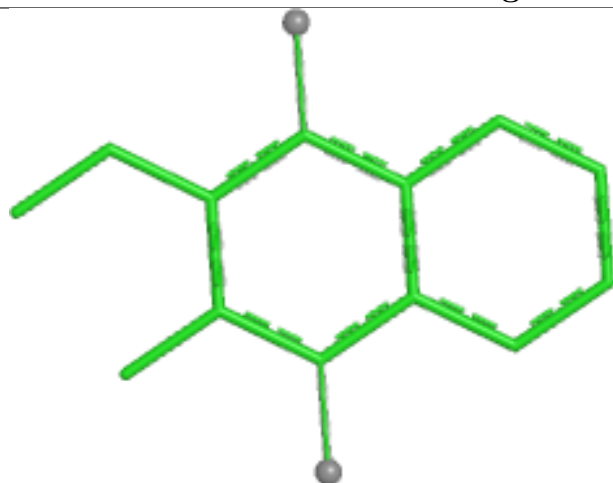




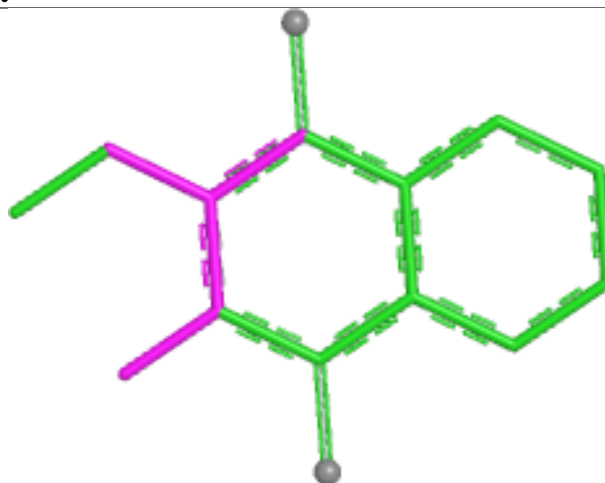
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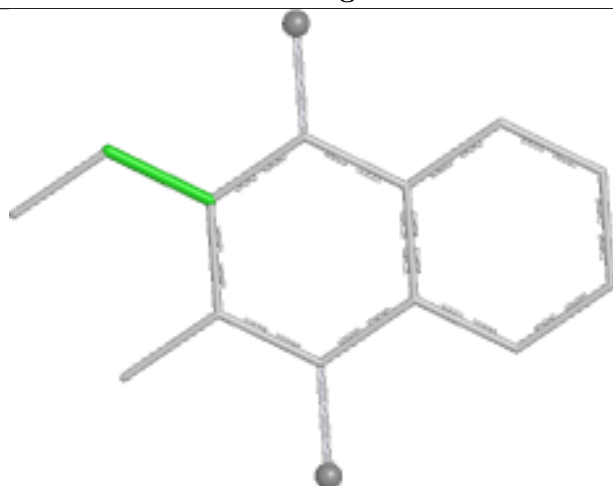
Ligand MQ7 G 1251



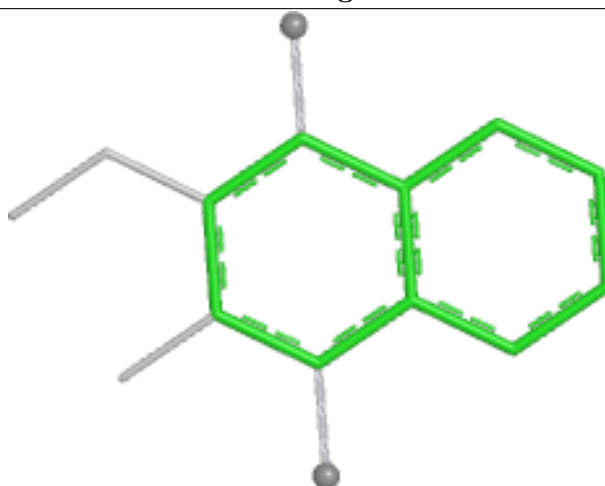
Bond lengths



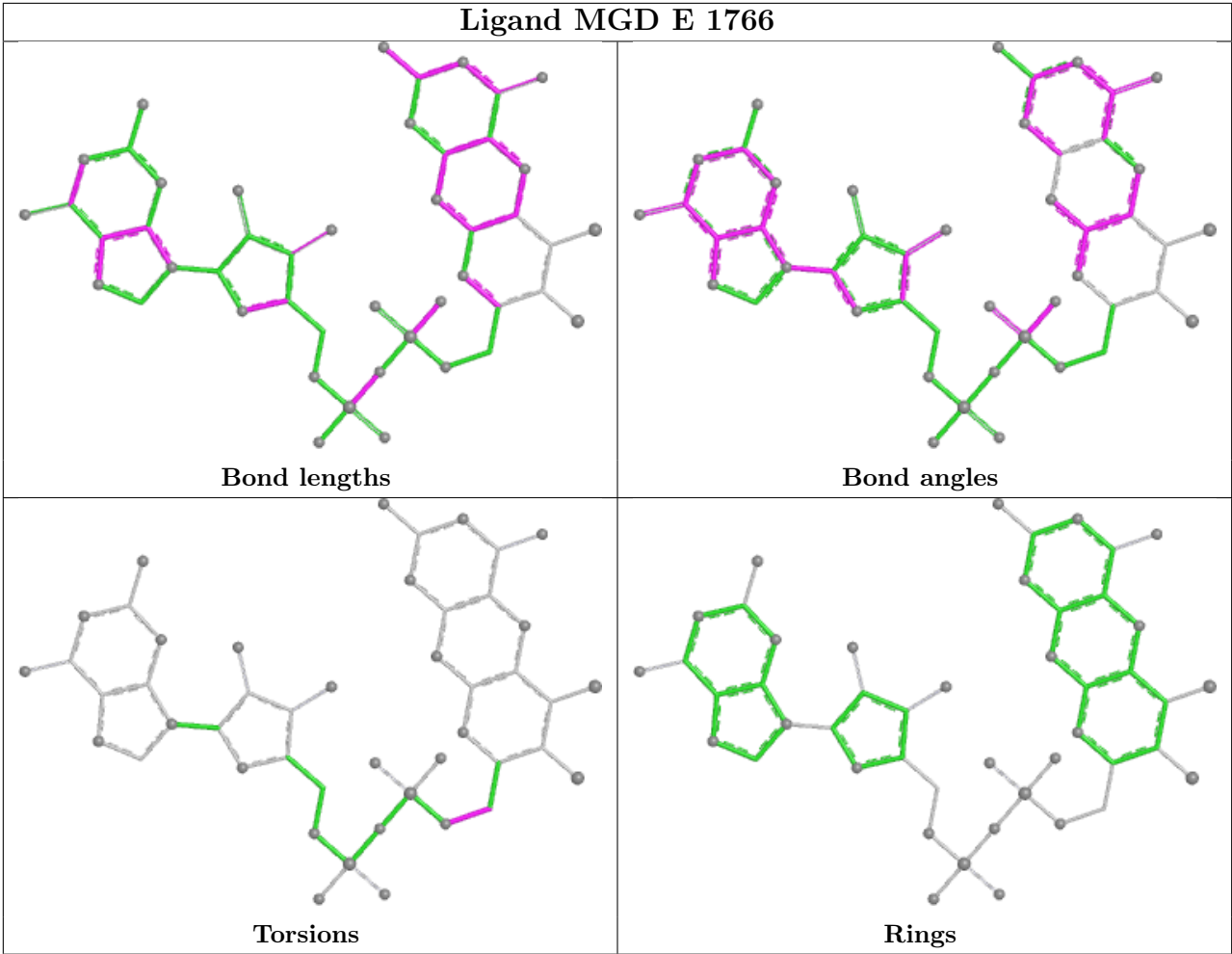
Bond angles



Torsions



Rings



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	2
1	A	1
3	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	583:PHE	C	584:GLY	N	1.71

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	323:LYS	C	324:PRO	N	1.66
1	G	109:LYS	C	110:GLY	N	1.05
1	E	387:GLY	C	388:CYS	N	0.66

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	735/765 (96%)	0.96	93 (12%) 8 4	48, 71, 103, 158	0
1	E	735/765 (96%)	0.90	74 (10%) 12 6	46, 70, 101, 161	0
2	B	194/195 (99%)	0.75	15 (7%) 19 10	50, 66, 88, 115	0
2	F	194/195 (99%)	1.08	27 (13%) 6 4	53, 71, 91, 114	0
3	C	251/253 (99%)	1.03	23 (9%) 14 8	55, 78, 105, 123	0
3	G	251/253 (99%)	1.54	71 (28%) 1 1	57, 86, 116, 131	0
All	All	2360/2426 (97%)	1.00	303 (12%) 7 4	46, 72, 105, 161	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	252	GLY	10.1
3	G	251	GLY	9.0
1	E	607	VAL	6.1
1	A	607	VAL	5.9
2	F	194	HIS	5.9
1	A	362	GLY	5.6
3	C	111	GLY	5.6
1	A	384	ALA	5.4
1	A	586	ALA	5.4
1	A	764	ARG	5.4
1	E	600	ALA	5.3
1	A	606	PRO	5.2
1	A	570	PRO	4.9
3	G	49	THR	4.9
1	A	583	PHE	4.8
1	E	764	ARG	4.8
1	E	592	LEU	4.7
3	C	95	GLY	4.5
3	G	27	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	66	GLU	4.3
1	E	393	GLY	4.3
1	E	730	GLY	4.3
3	G	101	THR	4.0
1	A	591	GLU	4.0
1	E	398	PRO	4.0
1	A	207	GLY	4.0
1	E	596	ARG	3.9
1	E	591	GLU	3.9
3	G	74	THR	3.8
1	A	589	LYS	3.7
1	E	599	GLU	3.7
3	G	36	LEU	3.7
1	A	585	THR	3.7
3	C	79	LEU	3.6
2	F	22	ALA	3.6
3	G	55	LEU	3.6
3	G	28	GLY	3.6
1	E	384	ALA	3.6
1	E	469	PRO	3.6
1	E	323	LYS	3.5
1	E	608	PHE	3.5
1	E	467	VAL	3.5
1	A	383	PRO	3.5
2	B	1	MET	3.5
3	G	221	TRP	3.5
3	G	157	VAL	3.5
1	E	383	PRO	3.4
1	E	593	TYR	3.4
3	C	75	THR	3.4
3	C	223	GLN	3.4
3	G	22	VAL	3.4
1	E	579	GLY	3.4
2	F	92	ALA	3.4
3	G	1	ALA	3.4
1	A	515	THR	3.4
3	G	250	LEU	3.3
1	A	288	GLU	3.3
1	A	569	LYS	3.3
1	A	387	GLY	3.3
1	A	395	ASP	3.3
2	B	46	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	468	LEU	3.3
3	G	17	ASN	3.3
1	A	678	GLY	3.3
1	E	30	ALA	3.3
1	E	397	GLU	3.3
1	A	608	PHE	3.3
1	A	685	THR	3.3
3	G	85	THR	3.3
3	C	26	GLY	3.3
3	G	69	ALA	3.2
1	A	391	PRO	3.2
1	A	730	GLY	3.2
1	E	584	GLY	3.2
3	C	114	ARG	3.2
2	F	71	PRO	3.2
3	G	163	ALA	3.2
2	B	44	GLY	3.1
1	E	133	GLU	3.1
2	F	131	CYS	3.1
1	A	535	PHE	3.1
3	G	78	LEU	3.1
3	G	104	LEU	3.1
3	G	162	LEU	3.1
1	A	588	GLY	3.1
1	A	48	PHE	3.1
1	A	656	ALA	3.0
3	G	66	GLU	3.0
3	G	18	ALA	3.0
3	G	10	GLN	3.0
1	E	597	PHE	3.0
2	F	2	PRO	3.0
1	E	595	GLN	3.0
1	E	391	PRO	3.0
3	G	169	PRO	3.0
1	E	389	SER	3.0
1	A	597	PHE	3.0
3	G	8	ASN	3.0
1	A	542	GLU	2.9
3	G	59	ASP	2.9
1	A	605	LEU	2.9
1	A	337	TYR	2.9
1	A	592	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	361	GLY	2.9
1	A	634	THR	2.9
3	G	45	ALA	2.9
1	E	478	VAL	2.9
1	A	285	GLY	2.9
1	E	421	ILE	2.9
3	G	75	HIS	2.8
1	A	587	SER	2.8
1	E	470	GLN	2.8
1	E	298	PRO	2.8
3	G	174	PRO	2.8
1	E	113	ARG	2.8
3	G	100	LEU	2.8
1	A	42	GLN	2.8
1	E	606	PRO	2.8
1	A	364	TYR	2.8
2	B	120	ALA	2.8
1	A	69	GLU	2.8
1	E	355	GLY	2.8
2	B	73	GLY	2.8
1	A	396	HIS	2.8
1	A	398	PRO	2.8
2	F	128	VAL	2.8
3	G	102	GLY	2.7
1	A	429	PRO	2.7
3	G	224	ARG	2.7
1	A	370	TYR	2.7
3	C	118	TRP	2.7
1	E	508	ALA	2.7
1	A	385	ALA	2.7
1	A	40	VAL	2.7
2	F	193	HIS	2.7
2	F	136	PRO	2.6
2	F	111	GLY	2.6
3	G	39	LEU	2.6
3	G	125	VAL	2.6
3	C	60	ASP	2.6
2	B	136	PRO	2.6
1	A	759	PRO	2.6
1	E	582	PRO	2.6
1	A	526	GLY	2.6
1	E	519	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
3	G	116	ALA	2.6
1	A	594	CYS	2.6
1	A	43	ILE	2.6
3	C	41	LYS	2.6
3	G	109	LYS	2.6
1	A	603	GLN	2.6
1	E	394	GLY	2.6
2	F	170	GLY	2.6
1	E	628	VAL	2.6
2	F	133	GLU	2.6
1	A	335	VAL	2.6
1	E	114	VAL	2.6
3	G	122	PHE	2.5
1	E	594	CYS	2.5
3	G	213	LEU	2.5
1	E	632	ALA	2.5
2	F	1	MET	2.5
3	C	112	SER	2.5
1	E	603	GLN	2.5
3	G	242	VAL	2.5
1	A	573	GLU	2.5
1	E	583	PHE	2.5
3	C	37	LEU	2.5
3	G	206	GLY	2.5
1	A	729	SER	2.5
1	E	392	SER	2.5
1	A	30	ALA	2.5
2	F	74	ALA	2.5
3	G	88	ILE	2.5
1	A	571	TRP	2.5
2	B	89	LYS	2.5
1	E	362	GLY	2.5
1	E	586	ALA	2.5
1	A	277	GLU	2.5
3	G	210	GLY	2.5
1	E	635	GLN	2.5
1	A	508	ALA	2.4
3	G	207	PHE	2.4
3	G	44	GLU	2.4
3	G	117	TRP	2.4
1	A	582	PRO	2.4
1	E	602	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
3	G	48	TYR	2.4
1	E	590	ILE	2.4
1	E	572	LEU	2.4
3	G	33	LEU	2.4
3	G	111	SER	2.4
1	A	537	TRP	2.4
1	A	484	THR	2.4
3	C	86	THR	2.4
3	G	30	VAL	2.4
1	A	295	ASP	2.4
3	G	171	ALA	2.4
1	E	286	PHE	2.4
2	F	104	ALA	2.3
3	C	172	ALA	2.3
3	G	107	LEU	2.3
1	E	36	GLU	2.3
2	F	85	VAL	2.3
1	A	523	ARG	2.3
3	G	38	HIS	2.3
3	G	99	PHE	2.3
2	F	185	GLY	2.3
3	G	53	LEU	2.3
1	A	663	GLU	2.3
1	E	386	GLY	2.3
1	E	387	GLY	2.3
3	G	64	TRP	2.3
3	G	226	ALA	2.3
2	B	123	LEU	2.3
3	G	214	LEU	2.3
2	F	46	TYR	2.3
1	A	595	GLN	2.3
1	E	588	GLY	2.3
1	E	268	LEU	2.3
2	B	75	SER	2.3
1	A	593	TYR	2.3
3	C	174	PHE	2.3
2	B	100	CYS	2.3
3	G	56	ILE	2.2
3	G	110	GLY	2.2
1	A	527	LEU	2.2
3	G	63	LEU	2.2
3	G	160	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	547	ARG	2.2
2	B	105	ARG	2.2
3	G	62	ILE	2.2
1	E	634	THR	2.2
2	F	72	THR	2.2
1	A	365	ILE	2.2
1	A	632	ALA	2.2
1	A	505	ARG	2.2
1	E	685	THR	2.2
1	A	728	ILE	2.2
1	E	616	GLU	2.2
3	C	224	GLU	2.2
1	A	388	CYS	2.2
1	E	115	ALA	2.2
2	F	173	PRO	2.2
1	A	339	ASP	2.2
3	G	77	TRP	2.2
1	E	396	HIS	2.2
3	G	119	LEU	2.2
3	G	158	LEU	2.2
3	G	68	PRO	2.2
1	A	47	CYS	2.2
2	F	3	ARG	2.2
3	G	13	TRP	2.2
1	A	721	THR	2.1
1	E	605	LEU	2.1
2	F	99	ALA	2.1
1	A	97	ARG	2.1
2	F	68	PRO	2.1
1	A	520	TRP	2.1
1	E	630	THR	2.1
1	E	622	LEU	2.1
1	A	531	LEU	2.1
1	A	539	THR	2.1
1	E	640	LEU	2.1
2	F	91	ILE	2.1
2	B	74	ALA	2.1
1	A	386	GLY	2.1
3	C	222	TRP	2.1
3	C	108	LEU	2.1
3	C	241	LEU	2.1
3	G	175	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	G	215	LEU	2.1
1	A	89	THR	2.1
1	E	489	TYR	2.1
3	G	52	ALA	2.1
1	A	434	GLY	2.1
1	A	511	PRO	2.1
2	B	124	GLU	2.1
2	F	115	LYS	2.1
3	C	110	LYS	2.1
2	F	97	ILE	2.1
2	B	58	CYS	2.1
3	C	119	ALA	2.1
1	E	604	PRO	2.1
1	E	523	ARG	2.0
1	E	280	ALA	2.0
2	F	116	CYS	2.0
3	G	35	ALA	2.0
1	A	390	GLY	2.0
1	A	80	PRO	2.0
1	E	48	PHE	2.0
1	E	67	GLY	2.0
2	B	127	LYS	2.0
1	A	381	LEU	2.0
1	A	70	ALA	2.0
1	A	686	ALA	2.0
1	A	530	GLY	2.0
1	A	538	LYS	2.0
1	A	284	VAL	2.0
1	A	95	LEU	2.0
1	E	531	LEU	2.0
3	C	40	LEU	2.0
1	A	590	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

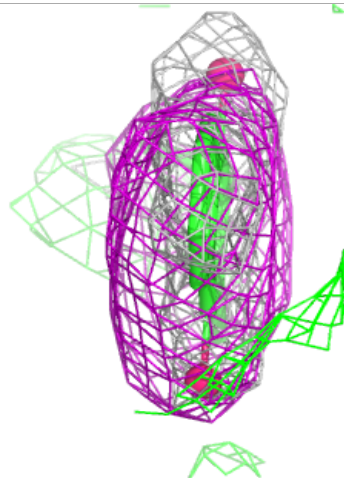
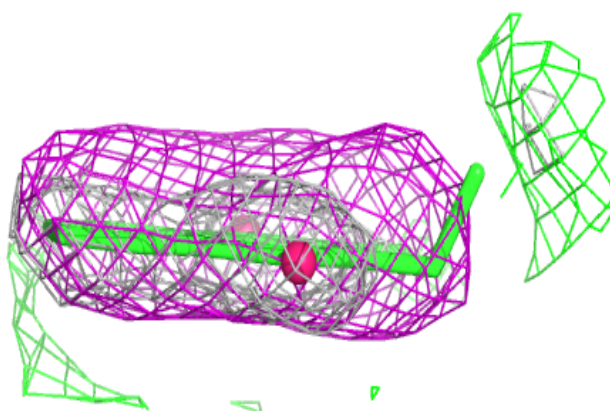
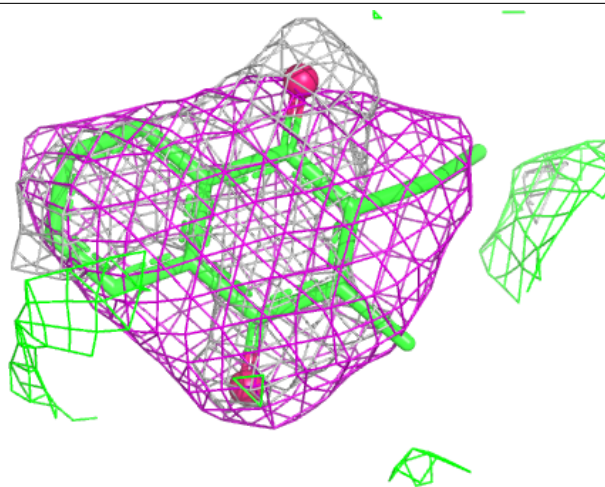
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MQ7	G	1251	15/48	0.74	0.43	27,31,36,42	0
7	MQ7	C	1252	15/48	0.75	0.41	26,27,28,29	0
4	SF4	B	1196	8/8	0.91	0.11	55,59,62,65	0
4	SF4	F	1197	8/8	0.93	0.09	68,72,73,75	0
5	MGD	E	1766	47/47	0.93	0.10	41,46,48,50	0
4	SF4	F	1195	8/8	0.93	0.09	70,71,74,75	0
4	SF4	F	1196	8/8	0.93	0.11	60,65,67,68	0
5	MGD	A	1765	47/47	0.94	0.11	48,52,55,58	0
4	SF4	F	1194	8/8	0.94	0.12	81,83,84,87	0
5	MGD	E	1765	47/47	0.95	0.11	46,53,56,56	0
4	SF4	B	1194	8/8	0.95	0.10	78,79,80,81	0
5	MGD	A	1766	47/47	0.96	0.09	37,46,48,52	0
6	MO	A	1767	1/1	0.98	0.04	54,54,54,54	0
4	SF4	B	1195	8/8	0.98	0.05	65,66,68,68	0
4	SF4	B	1197	8/8	0.98	0.05	57,60,61,63	0
4	SF4	E	1764	8/8	0.99	0.03	45,49,52,52	0
4	SF4	A	1764	8/8	0.99	0.03	44,46,48,49	0
6	MO	E	1767	1/1	1.00	0.03	60,60,60,60	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.

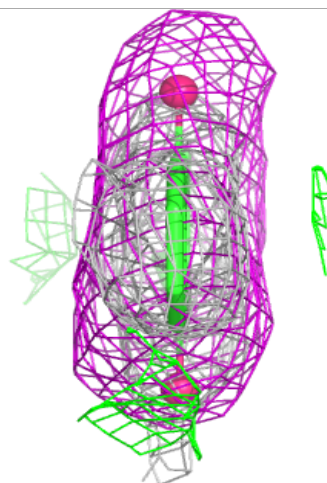
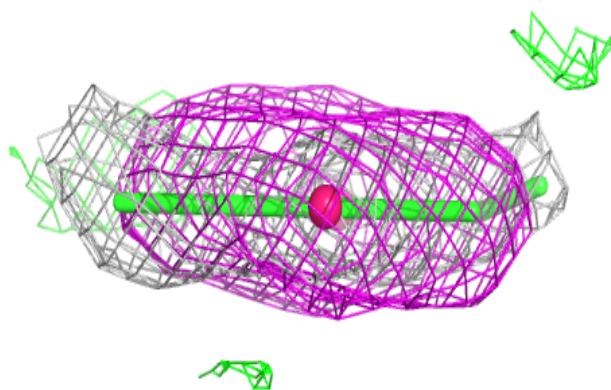
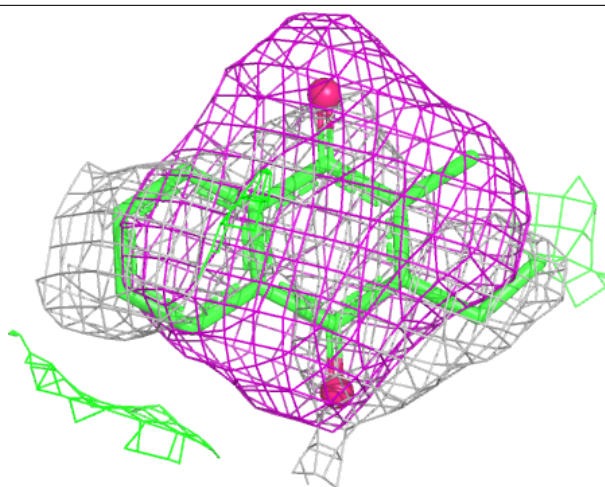
Electron density around MQ7 G 1251:

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



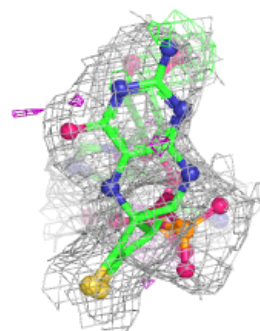
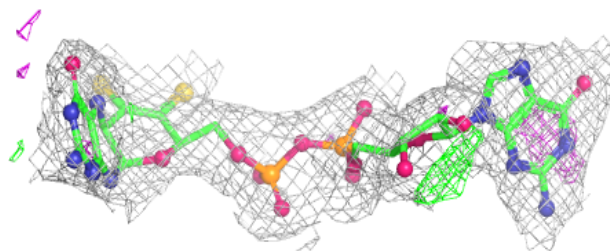
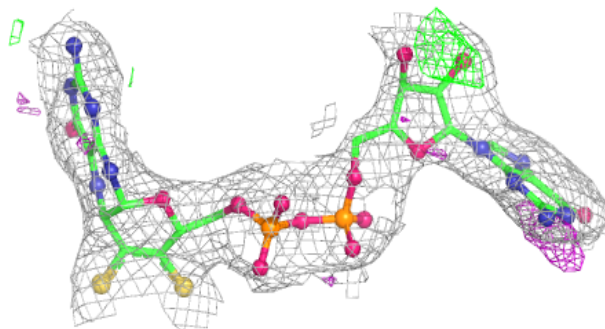
Electron density around MQ7 C 1252:

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

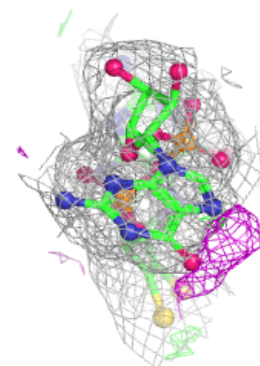
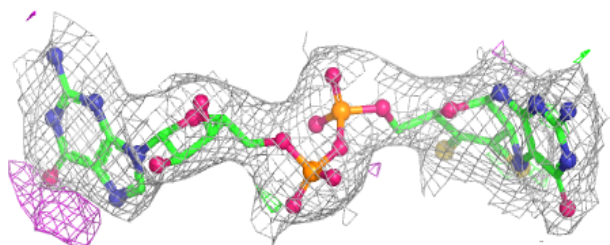
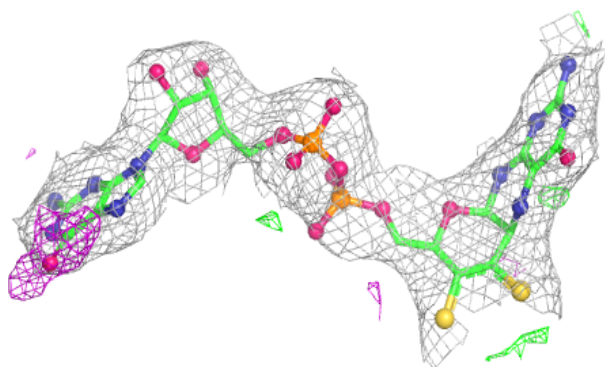


Electron density around MGD E 1766:

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

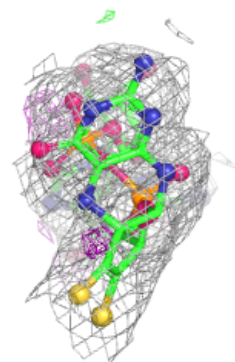
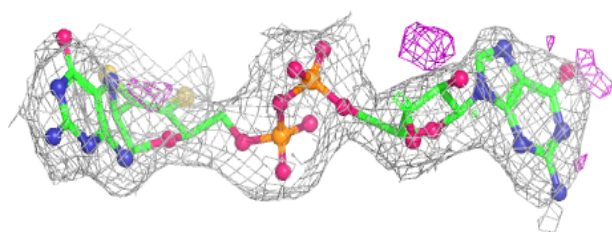
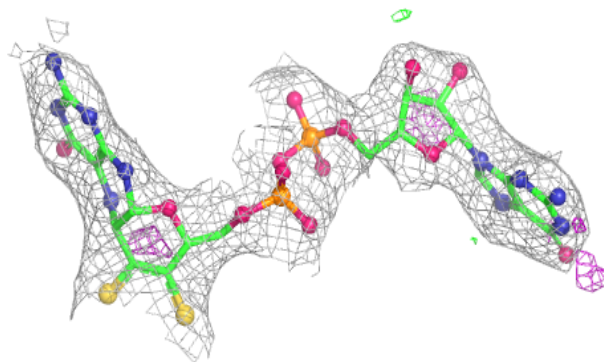
**Electron density around MGD A 1765:**

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

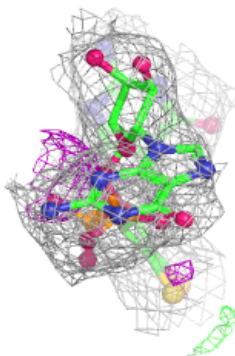
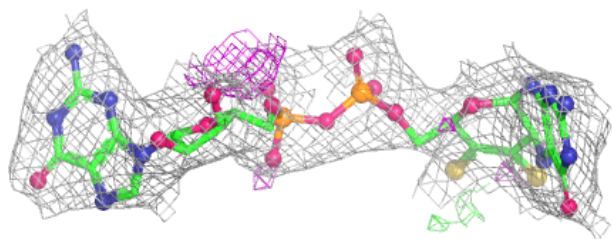
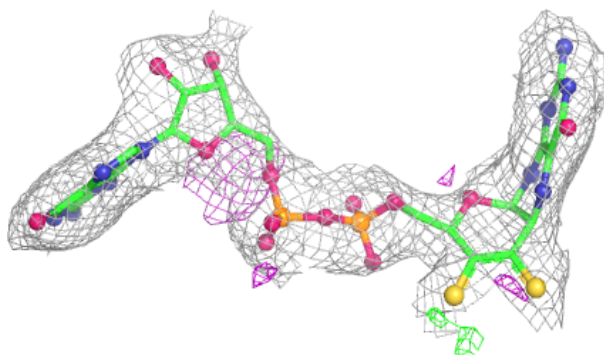


Electron density around MGD E 1765:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.