Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2024 – 08:09 pm BST

PDB ID	:	2VPZ
Title	:	Polysulfide reductase native structure
Authors	:	Jormakka, M.; Yokoyama, K.; Yano, T.; Tamakoshi, M.; Akimoto, S.; Shimamura, T.; Curmi, P.; Iwata, S.
Deposited on	:	2008-03-09
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

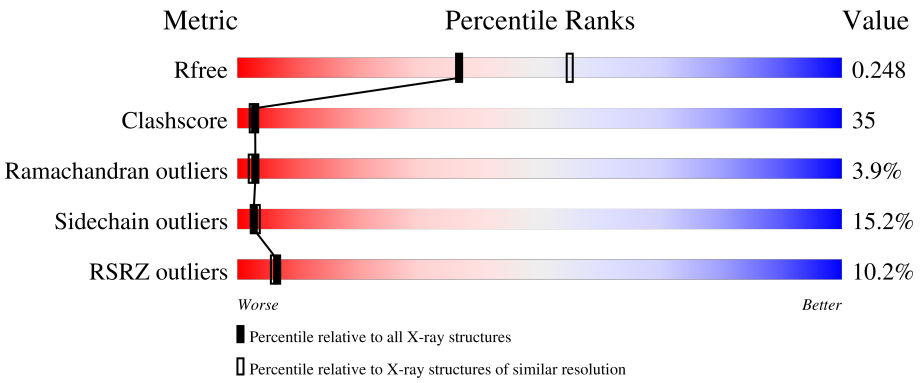
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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% 47% 33% 13% • •
1	E	765	11% 48% 33% 12% • •
2	B	195	7% 57% 33% 8% ••
2	F	195	5% 62% 28% 10% ••
3	C	253	9% 69% 22% 8% ••

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Mol	Chain	Length	Quality of chain
3	G	253	11% 61% 28% 8%

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	F	1194	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20193 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
			Total	C	N	O	S			
1	A	735	5896	3802	1032	1043	19	0	0	1
1	E	735	5896	3802	1032	1043	19	0	0	1

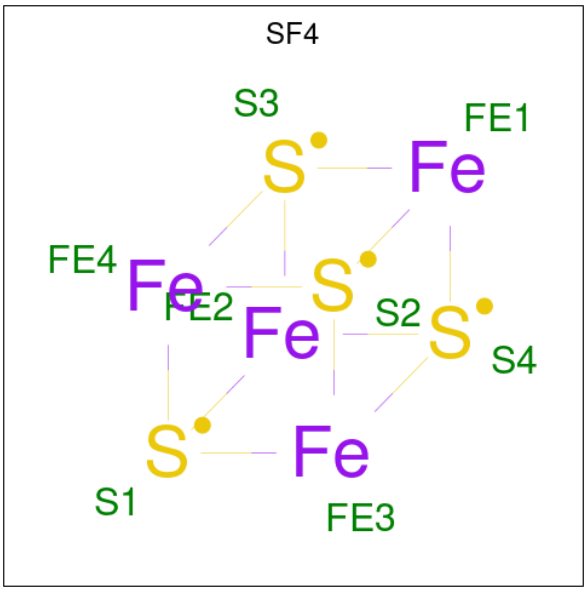
- Molecule 2 is a protein called NRFC PROTEIN.

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

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

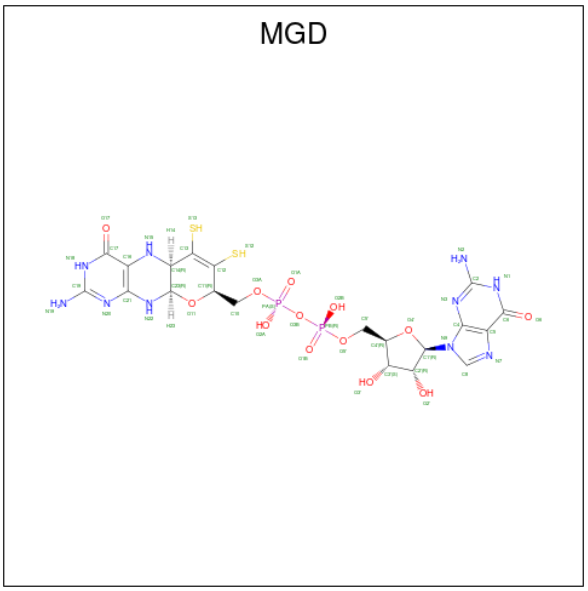
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	251	1948	1323	320	303	2	0	0	1
3	G	251	1948	1323	320	303	2	0	0	1

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



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

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



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

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	386	386	386	0	0
7	B	150	150	150	0	0
7	C	88	88	88	0	0

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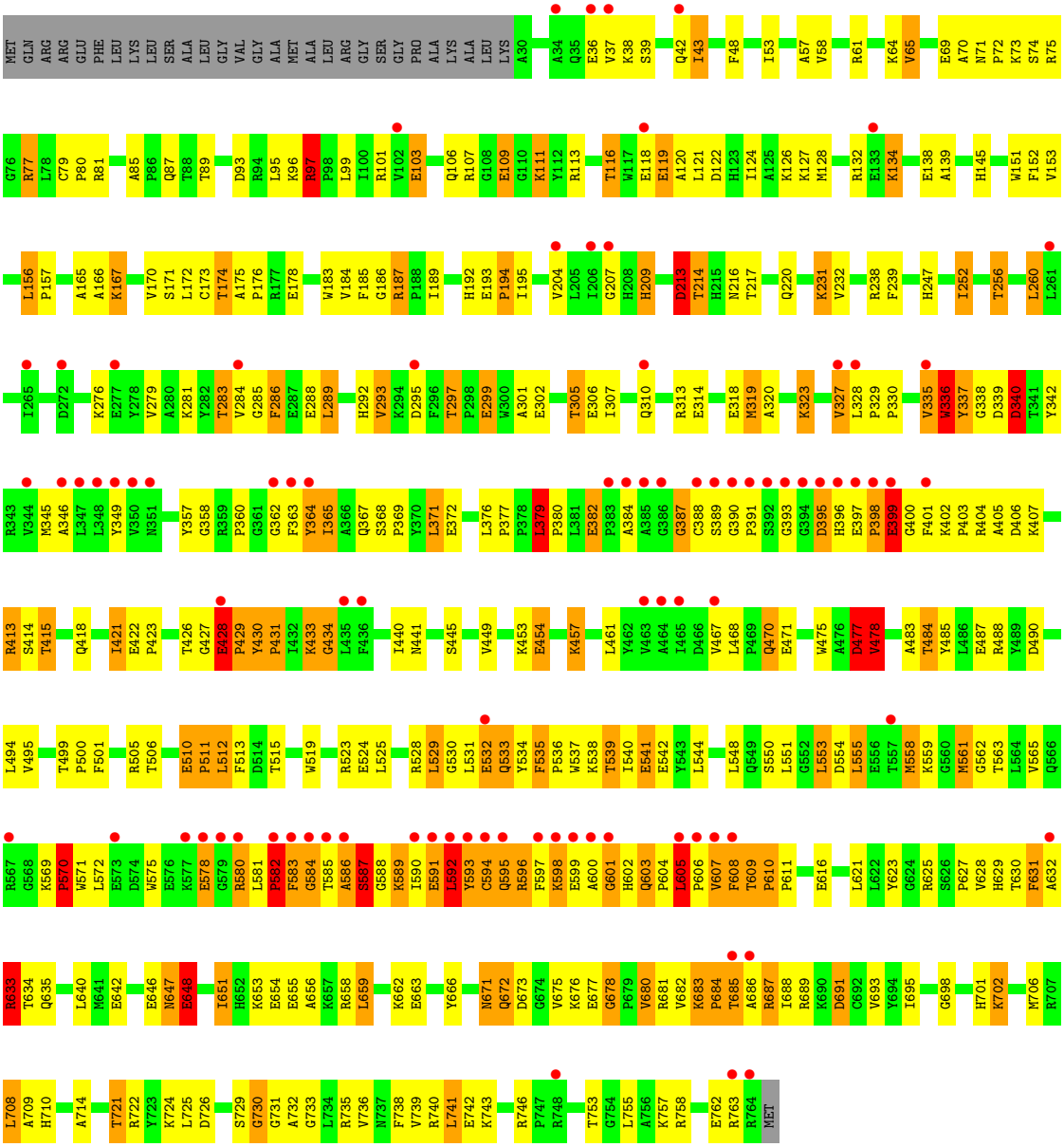
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	E	452	452	452	0	0
			Total	O		
7	F	130	130	130	0	0
			Total	O		
7	G	79	79	79	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

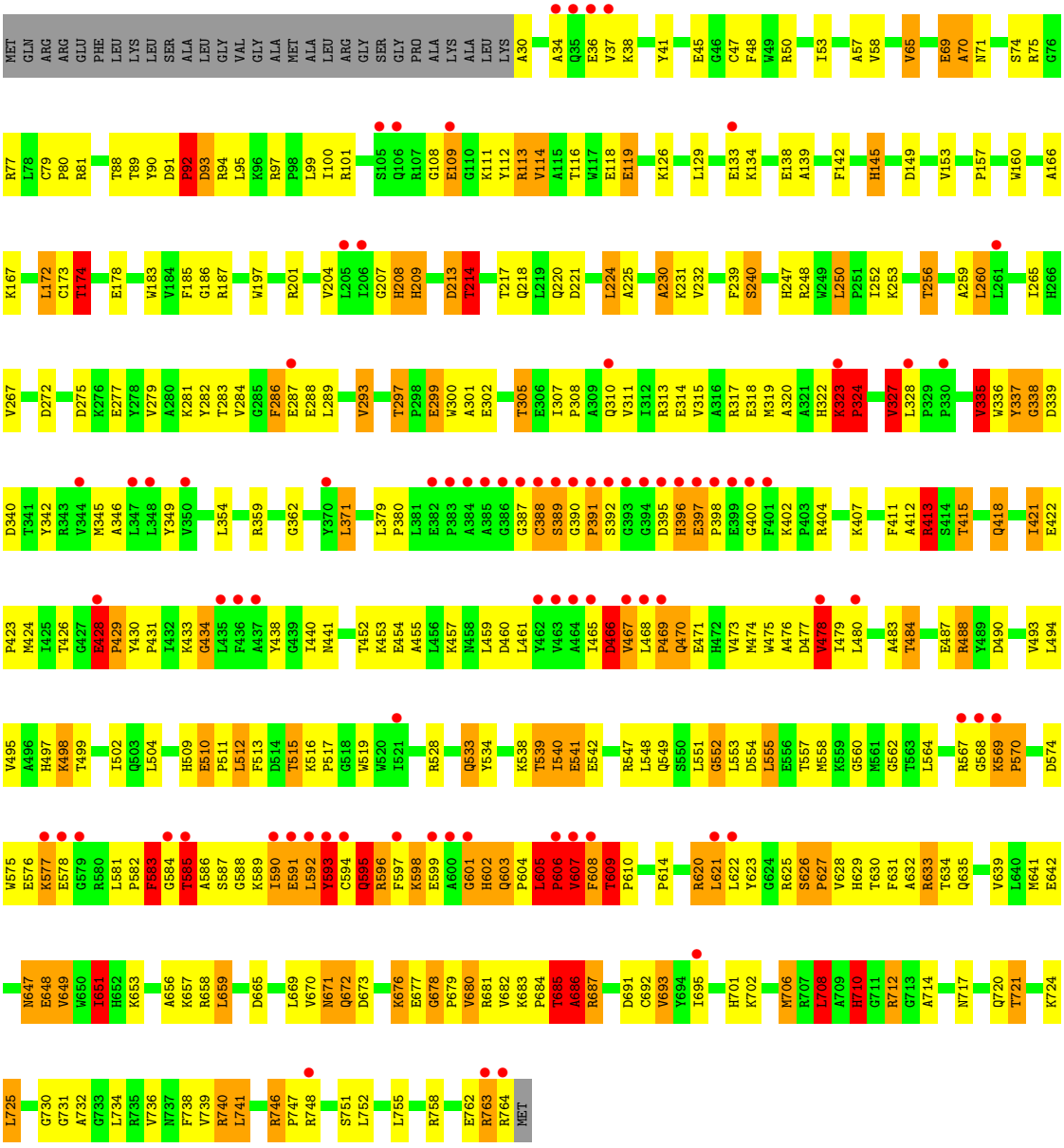
- Molecule 1: THIOSULFATE REDUCTASE

Chain A:



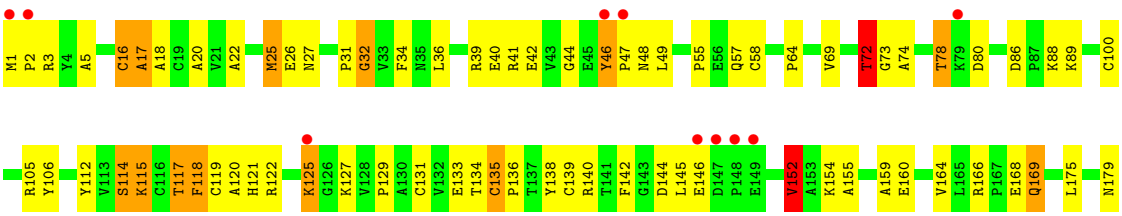
• Molecule 1: THIOSULFATE REDUCTASE

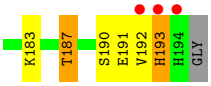
Chain E:



• Molecule 2: NRFC PROTEIN

Chain B:



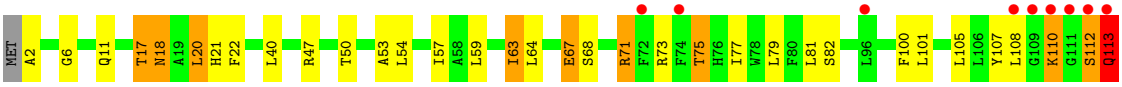


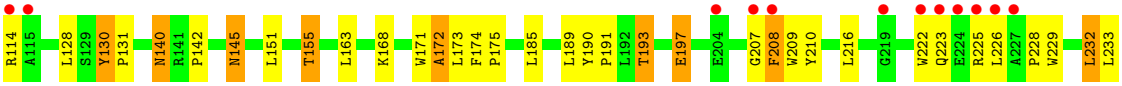
• Molecule 2: NRFC PROTEIN

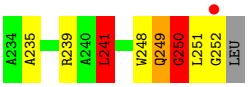
Chain F:

• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN

Chain C:

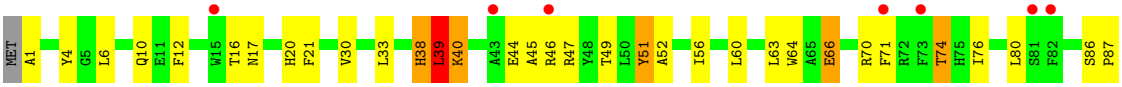


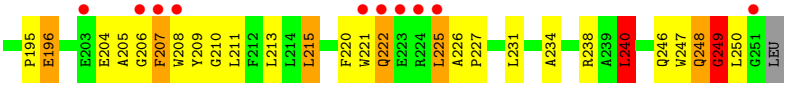




• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	118.41Å 166.26Å 246.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.40 29.83 – 2.25	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.83-2.40) 91.6 (29.83-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.253 0.241 , 0.248	Depositor DCC
R_{free} test set	4206 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 69.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20193	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.07	11/6079 (0.2%)	1.12	29/8267 (0.4%)
1	E	1.15	23/6079 (0.4%)	1.33	74/8267 (0.9%)
2	B	1.06	3/1512 (0.2%)	1.21	8/2058 (0.4%)
2	F	1.09	2/1512 (0.1%)	1.23	16/2058 (0.8%)
3	C	1.04	2/2016 (0.1%)	0.94	7/2764 (0.3%)
3	G	0.92	1/2016 (0.0%)	1.10	18/2764 (0.7%)
All	All	1.08	42/19214 (0.2%)	1.19	152/26178 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	3

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	324	PRO	N-CD	17.24	1.72	1.47
2	F	135	CYS	CB-SG	16.46	2.10	1.82
1	E	592	LEU	CG-CD1	15.44	2.08	1.51
3	C	114	ARG	NE-CZ	12.34	1.49	1.33
2	B	135	CYS	CB-SG	12.12	2.02	1.82
1	E	240	SER	CA-CB	-11.77	1.35	1.52
1	E	323	LYS	C-O	11.71	1.45	1.23
2	F	16	CYS	CB-SG	10.95	2.00	1.82
1	E	324	PRO	CA-C	10.34	1.73	1.52
1	A	648	GLU	CB-CG	10.21	1.71	1.52
1	A	399	GLU	CD-OE2	-9.79	1.14	1.25
2	B	16	CYS	CB-SG	9.57	1.98	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	324	PRO	CG-CD	9.00	1.80	1.50
3	C	114	ARG	CZ-NH1	8.28	1.43	1.33
1	E	324	PRO	N-CA	8.04	1.60	1.47
2	B	100	CYS	CB-SG	7.88	1.95	1.82
1	E	387	GLY	C-N	7.75	1.51	1.34
1	E	323	LYS	C-N	7.38	1.48	1.34
3	G	109	LYS	C-N	7.07	1.45	1.33
1	A	337	TYR	CB-CG	7.01	1.62	1.51
1	E	387	GLY	C-O	-6.95	1.12	1.23
1	E	648	GLU	CB-CG	6.73	1.65	1.52
1	E	388	CYS	CA-CB	-6.47	1.39	1.53
1	A	173	CYS	CB-SG	6.21	1.92	1.82
1	A	97	ARG	NE-CZ	6.17	1.41	1.33
1	E	478	VAL	CA-CB	6.00	1.67	1.54
1	E	231	LYS	CA-CB	-5.97	1.40	1.53
1	E	595	GLN	CA-CB	-5.95	1.40	1.53
1	E	173	CYS	CB-SG	5.88	1.92	1.82
1	A	336	TRP	CB-CG	-5.75	1.39	1.50
1	E	583	PHE	CA-C	5.51	1.67	1.52
1	A	583	PHE	C-O	5.51	1.33	1.23
1	E	594	CYS	C-O	-5.51	1.12	1.23
1	E	692	CYS	CB-SG	-5.50	1.72	1.81
1	E	685	THR	CA-C	5.50	1.67	1.52
1	A	648	GLU	CG-CD	5.47	1.60	1.51
1	E	594	CYS	CB-SG	5.43	1.91	1.82
1	A	364	TYR	C-O	-5.30	1.13	1.23
1	E	324	PRO	CB-CG	-5.29	1.23	1.50
1	A	401	PHE	N-CA	5.20	1.56	1.46
1	E	230	ALA	C-O	-5.20	1.13	1.23
1	A	601	GLY	CA-C	-5.15	1.43	1.51

All (152) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	323	LYS	C-N-CD	-27.55	59.98	120.60
1	E	324	PRO	CA-N-CD	-22.69	79.73	111.50
1	E	324	PRO	N-CA-CB	12.53	118.33	103.30
3	G	249	GLY	N-CA-C	12.02	143.14	113.10
1	E	387	GLY	CA-C-O	11.50	141.30	120.60
1	A	583	PHE	C-N-CA	11.19	145.79	122.30
1	E	323	LYS	O-C-N	-10.88	100.42	121.10
1	E	324	PRO	N-CA-C	-10.65	84.41	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	171	THR	N-CA-C	10.58	139.58	111.00
2	F	44	GLY	N-CA-C	10.03	138.18	113.10
2	B	46	TYR	N-CA-C	9.60	136.91	111.00
1	E	240	SER	N-CA-CB	-9.08	96.88	110.50
1	E	172	LEU	CA-CB-CG	-8.79	95.09	115.30
1	E	585	THR	CA-CB-CG2	-8.78	100.11	112.40
1	A	592	LEU	N-CA-C	8.65	134.34	111.00
1	A	691	ASP	CB-CA-C	-8.56	93.27	110.40
1	A	401	PHE	N-CA-C	8.43	133.76	111.00
1	E	725	LEU	CA-CB-CG	8.28	134.34	115.30
1	E	680	VAL	CB-CA-C	-8.23	95.77	111.40
3	G	207	PHE	CB-CA-C	-8.21	93.99	110.40
1	E	387	GLY	C-N-CA	-8.06	101.55	121.70
1	E	686	ALA	N-CA-C	8.04	132.70	111.00
1	E	388	CYS	N-CA-C	8.04	132.70	111.00
2	B	169	GLN	N-CA-C	-7.99	89.43	111.00
1	E	593	TYR	N-CA-CB	7.92	124.85	110.60
1	E	387	GLY	CA-C-N	-7.88	99.86	117.20
1	E	185	PHE	N-CA-C	-7.84	89.83	111.00
2	B	46	TYR	CB-CA-C	-7.82	94.77	110.40
1	E	327	VAL	CB-CA-C	-7.65	96.86	111.40
1	E	593	TYR	CB-CA-C	-7.61	95.18	110.40
1	E	583	PHE	N-CA-C	7.57	131.44	111.00
1	E	582	PRO	N-CA-C	7.57	131.77	112.10
1	E	731	GLY	N-CA-C	7.42	131.65	113.10
1	A	327	VAL	CB-CA-C	-7.41	97.32	111.40
1	E	585	THR	CB-CA-C	7.40	131.58	111.60
3	G	240	LEU	CA-CB-CG	7.32	132.13	115.30
1	E	659	LEU	N-CA-C	-7.31	91.27	111.00
1	E	323	LYS	CB-CA-C	7.22	124.85	110.40
1	E	685	THR	C-N-CA	7.22	139.75	121.70
3	C	113	GLN	N-CA-C	7.04	130.01	111.00
1	E	467	VAL	N-CA-C	6.98	129.85	111.00
1	E	595	GLN	N-CA-CB	-6.94	98.10	110.60
1	E	594	CYS	O-C-N	-6.90	111.66	122.70
1	E	708	LEU	CA-CB-CG	6.88	131.11	115.30
2	F	39	ARG	NE-CZ-NH2	-6.84	116.88	120.30
3	G	114	ALA	N-CA-C	-6.79	92.65	111.00
3	C	250	GLY	N-CA-C	6.75	129.96	113.10
1	A	648	GLU	N-CA-CB	-6.74	98.47	110.60
2	F	54	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	A	741	LEU	CA-CB-CG	6.73	130.79	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	390	GLY	N-CA-C	-6.66	96.44	113.10
1	E	603	GLN	N-CA-C	6.64	128.92	111.00
2	B	72	THR	N-CA-C	-6.57	93.26	111.00
2	F	145	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	582	PRO	N-CA-C	6.54	129.11	112.10
1	E	594	CYS	N-CA-C	6.52	128.60	111.00
1	A	340	ASP	N-CA-C	6.50	128.53	111.00
1	E	173	CYS	CA-CB-SG	6.46	125.62	114.00
2	F	152	VAL	CB-CA-C	-6.45	99.15	111.40
3	G	225	LEU	N-CA-C	-6.40	93.73	111.00
1	E	388	CYS	CA-CB-SG	6.38	125.49	114.00
1	A	185	PHE	C-N-CA	-6.32	109.03	122.30
1	E	323	LYS	CA-C-O	-6.28	106.91	120.10
1	E	428	GLU	N-CA-C	6.24	127.84	111.00
3	C	114	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	A	477	ASP	N-CA-C	-6.18	94.32	111.00
1	A	364	TYR	N-CA-C	6.16	127.63	111.00
1	A	379	LEU	CA-CB-CG	6.16	129.46	115.30
3	G	131	GLY	N-CA-C	-6.16	97.71	113.10
1	E	594	CYS	N-CA-CB	-6.13	99.56	110.60
1	A	213	ASP	N-CA-C	-6.09	94.56	111.00
1	E	34	ALA	C-N-CA	6.08	136.89	121.70
2	F	54	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	E	741	LEU	CA-CB-CG	6.05	129.23	115.30
1	E	593	TYR	CB-CG-CD2	6.05	124.63	121.00
2	F	16	CYS	N-CA-C	-6.04	94.68	111.00
1	E	92	PRO	N-CA-C	-6.04	96.38	112.10
3	C	226	LEU	CA-CB-CG	6.03	129.17	115.30
2	F	46	TYR	N-CA-C	6.01	127.22	111.00
1	E	213	ASP	N-CA-C	-5.99	94.84	111.00
1	E	593	TYR	CB-CG-CD1	-5.98	117.41	121.00
2	B	152	VAL	CB-CA-C	-5.97	100.06	111.40
1	E	590	ILE	CB-CA-C	-5.92	99.75	111.60
1	A	97	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	A	401	PHE	CA-C-O	-5.87	107.78	120.10
1	A	659	LEU	N-CA-C	-5.85	95.21	111.00
2	F	39	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	570	PRO	O-C-N	-5.83	113.38	122.70
1	E	710	HIS	C-N-CA	-5.82	110.08	122.30
3	G	109	LYS	CA-C-N	-5.82	104.57	116.20
1	E	214	THR	N-CA-CB	-5.79	99.30	110.30
3	C	241	LEU	CA-CB-CG	5.78	128.59	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	601	GLY	N-CA-C	5.76	127.51	113.10
3	G	248	GLN	N-CA-CB	-5.76	100.23	110.60
3	G	213	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	364	TYR	C-N-CA	5.74	136.04	121.70
1	A	109	GLU	N-CA-C	-5.72	95.54	111.00
1	E	379	LEU	CA-CB-CG	5.72	128.46	115.30
1	E	593	TYR	N-CA-C	-5.71	95.59	111.00
1	E	413	ARG	NE-CZ-NH2	5.68	123.14	120.30
3	G	4	TYR	N-CA-C	-5.68	95.67	111.00
1	A	319	MET	CA-CB-CG	5.66	122.92	113.30
2	F	43	VAL	N-CA-C	-5.66	95.72	111.00
1	E	606	PRO	N-CA-C	-5.64	97.45	112.10
1	A	433	LYS	N-CA-C	-5.63	95.81	111.00
1	E	594	CYS	C-N-CA	5.57	135.62	121.70
1	E	231	LYS	CA-CB-CG	5.56	125.63	113.40
3	G	6	LEU	CA-CB-CG	5.56	128.09	115.30
3	G	39	LEU	CA-CB-CG	5.54	128.04	115.30
1	E	710	HIS	CA-C-N	5.53	127.26	116.20
1	E	337	TYR	N-CA-C	5.53	125.93	111.00
1	E	712	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	E	335	VAL	CB-CA-C	5.49	121.84	111.40
1	E	260	LEU	CA-CB-CG	5.49	127.92	115.30
2	F	16	CYS	C-N-CA	-5.49	107.98	121.70
2	F	16	CYS	CA-C-N	5.48	129.25	117.20
1	A	376	LEU	CA-CB-CG	5.44	127.81	115.30
3	G	130	PRO	N-CA-C	-5.43	97.98	112.10
1	E	335	VAL	N-CA-CB	-5.40	99.61	111.50
1	E	213	ASP	CB-CG-OD1	5.40	123.16	118.30
3	C	114	ARG	N-CA-C	-5.39	96.45	111.00
3	G	109	LYS	O-C-N	5.37	132.32	123.20
1	E	338	GLY	N-CA-C	5.35	126.48	113.10
1	A	365	ILE	N-CA-CB	5.35	123.10	110.80
2	F	188	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	730	GLY	N-CA-C	5.32	126.41	113.10
1	E	400	GLY	N-CA-C	-5.32	99.80	113.10
3	G	225	LEU	N-CA-CB	5.32	121.04	110.40
2	B	32	GLY	N-CA-C	5.29	126.32	113.10
1	E	207	GLY	N-CA-C	-5.29	99.88	113.10
1	E	665	ASP	N-CA-C	5.29	125.28	111.00
1	E	651	ILE	CB-CA-C	-5.28	101.04	111.60
2	B	169	GLN	C-N-CA	-5.27	111.23	122.30
1	A	583	PHE	CB-CA-C	-5.23	99.94	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	710	HIS	N-CA-C	5.23	125.12	111.00
3	C	6	GLY	N-CA-C	-5.22	100.05	113.10
1	E	413	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	A	706	MET	N-CA-C	-5.18	97.00	111.00
1	E	692	CYS	CB-CA-C	-5.18	100.03	110.40
2	F	111	GLY	N-CA-C	5.17	126.01	113.10
2	F	36	LEU	CA-CB-CG	5.15	127.16	115.30
1	E	388	CYS	N-CA-CB	-5.13	101.36	110.60
1	E	555	LEU	CA-CB-CG	5.08	126.97	115.30
3	G	215	LEU	CA-CB-CG	5.07	126.97	115.30
1	A	260	LEU	CA-CB-CG	5.07	126.95	115.30
1	E	706	MET	N-CA-C	-5.06	97.33	111.00
1	A	570	PRO	N-CA-C	5.04	125.21	112.10
1	E	174	THR	N-CA-CB	-5.04	100.73	110.30
3	G	156	LEU	CA-CB-CG	5.03	126.87	115.30
3	G	171	ALA	N-CA-C	5.03	124.57	111.00
2	B	72	THR	N-CA-CB	-5.02	100.76	110.30
1	E	687	ARG	CB-CG-CD	-5.02	98.55	111.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	323	LYS	Mainchain,Peptide
1	E	428	GLU	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5896	0	5813	501	3
1	E	5896	0	5814	447	3
2	B	1475	0	1453	116	0
2	F	1475	0	1454	83	0
3	C	1948	0	2001	90	0
3	G	1948	0	2004	97	0
4	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	32	0	0	3	0
4	E	8	0	0	1	0
4	F	32	0	0	3	0
5	A	94	0	44	7	0
5	E	94	0	44	7	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	386	0	0	67	0
7	B	150	0	0	34	0
7	C	88	0	0	5	0
7	E	452	0	0	105	0
7	F	130	0	0	20	0
7	G	79	0	0	21	0
All	All	20193	0	18627	1302	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 35.

All (1302) 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:E:324:PRO:CD	1:E:324:PRO:CG	1.80	1.60
2:B:135:CYS:SG	2:B:135:CYS:CB	2.02	1.47
1:A:602:HIS:CE1	1:A:606:PRO:HG3	1.52	1.43
1:E:592:LEU:HA	1:E:603:GLN:NE2	1.27	1.41
2:F:135:CYS:CB	2:F:135:CYS:SG	2.10	1.40
1:E:605:LEU:H	1:E:605:LEU:CD2	1.28	1.39
1:A:591:GLU:OE2	1:A:604:PRO:HG3	1.26	1.34
1:A:186:GLY:HA3	1:A:583:PHE:C	1.47	1.32
1:A:184:VAL:CG2	1:A:592:LEU:HD23	1.61	1.30
1:A:582:PRO:HB2	7:A:2277:HOH:O	1.27	1.29
1:E:591:GLU:OE1	1:E:604:PRO:HB3	1.23	1.27
2:B:46:TYR:HB2	7:B:2032:HOH:O	1.33	1.26
1:E:323:LYS:O	7:E:2213:HOH:O	1.53	1.24
1:E:477:ASP:O	1:E:478:VAL:HG23	1.33	1.22
1:E:605:LEU:HD23	1:E:605:LEU:N	1.43	1.21
1:A:601:GLY:HA2	7:A:2285:HOH:O	1.06	1.20
1:A:604:PRO:O	1:A:606:PRO:HD2	1.40	1.20
1:E:388:CYS:HB2	1:E:593:TYR:OH	1.40	1.18
2:B:41:ARG:HH11	2:B:187:THR:CG2	1.56	1.18
1:E:36:GLU:O	1:E:58:VAL:HG22	1.01	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:207:PHE:CE2	3:G:211:LEU:HD13	1.78	1.18
3:C:171:TRP:O	3:C:171:TRP:CE3	1.98	1.17
1:E:602:HIS:CE1	1:E:606:PRO:HG3	1.81	1.15
1:E:562:GLY:O	7:E:2316:HOH:O	1.60	1.15
1:A:584:GLY:HA2	7:A:2278:HOH:O	0.97	1.14
1:A:337:TYR:O	1:A:340:ASP:OD2	1.62	1.14
1:E:477:ASP:O	1:E:478:VAL:CG2	1.96	1.13
1:E:36:GLU:O	1:E:58:VAL:CG2	1.96	1.13
1:E:592:LEU:CA	1:E:603:GLN:HE21	1.59	1.13
1:A:97:ARG:HH21	1:A:763:ARG:NH2	1.47	1.12
1:A:395:ASP:O	1:A:399:GLU:HB2	1.46	1.12
1:A:583:PHE:CE2	1:A:588:GLY:N	2.17	1.12
1:A:69:GLU:O	7:A:2034:HOH:O	1.66	1.12
2:B:134:THR:O	2:B:134:THR:CG2	1.98	1.12
2:B:134:THR:O	2:B:134:THR:HG23	1.48	1.11
1:A:42:GLN:O	1:A:53:ILE:HG13	1.51	1.10
1:E:116:THR:HG22	1:E:119:GLU:HB3	1.25	1.10
1:E:607:VAL:CG1	1:E:607:VAL:O	2.00	1.09
3:G:1:ALA:HB1	7:G:2001:HOH:O	1.52	1.09
1:A:601:GLY:CA	7:A:2285:HOH:O	1.69	1.09
2:F:57:GLN:NE2	2:F:140:ARG:HH22	1.49	1.09
1:A:284:VAL:O	1:A:590:ILE:HG22	1.51	1.09
1:A:397:GLU:HB3	1:A:398:PRO:HD3	1.18	1.09
1:E:607:VAL:O	1:E:607:VAL:HG12	1.49	1.08
1:A:395:ASP:HA	1:A:399:GLU:CG	1.83	1.08
1:E:591:GLU:OE1	1:E:604:PRO:CB	2.01	1.08
1:A:184:VAL:HG23	1:A:592:LEU:CD2	1.84	1.07
1:A:428:GLU:HB3	1:A:429:PRO:HD2	1.37	1.07
1:A:43:ILE:HG13	1:A:505:ARG:HB3	1.27	1.07
1:E:97:ARG:HG3	7:E:2194:HOH:O	1.53	1.07
1:A:604:PRO:O	1:A:606:PRO:CD	2.04	1.06
1:E:605:LEU:CD2	1:E:605:LEU:N	1.93	1.06
1:A:395:ASP:HA	1:A:399:GLU:HG3	1.06	1.05
1:A:77:ARG:NH1	2:B:138:TYR:HE2	1.54	1.04
1:E:323:LYS:HD3	1:E:354:LEU:CA	1.87	1.03
1:E:602:HIS:HE1	1:E:606:PRO:HG3	0.88	1.03
1:A:467:VAL:HB	7:A:2230:HOH:O	1.58	1.03
1:A:97:ARG:NH2	1:A:763:ARG:HH22	1.55	1.03
2:B:46:TYR:CD1	7:B:2032:HOH:O	2.10	1.03
1:A:186:GLY:HA3	1:A:583:PHE:O	1.59	1.02
1:A:288:GLU:HB3	1:A:591:GLU:HG3	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:GLU:OE2	1:A:604:PRO:CG	2.06	1.02
1:E:591:GLU:CD	1:E:604:PRO:HB3	1.77	1.02
1:E:602:HIS:CD2	1:E:604:PRO:HD2	1.93	1.02
1:E:602:HIS:NE2	1:E:604:PRO:HD2	1.75	1.02
1:A:632:ALA:O	1:A:635:GLN:HG2	1.61	1.01
1:E:323:LYS:HD3	1:E:354:LEU:HA	1.06	1.01
1:E:592:LEU:CA	1:E:603:GLN:NE2	2.20	1.01
1:E:763:ARG:HG2	7:E:2442:HOH:O	1.59	1.01
2:F:57:GLN:HE22	2:F:140:ARG:NH2	1.57	1.01
1:E:95:LEU:HD12	1:E:466:ASP:O	1.60	1.00
1:E:626:SER:HB2	7:E:2350:HOH:O	1.59	1.00
1:A:602:HIS:CE1	1:A:606:PRO:CG	2.44	1.00
3:G:207:PHE:HE2	3:G:211:LEU:HD13	1.14	1.00
1:A:685:THR:HB	2:B:42:GLU:OE2	1.62	1.00
3:C:17:THR:CG2	3:C:67:GLU:HG3	1.91	1.00
2:B:41:ARG:HD2	2:B:187:THR:HG21	1.40	0.99
1:E:511:PRO:HB3	1:E:515:THR:HG22	1.44	0.99
1:A:279:VAL:HG13	1:A:283:THR:HG21	1.42	0.99
1:E:339:ASP:HB2	1:E:607:VAL:HG11	1.44	0.99
1:E:429:PRO:HD2	7:E:2259:HOH:O	1.61	0.99
1:A:569:LYS:O	7:A:2271:HOH:O	1.81	0.99
2:B:41:ARG:HD2	2:B:187:THR:CG2	1.91	0.99
1:E:413:ARG:HD3	7:E:2250:HOH:O	1.62	0.98
1:A:165:ALA:O	1:A:415:THR:HG21	1.62	0.98
1:A:592:LEU:O	1:A:593:TYR:HB2	1.60	0.98
3:C:22:PHE:O	3:C:239:ARG:NH1	1.96	0.98
3:G:154:THR:CG2	3:G:238:ARG:HE	1.77	0.97
1:E:230:ALA:O	7:E:2141:HOH:O	1.80	0.97
3:G:38:HIS:HD2	3:G:45:ALA:HB1	1.28	0.97
1:E:598:LYS:HD2	7:E:2331:HOH:O	1.65	0.97
1:A:395:ASP:CA	1:A:399:GLU:HG3	1.93	0.97
1:A:603:GLN:HB3	1:A:604:PRO:HD3	1.43	0.97
1:E:47:CYS:HB2	7:E:2452:HOH:O	1.63	0.97
1:E:116:THR:CG2	1:E:119:GLU:H	1.78	0.97
1:E:608:PHE:O	7:E:2337:HOH:O	1.82	0.97
1:E:592:LEU:HD23	1:E:603:GLN:HE22	1.28	0.96
1:E:602:HIS:HE1	1:E:606:PRO:CG	1.78	0.96
1:A:583:PHE:HE2	1:A:588:GLY:N	1.59	0.96
1:A:172:LEU:HD13	1:A:445:SER:O	1.66	0.96
1:E:224:LEU:HD12	7:E:2135:HOH:O	1.64	0.96
1:A:763:ARG:HG2	7:A:2378:HOH:O	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ARG:HH11	2:B:187:THR:HG22	1.28	0.95
1:E:653:LYS:HD2	1:E:686:ALA:HB2	1.47	0.94
2:B:46:TYR:CE2	7:B:2029:HOH:O	2.20	0.94
3:C:171:TRP:O	3:C:171:TRP:CD2	2.20	0.94
1:A:170:VAL:O	1:A:175:ALA:HB2	1.65	0.94
2:F:57:GLN:NE2	2:F:140:ARG:NH2	2.15	0.94
1:E:342:TYR:CD1	1:E:607:VAL:HB	2.02	0.94
1:A:97:ARG:HH21	1:A:763:ARG:HH22	1.00	0.93
3:G:221:TRP:HE3	3:G:225:LEU:HD22	1.31	0.93
1:E:764:ARG:N	7:E:2446:HOH:O	2.01	0.93
2:B:192:VAL:HG21	7:B:2019:HOH:O	1.69	0.93
1:A:632:ALA:O	1:A:635:GLN:CG	2.16	0.93
1:E:590:ILE:HG13	7:E:2181:HOH:O	1.69	0.92
1:A:585:THR:O	1:A:586:ALA:HB3	1.70	0.92
1:E:428:GLU:O	1:E:430:TYR:N	2.02	0.92
2:F:41:ARG:HD2	2:F:187:THR:CG2	2.00	0.92
1:A:651:ILE:HD11	1:A:682:VAL:HG13	1.50	0.92
2:F:41:ARG:HD2	2:F:187:THR:HG23	1.49	0.92
1:A:42:GLN:O	1:A:53:ILE:CG1	2.17	0.91
3:C:155:THR:HG22	3:C:239:ARG:HE	1.35	0.91
3:G:206:GLY:O	3:G:209:TYR:N	2.03	0.91
1:A:531:LEU:O	1:A:534:TYR:O	1.88	0.91
1:A:116:THR:HG22	1:A:119:GLU:H	1.30	0.91
2:B:46:TYR:CB	7:B:2032:HOH:O	2.01	0.91
2:F:46:TYR:HB3	7:F:2036:HOH:O	1.69	0.91
3:G:111:SER:HB3	7:G:2036:HOH:O	1.69	0.91
1:A:360:PRO:HD3	1:A:571:TRP:CE3	2.06	0.90
1:A:599:GLU:O	7:A:2284:HOH:O	1.89	0.90
1:E:551:LEU:O	1:E:553:LEU:N	2.04	0.90
2:B:160:GLU:H	2:B:179:ASN:HD21	1.20	0.90
1:E:324:PRO:CD	1:E:324:PRO:CB	2.23	0.90
1:A:608:PHE:O	1:A:608:PHE:CD1	2.25	0.89
1:A:591:GLU:CD	1:A:604:PRO:HG3	1.93	0.89
1:E:112:TYR:OH	1:E:474:MET:O	1.91	0.89
1:A:184:VAL:HG23	1:A:592:LEU:HD23	0.91	0.89
3:C:207:GLY:O	3:C:210:TYR:N	2.04	0.89
1:E:349:TYR:OH	1:E:591:GLU:HA	1.73	0.89
1:A:186:GLY:CA	1:A:583:PHE:C	2.38	0.89
1:E:397:GLU:HB3	1:E:398:PRO:HD3	1.54	0.89
1:A:434:GLY:HA2	1:A:461:LEU:O	1.72	0.88
1:E:533:GLN:H	1:E:533:GLN:HE21	1.20	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:PRO:O	1:E:94:ARG:N	2.06	0.88
1:E:116:THR:HG23	1:E:119:GLU:H	1.39	0.88
1:A:680:VAL:HG11	7:A:2312:HOH:O	1.73	0.88
1:A:763:ARG:HB2	7:A:2380:HOH:O	1.72	0.88
1:A:580:ARG:CB	1:A:580:ARG:HH11	1.87	0.88
1:A:349:TYR:OH	1:A:591:GLU:O	1.92	0.87
1:A:335:VAL:CG1	1:A:732:ALA:O	2.23	0.87
1:A:591:GLU:HB3	1:A:603:GLN:NE2	1.88	0.87
1:E:604:PRO:O	1:E:606:PRO:HD3	1.75	0.87
1:A:729:SER:O	1:A:731:GLY:N	2.08	0.87
1:E:569:LYS:HD2	7:E:2322:HOH:O	1.73	0.87
1:A:77:ARG:HH11	2:B:138:TYR:HE2	1.04	0.86
2:B:146:GLU:HG2	7:B:2110:HOH:O	1.76	0.86
3:C:17:THR:HG21	3:C:67:GLU:HG3	1.56	0.86
1:A:116:THR:CG2	1:A:119:GLU:H	1.87	0.86
2:B:72:THR:HG22	2:B:74:ALA:H	1.38	0.86
1:A:186:GLY:HA3	1:A:584:GLY:N	1.91	0.86
1:A:276:LYS:HA	7:A:2152:HOH:O	1.75	0.86
1:E:297:THR:HG22	1:E:300:TRP:H	1.41	0.86
1:E:605:LEU:N	1:E:605:LEU:HD22	1.90	0.86
3:G:221:TRP:CE3	3:G:225:LEU:HD22	2.11	0.86
1:A:314:GLU:O	1:A:318:GLU:HG3	1.75	0.86
1:E:324:PRO:HD3	7:E:2170:HOH:O	1.74	0.85
1:E:635:GLN:O	1:E:641:MET:CG	2.23	0.85
2:F:41:ARG:HH11	2:F:187:THR:CG2	1.90	0.85
1:A:397:GLU:CB	1:A:398:PRO:HD3	2.06	0.85
1:A:607:VAL:HG12	1:A:607:VAL:O	1.77	0.85
2:B:16:CYS:O	2:B:16:CYS:SG	2.34	0.85
1:E:635:GLN:O	1:E:641:MET:HG3	1.77	0.85
1:E:95:LEU:CD1	1:E:466:ASP:O	2.24	0.85
1:E:493:VAL:HG13	7:E:2016:HOH:O	1.76	0.85
3:G:38:HIS:CD2	3:G:45:ALA:HB1	2.11	0.85
1:E:209:HIS:HE1	1:E:625:ARG:H	1.24	0.85
3:C:108:LEU:O	3:C:110:LYS:HG2	1.75	0.85
1:E:606:PRO:O	1:E:608:PHE:N	2.09	0.84
2:F:57:GLN:HE22	2:F:140:ARG:HH22	1.15	0.84
3:C:140:ASN:H	3:C:140:ASN:HD22	1.24	0.84
3:C:128:LEU:HB3	7:C:2061:HOH:O	1.75	0.84
2:F:160:GLU:H	2:F:179:ASN:HD21	1.23	0.84
2:B:159:ALA:O	2:F:183:LYS:HE2	1.78	0.83
1:A:601:GLY:N	7:A:2285:HOH:O	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:ARG:NH1	2:B:187:THR:CG2	2.41	0.83
3:C:168:LYS:HE2	7:C:2063:HOH:O	1.77	0.83
2:B:46:TYR:HD1	7:B:2032:HOH:O	1.51	0.83
3:G:139:ASN:H	3:G:139:ASN:HD22	1.27	0.83
1:A:42:GLN:NE2	1:A:505:ARG:HD3	1.92	0.83
1:E:590:ILE:CG1	7:E:2181:HOH:O	2.25	0.83
1:A:400:GLY:HA3	7:A:2196:HOH:O	1.79	0.83
1:E:614:PRO:HG2	7:E:2343:HOH:O	1.78	0.83
1:E:608:PHE:O	1:E:608:PHE:CD1	2.32	0.82
1:A:604:PRO:C	1:A:606:PRO:CD	2.48	0.82
3:G:196:GLU:HG2	7:G:2058:HOH:O	1.78	0.82
3:C:172:ALA:HA	3:C:175:PRO:HG2	1.60	0.82
1:E:116:THR:CG2	1:E:119:GLU:HB3	2.09	0.82
1:A:335:VAL:O	1:A:733:GLY:HA2	1.79	0.82
1:A:184:VAL:CG2	1:A:592:LEU:CD2	2.52	0.82
1:A:284:VAL:HG23	1:A:587:SER:HB3	1.61	0.82
1:E:498:LYS:HE2	7:E:2297:HOH:O	1.80	0.82
1:A:519:TRP:CE2	1:A:540:ILE:HG12	2.14	0.82
1:A:629:HIS:ND1	1:A:634:THR:HG23	1.93	0.82
3:G:206:GLY:O	3:G:210:GLY:N	2.12	0.82
2:F:47:PRO:HD2	7:F:2036:HOH:O	1.78	0.81
2:F:2:PRO:HD2	2:F:80:ASP:OD2	1.80	0.81
1:A:335:VAL:HG11	1:A:732:ALA:O	1.78	0.81
2:B:46:TYR:HE2	7:B:2029:HOH:O	1.59	0.81
1:E:510:GLU:HG3	7:E:2301:HOH:O	1.78	0.81
2:B:25:MET:CE	2:B:25:MET:HA	2.11	0.81
2:F:65:PRO:HD2	4:F:1196:SF4:S4	2.20	0.81
1:E:562:GLY:C	7:E:2316:HOH:O	2.08	0.81
1:A:97:ARG:NH2	1:A:763:ARG:NH2	2.19	0.81
2:B:117:THR:HG21	7:B:2095:HOH:O	1.81	0.81
1:A:653:LYS:HG3	1:A:684:PRO:O	1.81	0.81
3:G:154:THR:HG22	3:G:238:ARG:HE	1.45	0.80
1:A:607:VAL:HG13	1:A:609:THR:OG1	1.81	0.80
1:E:428:GLU:O	1:E:429:PRO:C	2.15	0.80
1:E:116:THR:HG22	1:E:119:GLU:CB	2.11	0.80
1:A:42:GLN:NE2	1:A:485:TYR:O	2.15	0.80
2:F:146:GLU:HG2	7:F:2004:HOH:O	1.80	0.80
1:E:283:THR:HG22	7:E:2182:HOH:O	1.80	0.80
1:A:207:GLY:O	5:A:1766:MGD:O5'	2.00	0.79
1:A:397:GLU:HB3	1:A:398:PRO:CD	2.06	0.79
1:E:388:CYS:SG	1:E:413:ARG:NE	2.55	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:GLY:CA	1:A:583:PHE:O	2.30	0.79
1:E:301:ALA:O	1:E:305:THR:HB	1.82	0.79
1:E:342:TYR:HD1	1:E:607:VAL:HB	1.46	0.79
1:E:494:LEU:HD22	1:E:502:ILE:HG12	1.65	0.79
1:A:48:PHE:CE1	1:A:145:HIS:CE1	2.71	0.79
1:A:429:PRO:O	1:A:430:TYR:CD2	2.35	0.79
1:A:604:PRO:C	1:A:606:PRO:HD3	2.03	0.78
1:A:686:ALA:HB3	7:A:2331:HOH:O	1.82	0.78
1:E:95:LEU:HD21	7:E:2278:HOH:O	1.82	0.78
1:A:183:TRP:CH2	1:A:596:ARG:HD3	2.17	0.78
1:A:413:ARG:H	1:A:413:ARG:CD	1.97	0.78
1:A:116:THR:HG22	1:A:119:GLU:HB3	1.64	0.78
3:C:53:ALA:O	3:C:57:ILE:HG13	1.81	0.78
1:A:583:PHE:HE2	1:A:588:GLY:H	1.25	0.78
1:A:591:GLU:HB3	1:A:603:GLN:HE22	1.48	0.78
1:A:602:HIS:HE1	1:A:606:PRO:HG3	1.03	0.78
7:B:2145:HOH:O	3:C:251:LEU:HD11	1.82	0.78
1:A:93:ASP:OD1	1:A:758:ARG:NH2	2.16	0.78
1:E:109:GLU:HG3	7:E:2068:HOH:O	1.83	0.78
1:A:605:LEU:HD23	1:A:605:LEU:H	1.48	0.78
1:E:608:PHE:CD1	1:E:608:PHE:C	2.57	0.78
1:A:602:HIS:ND1	1:A:606:PRO:HG3	1.98	0.78
2:F:72:THR:HG22	2:F:74:ALA:H	1.49	0.77
1:E:89:THR:OG1	1:E:484:THR:HG21	1.85	0.77
1:E:308:PRO:HB2	7:E:2198:HOH:O	1.84	0.77
1:A:591:GLU:O	1:A:592:LEU:HD12	1.83	0.77
1:A:740:ARG:NH1	7:A:2360:HOH:O	2.15	0.77
1:A:183:TRP:HH2	1:A:596:ARG:HD3	1.50	0.77
1:A:256:THR:HG21	1:A:305:THR:HA	1.67	0.77
1:E:648:GLU:HG2	1:E:681:ARG:HH12	1.47	0.77
1:A:585:THR:O	1:A:586:ALA:CB	2.32	0.77
1:E:305:THR:HG22	1:E:307:ILE:H	1.50	0.77
1:A:629:HIS:HA	1:A:634:THR:HG21	1.67	0.76
2:B:41:ARG:NH1	2:B:187:THR:HG22	2.00	0.76
1:A:70:ALA:O	7:A:2037:HOH:O	2.01	0.76
3:C:140:ASN:H	3:C:140:ASN:ND2	1.84	0.76
1:A:605:LEU:H	1:A:605:LEU:CD2	1.99	0.76
3:C:155:THR:HG21	3:C:239:ARG:HG2	1.68	0.76
1:A:633:ARG:HD2	5:A:1765:MGD:O2B	1.85	0.75
1:E:305:THR:CG2	1:E:307:ILE:H	1.99	0.75
3:C:155:THR:CG2	3:C:239:ARG:HE	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:HD2	1:A:220:GLN:HE22	1.49	0.75
1:E:629:HIS:ND1	1:E:634:THR:HG23	2.02	0.75
3:C:207:GLY:O	3:C:209:TRP:N	2.19	0.75
1:A:580:ARG:HH11	1:A:580:ARG:HB3	1.49	0.75
1:E:81:ARG:HG2	1:E:628:VAL:O	1.86	0.75
1:E:311:VAL:HB	7:E:2198:HOH:O	1.85	0.75
1:A:390:GLY:H	1:A:595:GLN:HE22	1.34	0.75
1:E:421:ILE:HG23	1:E:421:ILE:O	1.84	0.75
1:A:393:GLY:HA3	1:A:407:LYS:HE3	1.68	0.75
1:A:677:GLU:O	1:A:678:GLY:O	2.05	0.75
1:E:488:ARG:HD3	1:E:490:ASP:OD2	1.87	0.74
1:E:95:LEU:HD11	7:E:2278:HOH:O	1.85	0.74
1:E:438:TYR:HD2	7:E:2094:HOH:O	1.69	0.74
1:E:605:LEU:H	1:E:605:LEU:HD23	0.59	0.74
1:E:256:THR:HG21	1:E:305:THR:HA	1.68	0.74
1:A:279:VAL:HG13	1:A:283:THR:CG2	2.14	0.74
1:E:469:PRO:O	1:E:706:MET:HG3	1.87	0.74
1:E:685:THR:HG22	2:F:42:GLU:CD	2.07	0.74
1:A:138:GLU:OE2	1:A:402:LYS:HB2	1.87	0.74
3:C:173:LEU:HG	3:C:173:LEU:O	1.87	0.74
2:B:41:ARG:HH11	2:B:187:THR:HG23	1.51	0.74
3:G:111:SER:O	3:G:115:LEU:HD12	1.88	0.74
1:E:109:GLU:CG	7:E:2068:HOH:O	2.34	0.74
1:A:388:CYS:HA	1:A:593:TYR:OH	1.86	0.73
1:E:421:ILE:O	1:E:421:ILE:CG2	2.35	0.73
1:A:457:LYS:HA	7:A:2224:HOH:O	1.88	0.73
1:E:297:THR:HG23	1:E:299:GLU:H	1.52	0.73
1:A:42:GLN:HE22	1:A:505:ARG:HD3	1.52	0.73
1:E:592:LEU:CD2	1:E:603:GLN:HE22	2.02	0.73
2:B:57:GLN:HE22	2:B:140:ARG:HH22	1.34	0.73
2:F:1:MET:HA	7:F:2001:HOH:O	1.89	0.73
1:A:75:ARG:HH11	1:A:220:GLN:NE2	1.86	0.73
3:C:235:ALA:O	3:C:239:ARG:HG3	1.89	0.73
1:E:323:LYS:C	7:E:2213:HOH:O	2.17	0.73
1:E:453:LYS:HG2	1:E:475:TRP:CH2	2.24	0.73
1:A:320:ALA:O	1:A:323:LYS:HG2	1.90	0.72
1:A:651:ILE:HD11	1:A:682:VAL:CG1	2.19	0.72
1:E:277:GLU:O	1:E:281:LYS:HG2	1.88	0.72
1:E:539:THR:HG23	1:E:542:GLU:H	1.54	0.72
1:A:393:GLY:HA3	1:A:407:LYS:CE	2.20	0.72
1:E:397:GLU:HB3	1:E:398:PRO:CD	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:592:LEU:HD23	1:E:603:GLN:NE2	2.04	0.72
1:E:604:PRO:O	1:E:606:PRO:CD	2.37	0.72
3:G:234:ALA:O	3:G:238:ARG:HG3	1.88	0.72
3:C:155:THR:HG21	3:C:239:ARG:CG	2.20	0.72
2:B:16:CYS:O	2:B:18:ALA:N	2.21	0.72
3:C:241:LEU:C	3:C:241:LEU:HD12	2.10	0.72
1:A:153:VAL:HG11	1:A:167:LYS:HE2	1.71	0.72
1:A:647:ASN:C	1:A:648:GLU:HG3	2.11	0.72
1:A:395:ASP:O	1:A:399:GLU:CB	2.32	0.71
1:E:69:GLU:O	1:E:70:ALA:HB3	1.90	0.71
1:E:75:ARG:HH11	1:E:220:GLN:HE21	1.38	0.71
1:E:431:PRO:HD2	7:E:2262:HOH:O	1.90	0.71
1:E:239:PHE:HB3	1:E:687:ARG:HB3	1.72	0.71
1:A:285:GLY:O	1:A:590:ILE:HG23	1.90	0.71
1:A:170:VAL:O	1:A:175:ALA:CB	2.39	0.71
1:A:519:TRP:NE1	1:A:540:ILE:HG12	2.04	0.71
2:B:160:GLU:H	2:B:179:ASN:ND2	1.86	0.71
1:E:397:GLU:CB	1:E:398:PRO:HD3	2.21	0.71
1:A:428:GLU:HB3	1:A:429:PRO:CD	2.17	0.71
1:A:672:GLN:NE2	1:A:738:PHE:H	1.89	0.71
2:F:67:VAL:HB	2:F:68:PRO:HD3	1.71	0.71
1:E:473:VAL:HG11	7:E:2278:HOH:O	1.90	0.71
3:G:206:GLY:O	3:G:207:PHE:C	2.29	0.71
1:A:183:TRP:HE1	1:A:413:ARG:HH22	1.39	0.71
1:A:231:LYS:HA	1:A:247:HIS:CD2	2.25	0.70
1:A:342:TYR:CD1	1:A:607:VAL:HB	2.27	0.70
1:A:595:GLN:CG	1:A:595:GLN:O	2.39	0.70
2:F:117:THR:HG23	2:F:120:ALA:H	1.56	0.70
3:G:222:GLN:OE1	3:G:222:GLN:HA	1.91	0.70
1:A:427:GLY:O	1:A:428:GLU:O	2.08	0.70
1:E:38:LYS:HG3	7:E:2024:HOH:O	1.91	0.70
1:E:717:ASN:HD22	5:E:1765:MGD:H192	1.39	0.70
1:A:184:VAL:HG22	1:A:592:LEU:HD23	1.72	0.70
1:E:100:ILE:HG12	1:E:478:VAL:HG22	1.72	0.70
2:F:41:ARG:HH11	2:F:187:THR:HG23	1.55	0.70
3:G:107:LEU:O	3:G:109:LYS:N	2.23	0.70
1:E:113:ARG:NH1	1:E:114:VAL:HG13	2.06	0.70
1:E:478:VAL:HG23	7:E:2283:HOH:O	1.91	0.70
1:E:511:PRO:HB3	1:E:515:THR:CG2	2.21	0.70
1:A:721:THR:HG22	1:A:722:ARG:HG3	1.73	0.70
1:E:75:ARG:HH11	1:E:220:GLN:NE2	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:206:GLY:HA2	3:G:209:TYR:HB3	1.72	0.70
3:G:21:PHE:O	3:G:238:ARG:NH1	2.25	0.69
1:A:428:GLU:O	1:A:429:PRO:C	2.28	0.69
1:E:297:THR:CG2	1:E:299:GLU:H	2.04	0.69
1:A:510:GLU:HG3	7:A:2024:HOH:O	1.92	0.69
1:A:595:GLN:O	1:A:595:GLN:HG3	1.92	0.69
1:A:651:ILE:HD13	1:A:656:ALA:HB2	1.72	0.69
2:B:190:SER:HB3	3:C:252:GLY:N	2.06	0.69
3:C:171:TRP:O	3:C:172:ALA:HB2	1.92	0.69
1:E:339:ASP:CB	1:E:607:VAL:HG11	2.22	0.69
1:A:346:ALA:HB2	1:A:605:LEU:CD1	2.22	0.69
1:A:605:LEU:HD23	1:A:605:LEU:N	2.07	0.69
3:C:101:LEU:O	3:C:105:LEU:HD12	1.92	0.69
1:A:209:HIS:HE1	1:A:625:ARG:H	1.41	0.69
1:A:625:ARG:HH22	5:A:1765:MGD:H15	1.41	0.69
1:A:377:PRO:HG2	1:A:533:GLN:HG3	1.75	0.69
1:A:608:PHE:CD1	1:A:608:PHE:C	2.66	0.69
1:E:635:GLN:NE2	1:E:635:GLN:H	1.91	0.69
1:A:561:MET:O	1:A:563:THR:N	2.25	0.69
1:A:390:GLY:N	1:A:595:GLN:HE22	1.91	0.68
1:A:467:VAL:HG13	7:A:2050:HOH:O	1.93	0.68
2:B:41:ARG:HD2	2:B:187:THR:HG23	1.75	0.68
3:C:108:LEU:O	3:C:110:LYS:CG	2.42	0.68
1:E:116:THR:HG21	7:E:2074:HOH:O	1.93	0.68
1:E:671:ASN:C	1:E:671:ASN:HD22	1.96	0.68
1:A:611:PRO:HB3	7:A:2138:HOH:O	1.91	0.68
1:A:629:HIS:CA	1:A:634:THR:HG21	2.23	0.68
1:A:729:SER:O	1:A:729:SER:OG	2.03	0.68
1:E:183:TRP:HH2	1:E:596:ARG:HD3	1.57	0.68
1:A:367:GLN:HG3	7:A:2272:HOH:O	1.93	0.68
3:C:21:HIS:HE1	3:C:64:LEU:HD11	1.59	0.68
1:E:91:ASP:O	1:E:92:PRO:O	2.12	0.68
1:A:393:GLY:HA3	1:A:407:LYS:NZ	2.07	0.68
3:C:197:GLU:HG2	7:C:2073:HOH:O	1.92	0.68
2:F:40:GLU:HB2	7:F:2022:HOH:O	1.94	0.68
1:E:591:GLU:OE2	1:E:604:PRO:HG3	1.94	0.68
3:G:139:ASN:H	3:G:139:ASN:ND2	1.92	0.68
1:A:232:VAL:H	1:A:247:HIS:HD2	1.40	0.68
1:E:100:ILE:HG23	1:E:478:VAL:HG22	1.74	0.68
1:E:673:ASP:OD2	1:E:721:THR:CG2	2.42	0.68
1:A:166:ALA:HB2	1:A:415:THR:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:539:THR:HG22	1:E:542:GLU:CB	2.24	0.67
3:G:76:ILE:O	3:G:80:LEU:HG	1.94	0.67
3:C:145:ASN:C	3:C:145:ASN:HD22	1.95	0.67
1:E:69:GLU:O	1:E:70:ALA:CB	2.42	0.67
1:A:382:GLU:HA	7:A:2188:HOH:O	1.93	0.67
7:A:2015:HOH:O	2:B:25:MET:HE1	1.93	0.67
1:E:577:LYS:HE2	7:E:2323:HOH:O	1.94	0.67
2:F:72:THR:HG23	2:F:89:LYS:HB3	1.77	0.67
2:F:169:GLN:NE2	7:F:2108:HOH:O	2.27	0.67
1:A:77:ARG:NH1	2:B:138:TYR:CE2	2.39	0.67
1:A:422:GLU:HB3	1:A:423:PRO:HD3	1.76	0.67
1:A:79:CYS:HB2	1:A:80:PRO:HD2	1.77	0.67
2:B:47:PRO:O	2:B:48:ASN:OD1	2.13	0.67
1:A:604:PRO:C	1:A:606:PRO:HD2	2.12	0.67
2:B:25:MET:HA	2:B:25:MET:HE2	1.77	0.67
1:E:88:THR:HG23	1:E:468:LEU:HD21	1.76	0.67
1:E:648:GLU:HG2	1:E:681:ARG:NH1	2.10	0.67
1:E:734:LEU:HD22	7:E:2420:HOH:O	1.94	0.67
1:A:653:LYS:HD2	1:A:686:ALA:H	1.59	0.66
1:E:118:GLU:HG3	7:E:2307:HOH:O	1.95	0.66
1:A:36:GLU:O	1:A:58:VAL:HG22	1.96	0.66
1:A:209:HIS:O	1:A:213:ASP:HB3	1.94	0.66
1:E:762:GLU:HB2	7:E:2445:HOH:O	1.94	0.66
2:F:3:ARG:HG2	7:F:2003:HOH:O	1.95	0.66
3:G:51:TYR:N	7:G:2015:HOH:O	2.29	0.66
2:F:55:PRO:HG2	4:F:1194:SF4:S2	2.34	0.66
3:G:206:GLY:HA2	3:G:209:TYR:CB	2.25	0.66
1:A:673:ASP:OD2	1:A:721:THR:HG21	1.95	0.66
1:E:183:TRP:CH2	1:E:596:ARG:HD3	2.31	0.66
1:E:438:TYR:CD2	7:E:2094:HOH:O	2.47	0.66
1:E:465:ILE:O	1:E:466:ASP:HB3	1.94	0.66
2:F:117:THR:HG21	7:F:2078:HOH:O	1.94	0.66
3:G:115:LEU:HD13	7:G:2032:HOH:O	1.95	0.66
1:E:259:ALA:HB3	7:E:2196:HOH:O	1.96	0.66
1:E:297:THR:CG2	1:E:299:GLU:HG2	2.26	0.66
3:G:12:PHE:CZ	3:G:246:GLN:HG2	2.30	0.66
1:A:301:ALA:O	1:A:305:THR:HB	1.96	0.66
1:A:413:ARG:H	1:A:413:ARG:HD2	1.59	0.66
2:B:46:TYR:CE2	7:B:2033:HOH:O	2.49	0.66
1:E:746:ARG:HG3	1:E:746:ARG:HH11	1.61	0.66
1:A:89:THR:OG1	1:A:484:THR:HG21	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TYR:HD1	1:A:607:VAL:HB	1.60	0.65
1:A:429:PRO:O	1:A:430:TYR:CG	2.49	0.65
2:F:43:VAL:HG23	7:F:2122:HOH:O	1.96	0.65
2:F:72:THR:HG21	2:F:89:LYS:O	1.95	0.65
2:B:47:PRO:HD3	7:B:2034:HOH:O	1.96	0.65
2:B:72:THR:HG21	2:B:89:LYS:O	1.96	0.65
1:E:591:GLU:O	1:E:591:GLU:HG3	1.96	0.65
1:A:286:PHE:HA	1:A:590:ILE:HG21	1.78	0.65
2:F:57:GLN:HE21	2:F:140:ARG:HH22	1.44	0.65
1:A:186:GLY:H	1:A:583:PHE:HA	1.62	0.65
3:C:21:HIS:CE1	3:C:64:LEU:HD21	2.32	0.65
1:A:293:VAL:HG13	1:A:293:VAL:O	1.95	0.65
1:A:632:ALA:O	1:A:635:GLN:HG3	1.95	0.65
3:C:21:HIS:ND1	3:C:64:LEU:HG	2.11	0.65
1:E:673:ASP:OD2	1:E:721:THR:HG21	1.96	0.65
1:A:330:PRO:HD2	7:A:2168:HOH:O	1.96	0.65
1:A:396:HIS:HB3	1:A:403:PRO:HB3	1.78	0.65
1:A:305:THR:O	1:A:306:GLU:HB2	1.96	0.65
3:G:129:TYR:CD2	3:G:130:PRO:HD3	2.31	0.65
1:E:589:LYS:HB3	1:E:592:LEU:HB2	1.78	0.64
1:A:174:THR:HG23	1:A:178:GLU:HG2	1.80	0.64
1:A:400:GLY:CA	7:A:2196:HOH:O	2.39	0.64
1:A:606:PRO:O	1:A:608:PHE:N	2.29	0.64
1:E:97:ARG:NH2	1:E:763:ARG:HD2	2.11	0.64
1:E:139:ALA:O	1:E:433:LYS:O	2.15	0.64
1:E:602:HIS:CD2	1:E:604:PRO:CD	2.75	0.64
2:F:47:PRO:CD	7:F:2036:HOH:O	2.40	0.64
1:A:134:LYS:HE2	7:A:2079:HOH:O	1.96	0.64
1:E:232:VAL:H	1:E:247:HIS:CD2	2.16	0.64
1:A:395:ASP:C	1:A:399:GLU:HB2	2.18	0.64
1:E:305:THR:HG23	1:E:307:ILE:HG12	1.79	0.64
1:E:589:LYS:NZ	7:E:2326:HOH:O	2.29	0.64
1:E:639:VAL:HG11	2:F:25:MET:HE3	1.78	0.64
2:F:3:ARG:HD2	2:F:62:GLU:OE2	1.96	0.64
3:G:150:LEU:O	3:G:154:THR:HB	1.98	0.64
2:B:25:MET:HA	2:B:25:MET:HE3	1.79	0.64
1:E:232:VAL:H	1:E:247:HIS:HD2	1.46	0.64
1:E:311:VAL:CB	7:E:2198:HOH:O	2.45	0.64
1:E:323:LYS:CD	1:E:354:LEU:HA	2.02	0.64
1:E:589:LYS:HG2	1:E:592:LEU:HD12	1.80	0.64
1:A:642:GLU:HG2	2:B:34:PHE:HZ	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ASN:HD22	1:E:74:SER:H	1.45	0.64
1:E:116:THR:HG22	1:E:119:GLU:H	1.59	0.64
1:E:346:ALA:N	1:E:605:LEU:HD12	2.13	0.64
1:E:153:VAL:HG11	1:E:167:LYS:HE2	1.80	0.64
3:G:154:THR:HG21	3:G:238:ARG:HG2	1.80	0.64
1:A:483:ALA:HA	1:A:515:THR:CG2	2.27	0.64
1:A:519:TRP:CE2	1:A:540:ILE:CG1	2.80	0.64
1:E:575:TRP:O	1:E:578:GLU:HB2	1.97	0.64
3:G:225:LEU:HB3	7:G:2070:HOH:O	1.97	0.64
1:E:686:ALA:HB1	7:E:2386:HOH:O	1.97	0.63
1:E:708:LEU:HA	7:E:2408:HOH:O	1.98	0.63
3:G:154:THR:CG2	3:G:238:ARG:NE	2.58	0.63
1:E:434:GLY:HA2	1:E:461:LEU:O	1.97	0.63
1:A:349:TYR:CE2	1:A:590:ILE:O	2.52	0.63
1:E:100:ILE:HG23	1:E:478:VAL:CG2	2.28	0.63
1:E:465:ILE:O	1:E:466:ASP:CB	2.47	0.63
1:A:152:PHE:O	1:A:157:PRO:HD3	1.98	0.63
1:A:336:TRP:HD1	1:A:336:TRP:H	1.46	0.63
1:A:73:LYS:NZ	1:A:192:HIS:HD2	1.95	0.63
1:A:238:ARG:HG3	1:A:688:ILE:HD12	1.80	0.63
1:A:488:ARG:NH2	5:A:1765:MGD:O6	2.31	0.63
1:A:349:TYR:HE1	1:A:605:LEU:HD21	1.64	0.63
1:A:602:HIS:ND1	1:A:606:PRO:CG	2.58	0.63
2:B:17:ALA:HB1	2:B:20:ALA:HB3	1.81	0.63
1:E:97:ARG:HH21	1:E:763:ARG:NH1	1.95	0.63
1:E:651:ILE:HD11	1:E:682:VAL:CG1	2.29	0.63
1:A:495:VAL:HG13	7:A:2020:HOH:O	1.98	0.63
1:A:511:PRO:HB3	1:A:515:THR:HG22	1.80	0.63
2:B:134:THR:O	2:B:134:THR:HG22	1.93	0.62
3:C:222:TRP:CG	3:C:223:GLN:N	2.62	0.62
1:E:470:GLN:HG2	1:E:706:MET:SD	2.38	0.62
2:F:160:GLU:H	2:F:179:ASN:ND2	1.96	0.62
1:A:37:VAL:HG12	1:A:38:LYS:N	2.13	0.62
1:A:484:THR:HG22	1:A:487:GLU:HG3	1.81	0.62
1:E:424:MET:HG2	1:E:459:LEU:HD21	1.81	0.62
3:G:206:GLY:O	3:G:209:TYR:CA	2.46	0.62
1:A:166:ALA:HB2	1:A:415:THR:CG2	2.28	0.62
1:A:642:GLU:OE2	2:B:31:PRO:O	2.17	0.62
1:E:30:ALA:HB3	7:E:2002:HOH:O	1.98	0.62
1:E:632:ALA:O	1:E:635:GLN:NE2	2.32	0.62
1:A:127:LYS:HE2	7:A:2227:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:HIS:HE1	1:E:625:ARG:N	1.94	0.62
1:E:622:LEU:HD22	5:E:1766:MGD:H8	1.80	0.62
1:E:253:LYS:O	1:E:256:THR:HB	1.99	0.62
1:E:588:GLY:HA3	7:E:2178:HOH:O	1.99	0.62
1:A:95:LEU:HD11	1:A:468:LEU:O	1.99	0.62
1:E:75:ARG:HD2	1:E:220:GLN:HE22	1.65	0.62
2:F:45:GLU:HB2	7:F:2029:HOH:O	1.99	0.62
1:E:658:ARG:C	1:E:659:LEU:O	2.37	0.61
1:E:720:GLN:HB3	7:E:2420:HOH:O	2.00	0.61
1:A:75:ARG:HH11	1:A:220:GLN:HE21	1.47	0.61
1:A:195:ILE:HA	1:A:362:GLY:O	2.00	0.61
2:B:78:THR:HG21	7:B:2067:HOH:O	2.00	0.61
1:A:647:ASN:H	1:A:647:ASN:HD22	1.46	0.61
2:B:121:HIS:O	2:B:125:LYS:HE2	2.00	0.61
1:E:391:PRO:O	1:E:413:ARG:HG2	2.00	0.61
1:E:551:LEU:O	1:E:553:LEU:HB2	2.00	0.61
2:B:46:TYR:O	7:B:2030:HOH:O	2.15	0.61
3:C:18:ASN:OD1	3:C:67:GLU:OE2	2.17	0.61
2:F:78:THR:HG21	7:F:2060:HOH:O	2.00	0.61
7:E:2386:HOH:O	2:F:49:LEU:HD11	2.01	0.61
1:A:183:TRP:CB	1:A:592:LEU:HD22	2.30	0.61
1:A:339:ASP:HB3	1:A:607:VAL:HG11	1.82	0.61
1:A:578:GLU:HB3	1:A:580:ARG:HD3	1.82	0.61
1:A:603:GLN:HB3	1:A:604:PRO:CD	2.27	0.61
2:B:44:GLY:O	2:B:49:LEU:HD13	2.01	0.61
1:E:589:LYS:HG2	1:E:592:LEU:CD1	2.31	0.61
1:A:387:GLY:O	1:A:593:TYR:CE1	2.54	0.61
1:A:581:LEU:HD11	7:A:2275:HOH:O	2.00	0.61
1:A:604:PRO:O	1:A:606:PRO:HD3	1.95	0.61
2:F:193:HIS:HB2	7:F:2130:HOH:O	2.00	0.61
1:A:581:LEU:CD1	7:A:2275:HOH:O	2.49	0.60
1:E:488:ARG:HB2	1:E:517:PRO:HB3	1.82	0.60
2:F:88:LYS:O	3:G:74:THR:HG22	2.00	0.60
1:A:687:ARG:NH2	2:B:40:GLU:OE2	2.33	0.60
1:A:232:VAL:H	1:A:247:HIS:CD2	2.18	0.60
1:A:293:VAL:O	1:A:293:VAL:CG1	2.48	0.60
1:A:635:GLN:O	1:A:709:ALA:HB2	2.01	0.60
2:F:41:ARG:HD2	2:F:187:THR:HG21	1.80	0.60
1:A:580:ARG:HH11	1:A:580:ARG:HB2	1.67	0.60
1:A:672:GLN:HE22	1:A:738:PHE:H	1.46	0.60
1:E:174:THR:HG23	1:E:178:GLU:HG2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:ASP:C	1:E:478:VAL:HG23	2.15	0.60
1:E:633:ARG:HD2	5:E:1765:MGD:O2B	2.01	0.60
1:A:95:LEU:HD12	1:A:467:VAL:C	2.22	0.60
1:A:239:PHE:HB3	1:A:687:ARG:HB3	1.84	0.60
1:A:314:GLU:HG2	7:A:2165:HOH:O	2.01	0.60
1:A:346:ALA:HB2	1:A:605:LEU:HD13	1.82	0.60
2:B:117:THR:HG22	2:B:119:CYS:N	2.16	0.60
1:A:305:THR:HG22	1:A:307:ILE:H	1.67	0.60
1:E:569:LYS:CD	7:E:2322:HOH:O	2.40	0.60
1:A:71:ASN:HD22	1:A:74:SER:H	1.47	0.60
1:A:338:GLY:O	1:A:726:ASP:HA	2.02	0.60
1:A:349:TYR:CE1	1:A:605:LEU:HD21	2.37	0.60
1:A:428:GLU:O	1:A:430:TYR:N	2.35	0.60
1:E:297:THR:HG21	7:E:2087:HOH:O	2.01	0.60
2:B:2:PRO:HB3	2:B:144:ASP:CG	2.22	0.60
3:C:47:ARG:NH1	3:C:107:TYR:O	2.35	0.60
1:E:267:VAL:HG22	7:E:2200:HOH:O	2.01	0.60
2:F:117:THR:HG22	2:F:119:CYS:H	1.66	0.59
1:A:153:VAL:CG1	1:A:167:LYS:HE2	2.33	0.59
3:C:241:LEU:C	3:C:241:LEU:CD1	2.69	0.59
1:E:284:VAL:HG12	1:E:592:LEU:CD1	2.32	0.59
1:A:139:ALA:O	1:A:433:LYS:O	2.20	0.59
1:A:580:ARG:CB	1:A:580:ARG:NH1	2.63	0.59
3:C:171:TRP:O	3:C:171:TRP:HE3	1.81	0.59
1:A:231:LYS:HA	1:A:247:HIS:NE2	2.17	0.59
1:A:284:VAL:O	1:A:590:ILE:CG2	2.38	0.59
1:A:391:PRO:O	1:A:413:ARG:HB3	2.03	0.59
1:A:183:TRP:HB2	1:A:592:LEU:HD22	1.85	0.59
2:B:44:GLY:O	2:B:49:LEU:CD1	2.50	0.59
2:B:47:PRO:CD	7:B:2034:HOH:O	2.50	0.59
1:E:553:LEU:HD21	1:E:557:THR:HG21	1.85	0.59
1:E:608:PHE:C	7:E:2337:HOH:O	2.33	0.59
1:E:79:CYS:HB2	1:E:80:PRO:HD2	1.85	0.59
1:A:335:VAL:HG13	1:A:732:ALA:O	2.00	0.59
1:A:428:GLU:CB	1:A:429:PRO:HD2	2.24	0.59
1:A:642:GLU:HG2	2:B:34:PHE:CZ	2.37	0.59
1:E:318:GLU:O	1:E:322:HIS:HD2	1.86	0.59
1:E:539:THR:CG2	1:E:542:GLU:H	2.16	0.59
1:E:740:ARG:NH1	7:E:2427:HOH:O	2.35	0.59
1:E:585:THR:OG1	1:E:589:LYS:HE3	2.02	0.58
1:A:360:PRO:HD3	1:A:571:TRP:CZ3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:607:VAL:O	1:E:607:VAL:HG13	1.98	0.58
1:A:99:LEU:O	1:A:478:VAL:HA	2.04	0.58
1:E:495:VAL:CG2	7:E:2299:HOH:O	2.51	0.58
1:E:597:PHE:HB3	7:E:2327:HOH:O	2.02	0.58
3:G:105:LEU:HG	7:G:2032:HOH:O	2.01	0.58
3:G:207:PHE:HE2	3:G:211:LEU:CD1	2.03	0.58
1:A:152:PHE:O	1:A:157:PRO:CD	2.52	0.58
1:A:539:THR:CG2	1:A:541:GLU:HG2	2.34	0.58
1:A:685:THR:HB	2:B:42:GLU:CD	2.23	0.58
2:F:43:VAL:CG2	7:F:2122:HOH:O	2.52	0.58
1:E:282:TYR:O	1:E:587:SER:HB3	2.03	0.58
1:E:490:ASP:O	7:E:2290:HOH:O	2.17	0.58
2:F:194:HIS:N	7:F:2129:HOH:O	2.35	0.58
3:G:105:LEU:HB3	7:G:2011:HOH:O	2.04	0.58
1:E:310:GLN:NE2	1:E:314:GLU:OE2	2.36	0.58
1:E:708:LEU:O	1:E:712:ARG:HD2	2.04	0.58
1:A:413:ARG:H	1:A:413:ARG:NE	2.00	0.58
2:B:192:VAL:HG12	2:B:193:HIS:N	2.19	0.58
1:A:335:VAL:HG13	1:A:732:ALA:C	2.23	0.58
1:A:603:GLN:CB	1:A:604:PRO:HD3	2.27	0.58
1:A:755:LEU:O	1:A:758:ARG:HD3	2.04	0.58
2:B:117:THR:HB	7:B:2010:HOH:O	2.03	0.58
2:F:41:ARG:HH11	2:F:187:THR:HG22	1.68	0.58
1:A:53:ILE:HD12	1:A:65:VAL:HG22	1.86	0.57
1:A:583:PHE:CE2	1:A:587:SER:C	2.77	0.57
1:A:653:LYS:CG	1:A:684:PRO:O	2.52	0.57
3:C:171:TRP:O	3:C:172:ALA:CB	2.51	0.57
1:E:670:VAL:HG22	1:E:676:LYS:HG3	1.85	0.57
1:E:672:GLN:NE2	1:E:738:PHE:H	2.02	0.57
1:A:116:THR:HG22	1:A:119:GLU:N	2.10	0.57
1:A:388:CYS:HA	1:A:593:TYR:CE1	2.39	0.57
1:A:631:PHE:O	1:A:698:GLY:HA3	2.04	0.57
1:E:606:PRO:CD	1:E:607:VAL:H	2.15	0.57
1:A:121:LEU:HD13	1:A:524:GLU:HB3	1.86	0.57
1:E:108:GLY:HA3	7:E:2066:HOH:O	2.03	0.57
3:G:221:TRP:HZ3	3:G:225:LEU:HD13	1.69	0.57
2:F:78:THR:HG22	2:F:80:ASP:H	1.69	0.57
1:A:120:ALA:HB3	7:A:2068:HOH:O	2.04	0.57
1:A:109:GLU:OE2	1:A:111:LYS:HE2	2.03	0.57
1:E:649:VAL:HG13	1:E:695:ILE:CG2	2.35	0.57
1:E:297:THR:HG23	1:E:299:GLU:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:TYR:CD2	3:C:131:PRO:HD3	2.39	0.57
1:E:209:HIS:CE1	1:E:625:ARG:H	2.15	0.57
3:G:38:HIS:CE1	7:G:2011:HOH:O	2.57	0.57
1:A:427:GLY:O	1:A:430:TYR:O	2.23	0.57
1:E:539:THR:HG22	1:E:542:GLU:HB2	1.87	0.57
1:A:292:HIS:NE2	1:A:604:PRO:HB2	2.20	0.56
3:C:128:LEU:HD22	7:C:2061:HOH:O	2.05	0.56
1:E:669:LEU:CD2	1:E:741:LEU:HD22	2.35	0.56
1:A:594:CYS:O	1:A:598:LYS:HG3	2.05	0.56
1:A:630:THR:H	1:A:634:THR:HG21	1.70	0.56
3:C:171:TRP:O	3:C:171:TRP:CG	2.58	0.56
1:A:345:MET:HE3	1:A:592:LEU:HD11	1.87	0.56
1:A:607:VAL:O	1:A:607:VAL:CG1	2.48	0.56
2:B:117:THR:CG2	2:B:120:ALA:H	2.18	0.56
3:C:207:GLY:O	3:C:208:PHE:C	2.41	0.56
1:E:418:GLN:H	1:E:418:GLN:NE2	2.03	0.56
1:E:479:ILE:O	1:E:480:LEU:HD23	2.06	0.56
1:E:642:GLU:HG3	7:E:2436:HOH:O	2.05	0.56
1:A:583:PHE:HE2	1:A:588:GLY:CA	2.17	0.56
1:A:646:GLU:O	1:A:648:GLU:OE2	2.23	0.56
2:B:36:LEU:HD11	7:B:2104:HOH:O	2.05	0.56
7:B:2027:HOH:O	3:C:2:ALA:HB1	2.05	0.56
1:A:382:GLU:HB3	7:A:2189:HOH:O	2.05	0.56
1:A:534:TYR:O	1:A:535:PHE:HB2	2.05	0.56
1:E:591:GLU:O	1:E:603:GLN:NE2	2.39	0.56
1:E:647:ASN:HD21	1:E:714:ALA:H	1.52	0.56
2:B:57:GLN:O	2:B:58:CYS:C	2.43	0.56
1:A:252:ILE:CD1	1:A:256:THR:HG22	2.35	0.56
1:A:428:GLU:O	1:A:430:TYR:O	2.24	0.56
2:B:88:LYS:O	3:C:75:THR:HG22	2.05	0.56
3:C:59:LEU:O	3:C:63:ILE:HG23	2.06	0.56
1:E:511:PRO:CB	1:E:515:THR:HG22	2.28	0.56
1:E:539:THR:HG22	1:E:542:GLU:HB3	1.87	0.56
1:A:558:MET:HE2	1:A:558:MET:HA	1.87	0.56
1:E:311:VAL:CG2	7:E:2198:HOH:O	2.54	0.56
1:A:37:VAL:HG13	1:A:57:ALA:O	2.07	0.56
1:A:633:ARG:CD	5:A:1765:MGD:O2B	2.54	0.56
3:C:155:THR:CG2	3:C:239:ARG:NE	2.69	0.56
1:A:335:VAL:HG13	1:A:733:GLY:HA2	1.88	0.55
1:A:345:MET:HG2	1:A:592:LEU:HD21	1.88	0.55
2:B:27:ASN:HD21	2:B:121:HIS:CE1	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:THR:HG23	2:B:89:LYS:HB3	1.88	0.55
1:E:647:ASN:H	1:E:647:ASN:HD22	1.52	0.55
2:B:3:ARG:HG2	7:B:2001:HOH:O	2.06	0.55
2:B:57:GLN:NE2	7:B:2045:HOH:O	2.39	0.55
3:C:239:ARG:NH2	7:C:2082:HOH:O	2.37	0.55
1:E:474:MET:HE2	7:E:2070:HOH:O	2.05	0.55
3:G:196:GLU:CD	3:G:196:GLU:H	2.07	0.55
2:B:142:PHE:C	2:B:152:VAL:HG22	2.26	0.55
3:C:17:THR:CG2	3:C:67:GLU:CG	2.77	0.55
3:C:197:GLU:CD	3:C:197:GLU:H	2.10	0.55
1:E:77:ARG:NE	7:E:2048:HOH:O	2.39	0.55
2:F:164:VAL:HG22	2:F:173:PRO:HB2	1.88	0.55
1:A:39:SER:HB2	7:A:2005:HOH:O	2.06	0.55
2:B:166:ARG:NH2	3:C:249:GLN:NE2	2.54	0.55
3:C:140:ASN:HD22	3:C:140:ASN:N	2.02	0.55
1:A:319:MET:CE	1:A:328:LEU:HD11	2.36	0.55
1:E:590:ILE:HB	7:E:2181:HOH:O	2.06	0.55
1:E:687:ARG:NH2	2:F:40:GLU:OE2	2.40	0.55
3:G:220:PHE:HD1	7:G:2066:HOH:O	1.90	0.55
1:A:635:GLN:HG3	1:A:701:HIS:NE2	2.22	0.55
1:E:671:ASN:ND2	1:E:673:ASP:H	2.05	0.55
1:E:679:PRO:HG2	1:E:747:PRO:HB3	1.89	0.55
1:A:658:ARG:C	1:A:659:LEU:O	2.39	0.55
2:B:166:ARG:HH22	3:C:249:GLN:NE2	2.04	0.55
1:E:686:ALA:CB	7:E:2386:HOH:O	2.54	0.55
3:G:30:VAL:HG12	3:G:52:ALA:HB2	1.89	0.55
1:A:42:GLN:O	1:A:53:ILE:HG12	2.06	0.55
1:E:604:PRO:C	1:E:606:PRO:HD3	2.28	0.55
3:G:208:TRP:HA	3:G:208:TRP:CE3	2.42	0.55
1:A:609:THR:O	1:A:610:PRO:C	2.45	0.54
1:E:90:TYR:OH	1:E:509:HIS:HE1	1.90	0.54
1:E:549:GLN:HG3	7:E:2313:HOH:O	2.08	0.54
1:A:519:TRP:CZ2	1:A:540:ILE:HG13	2.43	0.54
1:A:364:TYR:HB2	1:A:570:PRO:HB3	1.89	0.54
1:A:426:THR:HG23	7:A:2052:HOH:O	2.07	0.54
2:B:114:SER:O	2:B:115:LYS:HB3	2.07	0.54
1:E:204:VAL:HB	1:E:328:LEU:HG	1.90	0.54
1:E:345:MET:HB2	1:E:605:LEU:HD13	1.89	0.54
1:E:418:GLN:H	1:E:418:GLN:HE21	1.54	0.54
1:E:724:LYS:HG2	7:E:2424:HOH:O	2.07	0.54
1:E:116:THR:CG2	1:E:119:GLU:N	2.60	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:PRO:HG3	1:E:411:PHE:CZ	2.43	0.54
2:F:44:GLY:O	2:F:45:GLU:HB2	2.08	0.54
1:A:367:GLN:O	1:A:500:PRO:HG3	2.07	0.54
1:A:708:LEU:HD22	1:A:755:LEU:HB3	1.89	0.54
3:G:49:THR:HG21	7:G:2011:HOH:O	2.06	0.54
1:A:75:ARG:NH1	1:A:220:GLN:NE2	2.54	0.54
1:A:204:VAL:HB	1:A:328:LEU:HG	1.90	0.54
1:A:319:MET:HE1	1:A:328:LEU:HD11	1.89	0.54
1:A:384:ALA:N	7:A:2190:HOH:O	2.32	0.54
1:A:558:MET:CE	1:A:561:MET:SD	2.96	0.54
2:B:57:GLN:HE22	2:B:140:ARG:NH2	2.03	0.54
3:C:112:SER:O	3:C:113:GLN:HG2	2.08	0.54
1:E:483:ALA:N	1:E:516:LYS:O	2.30	0.54
1:E:551:LEU:O	1:E:552:GLY:C	2.47	0.54
1:A:80:PRO:HD3	2:B:18:ALA:HB2	1.90	0.53
1:A:107:ARG:HG2	1:A:475:TRP:O	2.07	0.53
1:A:256:THR:CG2	1:A:305:THR:HA	2.36	0.53
1:A:483:ALA:HA	1:A:515:THR:HG21	1.90	0.53
3:G:156:LEU:HD12	3:G:178:LEU:HD13	1.91	0.53
1:E:470:GLN:NE2	7:E:2279:HOH:O	2.41	0.53
1:A:471:GLU:O	1:A:471:GLU:HG2	2.09	0.53
1:A:540:ILE:O	1:A:544:LEU:HG	2.08	0.53
1:A:467:VAL:CG2	7:A:2230:HOH:O	2.56	0.53
1:A:582:PRO:C	7:A:2277:HOH:O	2.46	0.53
1:E:129:LEU:O	1:E:133:GLU:HG2	2.07	0.53
1:E:320:ALA:O	1:E:323:LYS:HB2	2.08	0.53
2:F:41:ARG:CD	2:F:187:THR:HG23	2.33	0.53
3:G:115:LEU:HB3	7:G:2032:HOH:O	2.08	0.53
1:A:81:ARG:HE	1:A:214:THR:HG22	1.73	0.53
1:A:592:LEU:O	1:A:593:TYR:CB	2.40	0.53
1:E:109:GLU:HG2	7:E:2068:HOH:O	2.04	0.53
1:E:342:TYR:HD1	1:E:607:VAL:CB	2.18	0.53
2:F:39:ARG:HD2	2:F:56:GLU:OE2	2.08	0.53
3:G:189:TYR:O	3:G:192:THR:HB	2.09	0.53
1:A:380:PRO:HD3	1:A:534:TYR:OH	2.08	0.53
1:E:186:GLY:HA3	1:E:584:GLY:N	2.24	0.53
1:E:339:ASP:HB2	1:E:607:VAL:CG1	2.27	0.53
1:E:346:ALA:H	1:E:605:LEU:HD12	1.73	0.53
1:E:591:GLU:OE1	1:E:604:PRO:CA	2.56	0.53
2:F:166:ARG:HH22	3:G:248:GLN:HE21	1.57	0.53
3:G:206:GLY:C	3:G:209:TYR:H	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:HA	1:A:363:PHE:HB2	1.90	0.53
1:E:590:ILE:O	1:E:592:LEU:HG	2.09	0.53
1:A:122:ASP:OD1	1:A:528:ARG:NH1	2.41	0.53
1:A:193:GLU:HG2	7:A:2120:HOH:O	2.09	0.53
1:A:346:ALA:HB2	1:A:605:LEU:HD12	1.91	0.53
1:A:519:TRP:CD1	1:A:540:ILE:HG21	2.44	0.53
1:A:602:HIS:CD2	1:A:604:PRO:HD2	2.44	0.53
3:C:207:GLY:HA2	3:C:210:TYR:HB3	1.91	0.53
1:E:651:ILE:HD13	1:E:656:ALA:HB2	1.89	0.52
1:A:231:LYS:HB2	1:A:247:HIS:CD2	2.45	0.52
1:A:428:GLU:OE2	1:A:428:GLU:HA	2.03	0.52
2:B:57:GLN:NE2	2:B:140:ARG:HH22	2.05	0.52
1:E:607:VAL:HG23	7:E:2149:HOH:O	2.09	0.52
1:A:388:CYS:HA	1:A:593:TYR:CZ	2.44	0.52
1:A:607:VAL:HG13	1:A:609:THR:CB	2.38	0.52
3:G:226:ALA:HB3	3:G:227:PRO:HD3	1.90	0.52
1:A:583:PHE:CZ	1:A:587:SER:HA	2.45	0.52
2:B:117:THR:HG22	2:B:119:CYS:H	1.75	0.52
1:E:286:PHE:CB	7:E:2181:HOH:O	2.57	0.52
1:E:519:TRP:CE2	1:E:540:ILE:CG1	2.92	0.52
1:A:53:ILE:HD12	1:A:65:VAL:CG2	2.40	0.52
1:A:186:GLY:C	1:A:583:PHE:O	2.48	0.52
1:A:295:ASP:HB2	7:A:2160:HOH:O	2.09	0.52
1:A:413:ARG:HD2	1:A:413:ARG:N	2.24	0.52
3:G:70:ARG:HG2	3:G:71:PHE:H	1.74	0.52
3:G:39:LEU:HD13	3:G:116:ALA:HB3	1.92	0.52
3:C:145:ASN:C	3:C:145:ASN:ND2	2.62	0.52
1:E:279:VAL:O	1:E:283:THR:HB	2.09	0.52
1:E:586:ALA:HB3	7:E:2326:HOH:O	2.09	0.52
1:E:622:LEU:HD22	7:E:2426:HOH:O	2.09	0.52
1:A:422:GLU:HB2	7:A:2205:HOH:O	2.09	0.52
1:E:81:ARG:HE	1:E:214:THR:HG22	1.75	0.51
1:A:678:GLY:HA3	7:A:2329:HOH:O	2.10	0.51
1:E:539:THR:HG23	1:E:541:GLU:HG2	1.93	0.51
1:A:708:LEU:HD23	1:A:708:LEU:N	2.25	0.51
2:B:140:ARG:NH2	7:B:2045:HOH:O	2.43	0.51
1:E:209:HIS:CG	5:E:1766:MGD:H5'1	2.46	0.51
1:A:187:ARG:NH2	1:A:367:GLN:NE2	2.58	0.51
1:A:286:PHE:CA	1:A:590:ILE:HG21	2.40	0.51
2:B:192:VAL:HG12	2:B:193:HIS:H	1.75	0.51
1:E:93:ASP:OD1	1:E:758:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:LYS:HG3	1:E:282:TYR:CE1	2.46	0.51
1:A:630:THR:N	1:A:634:THR:HG21	2.26	0.51
1:E:345:MET:CB	1:E:605:LEU:HD13	2.41	0.51
1:A:42:GLN:CD	1:A:505:ARG:HB2	2.31	0.51
1:A:134:LYS:CE	7:A:2079:HOH:O	2.56	0.51
1:A:358:GLY:O	1:A:571:TRP:HA	2.11	0.51
1:A:379:LEU:O	1:A:380:PRO:C	2.49	0.51
2:B:183:LYS:HE3	7:B:2143:HOH:O	2.11	0.51
1:E:45:GLU:HG3	7:E:2012:HOH:O	2.10	0.51
1:E:359:ARG:HD3	7:E:2101:HOH:O	2.10	0.51
1:E:635:GLN:O	1:E:641:MET:HG2	2.05	0.51
1:E:635:GLN:NE2	1:E:635:GLN:N	2.56	0.51
1:E:642:GLU:OE2	2:F:32:GLY:N	2.28	0.51
3:G:207:PHE:O	3:G:211:LEU:N	2.44	0.51
1:A:113:ARG:NH2	7:A:2066:HOH:O	2.43	0.51
1:A:421:ILE:HG22	1:A:421:ILE:O	2.10	0.51
1:A:457:LYS:HD3	7:A:2225:HOH:O	2.11	0.51
3:C:67:GLU:O	3:C:67:GLU:HG2	2.11	0.51
3:C:140:ASN:O	3:C:142:PRO:HD3	2.11	0.51
1:E:519:TRP:CE2	1:E:540:ILE:HG13	2.46	0.51
1:A:345:MET:CE	1:A:592:LEU:HD11	2.41	0.51
1:A:519:TRP:CG	1:A:540:ILE:HG21	2.46	0.51
2:B:2:PRO:HB3	2:B:144:ASP:HB2	1.93	0.51
2:F:67:VAL:CB	2:F:68:PRO:HD3	2.41	0.51
1:A:535:PHE:N	1:A:536:PRO:CD	2.74	0.50
1:A:151:TRP:O	1:A:156:LEU:HB2	2.11	0.50
1:A:336:TRP:O	1:A:735:ARG:HB2	2.10	0.50
1:A:580:ARG:HB2	1:A:580:ARG:NH1	2.25	0.50
1:E:315:VAL:HG12	1:E:319:MET:HE3	1.93	0.50
1:E:396:HIS:CE1	1:E:404:ARG:H	2.29	0.50
1:E:553:LEU:CD2	1:E:557:THR:HG21	2.40	0.50
2:F:2:PRO:HB3	2:F:144:ASP:CG	2.31	0.50
3:G:66:GLU:O	3:G:66:GLU:HG2	2.12	0.50
2:B:2:PRO:HD2	2:B:80:ASP:OD2	2.10	0.50
2:B:121:HIS:O	2:B:125:LYS:CE	2.58	0.50
3:C:207:GLY:C	3:C:209:TRP:N	2.64	0.50
1:E:684:PRO:O	1:E:685:THR:C	2.49	0.50
1:E:99:LEU:O	1:E:478:VAL:HA	2.12	0.50
1:E:388:CYS:HB2	1:E:593:TYR:HH	1.66	0.50
1:E:422:GLU:H	1:E:423:PRO:HD2	1.76	0.50
1:E:396:HIS:HB3	1:E:407:LYS:HE3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:568:GLY:O	1:E:570:PRO:HD3	2.12	0.50
1:A:483:ALA:CA	1:A:515:THR:HG23	2.42	0.50
1:A:605:LEU:N	1:A:606:PRO:CD	2.73	0.50
2:B:72:THR:CG2	2:B:74:ALA:H	2.18	0.50
1:E:397:GLU:CG	1:E:398:PRO:HD3	2.42	0.50
3:G:46:ARG:HG3	7:G:2014:HOH:O	2.10	0.50
1:A:152:PHE:O	1:A:157:PRO:CG	2.60	0.50
1:E:336:TRP:O	1:E:340:ASP:OD1	2.30	0.50
3:G:189:TYR:HB3	3:G:190:PRO:HD3	1.94	0.50
1:E:37:VAL:HA	1:E:57:ALA:O	2.12	0.49
1:E:284:VAL:HG12	1:E:592:LEU:HD12	1.93	0.49
3:G:76:ILE:HG12	3:G:80:LEU:HD11	1.94	0.49
1:A:558:MET:HE2	1:A:561:MET:SD	2.53	0.49
2:B:32:GLY:N	7:B:2011:HOH:O	2.43	0.49
2:B:117:THR:O	2:B:117:THR:HG23	2.12	0.49
1:E:88:THR:HG21	1:E:467:VAL:HG11	1.92	0.49
1:A:415:THR:HG22	7:A:2204:HOH:O	2.13	0.49
1:A:689:ARG:NH2	1:A:691:ASP:OD2	2.41	0.49
1:E:209:HIS:CD2	5:E:1766:MGD:H5'1	2.48	0.49
1:A:79:CYS:CB	1:A:80:PRO:HD2	2.42	0.49
1:A:427:GLY:C	1:A:428:GLU:O	2.51	0.49
1:A:536:PRO:HG2	1:A:537:TRP:H	1.77	0.49
1:A:647:ASN:HD21	1:A:714:ALA:H	1.61	0.49
2:B:2:PRO:HB3	2:B:144:ASP:CB	2.42	0.49
1:E:208:HIS:HE1	1:E:218:GLN:NE2	2.10	0.49
1:E:635:GLN:H	1:E:635:GLN:HE21	1.60	0.49
2:F:72:THR:HG22	2:F:74:ALA:N	2.23	0.49
3:G:207:PHE:C	3:G:207:PHE:CD2	2.84	0.49
1:A:388:CYS:O	1:A:391:PRO:HD3	2.12	0.49
1:A:525:LEU:O	1:A:529:LEU:HG	2.12	0.49
2:B:117:THR:CG2	2:B:117:THR:O	2.60	0.49
1:E:311:VAL:HG23	7:E:2198:HOH:O	2.10	0.49
1:A:320:ALA:O	1:A:323:LYS:CG	2.60	0.49
3:C:20:LEU:HD13	3:C:63:ILE:HD13	1.94	0.49
1:A:395:ASP:CA	1:A:399:GLU:CG	2.72	0.49
1:A:554:ASP:OD2	1:A:554:ASP:N	2.46	0.49
1:A:583:PHE:CE2	1:A:588:GLY:CA	2.93	0.49
1:E:324:PRO:HD2	7:E:2213:HOH:O	2.10	0.49
1:E:591:GLU:CD	1:E:604:PRO:CB	2.63	0.49
1:A:36:GLU:O	1:A:36:GLU:HG2	2.13	0.49
7:E:2167:HOH:O	2:F:46:TYR:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:PHE:HE1	1:A:145:HIS:CE1	2.30	0.49
2:B:22:ALA:HB2	2:B:134:THR:HG21	1.95	0.49
1:E:69:GLU:HA	7:E:2042:HOH:O	2.11	0.49
1:E:598:LYS:HB3	1:E:599:GLU:OE1	2.13	0.49
3:G:144:ASN:OD1	3:G:192:THR:CG2	2.61	0.49
1:A:558:MET:HE1	1:A:561:MET:SD	2.53	0.49
3:G:240:LEU:C	3:G:240:LEU:HD12	2.33	0.49
1:E:621:LEU:HD22	1:E:622:LEU:O	2.12	0.48
1:A:345:MET:HE1	1:A:605:LEU:HD22	1.94	0.48
1:A:710:HIS:O	7:A:2345:HOH:O	2.20	0.48
1:E:186:GLY:H	1:E:583:PHE:HA	1.78	0.48
1:E:81:ARG:HD2	1:E:630:THR:OG1	2.13	0.48
1:E:454:GLU:HG2	7:E:2274:HOH:O	2.13	0.48
1:E:467:VAL:HG12	1:E:468:LEU:HG	1.94	0.48
1:E:519:TRP:NE1	1:E:540:ILE:HG12	2.28	0.48
3:G:38:HIS:CE1	3:G:105:LEU:HD22	2.48	0.48
1:A:572:LEU:HD22	7:A:2275:HOH:O	2.13	0.48
1:E:671:ASN:C	1:E:671:ASN:ND2	2.66	0.48
1:E:685:THR:HG22	2:F:42:GLU:OE2	2.13	0.48
1:A:81:ARG:HE	1:A:214:THR:CG2	2.27	0.48
1:A:96:LYS:HB3	1:A:513:PHE:HB3	1.96	0.48
3:G:221:TRP:HD1	7:G:2035:HOH:O	1.96	0.48
3:G:225:LEU:CB	7:G:2070:HOH:O	2.59	0.48
1:A:81:ARG:HH21	1:A:214:THR:HG22	1.77	0.48
1:A:284:VAL:CG2	1:A:587:SER:HB3	2.38	0.48
1:E:225:ALA:O	1:E:230:ALA:HB3	2.14	0.48
1:E:342:TYR:CE1	1:E:607:VAL:HB	2.46	0.48
1:E:371:LEU:HD13	1:E:547:ARG:CZ	2.42	0.48
1:E:497:HIS:O	1:E:498:LYS:C	2.51	0.48
1:E:512:LEU:O	1:E:515:THR:HB	2.14	0.48
3:G:206:GLY:CA	3:G:209:TYR:CB	2.90	0.48
1:E:100:ILE:HG12	1:E:478:VAL:CG2	2.42	0.48
1:E:345:MET:HB3	1:E:605:LEU:CD1	2.44	0.48
1:E:632:ALA:C	1:E:635:GLN:NE2	2.66	0.48
3:G:40:LYS:HG3	3:G:40:LYS:O	2.14	0.48
1:A:183:TRP:HB3	1:A:592:LEU:HD22	1.95	0.48
1:A:519:TRP:CZ2	1:A:540:ILE:CG1	2.97	0.48
1:A:585:THR:O	1:A:585:THR:HG22	2.12	0.48
2:B:122:ARG:HB3	2:B:127:LYS:HB2	1.95	0.48
3:C:174:PHE:H	3:C:175:PRO:HD2	1.79	0.48
1:E:41:TYR:HE1	1:E:560:GLY:O	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:PRO:HG2	1:E:392:SER:H	1.77	0.48
1:E:701:HIS:O	1:E:710:HIS:O	2.30	0.48
1:A:71:ASN:HD21	1:A:73:LYS:HB2	1.78	0.48
1:A:454:GLU:HG2	7:A:2101:HOH:O	2.14	0.48
1:A:673:ASP:OD2	1:A:721:THR:CG2	2.61	0.48
2:B:155:ALA:HB1	7:B:2113:HOH:O	2.14	0.48
3:C:140:ASN:ND2	3:C:140:ASN:N	2.59	0.48
1:E:286:PHE:C	1:E:288:GLU:H	2.16	0.48
3:G:172:LEU:O	3:G:176:ARG:HG3	2.14	0.48
1:A:591:GLU:CB	1:A:603:GLN:HE22	2.23	0.48
1:A:599:GLU:HB2	7:A:2281:HOH:O	2.14	0.48
1:E:91:ASP:C	1:E:92:PRO:O	2.52	0.48
2:F:115:LYS:HG3	2:F:116:CYS:O	2.14	0.47
1:A:393:GLY:HA3	1:A:407:LYS:HZ1	1.80	0.47
2:B:36:LEU:CD1	7:B:2104:HOH:O	2.62	0.47
1:A:285:GLY:C	1:A:590:ILE:HG23	2.34	0.47
1:A:305:THR:HG23	1:A:307:ILE:HD12	1.96	0.47
1:A:390:GLY:H	1:A:595:GLN:NE2	2.09	0.47
1:A:422:GLU:HB3	1:A:423:PRO:CD	2.43	0.47
2:B:27:ASN:HD21	2:B:121:HIS:HE1	1.61	0.47
1:A:276:LYS:CA	7:A:2152:HOH:O	2.49	0.47
1:A:428:GLU:CB	1:A:429:PRO:CD	2.89	0.47
1:A:73:LYS:NZ	1:A:192:HIS:CD2	2.79	0.47
1:E:606:PRO:CG	1:E:607:VAL:N	2.77	0.47
1:A:239:PHE:O	1:A:687:ARG:HD2	2.15	0.47
1:A:364:TYR:HB2	1:A:570:PRO:CB	2.45	0.47
1:A:671:ASN:HD21	1:A:675:VAL:H	1.63	0.47
7:B:2075:HOH:O	3:C:82:SER:HB3	2.14	0.47
1:E:160:TRP:O	1:E:160:TRP:CG	2.67	0.47
1:A:654:GLU:HG3	7:A:2317:HOH:O	2.14	0.47
1:E:36:GLU:HB3	7:E:2005:HOH:O	2.14	0.47
1:E:81:ARG:HE	1:E:214:THR:CG2	2.27	0.47
1:E:81:ARG:NE	1:E:214:THR:HG22	2.29	0.47
1:E:100:ILE:HG12	1:E:478:VAL:HG13	1.96	0.47
1:E:201:ARG:HD3	7:E:2124:HOH:O	2.14	0.47
2:F:190:SER:O	2:F:194:HIS:N	2.47	0.47
1:A:195:ILE:HG12	1:A:329:PRO:HB3	1.97	0.47
1:A:683:LYS:HA	1:A:684:PRO:HD2	1.67	0.47
2:F:16:CYS:SG	2:F:16:CYS:O	2.73	0.47
3:G:70:ARG:HG2	3:G:71:PHE:N	2.29	0.47
1:A:118:GLU:H	1:A:118:GLU:CD	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:HIS:CB	1:A:403:PRO:HB3	2.44	0.47
1:E:677:GLU:O	1:E:678:GLY:O	2.33	0.47
1:A:214:THR:HG23	1:A:214:THR:O	2.15	0.47
1:A:336:TRP:CD1	1:A:336:TRP:N	2.73	0.47
7:A:2041:HOH:O	2:B:133:GLU:HG3	2.15	0.47
1:E:119:GLU:HG2	7:E:2076:HOH:O	2.15	0.47
1:E:519:TRP:CE2	1:E:540:ILE:HG12	2.49	0.47
1:A:103:GLU:HA	1:A:103:GLU:OE1	2.15	0.46
1:A:519:TRP:CG	1:A:540:ILE:CG2	2.97	0.46
2:B:47:PRO:CG	7:B:2034:HOH:O	2.63	0.46
2:F:78:THR:CG2	2:F:79:LYS:N	2.79	0.46
1:A:289:LEU:HD12	1:A:590:ILE:HD11	1.97	0.46
1:A:470:GLN:HE21	1:A:470:GLN:HB3	1.39	0.46
2:B:86:ASP:OD1	2:B:88:LYS:HB2	2.15	0.46
1:E:606:PRO:HG2	1:E:607:VAL:N	2.31	0.46
2:F:172:ARG:N	2:F:173:PRO:HD3	2.30	0.46
1:A:345:MET:HE1	1:A:605:LEU:CD2	2.44	0.46
1:A:530:GLY:HA2	1:A:532:GLU:OE2	2.15	0.46
1:A:592:LEU:O	1:A:592:LEU:HD13	2.15	0.46
2:B:46:TYR:CD2	7:B:2033:HOH:O	2.68	0.46
1:A:187:ARG:HH22	1:A:367:GLN:NE2	2.13	0.46
1:A:231:LYS:CA	1:A:247:HIS:CD2	2.98	0.46
3:C:17:THR:HG22	3:C:18:ASN:N	2.31	0.46
3:C:68:SER:O	3:C:71:ARG:HB3	2.16	0.46
3:C:151:LEU:O	3:C:155:THR:HB	2.16	0.46
1:E:142:PHE:CG	1:E:157:PRO:HG3	2.50	0.46
1:E:755:LEU:O	1:E:758:ARG:HD3	2.15	0.46
1:A:93:ASP:CG	1:A:758:ARG:HH22	2.18	0.46
1:E:651:ILE:HD11	1:E:682:VAL:HG13	1.96	0.46
2:F:29:VAL:HA	2:F:30:PRO:HD3	1.71	0.46
2:F:166:ARG:HH22	3:G:248:GLN:NE2	2.12	0.46
1:A:231:LYS:HB2	1:A:247:HIS:CG	2.50	0.46
1:A:429:PRO:C	1:A:430:TYR:CD2	2.88	0.46
1:A:635:GLN:C	1:A:709:ALA:HB2	2.36	0.46
1:A:132:ARG:CD	7:A:2077:HOH:O	2.63	0.46
1:E:424:MET:CE	1:E:455:ALA:HB1	2.45	0.46
1:E:627:PRO:HB2	2:F:16:CYS:HA	1.97	0.46
1:E:630:THR:HG23	7:E:2452:HOH:O	2.15	0.46
1:A:523:ARG:HG3	1:A:535:PHE:HB3	1.97	0.46
2:B:139:CYS:SG	4:B:1194:SF4:S3	3.13	0.46
1:E:724:LYS:CG	7:E:2424:HOH:O	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:70:ARG:CG	3:G:71:PHE:N	2.78	0.46
1:A:75:ARG:HD2	1:A:220:GLN:NE2	2.25	0.46
1:A:195:ILE:N	1:A:195:ILE:HD12	2.30	0.46
1:A:231:LYS:HB3	1:A:231:LYS:HE3	1.68	0.46
1:A:310:GLN:HG3	7:A:2164:HOH:O	2.16	0.46
1:A:519:TRP:CD2	1:A:540:ILE:HG23	2.50	0.46
1:E:252:ILE:HG12	1:E:256:THR:HG22	1.98	0.46
1:E:336:TRP:O	1:E:338:GLY:N	2.49	0.46
3:G:144:ASN:C	3:G:144:ASN:HD22	2.19	0.46
3:G:222:GLN:C	7:G:2070:HOH:O	2.53	0.46
1:A:627:PRO:HB2	2:B:16:CYS:HA	1.98	0.45
1:E:153:VAL:CG1	1:E:167:LYS:HE2	2.46	0.45
1:E:495:VAL:HG21	7:E:2299:HOH:O	2.15	0.45
2:F:35:ASN:HD22	2:F:106:TYR:HE2	1.64	0.45
7:B:2081:HOH:O	3:C:251:LEU:HD11	2.15	0.45
3:C:50:THR:O	3:C:54:LEU:HG	2.16	0.45
1:E:97:ARG:HH22	1:E:763:ARG:HD2	1.80	0.45
1:E:305:THR:HG23	1:E:307:ILE:H	1.78	0.45
1:E:345:MET:CB	1:E:605:LEU:CD1	2.94	0.45
1:E:247:HIS:CE1	7:E:2150:HOH:O	2.69	0.45
1:A:183:TRP:HB3	1:A:592:LEU:O	2.16	0.45
1:E:81:ARG:NH1	1:E:630:THR:OG1	2.39	0.45
1:E:166:ALA:HB2	1:E:415:THR:CG2	2.45	0.45
1:E:647:ASN:HD22	1:E:647:ASN:N	2.10	0.45
1:A:647:ASN:HD22	1:A:647:ASN:N	2.10	0.45
1:E:397:GLU:HB3	7:E:2242:HOH:O	2.16	0.45
1:E:591:GLU:OE2	1:E:604:PRO:HB3	2.15	0.45
1:E:592:LEU:HA	1:E:603:GLN:HE21	0.65	0.45
3:G:139:ASN:ND2	7:G:2043:HOH:O	2.49	0.45
1:A:299:GLU:OE2	1:A:313:ARG:NH2	2.30	0.45
1:A:369:PRO:HG2	1:A:494:LEU:HB3	1.99	0.45
1:A:483:ALA:HA	1:A:515:THR:HG23	1.95	0.45
1:E:93:ASP:O	1:E:469:PRO:HD3	2.16	0.45
1:E:149:ASP:CB	7:E:2094:HOH:O	2.64	0.45
1:E:335:VAL:HG13	1:E:732:ALA:O	2.17	0.45
1:A:37:VAL:CG1	1:A:38:LYS:N	2.78	0.45
1:A:305:THR:CG2	1:A:307:ILE:HB	2.47	0.45
2:B:41:ARG:NH1	2:B:187:THR:HG23	2.21	0.45
1:E:265:ILE:HD11	1:E:349:TYR:HB2	1.98	0.45
2:F:35:ASN:ND2	2:F:106:TYR:HE2	2.15	0.45
2:F:46:TYR:CD1	2:F:46:TYR:C	2.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:591:GLU:OE2	1:E:604:PRO:CG	2.64	0.45
2:F:88:LYS:O	3:G:74:THR:CG2	2.63	0.45
1:A:285:GLY:C	1:A:590:ILE:CG2	2.86	0.45
1:A:345:MET:CE	1:A:605:LEU:HD22	2.47	0.45
2:B:57:GLN:CD	7:B:2045:HOH:O	2.56	0.45
3:G:100:LEU:HB3	7:G:2031:HOH:O	2.17	0.45
1:A:337:TYR:O	1:A:340:ASP:CG	2.47	0.45
1:A:548:LEU:HD13	1:A:558:MET:HB2	1.99	0.45
2:B:55:PRO:HB2	7:B:2104:HOH:O	2.16	0.45
3:C:77:ILE:HG12	3:C:81:LEU:HD11	1.99	0.45
3:C:108:LEU:HB3	3:C:110:LYS:HG3	1.99	0.45
3:C:190:TYR:HB3	3:C:191:PRO:HD3	1.99	0.45
1:E:553:LEU:HD21	1:E:557:THR:CG2	2.47	0.45
3:G:132:LEU:O	3:G:136:VAL:HB	2.17	0.45
1:A:256:THR:HG23	1:A:256:THR:O	2.17	0.44
1:A:335:VAL:HG13	1:A:733:GLY:CA	2.46	0.44
1:E:97:ARG:HH21	1:E:763:ARG:CZ	2.31	0.44
1:E:380:PRO:HD3	1:E:534:TYR:OH	2.16	0.44
1:E:632:ALA:C	1:E:635:GLN:HE22	2.20	0.44
3:G:206:GLY:HA2	3:G:209:TYR:HB2	1.98	0.44
2:B:191:GLU:HG3	7:B:2144:HOH:O	2.17	0.44
3:C:21:HIS:CE1	3:C:64:LEU:CG	3.00	0.44
1:E:397:GLU:CB	1:E:398:PRO:CD	2.88	0.44
1:E:591:GLU:O	1:E:591:GLU:CG	2.64	0.44
1:A:64:LYS:HE2	2:B:26:GLU:HB2	1.98	0.44
1:A:107:ARG:HB2	7:A:2224:HOH:O	2.16	0.44
2:B:168:GLU:C	2:B:169:GLN:O	2.52	0.44
1:E:651:ILE:HD11	1:E:682:VAL:HG12	1.99	0.44
3:C:248:TRP:CE2	3:C:250:GLY:HA3	2.53	0.44
1:E:48:PHE:CZ	1:E:145:HIS:CE1	3.05	0.44
1:E:620:ARG:HB3	7:E:2392:HOH:O	2.17	0.44
1:A:449:VAL:O	1:A:453:LYS:HG3	2.17	0.44
1:A:512:LEU:O	1:A:515:THR:HB	2.17	0.44
1:A:686:ALA:CB	7:A:2331:HOH:O	2.52	0.44
1:E:308:PRO:CB	7:E:2198:HOH:O	2.53	0.44
1:E:639:VAL:HG21	2:F:25:MET:HE3	1.98	0.44
1:A:64:LYS:CE	2:B:26:GLU:HB2	2.47	0.44
1:E:197:TRP:CG	1:E:221:ASP:HB3	2.53	0.44
3:C:172:ALA:CA	3:C:175:PRO:HG2	2.39	0.44
1:E:469:PRO:O	1:E:706:MET:CG	2.63	0.44
3:G:52:ALA:O	3:G:56:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HG23	1:A:118:GLU:N	2.33	0.44
1:A:305:THR:CG2	1:A:307:ILE:H	2.31	0.44
1:A:540:ILE:HG13	1:A:540:ILE:H	1.63	0.44
1:E:519:TRP:CZ2	1:E:540:ILE:HG13	2.53	0.44
1:A:75:ARG:NH1	1:A:220:GLN:HE21	2.11	0.44
1:A:81:ARG:HH21	1:A:214:THR:CG2	2.30	0.44
1:A:232:VAL:N	1:A:247:HIS:HD2	2.11	0.44
1:E:75:ARG:NH1	1:E:220:GLN:HE21	2.11	0.44
1:E:239:PHE:CB	1:E:687:ARG:HB3	2.44	0.44
1:E:327:VAL:HG13	1:E:362:GLY:HA2	1.99	0.44
1:E:428:GLU:O	1:E:430:TYR:CA	2.65	0.44
1:A:43:ILE:HB	1:A:505:ARG:HH21	1.83	0.43
1:A:116:THR:HG22	1:A:119:GLU:CB	2.43	0.43
1:A:124:ILE:HD11	1:A:478:VAL:HG11	2.00	0.43
1:A:404:ARG:HG3	1:A:406:ASP:OD2	2.18	0.43
1:A:534:TYR:O	1:A:535:PHE:CB	2.66	0.43
1:A:569:LYS:HA	1:A:570:PRO:HD3	1.76	0.43
1:E:256:THR:CG2	1:E:305:THR:HA	2.42	0.43
1:E:412:ALA:HB1	1:E:413:ARG:NH1	2.33	0.43
3:C:21:HIS:CD2	3:C:21:HIS:C	2.92	0.43
1:E:214:THR:HG21	1:E:627:PRO:O	2.17	0.43
1:E:287:GLU:OE1	1:E:287:GLU:N	2.51	0.43
1:E:601:GLY:HA2	7:E:2334:HOH:O	2.18	0.43
1:E:606:PRO:CG	1:E:607:VAL:H	2.31	0.43
1:E:606:PRO:CD	1:E:607:VAL:N	2.81	0.43
1:E:623:TYR:HA	1:E:695:ILE:O	2.18	0.43
1:A:284:VAL:HG12	1:A:285:GLY:N	2.33	0.43
1:A:548:LEU:O	1:A:553:LEU:O	2.36	0.43
3:C:222:TRP:CD1	3:C:223:GLN:N	2.86	0.43
2:F:63:ASN:HB2	7:F:2111:HOH:O	2.18	0.43
1:A:483:ALA:CA	1:A:515:THR:CG2	2.95	0.43
1:E:299:GLU:OE2	1:E:313:ARG:NH2	2.29	0.43
1:E:609:THR:HG23	7:E:2338:HOH:O	2.18	0.43
1:E:672:GLN:NE2	1:E:672:GLN:H	2.17	0.43
3:G:227:PRO:O	3:G:231:LEU:HB2	2.18	0.43
1:A:430:TYR:HB2	1:A:431:PRO:HD3	2.01	0.43
3:C:21:HIS:CE1	3:C:64:LEU:HD11	2.45	0.43
1:E:81:ARG:HB2	4:E:1764:SF4:S3	2.58	0.43
1:E:112:TYR:CZ	1:E:474:MET:O	2.71	0.43
1:E:315:VAL:HG12	1:E:319:MET:CE	2.49	0.43
3:G:46:ARG:CG	7:G:2014:HOH:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:PHE:CZ	1:A:587:SER:CA	3.01	0.43
1:A:591:GLU:O	1:A:592:LEU:CD1	2.62	0.43
1:A:596:ARG:NH1	1:A:600:ALA:CB	2.81	0.43
1:E:95:LEU:CD1	7:E:2278:HOH:O	2.58	0.43
1:E:116:THR:HG23	1:E:119:GLU:N	2.19	0.43
1:E:149:ASP:HA	7:E:2094:HOH:O	2.17	0.43
1:E:313:ARG:HD3	1:E:317:ARG:NH2	2.34	0.43
1:E:647:ASN:H	1:E:647:ASN:ND2	2.17	0.43
2:F:117:THR:HG23	2:F:117:THR:O	2.17	0.43
3:G:207:PHE:HB3	3:G:208:TRP:H	1.43	0.43
1:A:592:LEU:HD13	1:A:592:LEU:C	2.38	0.43
1:A:605:LEU:CD2	1:A:605:LEU:N	2.70	0.43
1:E:622:LEU:HB2	1:E:693:VAL:O	2.19	0.43
2:F:147:ASP:O	2:F:150:SER:HB2	2.17	0.43
1:A:193:GLU:CG	7:A:2120:HOH:O	2.65	0.43
1:A:286:PHE:HA	1:A:590:ILE:CG2	2.47	0.43
1:E:346:ALA:N	1:E:605:LEU:CD1	2.79	0.43
1:E:453:LYS:HG2	1:E:475:TRP:CZ2	2.53	0.43
1:E:620:ARG:O	1:E:620:ARG:CG	2.66	0.43
1:E:708:LEU:HD22	7:E:2408:HOH:O	2.18	0.43
1:E:717:ASN:ND2	5:E:1765:MGD:H192	2.11	0.43
1:A:342:TYR:CD2	1:A:605:LEU:HA	2.54	0.43
1:E:466:ASP:HA	5:E:1765:MGD:N2	2.34	0.43
1:E:669:LEU:HD23	1:E:741:LEU:HD22	1.99	0.43
2:F:55:PRO:CG	4:F:1194:SF4:S2	3.05	0.43
1:A:488:ARG:HD3	1:A:490:ASP:OD2	2.19	0.43
1:E:574:ASP:HA	1:E:577:LYS:HD3	2.00	0.43
1:E:683:LYS:HE2	1:E:685:THR:HB	1.99	0.43
1:A:122:ASP:HB2	7:A:2071:HOH:O	2.18	0.42
1:A:483:ALA:HB2	1:A:515:THR:CG2	2.49	0.42
1:A:555:LEU:O	1:A:559:LYS:HG3	2.18	0.42
3:C:57:ILE:HG21	3:C:100:PHE:HB2	2.01	0.42
1:E:397:GLU:CB	7:E:2242:HOH:O	2.67	0.42
1:E:468:LEU:HB3	1:E:469:PRO:HD2	2.00	0.42
1:A:85:ALA:HA	7:A:2044:HOH:O	2.18	0.42
1:A:124:ILE:O	1:A:128:MET:HG3	2.19	0.42
1:A:184:VAL:HG22	1:A:592:LEU:CG	2.49	0.42
1:A:533:GLN:HG2	1:A:534:TYR:N	2.33	0.42
1:A:623:TYR:HA	1:A:695:ILE:O	2.19	0.42
1:A:702:LYS:HG3	7:A:2232:HOH:O	2.18	0.42
3:C:155:THR:CG2	3:C:239:ARG:CG	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:148:ALA:HA	7:G:2049:HOH:O	2.19	0.42
3:G:205:ALA:HB1	3:G:240:LEU:CD2	2.49	0.42
1:A:548:LEU:C	1:A:553:LEU:O	2.58	0.42
1:E:302:GLU:O	1:E:302:GLU:HG2	2.19	0.42
2:F:57:GLN:HE22	2:F:140:ARG:HH21	1.58	0.42
3:G:160:LEU:HB3	3:G:175:LEU:HB2	2.00	0.42
1:A:595:GLN:HA	1:A:598:LYS:HD2	2.02	0.42
1:A:647:ASN:H	1:A:647:ASN:ND2	2.14	0.42
1:E:100:ILE:CG2	1:E:478:VAL:HG22	2.48	0.42
1:E:433:LYS:HB3	1:E:460:ASP:HB2	2.01	0.42
1:E:553:LEU:HD23	1:E:553:LEU:HA	1.86	0.42
2:F:135:CYS:HA	2:F:136:PRO:HD3	1.76	0.42
1:A:209:HIS:CE1	1:A:625:ARG:H	2.29	0.42
1:A:586:ALA:O	1:A:587:SER:CB	2.66	0.42
2:F:125:LYS:HE2	7:F:2079:HOH:O	2.20	0.42
3:G:91:GLY:O	3:G:95:LEU:HD12	2.19	0.42
3:G:206:GLY:CA	3:G:209:TYR:HB2	2.49	0.42
1:A:391:PRO:O	1:A:413:ARG:CB	2.67	0.42
2:B:106:TYR:CE1	2:B:114:SER:HB3	2.54	0.42
1:E:79:CYS:CB	1:E:80:PRO:HD2	2.49	0.42
1:E:275:ASP:N	1:E:323:LYS:HE3	2.34	0.42
2:F:118:PHE:HD1	2:F:118:PHE:HA	1.63	0.42
7:F:2030:HOH:O	3:G:250:LEU:HD12	2.18	0.42
3:G:206:GLY:O	3:G:209:TYR:CB	2.68	0.42
1:A:77:ARG:NH2	7:A:2041:HOH:O	2.42	0.42
1:A:671:ASN:ND2	1:A:675:VAL:H	2.17	0.42
1:E:48:PHE:CE1	1:E:145:HIS:CE1	3.08	0.42
7:E:2135:HOH:O	2:F:138:TYR:CE1	2.73	0.42
1:A:682:VAL:HG12	1:A:684:PRO:HD3	2.02	0.42
3:G:247:TRP:CE2	3:G:249:GLY:HA3	2.55	0.42
1:A:72:PRO:HG2	1:A:501:PHE:CD2	2.54	0.42
1:A:422:GLU:N	1:A:423:PRO:HD2	2.34	0.42
1:A:628:VAL:HG13	1:A:640:LEU:HD22	2.02	0.42
1:E:166:ALA:HB2	1:E:415:THR:HG21	2.02	0.42
1:A:655:GLU:CD	1:A:658:ARG:HH22	2.23	0.41
2:B:5:ALA:HB3	2:B:145:LEU:HD13	2.02	0.41
2:B:64:PRO:HB3	4:B:1196:SF4:S3	2.60	0.41
2:B:88:LYS:O	3:C:75:THR:CG2	2.67	0.41
1:E:297:THR:HG21	1:E:299:GLU:HG2	2.00	0.41
1:E:730:GLY:HA3	7:E:2253:HOH:O	2.19	0.41
1:E:734:LEU:CD2	7:E:2420:HOH:O	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:HB2	1:A:477:ASP:HA	2.02	0.41
1:A:156:LEU:HB3	1:A:157:PRO:HD3	2.02	0.41
1:E:250:LEU:HD13	1:E:307:ILE:HG21	2.02	0.41
2:B:78:THR:HG22	2:B:80:ASP:H	1.86	0.41
3:C:21:HIS:CE1	3:C:64:LEU:CD2	3.00	0.41
1:E:256:THR:HG23	7:E:2196:HOH:O	2.19	0.41
1:E:569:LYS:HA	1:E:570:PRO:HD3	1.85	0.41
1:E:576:GLU:C	1:E:578:GLU:H	2.23	0.41
2:F:166:ARG:HD2	7:F:2106:HOH:O	2.20	0.41
1:A:113:ARG:NE	7:A:2066:HOH:O	2.54	0.41
1:A:194:PRO:O	1:A:363:PHE:HA	2.20	0.41
1:A:676:LYS:NZ	1:A:742:GLU:OE1	2.53	0.41
1:E:112:TYR:OH	1:E:476:ALA:O	2.38	0.41
1:E:247:HIS:CD2	1:E:247:HIS:N	2.87	0.41
1:E:651:ILE:HD12	1:E:684:PRO:HA	2.02	0.41
3:G:208:TRP:HA	3:G:208:TRP:HE3	1.85	0.41
2:B:129:PRO:HB3	4:B:1195:SF4:S3	2.61	0.41
3:C:229:TRP:O	3:C:233:LEU:HG	2.19	0.41
1:E:116:THR:HG22	1:E:119:GLU:N	2.30	0.41
1:E:293:VAL:O	1:E:293:VAL:HG13	2.19	0.41
1:E:412:ALA:HB1	1:E:413:ARG:HH12	1.85	0.41
1:E:484:THR:HB	1:E:487:GLU:OE1	2.20	0.41
2:F:117:THR:HB	7:F:2012:HOH:O	2.19	0.41
1:A:575:TRP:O	1:A:580:ARG:HG2	2.21	0.41
1:E:248:ARG:NH1	1:E:318:GLU:OE2	2.54	0.41
1:E:533:GLN:HE21	1:E:533:GLN:N	2.02	0.41
1:A:69:GLU:C	7:A:2034:HOH:O	2.37	0.41
1:A:252:ILE:HG13	1:A:307:ILE:HD11	2.02	0.41
3:C:173:LEU:O	3:C:173:LEU:CG	2.65	0.41
1:E:100:ILE:CG1	1:E:478:VAL:HG22	2.48	0.41
1:E:113:ARG:HB3	7:E:2046:HOH:O	2.21	0.41
1:E:142:PHE:CD1	1:E:157:PRO:HB3	2.56	0.41
1:A:295:ASP:O	1:A:297:THR:HG22	2.21	0.41
2:B:46:TYR:HE2	7:B:2033:HOH:O	1.96	0.41
2:B:72:THR:CG2	2:B:73:GLY:N	2.84	0.41
1:E:421:ILE:HD11	1:E:452:THR:HG23	2.03	0.41
1:E:424:MET:HE2	1:E:455:ALA:HB1	2.02	0.41
1:A:42:GLN:OE1	1:A:506:THR:N	2.53	0.41
1:A:175:ALA:HB3	1:A:176:PRO:HD3	2.02	0.41
1:A:284:VAL:HB	1:A:589:LYS:HA	2.03	0.41
1:A:499:THR:HB	1:A:565:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:GLU:HG3	1:A:510:GLU:H	1.77	0.41
2:B:118:PHE:HD1	2:B:118:PHE:HA	1.72	0.41
2:B:135:CYS:HA	2:B:136:PRO:HD3	1.89	0.41
2:B:190:SER:CB	3:C:252:GLY:N	2.81	0.41
3:C:185:LEU:O	3:C:189:LEU:HG	2.20	0.41
1:E:88:THR:CG2	1:E:467:VAL:HG11	2.51	0.41
1:E:97:ARG:NH2	1:E:763:ARG:NH1	2.64	0.41
1:E:288:GLU:HG3	7:E:2186:HOH:O	2.21	0.41
1:E:622:LEU:O	1:E:623:TYR:HB3	2.21	0.41
1:A:116:THR:HG23	1:A:118:GLU:H	1.85	0.41
1:A:279:VAL:HA	1:A:283:THR:HB	2.03	0.41
1:E:50:ARG:HD2	7:E:2016:HOH:O	2.20	0.41
1:E:204:VAL:HG21	1:E:319:MET:CE	2.50	0.41
3:G:16:THR:HG21	3:G:66:GLU:HB2	2.03	0.41
3:G:195:PRO:HD2	3:G:196:GLU:OE2	2.20	0.41
1:E:239:PHE:O	1:E:687:ARG:HD2	2.21	0.40
1:E:591:GLU:O	1:E:603:GLN:HG2	2.20	0.40
3:G:86:SER:O	3:G:87:PRO:C	2.57	0.40
1:A:587:SER:O	1:A:589:LYS:HE2	2.21	0.40
1:A:666:TYR:CZ	1:A:681:ARG:HG3	2.56	0.40
1:A:753:THR:CG2	1:A:757:LYS:HE2	2.51	0.40
2:B:112:TYR:HB3	3:C:73:ARG:NH2	2.35	0.40
3:C:145:ASN:OD1	3:C:193:THR:CG2	2.68	0.40
3:C:207:GLY:HA2	3:C:210:TYR:CB	2.52	0.40
3:C:208:PHE:C	3:C:208:PHE:CD2	2.93	0.40
3:C:222:TRP:CD1	3:C:222:TRP:C	2.94	0.40
1:E:53:ILE:HD12	1:E:65:VAL:HG22	2.03	0.40
2:F:35:ASN:ND2	2:F:106:TYR:CE2	2.88	0.40
3:G:112:GLN:N	7:G:2036:HOH:O	2.53	0.40
3:G:205:ALA:HB1	3:G:240:LEU:HD22	2.02	0.40
1:A:43:ILE:HB	1:A:505:ARG:NH2	2.36	0.40
1:A:371:LEU:HD23	1:A:551:LEU:CD1	2.52	0.40
1:A:405:ALA:HB2	1:A:430:TYR:CZ	2.57	0.40
2:B:25:MET:CE	2:B:25:MET:CA	2.92	0.40
2:B:166:ARG:HG2	7:B:2145:HOH:O	2.22	0.40
3:C:174:PHE:N	3:C:175:PRO:HD2	2.37	0.40
3:C:228:PRO:O	3:C:232:LEU:HD12	2.22	0.40
1:E:553:LEU:CD2	1:E:557:THR:CG2	2.99	0.40
1:A:207:GLY:O	5:A:1766:MGD:PB	2.79	0.40
1:E:95:LEU:CD2	7:E:2278:HOH:O	2.53	0.40
1:E:548:LEU:HD23	1:E:548:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:44:GLU:OE1	3:G:47:ARG:NH1	2.54	0.40
1:A:113:ARG:CZ	7:A:2066:HOH:O	2.70	0.40
1:A:170:VAL:HG12	1:A:171:SER:N	2.36	0.40
1:A:209:HIS:HD2	5:A:1766:MGD:O2A	2.04	0.40
1:A:506:THR:CG2	7:A:2248:HOH:O	2.69	0.40
1:E:426:THR:C	1:E:428:GLU:N	2.75	0.40
1:E:595:GLN:O	1:E:595:GLN:HG3	2.21	0.40
1:E:746:ARG:HH11	1:E:746:ARG:CG	2.32	0.40
2:F:117:THR:HG22	2:F:119:CYS:N	2.34	0.40
3:G:33:LEU:HD23	3:G:33:LEU:HA	1.75	0.40
3:G:60:LEU:HD23	3:G:63:LEU:HD12	2.02	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:134:LYS:N[2_674]	1.60	0.60
1:A:399:GLU:OE2	1:E:133:GLU:C[2_674]	1.61	0.59
1:A:399:GLU:OE2	1:E:133:GLU:O[2_674]	2.10	0.10

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	733/765 (96%)	651 (89%)	46 (6%)	36 (5%)	2 1
1	E	733/765 (96%)	634 (86%)	63 (9%)	36 (5%)	2 1
2	B	192/195 (98%)	176 (92%)	13 (7%)	3 (2%)	9 13
2	F	192/195 (98%)	179 (93%)	9 (5%)	4 (2%)	7 8
3	C	249/253 (98%)	231 (93%)	13 (5%)	5 (2%)	7 9
3	G	249/253 (98%)	220 (88%)	22 (9%)	7 (3%)	5 4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2348/2426 (97%)	2091 (89%)	166 (7%)	91 (4%)	3 2

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	TRP
1	A	340	ASP
1	A	428	GLU
1	A	429	PRO
1	A	431	PRO
1	A	535	PHE
1	A	562	GLY
1	A	570	PRO
1	A	586	ALA
1	A	587	SER
1	A	593	TYR
1	A	605	LEU
1	A	678	GLY
1	A	687	ARG
1	A	730	GLY
2	B	17	ALA
3	C	208	PHE
3	C	250	GLY
1	E	92	PRO
1	E	93	ASP
1	E	109	GLU
1	E	324	PRO
1	E	396	HIS
1	E	397	GLU
1	E	428	GLU
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	113	ARG
3	G	222	GLN

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Mol	Chain	Res	Type
1	A	365	ILE
1	A	399	GLU
1	A	430	TYR
1	A	434	GLY
1	A	582	PRO
1	A	592	LEU
1	A	607	VAL
1	A	631	PHE
1	A	633	ARG
2	B	193	HIS
3	C	112	SER
3	C	172	ALA
1	E	337	TYR
1	E	391	PRO
1	E	606	PRO
1	E	685	THR
2	F	178	LEU
2	F	179	ASN
3	G	39	LEU
3	G	51	TYR
3	G	249	GLY
1	A	216	ASN
1	A	389	SER
1	A	398	PRO
1	E	389	SER
1	E	429	PRO
1	E	466	ASP
1	E	469	PRO
1	E	471	GLU
1	E	513	PHE
1	E	570	PRO
2	F	45	GLU
1	A	478	VAL
2	B	115	LYS
1	E	478	VAL
1	E	627	PRO
1	E	710	HIS
1	E	763	ARG
3	G	38	HIS
1	A	387	GLY
3	C	113	GLN
1	E	70	ALA

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Mol	Chain	Res	Type
1	A	598	LYS
1	A	609	THR
1	A	610	PRO
1	A	684	PRO
1	E	138	GLU
1	E	610	PRO
1	A	584	GLY
1	E	605	LEU
1	A	194	PRO
1	E	434	GLY
1	A	511	PRO
1	E	609	THR

5.3.2 Protein sidechains (i)

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%)	500 (82%)	110 (18%)	1 2
1	E	610/632 (96%)	508 (83%)	102 (17%)	2 2
2	B	162/163 (99%)	145 (90%)	17 (10%)	7 9
2	F	162/163 (99%)	146 (90%)	16 (10%)	8 11
3	C	185/187 (99%)	162 (88%)	23 (12%)	4 5
3	G	185/187 (99%)	163 (88%)	22 (12%)	5 6
All	All	1914/1964 (98%)	1624 (85%)	290 (15%)	3 3

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	61	ARG
1	A	65	VAL
1	A	77	ARG
1	A	87	GLN
1	A	97	ARG

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Mol	Chain	Res	Type
1	A	103	GLU
1	A	106	GLN
1	A	111	LYS
1	A	116	THR
1	A	119	GLU
1	A	126	LYS
1	A	134	LYS
1	A	156	LEU
1	A	167	LYS
1	A	174	THR
1	A	187	ARG
1	A	189	ILE
1	A	209	HIS
1	A	213	ASP
1	A	214	THR
1	A	217	THR
1	A	231	LYS
1	A	252	ILE
1	A	256	THR
1	A	260	LEU
1	A	281	LYS
1	A	283	THR
1	A	286	PHE
1	A	289	LEU
1	A	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	368	SER
1	A	371	LEU
1	A	372	GLU
1	A	379	LEU
1	A	382	GLU
1	A	395	ASP
1	A	413	ARG
1	A	414	SER
1	A	415	THR
1	A	418	GLN

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Mol	Chain	Res	Type
1	A	421	ILE
1	A	428	GLU
1	A	440	ILE
1	A	441	ASN
1	A	454	GLU
1	A	457	LYS
1	A	470	GLN
1	A	477	ASP
1	A	478	VAL
1	A	484	THR
1	A	510	GLU
1	A	512	LEU
1	A	529	LEU
1	A	532	GLU
1	A	533	GLN
1	A	538	LYS
1	A	539	THR
1	A	541	GLU
1	A	542	GLU
1	A	550	SER
1	A	553	LEU
1	A	555	LEU
1	A	558	MET
1	A	561	MET
1	A	578	GLU
1	A	580	ARG
1	A	587	SER
1	A	589	LYS
1	A	591	GLU
1	A	592	LEU
1	A	594	CYS
1	A	595	GLN
1	A	596	ARG
1	A	597	PHE
1	A	603	GLN
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

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Mol	Chain	Res	Type
1	A	651	ILE
1	A	662	LYS
1	A	663	GLU
1	A	671	ASN
1	A	672	GLN
1	A	680	VAL
1	A	683	LYS
1	A	685	THR
1	A	693	VAL
1	A	702	LYS
1	A	708	LEU
1	A	721	THR
1	A	724	LYS
1	A	725	LEU
1	A	736	VAL
1	A	739	VAL
1	A	741	LEU
1	A	743	LYS
1	A	746	ARG
1	A	762	GLU
2	B	1	MET
2	B	25	MET
2	B	39	ARG
2	B	69	VAL
2	B	72	THR
2	B	78	THR
2	B	105	ARG
2	B	114	SER
2	B	117	THR
2	B	118	PHE
2	B	125	LYS
2	B	131	CYS
2	B	152	VAL
2	B	154	LYS
2	B	164	VAL
2	B	175	LEU
2	B	187	THR
3	C	11	GLN
3	C	17	THR
3	C	18	ASN
3	C	20	LEU
3	C	40	LEU

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Mol	Chain	Res	Type
3	C	63	ILE
3	C	67	GLU
3	C	71	ARG
3	C	75	THR
3	C	79	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	111	LYS
1	E	113	ARG
1	E	114	VAL
1	E	119	GLU
1	E	126	LYS
1	E	145	HIS
1	E	172	LEU
1	E	174	THR
1	E	187	ARG
1	E	208	HIS
1	E	209	HIS
1	E	213	ASP
1	E	214	THR
1	E	217	THR
1	E	224	LEU
1	E	240	SER
1	E	250	LEU
1	E	256	THR
1	E	260	LEU
1	E	272	ASP
1	E	286	PHE

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Mol	Chain	Res	Type
1	E	289	LEU
1	E	293	VAL
1	E	297	THR
1	E	299	GLU
1	E	305	THR
1	E	327	VAL
1	E	335	VAL
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	470	GLN
1	E	484	THR
1	E	488	ARG
1	E	498	LYS
1	E	499	THR
1	E	504	LEU
1	E	510	GLU
1	E	512	LEU
1	E	515	THR
1	E	528	ARG
1	E	533	GLN
1	E	538	LYS
1	E	539	THR
1	E	540	ILE
1	E	541	GLU
1	E	554	ASP
1	E	555	LEU
1	E	558	MET
1	E	564	LEU
1	E	569	LYS
1	E	577	LYS
1	E	581	LEU

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Mol	Chain	Res	Type
1	E	585	THR
1	E	591	GLU
1	E	595	GLN
1	E	596	ARG
1	E	598	LYS
1	E	602	HIS
1	E	605	LEU
1	E	607	VAL
1	E	608	PHE
1	E	609	THR
1	E	620	ARG
1	E	621	LEU
1	E	626	SER
1	E	633	ARG
1	E	647	ASN
1	E	649	VAL
1	E	651	ILE
1	E	657	LYS
1	E	671	ASN
1	E	672	GLN
1	E	676	LYS
1	E	680	VAL
1	E	685	THR
1	E	691	ASP
1	E	693	VAL
1	E	702	LYS
1	E	708	LEU
1	E	721	THR
1	E	725	LEU
1	E	736	VAL
1	E	739	VAL
1	E	740	ARG
1	E	746	ARG
1	E	748	ARG
1	E	751	SER
1	E	752	LEU
2	F	49	LEU
2	F	69	VAL
2	F	72	THR
2	F	80	ASP
2	F	88	LYS
2	F	114	SER

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Mol	Chain	Res	Type
2	F	117	THR
2	F	118	PHE
2	F	133	GLU
2	F	145	LEU
2	F	150	SER
2	F	152	VAL
2	F	164	VAL
2	F	171	THR
2	F	175	LEU
2	F	187	THR
3	G	10	GLN
3	G	17	ASN
3	G	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	113	ARG
3	G	129	TYR
3	G	136	VAL
3	G	139	ASN
3	G	144	ASN
3	G	154	THR
3	G	162	LEU
3	G	167	LYS
3	G	192	THR
3	G	196	GLU
3	G	204	GLU
3	G	215	LEU
3	G	240	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	71	ASN
1	A	83	GLN
1	A	192	HIS
1	A	209	HIS
1	A	220	GLN

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Mol	Chain	Res	Type
1	A	247	HIS
1	A	322	HIS
1	A	367	GLN
1	A	441	ASN
1	A	470	GLN
1	A	472	HIS
1	A	509	HIS
1	A	533	GLN
1	A	595	GLN
1	A	602	HIS
1	A	603	GLN
1	A	647	ASN
1	A	671	ASN
1	A	672	GLN
1	A	717	ASN
2	B	27	ASN
2	B	35	ASN
2	B	57	GLN
2	B	77	GLN
2	B	179	ASN
3	C	9	ASN
3	C	11	GLN
3	C	21	HIS
3	C	84	HIS
3	C	140	ASN
3	C	249	GLN
1	E	60	ASN
1	E	71	ASN
1	E	83	GLN
1	E	192	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

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Mol	Chain	Res	Type
1	E	602	HIS
1	E	603	GLN
1	E	635	GLN
1	E	647	ASN
1	E	671	ASN
1	E	672	GLN
1	E	717	ASN
2	F	27	ASN
2	F	35	ASN
2	F	57	GLN
2	F	77	GLN
2	F	179	ASN
3	G	8	ASN
3	G	38	HIS
3	G	137	ASN
3	G	139	ASN
3	G	248	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	1194	2	0,12,12	-	-	-		
5	MGD	A	1766	6	41,52,52	1.87	12 (29%)	40,81,81	2.91	12 (30%)
4	SF4	B	1195	2	0,12,12	-	-	-		
4	SF4	B	1197	2	0,12,12	-	-	-		
4	SF4	A	1764	1	0,12,12	-	-	-		
5	MGD	A	1765	6	41,52,52	1.77	8 (19%)	40,81,81	2.73	11 (27%)
4	SF4	F	1195	2	0,12,12	-	-	-		
4	SF4	F	1196	2	0,12,12	-	-	-		
5	MGD	E	1765	6	41,52,52	1.64	7 (17%)	40,81,81	2.64	15 (37%)
5	MGD	E	1766	6	41,52,52	1.99	9 (21%)	40,81,81	2.52	12 (30%)
4	SF4	F	1194	2	0,12,12	-	-	-		
4	SF4	F	1197	2	0,12,12	-	-	-		
4	SF4	B	1196	2	0,12,12	-	-	-		
4	SF4	E	1764	1	0,12,12	-	-	-		

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
5	MGD	A	1766	6	-	1/18/66/66	0/6/6/6
4	SF4	B	1195	2	-	-	0/6/5/5
4	SF4	B	1197	2	-	-	0/6/5/5
4	SF4	A	1764	1	-	-	0/6/5/5
5	MGD	E	1766	6	-	1/18/66/66	0/6/6/6
5	MGD	E	1765	6	-	2/18/66/66	0/6/6/6
5	MGD	A	1765	6	-	6/18/66/66	0/6/6/6
4	SF4	F	1195	2	-	-	0/6/5/5
4	SF4	F	1196	2	-	-	0/6/5/5
4	SF4	F	1194	2	-	-	0/6/5/5
4	SF4	F	1197	2	-	-	0/6/5/5
4	SF4	B	1196	2	-	-	0/6/5/5
4	SF4	E	1764	1	-	-	0/6/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1765	MGD	C16-C21	6.61	1.49	1.38
5	E	1766	MGD	C21-N22	-5.84	1.29	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1766	MGD	C16-C21	5.49	1.48	1.38
5	A	1765	MGD	C16-C21	5.45	1.47	1.38
5	A	1766	MGD	C16-C21	5.05	1.47	1.38
5	A	1766	MGD	O11-C23	4.61	1.50	1.43
5	A	1765	MGD	C23-C14	-4.26	1.50	1.53
5	E	1766	MGD	O3'-C3'	4.12	1.52	1.43
5	A	1765	MGD	O4'-C1'	3.92	1.46	1.41
5	A	1766	MGD	C14-N15	-3.84	1.42	1.46
5	A	1766	MGD	C16-C17	3.40	1.51	1.42
5	E	1766	MGD	C5-C4	3.14	1.51	1.43
5	E	1765	MGD	C10-C11	-3.06	1.47	1.52
5	A	1765	MGD	C5-C6	2.99	1.53	1.47
5	E	1766	MGD	O4'-C1'	2.88	1.45	1.41
5	A	1766	MGD	C6-N1	-2.85	1.33	1.37
5	E	1766	MGD	C19-N20	2.82	1.39	1.33
5	E	1766	MGD	C14-N15	-2.69	1.43	1.46
5	A	1765	MGD	C17-N18	-2.68	1.33	1.38
5	E	1765	MGD	C16-C17	2.66	1.49	1.42
5	A	1765	MGD	C14-N15	2.64	1.49	1.46
5	A	1765	MGD	O6-C6	2.60	1.28	1.23
5	E	1766	MGD	C19-N18	-2.59	1.31	1.37
5	A	1766	MGD	C21-N22	-2.56	1.32	1.35
5	E	1765	MGD	O4'-C1'	2.46	1.44	1.41
5	E	1766	MGD	C19-N19	-2.42	1.28	1.34
5	A	1766	MGD	O4'-C1'	2.36	1.44	1.41
5	A	1765	MGD	C5-C4	2.34	1.49	1.43
5	E	1765	MGD	C8-N7	2.33	1.39	1.35
5	A	1766	MGD	C5-C4	2.26	1.48	1.43
5	A	1766	MGD	PB-O2B	-2.23	1.44	1.55
5	E	1765	MGD	C5-C4	2.22	1.48	1.43
5	E	1765	MGD	C2'-C1'	-2.15	1.50	1.53
5	A	1766	MGD	C23-C14	-2.07	1.52	1.53
5	A	1766	MGD	C19-N20	2.01	1.38	1.33
5	A	1766	MGD	PA-O2A	-2.01	1.45	1.55

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1766	MGD	O11-C23-C14	14.07	118.35	108.96
5	A	1765	MGD	O11-C23-C14	12.57	117.35	108.96
5	E	1766	MGD	O11-C23-C14	10.62	116.05	108.96
5	E	1765	MGD	O11-C23-N22	-9.81	98.49	108.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1765	MGD	O11-C23-C14	-7.04	104.27	108.96
5	E	1766	MGD	O17-C17-C16	-5.86	113.82	127.24
5	E	1765	MGD	C19-N20-C21	5.77	123.84	113.43
5	A	1765	MGD	C19-N20-C21	5.31	123.01	113.43
5	A	1765	MGD	O4'-C1'-C2'	-3.94	101.17	106.93
5	E	1766	MGD	C19-N20-C21	3.93	120.53	113.43
5	A	1766	MGD	O11-C23-N22	3.91	112.59	108.57
5	A	1765	MGD	C17-C16-N15	3.81	126.97	116.76
5	A	1766	MGD	C19-N18-C17	-3.69	118.37	125.10
5	A	1766	MGD	O6-C6-C5	-3.65	117.25	124.37
5	A	1766	MGD	O17-C17-C16	-3.44	119.36	127.24
5	E	1765	MGD	C17-C16-N15	3.37	125.81	116.76
5	E	1766	MGD	C16-C17-N18	3.25	121.98	112.31
5	A	1765	MGD	N2-C2-N1	3.14	123.39	116.71
5	E	1765	MGD	C8-N7-C5	3.13	108.96	102.99
5	A	1766	MGD	C17-C16-N15	3.13	125.16	116.76
5	A	1766	MGD	C5-C6-N1	2.98	119.22	113.95
5	A	1765	MGD	O17-C17-C16	-2.91	120.57	127.24
5	E	1766	MGD	O2A-PA-O1A	2.89	126.50	112.24
5	E	1765	MGD	C16-C17-N18	2.79	120.61	112.31
5	A	1766	MGD	O5'-C5'-C4'	-2.74	99.54	108.99
5	E	1766	MGD	O11-C23-N22	-2.73	105.77	108.57
5	E	1765	MGD	O3'-C3'-C4'	-2.70	103.23	111.05
5	E	1766	MGD	C2-N1-C6	-2.70	120.12	125.10
5	E	1766	MGD	O3'-C3'-C4'	2.69	118.82	111.05
5	E	1766	MGD	C19-N18-C17	-2.68	120.21	125.10
5	E	1765	MGD	O4'-C1'-C2'	-2.63	103.08	106.93
5	A	1765	MGD	O4'-C4'-C5'	-2.59	100.85	109.37
5	E	1765	MGD	O17-C17-C16	-2.53	121.45	127.24
5	A	1765	MGD	N19-C19-N18	2.49	122.02	116.71
5	A	1766	MGD	C16-C17-N18	2.47	119.67	112.31
5	E	1766	MGD	C5-C6-N1	2.39	118.17	113.95
5	E	1766	MGD	O6-C6-C5	-2.38	119.72	124.37
5	E	1765	MGD	O2B-PB-O1B	2.37	123.95	112.24
5	A	1765	MGD	C23-C14-C13	-2.33	105.31	110.53
5	A	1766	MGD	C19-N20-C21	2.33	117.63	113.43
5	A	1765	MGD	PA-O3B-PB	2.32	140.79	132.83
5	A	1766	MGD	O6-C6-N1	2.29	123.35	120.65
5	E	1765	MGD	C5-C6-N1	2.27	117.96	113.95
5	A	1766	MGD	O4'-C4'-C5'	-2.26	101.93	109.37
5	E	1765	MGD	C19-N18-C17	-2.26	120.98	125.10
5	E	1765	MGD	O6-C6-C5	-2.17	120.14	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1765	MGD	C8-N7-C5	2.16	107.11	102.99
5	E	1765	MGD	O2A-PA-O1A	2.15	122.84	112.24
5	E	1766	MGD	O17-C17-N18	2.10	124.15	120.12
5	E	1765	MGD	N2-C2-N1	2.10	121.18	116.71

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1765	MGD	C5'-O5'-PB-O2B
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-O3B
5	E	1766	MGD	C11-C10-O3A-PA
5	A	1765	MGD	C5'-O5'-PB-O1B
5	A	1765	MGD	PA-O3B-PB-O1B
5	A	1765	MGD	O4'-C4'-C5'-O5'

There are no ring outliers.

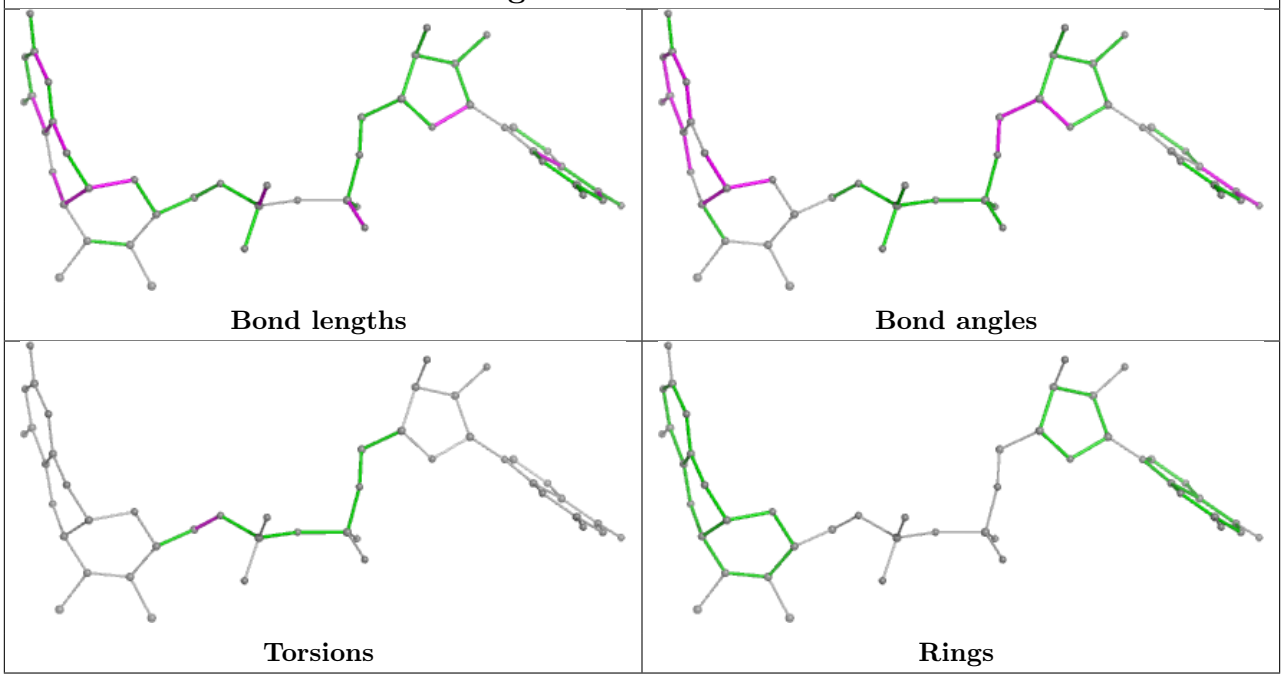
10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1194	SF4	1	0
5	A	1766	MGD	3	0
4	B	1195	SF4	1	0
5	A	1765	MGD	4	0
4	F	1196	SF4	1	0
5	E	1765	MGD	4	0
5	E	1766	MGD	3	0
4	F	1194	SF4	2	0
4	B	1196	SF4	1	0
4	E	1764	SF4	1	0

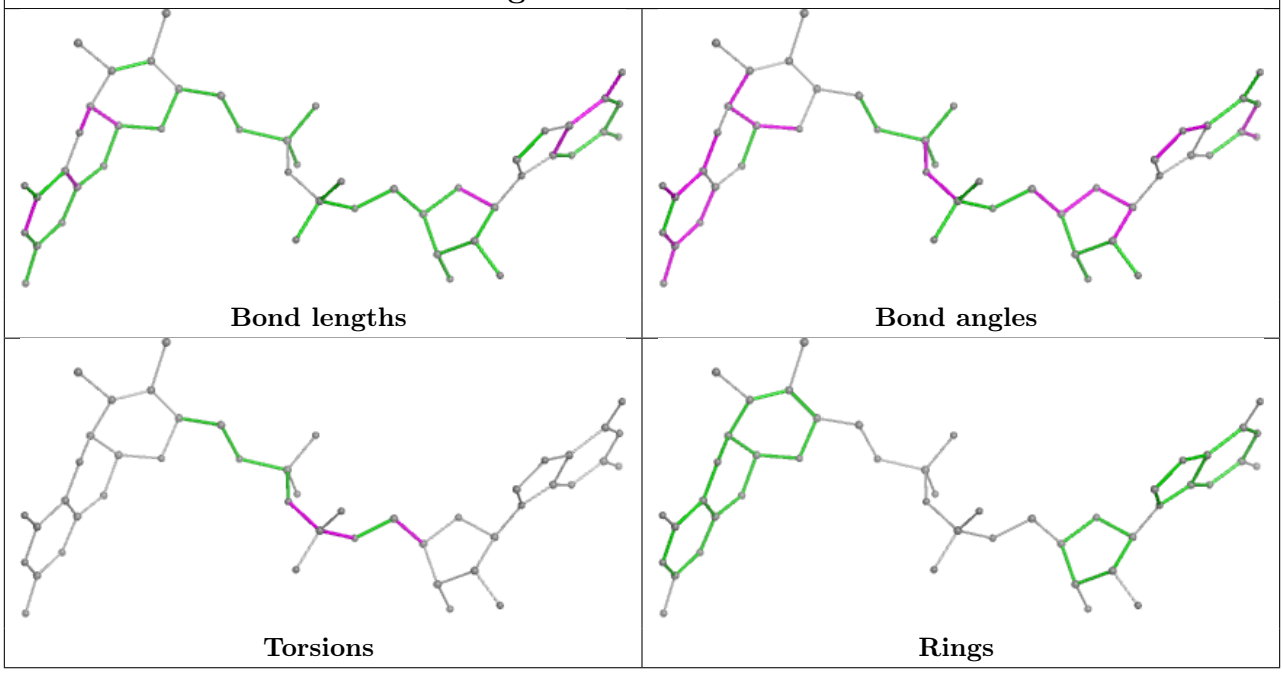
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

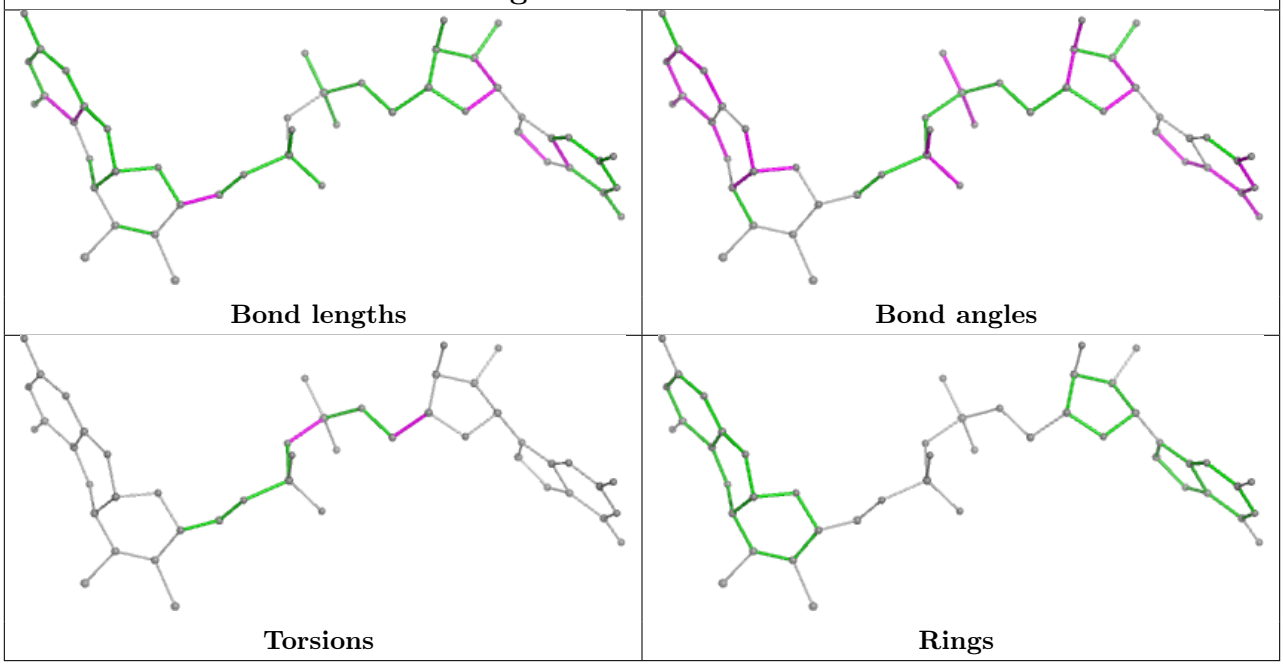
Ligand MGD A 1766



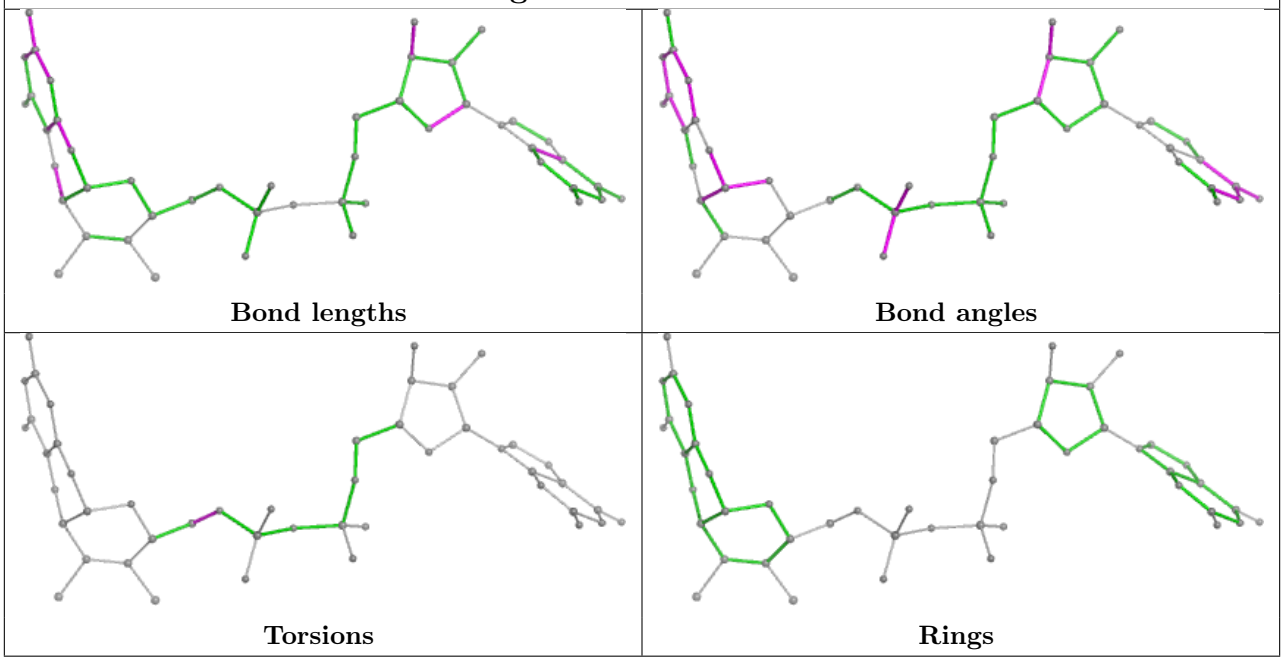
Ligand MGD A 1765



Ligand MGD E 1765



Ligand MGD E 1766



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.49	88 (11%)	4	3	25, 48, 80, 134	0
1	E	735/765 (96%)	0.43	81 (11%)	5	5	25, 46, 78, 136	0
2	B	194/195 (99%)	0.09	13 (6%)	17	16	29, 42, 63, 90	0
2	F	194/195 (99%)	0.07	9 (4%)	32	31	31, 46, 67, 90	0
3	C	251/253 (99%)	0.21	22 (8%)	10	9	32, 54, 81, 99	0
3	G	251/253 (99%)	0.50	28 (11%)	5	4	34, 62, 91, 107	0
All	All	2360/2426 (97%)	0.38	241 (10%)	6	6	25, 48, 80, 136	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	PHE	13.1
3	C	252	GLY	11.3
2	F	1	MET	11.3
1	E	390	GLY	10.6
3	G	251	GLY	10.6
2	B	1	MET	10.4
1	A	607	VAL	10.2
1	E	398	PRO	9.7
3	G	111	SER	9.7
1	E	388	CYS	9.7
3	C	111	GLY	9.2
1	A	388	CYS	9.1
1	E	396	HIS	9.1
1	A	392	SER	9.0
1	A	398	PRO	8.9
2	F	194	HIS	8.8
1	A	393	GLY	8.7
1	A	764	ARG	8.5
1	E	592	LEU	8.3

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Mol	Chain	Res	Type	RSRZ
1	E	394	GLY	8.2
1	A	401	PHE	8.1
1	A	389	SER	8.1
1	A	396	HIS	8.0
1	A	385	ALA	7.8
3	G	112	GLN	7.6
1	A	397	GLU	7.6
1	E	385	ALA	7.5
1	E	392	SER	7.5
1	E	393	GLY	7.5
1	E	389	SER	7.4
1	A	391	PRO	7.2
1	E	386	GLY	7.2
1	E	607	VAL	7.2
1	A	586	ALA	6.9
1	E	387	GLY	6.9
1	E	384	ALA	6.9
1	E	391	PRO	6.7
3	G	110	GLY	6.7
1	E	600	ALA	6.7
2	F	193	HIS	6.5
1	A	390	GLY	6.4
3	G	221	TRP	6.4
1	E	395	ASP	6.3
1	E	36	GLU	6.2
1	E	597	PHE	6.1
3	C	222	TRP	5.7
1	E	397	GLU	5.6
1	A	597	PHE	5.6
1	A	399	GLU	5.6
1	E	593	TYR	5.5
1	E	400	GLY	5.5
1	E	34	ALA	5.4
1	A	590	ILE	5.4
1	E	764	ARG	5.4
3	G	224	ARG	5.3
3	C	110	LYS	5.3
3	G	206	GLY	5.3
1	A	395	ASP	5.3
1	A	600	ALA	5.2
1	E	590	ILE	5.0
2	B	193	HIS	4.9

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Mol	Chain	Res	Type	RSRZ
3	G	225	LEU	4.9
2	B	46	TYR	4.9
3	C	112	SER	4.9
3	G	222	GLN	4.8
1	A	347	LEU	4.8
1	E	399	GLU	4.7
3	C	74	PHE	4.5
3	C	223	GLN	4.5
3	G	207	PHE	4.5
1	A	685	THR	4.4
1	E	133	GLU	4.4
1	E	465	ILE	4.3
1	A	348	LEU	4.3
1	A	606	PRO	4.2
1	E	591	GLU	4.1
1	A	384	ALA	4.1
1	E	599	GLU	4.1
1	A	328	LEU	4.0
1	A	577	LYS	4.0
1	E	383	PRO	4.0
2	B	2	PRO	4.0
1	A	584	GLY	4.0
1	A	284	VAL	3.9
3	G	109	LYS	3.9
3	C	226	LEU	3.9
2	F	2	PRO	3.8
1	A	350	VAL	3.8
3	C	108	LEU	3.8
1	A	346	ALA	3.7
2	B	194	HIS	3.7
1	A	36	GLU	3.7
1	A	207	GLY	3.7
1	A	592	LEU	3.7
3	C	225	ARG	3.6
3	G	169	PRO	3.6
1	A	599	GLU	3.6
3	C	109	GLY	3.5
1	A	335	VAL	3.5
1	A	594	CYS	3.5
1	E	435	LEU	3.5
3	G	73	PHE	3.5
1	A	383	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
3	G	167	LYS	3.4
1	A	206	ILE	3.3
1	E	464	ALA	3.3
1	A	428	GLU	3.2
1	A	582	PRO	3.2
3	G	15	TRP	3.2
1	E	577	LYS	3.2
1	A	567	ARG	3.1
1	A	42	GLN	3.1
1	E	382	GLU	3.1
1	A	261	LEU	3.1
1	A	386	GLY	3.1
1	E	105	SER	3.1
1	E	478	VAL	3.1
2	F	79	LYS	3.0
1	E	436	PHE	3.0
1	E	463	VAL	3.0
1	A	632	ALA	3.0
1	E	468	LEU	3.0
1	A	585	THR	3.0
1	A	362	GLY	3.0
1	E	350	VAL	3.0
1	E	594	CYS	2.9
1	E	568	GLY	2.9
3	C	224	GLU	2.9
1	A	102	VAL	2.9
3	C	204	GLU	2.9
1	E	584	GLY	2.9
3	G	113	ARG	2.9
1	A	344	VAL	2.9
2	B	149	GLU	2.9
1	E	323	LYS	2.9
1	E	622	LEU	2.9
2	B	147	ASP	2.8
3	G	114	ALA	2.8
1	A	580	ARG	2.8
1	A	686	ALA	2.8
1	E	347	LEU	2.8
1	E	480	LEU	2.8
1	A	295	ASP	2.8
1	E	578	GLU	2.8
2	F	149	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	208	PHE	2.7
3	G	107	LEU	2.7
1	E	467	VAL	2.7
3	G	108	GLY	2.7
1	E	567	ARG	2.7
3	C	114	ARG	2.7
3	G	106	TYR	2.7
1	E	109	GLU	2.7
1	A	593	TYR	2.7
1	E	469	PRO	2.7
1	E	606	PRO	2.7
3	C	207	GLY	2.7
1	E	37	VAL	2.7
2	B	148	PRO	2.7
2	F	147	ASP	2.7
1	E	428	GLU	2.7
1	A	465	ILE	2.6
3	G	71	PHE	2.6
2	B	192	VAL	2.6
1	E	261	LEU	2.6
1	E	748	ARG	2.6
3	G	43	ALA	2.6
1	A	277	GLU	2.6
2	B	125	LYS	2.6
1	E	106	GLN	2.6
1	E	437	ALA	2.6
1	A	363	PHE	2.6
1	E	370	TYR	2.6
1	E	287	GLU	2.6
1	A	435	LEU	2.5
3	G	46	ARG	2.5
1	A	349	TYR	2.5
1	A	133	GLU	2.5
3	G	223	GLU	2.5
1	E	608	PHE	2.5
1	A	763	ARG	2.5
1	E	206	ILE	2.5
1	A	598	LYS	2.5
1	A	748	ARG	2.4
1	A	467	VAL	2.4
1	E	344	VAL	2.4
2	F	16	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	464	ALA	2.4
3	C	72	PHE	2.4
1	A	34	ALA	2.4
3	C	113	GLN	2.4
1	A	579	GLY	2.3
1	E	348	LEU	2.3
1	E	621	LEU	2.3
1	E	569	LYS	2.3
3	G	82	PHE	2.3
3	G	81	SER	2.3
1	A	394	GLY	2.3
1	A	601	GLY	2.3
1	E	579	GLY	2.3
1	E	310	GLN	2.3
1	A	204	VAL	2.3
1	E	763	ARG	2.3
1	A	37	VAL	2.2
1	A	557	THR	2.2
1	A	532	GLU	2.2
3	C	227	ALA	2.2
1	E	330	PRO	2.2
1	A	595	GLN	2.2
2	B	146	GLU	2.2
1	A	265	ILE	2.2
1	E	695	ILE	2.2
1	E	401	PHE	2.2
1	E	585	THR	2.2
2	F	125	LYS	2.2
1	E	601	GLY	2.2
3	C	96	LEU	2.2
1	A	327	VAL	2.2
1	A	310	GLN	2.1
1	A	605	LEU	2.1
1	A	463	VAL	2.1
1	A	118	GLU	2.1
1	A	573	GLU	2.1
1	A	436	PHE	2.1
1	A	364	TYR	2.1
1	E	328	LEU	2.1
1	E	462	TYR	2.1
1	A	272	ASP	2.1
1	A	578	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	591	GLU	2.1
1	E	35	GLN	2.1
3	G	203	GLU	2.1
3	C	115	ALA	2.1
3	G	208	TRP	2.0
1	E	205	LEU	2.0
1	E	521	ILE	2.0
3	C	219	GLY	2.0
2	B	79	LYS	2.0
1	A	351	ASN	2.0
1	A	608	PHE	2.0
2	B	47	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SF4	B	1194	8/8	0.87	0.11	49,52,53,54	0
4	SF4	F	1194	8/8	0.87	0.15	59,63,70,71	0
4	SF4	B	1196	8/8	0.88	0.14	43,45,50,51	0
4	SF4	B	1195	8/8	0.95	0.09	46,48,52,55	0
4	SF4	F	1196	8/8	0.95	0.08	40,42,43,43	0
5	MGD	E	1766	47/47	0.95	0.14	25,32,36,39	0
5	MGD	E	1765	47/47	0.96	0.14	31,38,40,41	0
4	SF4	E	1764	8/8	0.96	0.09	33,38,40,42	0
4	SF4	A	1764	8/8	0.97	0.09	32,37,40,41	0
4	SF4	F	1197	8/8	0.97	0.05	44,46,48,49	0
5	MGD	A	1766	47/47	0.97	0.13	23,33,40,40	0

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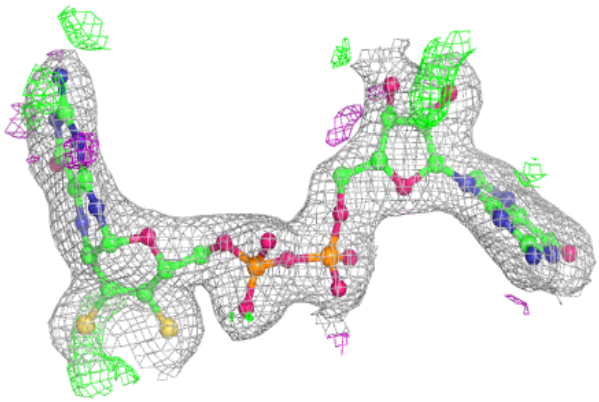
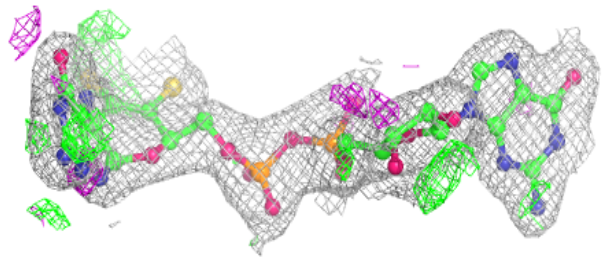
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SF4	B	1197	8/8	0.97	0.07	36,39,43,43	0
4	SF4	F	1195	8/8	0.97	0.07	42,43,43,44	0
5	MGD	A	1765	47/47	0.98	0.14	28,39,42,45	0
6	MO	A	1767	1/1	0.99	0.10	35,35,35,35	0
6	MO	E	1767	1/1	1.00	0.10	31,31,31,31	0

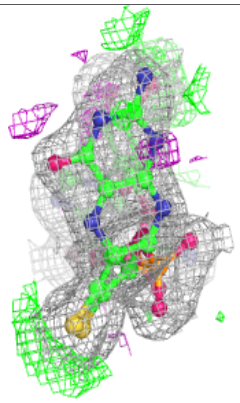
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MGD E 1766:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

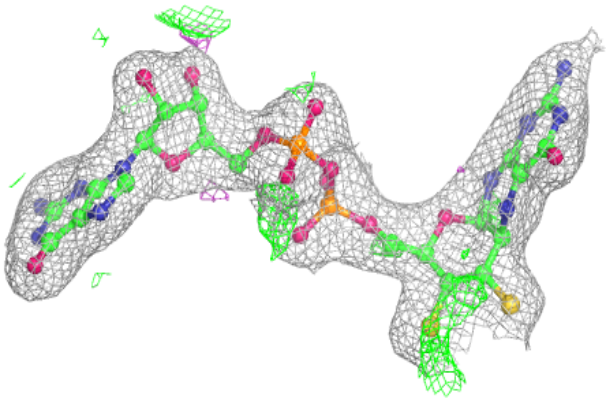


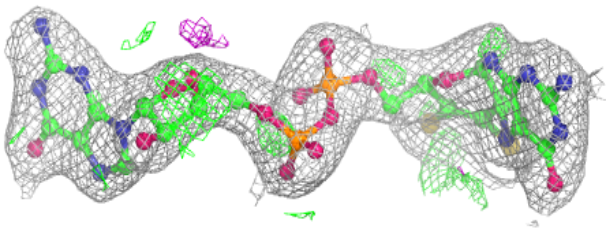


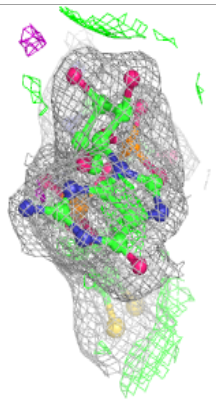


Electron density around MGD E 1765:

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

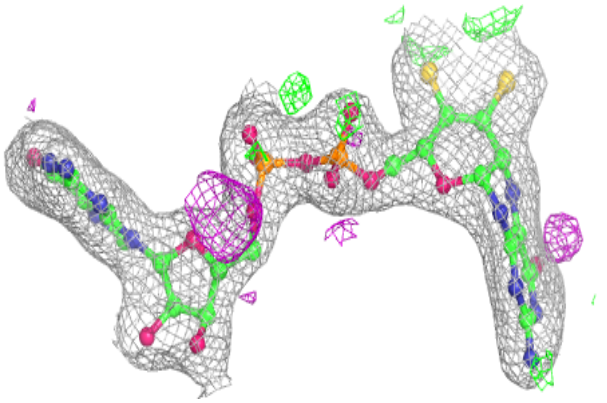


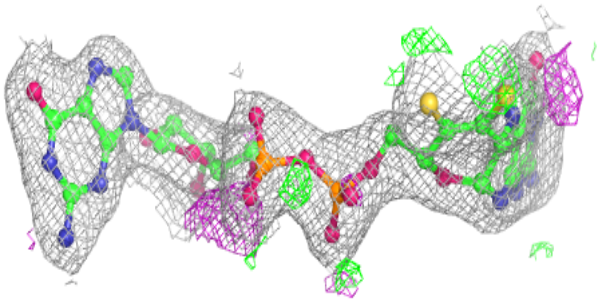


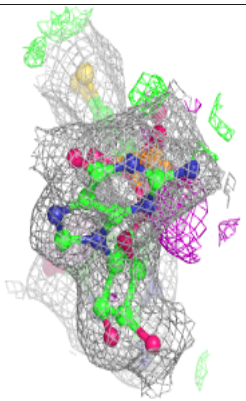


Electron density around MGD A 1766:

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

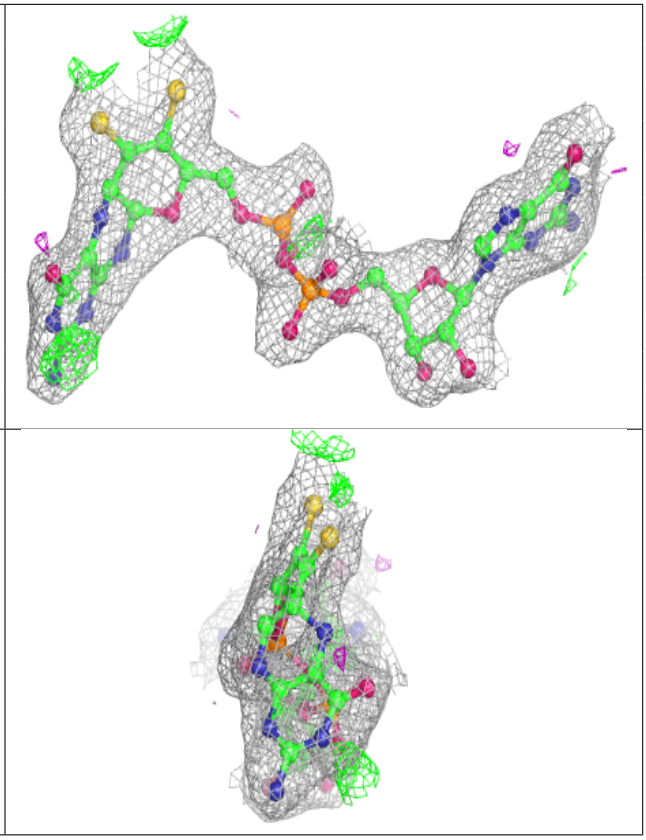






Electron density around MGD A 1765:

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



6.5 Other polymers (i)

There are no such residues in this entry.