Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2022 – 12:55 pm GMT

PDB ID	:	7Z04
Title	:	10 mM Rb+ soak of beryllium fluoride inhibited Na+,K+-ATPase, E2-BeFx (rigid body model)
Authors	:	Fruergaard, M.U.; Dach, I.; Andersen, J.L.; Ozol, M.; Shasavar, A.; Quistgaard, E.M.; Poulsen, H.; Fedosova, N.U.; Nissen, P.
Deposited on	:	2022-02-22
Resolution	:	7.50 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

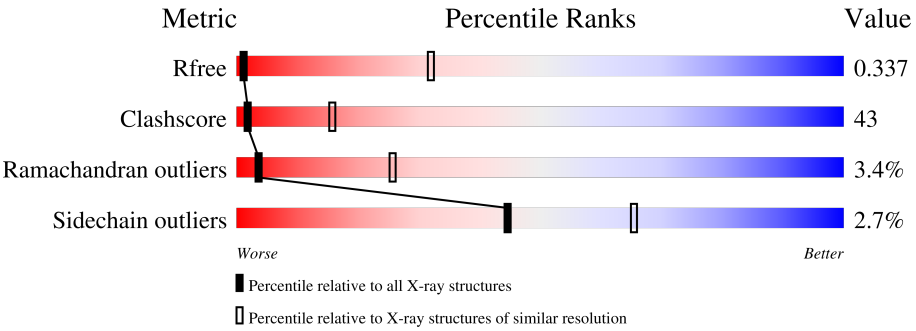
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 7.50 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	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)

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%

Mol	Chain	Length	Quality of chain
1	A	1020	46% 49%
1	C	1020	42% 51% 5%
2	B	302	44% 44% 8%
2	D	302	41% 49% 5%
3	E	64	27% 23% 50%
3	G	64	34% 14% 50%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20708 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 Sodium/potassium-transporting ATPase subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	996	Total	C	N	O	S	0	0	0
			7726	4922	1301	1456	47			
1	C	996	Total	C	N	O	S	0	0	0
			7726	4922	1301	1456	47			

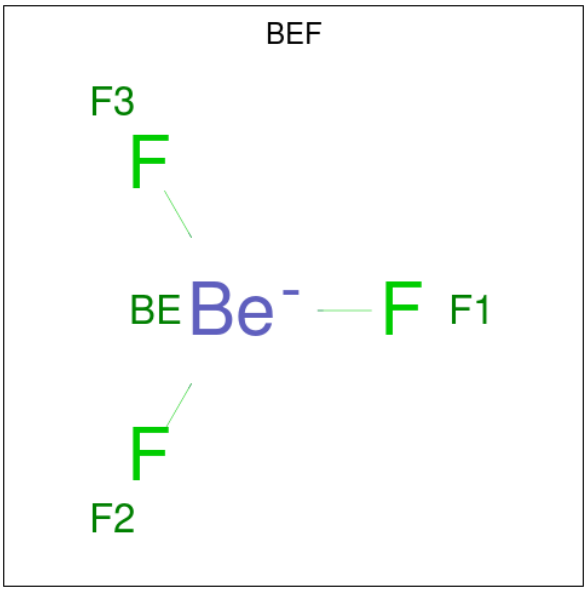
- Molecule 2 is a protein called Sodium/potassium-transporting ATPase subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	0	0	0
			2368	1534	386	435	13			
2	D	289	Total	C	N	O	S	0	0	0
			2368	1534	386	435	13			

- Molecule 3 is a protein called FXYD domain-containing ion transport regulator.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	32	Total	C	N	O	0	0	0
			255	174	37	44			
3	E	32	Total	C	N	O	0	0	0
			255	174	37	44			

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Be F 4 1 3	0	0
4	C	1	Total Be F 4 1 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

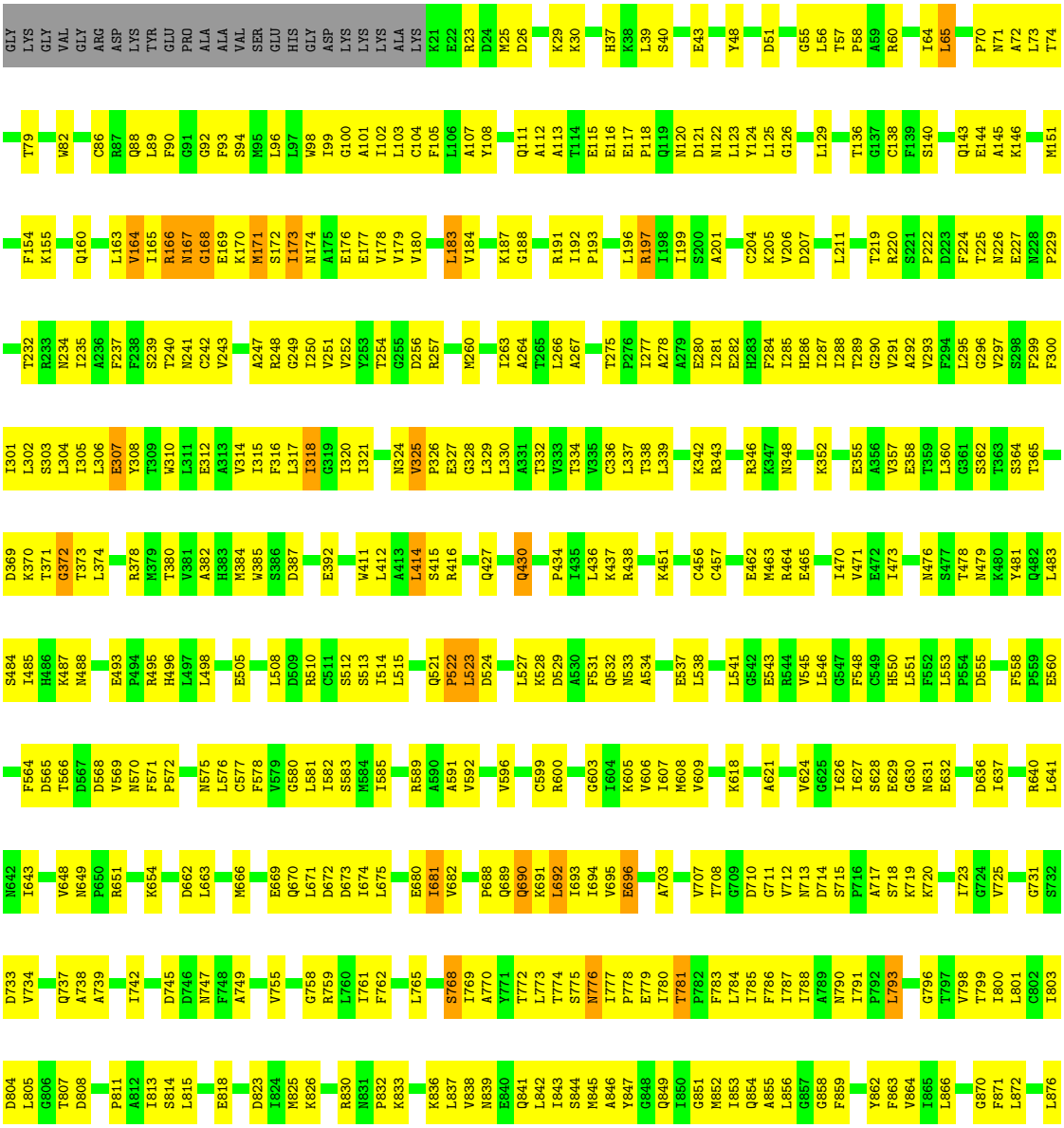
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

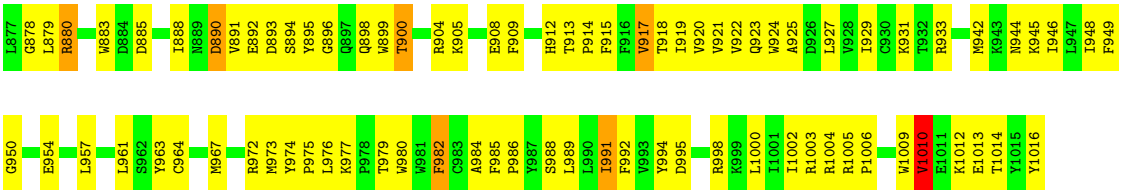
3 Residue-property plots (i)

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. 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. 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: Sodium/potassium-transporting ATPase subunit alpha-1

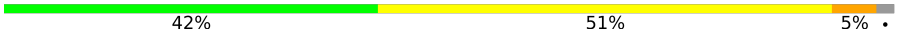
Chain A:

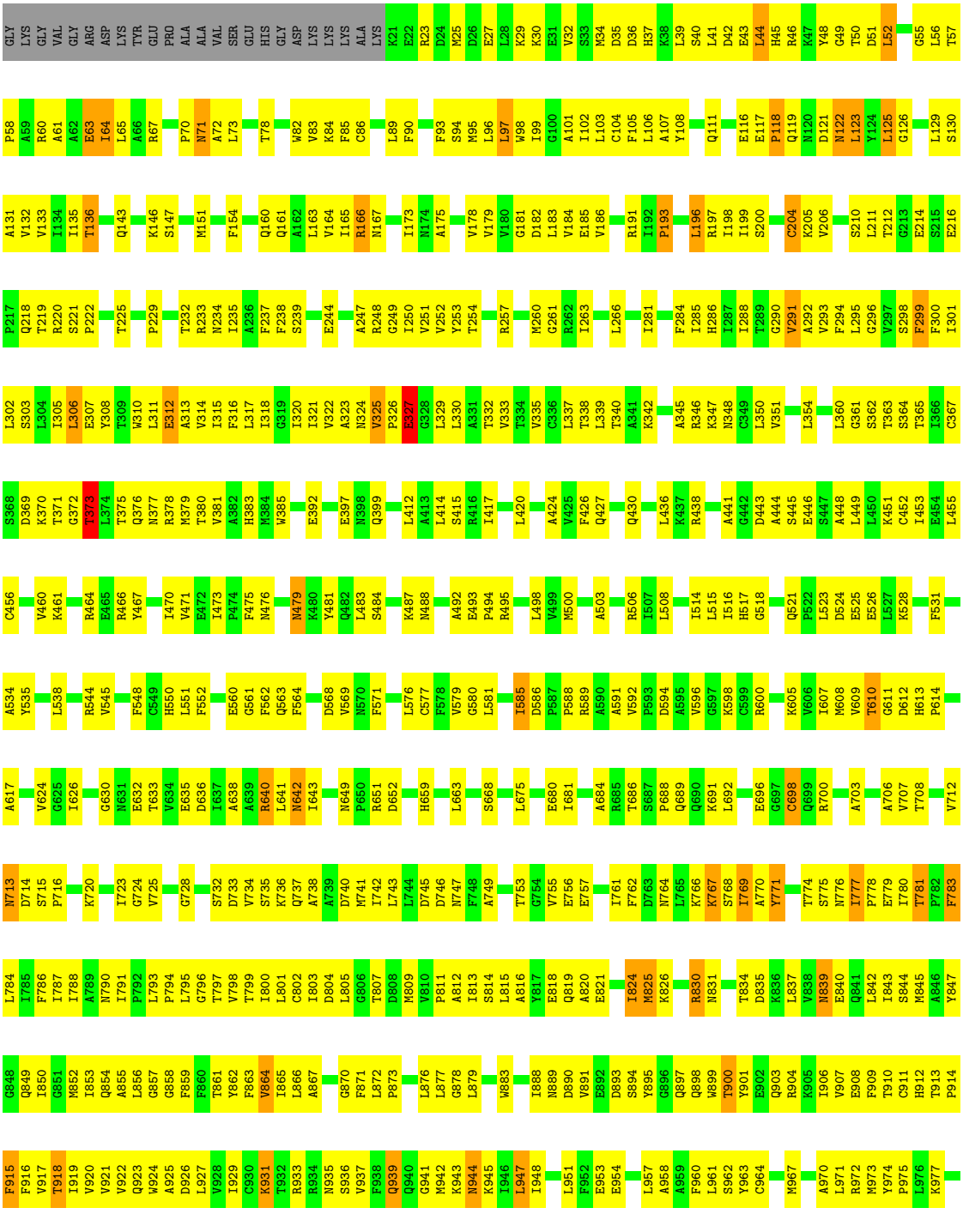


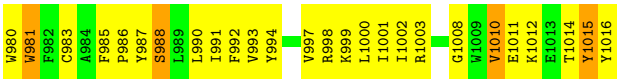


• Molecule 1: Sodium/potassium-transporting ATPase subunit alpha-1

Chain C:

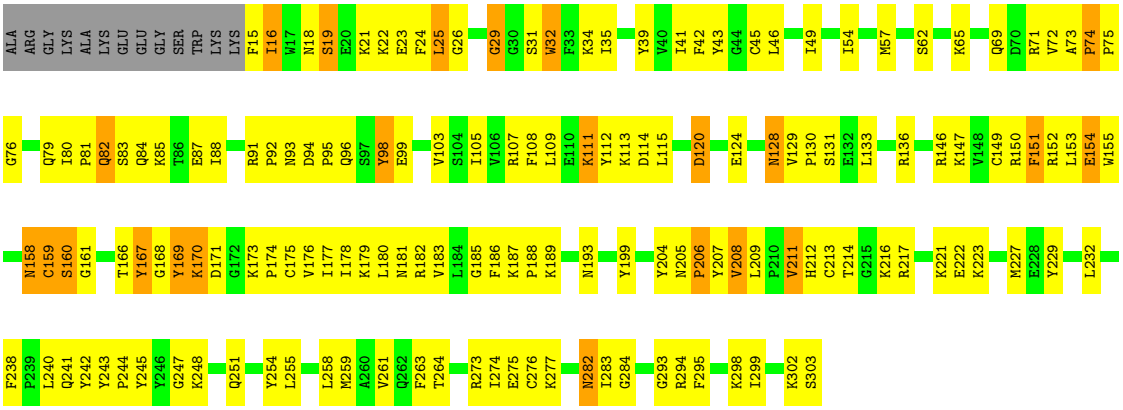






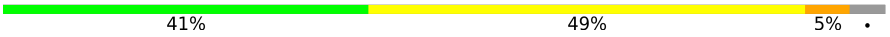
• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

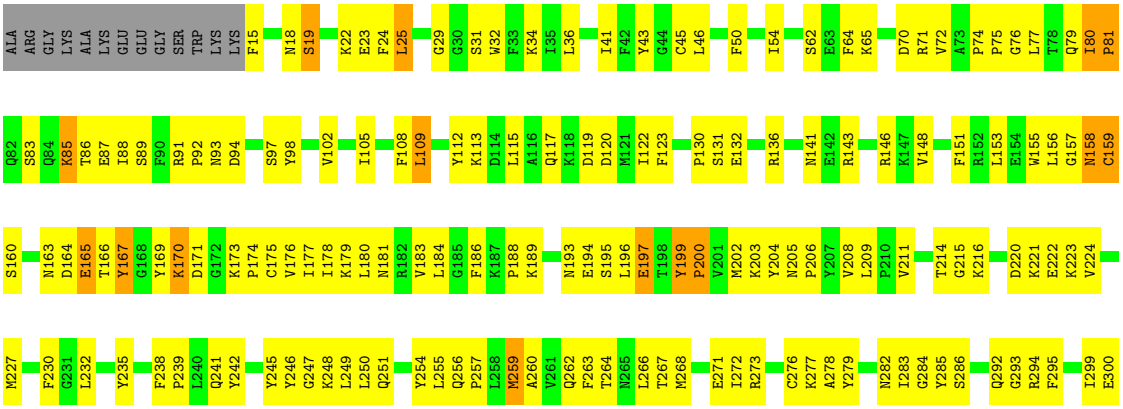
Chain B:



• Molecule 2: Sodium/potassium-transporting ATPase subunit beta-1

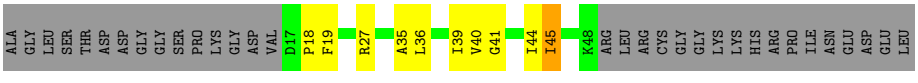
Chain D:





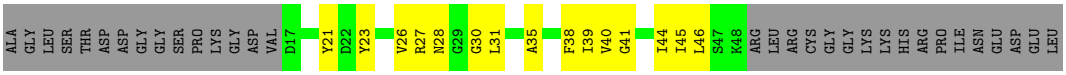
• Molecule 3: FXYD domain-containing ion transport regulator

Chain G:



• Molecule 3: FXYD domain-containing ion transport regulator

Chain E:


ALA GLY LEU SER THR ASP ASP GLY GLY SER PRO LYS GLY ASP VAL D17 Y21 D22 Y23 V26 R27 N28 G29 G30 L31 A35 F38 I39 V40 G41 I44 I45 L46 S47 K48 ARG LEU ARG CYS GLY GLY LYS LYS HIS ARG PRO ILE ASN GLU ASP GLU LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	119.00Å 119.15Å 498.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 7.50 48.98 – 7.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (25.00-7.50) 99.9 (48.98-7.50)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 7.37Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.302 , 0.338 0.318 , 0.337	Depositor DCC
R_{free} test set	943 reflections (9.81%)	wwPDB-VP
Wilson B-factor (Å^2)	373.0	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.058 for k,h,-l	Xtriage
F_o,F_c correlation	0.50	EDS
Total number of atoms	20708	wwPDB-VP
Average B, all atoms (Å^2)	480.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.67	6/7876 (0.1%)	0.80	13/10688 (0.1%)
1	C	0.65	6/7876 (0.1%)	0.78	12/10688 (0.1%)
2	B	0.67	2/2431 (0.1%)	0.79	1/3279 (0.0%)
2	D	0.64	0/2431	0.76	2/3279 (0.1%)
3	E	0.62	0/261	0.83	0/354
3	G	0.62	0/261	0.78	1/354 (0.3%)
All	All	0.66	14/21136 (0.1%)	0.79	29/28642 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	325	VAL	C-N	8.50	1.50	1.34
1	A	325	VAL	C-N	8.42	1.50	1.34
2	B	159	CYS	CB-SG	7.75	1.95	1.82
2	B	282	ASN	CA-C	-6.52	1.35	1.52
1	C	63	GLU	CD-OE1	-6.30	1.18	1.25
1	C	122	ASN	CB-CG	6.12	1.65	1.51
1	A	169	GLU	CG-CD	6.08	1.61	1.51
1	A	169	GLU	CB-CG	5.90	1.63	1.52
1	A	690	GLN	CB-CG	5.19	1.66	1.52
1	C	783	PHE	CB-CG	5.16	1.60	1.51
1	C	82	TRP	CB-CG	5.14	1.59	1.50
1	C	981	TRP	CB-CG	-5.08	1.41	1.50
1	A	696	GLU	CG-CD	5.03	1.59	1.51
1	A	696	GLU	CB-CG	5.00	1.61	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	125	LEU	CA-CB-CG	8.91	135.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	171	MET	CA-CB-CG	8.34	127.47	113.30
2	B	98	TYR	CA-CB-CG	7.77	128.17	113.40
1	A	73	LEU	CA-CB-CG	6.97	131.33	115.30
1	C	123	LEU	CA-CB-CG	-6.79	99.69	115.30
1	C	52	LEU	CA-CB-CG	6.76	130.86	115.30
1	C	196	LEU	CA-CB-CG	6.13	129.41	115.30
1	C	325	VAL	C-N-CD	-6.06	107.27	120.60
1	C	44	LEU	CA-CB-CG	-6.04	101.41	115.30
1	C	311	LEU	N-CA-C	5.94	127.04	111.00
1	C	915	PHE	N-CA-C	-5.80	95.34	111.00
2	D	109	LEU	CA-CB-CG	5.70	128.41	115.30
1	C	663	LEU	CA-CB-CG	5.68	128.36	115.30
1	A	523	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	65	LEU	CA-CB-CG	5.56	128.09	115.30
1	A	546	LEU	CA-CB-CG	5.56	128.09	115.30
2	D	164	ASP	C-N-CA	5.56	135.59	121.70
3	G	45	ILE	CB-CA-C	-5.40	100.81	111.60
1	A	414	LEU	CA-CB-CG	5.38	127.68	115.30
1	A	183	LEU	CA-CB-CG	5.36	127.63	115.30
1	A	890	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	167	ASN	C-N-CA	5.19	133.21	122.30
1	A	166	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	A	138	CYS	CA-CB-SG	5.10	123.18	114.00
1	C	97	LEU	CA-CB-CG	5.09	127.00	115.30
1	C	825	MET	CG-SD-CE	5.07	108.32	100.20
1	A	773	LEU	CA-CB-CG	5.06	126.93	115.30
1	C	508	LEU	CA-CB-CG	5.02	126.86	115.30
1	A	825	MET	CG-SD-CE	5.00	108.20	100.20

There are no chirality outliers.

There are no planarity outliers.

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	7726	0	7778	647	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7726	0	7778	734	0
2	B	2368	0	2338	237	0
2	D	2368	0	2338	175	0
3	E	255	0	259	11	0
3	G	255	0	259	13	0
4	A	4	0	0	1	0
4	C	4	0	0	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
All	All	20708	0	20750	1769	0

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 43.

All (1769) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:PHE:CD1	1:C:317:LEU:HB2	1.14	1.61
1:A:96:LEU:CD1	1:A:285:ILE:HD13	1.34	1.58
2:D:102:VAL:CG1	2:D:169:TYR:CE2	1.87	1.54
1:C:302:LEU:HA	1:C:305:ILE:CG2	1.39	1.52
1:A:783:PHE:CE2	1:A:800:ILE:HD11	1.42	1.49
2:D:102:VAL:HG13	2:D:169:TYR:CD2	1.45	1.49
1:A:297:VAL:HA	1:A:300:PHE:CE2	1.45	1.47
1:C:300:PHE:CZ	1:C:313:ALA:HB1	1.46	1.47
1:A:96:LEU:HD13	1:A:285:ILE:CG2	1.39	1.46
1:C:300:PHE:CE1	1:C:313:ALA:HB1	1.47	1.46
1:C:300:PHE:CD1	1:C:317:LEU:CB	2.00	1.44
2:D:102:VAL:HG13	2:D:169:TYR:CE2	1.46	1.42
1:C:323:ALA:O	1:C:780:ILE:CD1	1.67	1.41
1:A:783:PHE:HE2	1:A:800:ILE:CD1	1.36	1.38
1:A:96:LEU:CD1	1:A:285:ILE:HG21	1.54	1.38
1:A:92:GLY:O	1:A:96:LEU:CG	1.71	1.36
1:A:783:PHE:CE2	1:A:800:ILE:CD1	2.08	1.35
1:C:302:LEU:CA	1:C:305:ILE:HG22	1.58	1.33
2:D:102:VAL:CG1	2:D:169:TYR:CD2	2.04	1.33
1:C:64:ILE:HG23	1:C:67:ARG:CD	1.60	1.31
1:A:92:GLY:O	1:A:96:LEU:CD1	1.80	1.29
1:C:1008:GLY:O	1:C:1012:LYS:CG	1.79	1.29
1:A:92:GLY:O	1:A:96:LEU:HG	1.16	1.29
2:B:185:GLY:O	2:B:244:PRO:HG3	1.36	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:GLY:C	2:B:244:PRO:CB	2.04	1.24
1:C:64:ILE:CG2	1:C:67:ARG:HD3	1.66	1.24
2:B:186:PHE:C	2:B:244:PRO:HB3	1.57	1.23
1:A:329:LEU:HD21	1:A:772:THR:CB	1.68	1.23
1:A:136:THR:HG21	1:A:330:LEU:CG	1.69	1.22
1:A:297:VAL:CA	1:A:300:PHE:CE2	2.22	1.21
1:C:151:MET:CE	1:C:742:ILE:HG13	1.69	1.21
1:C:64:ILE:O	1:C:67:ARG:HG2	1.40	1.21
1:A:96:LEU:CD1	1:A:285:ILE:CD1	2.20	1.18
1:C:300:PHE:CE1	1:C:317:LEU:CB	2.25	1.18
1:C:1008:GLY:O	1:C:1012:LYS:HG2	1.01	1.18
1:A:297:VAL:CA	1:A:300:PHE:HE2	1.54	1.17
1:C:151:MET:SD	1:C:350:LEU:HD23	1.84	1.16
1:C:300:PHE:CG	1:C:317:LEU:HB2	1.79	1.16
1:C:1011:GLU:OE2	1:C:1015:TYR:CD2	1.99	1.16
1:C:300:PHE:CZ	1:C:313:ALA:CB	2.29	1.15
1:C:56:LEU:CB	1:C:60:ARG:HD2	1.74	1.15
1:A:899:TRP:CH2	2:B:72:VAL:HG23	1.80	1.14
1:C:323:ALA:C	1:C:780:ILE:HD11	1.67	1.14
1:A:56:LEU:HD11	1:A:60:ARG:CG	1.76	1.13
2:B:186:PHE:N	2:B:244:PRO:HB3	1.63	1.13
1:C:609:VAL:HG12	1:C:691:LYS:HE2	1.27	1.13
1:C:302:LEU:HA	1:C:305:ILE:HG21	1.26	1.13
2:B:186:PHE:N	2:B:244:PRO:CB	2.11	1.12
2:D:102:VAL:HG11	2:D:169:TYR:CE2	1.71	1.11
1:A:136:THR:HG21	1:A:330:LEU:CD1	1.80	1.11
2:B:79:GLN:O	2:B:82:GLN:NE2	1.83	1.11
1:A:99:ILE:HG22	1:A:103:LEU:HD11	1.32	1.11
1:C:93:PHE:CG	1:C:330:LEU:HD13	1.86	1.10
1:C:300:PHE:CE2	1:C:317:LEU:HD22	1.86	1.10
1:A:56:LEU:CD1	1:A:60:ARG:HG2	1.81	1.09
1:C:300:PHE:CE1	1:C:317:LEU:HB3	1.83	1.09
1:A:329:LEU:HD21	1:A:772:THR:HB	1.26	1.09
1:C:300:PHE:CE1	1:C:313:ALA:CB	2.35	1.08
1:A:320:ILE:HD13	1:A:787:ILE:HD11	1.12	1.08
1:C:302:LEU:C	1:C:305:ILE:HG22	1.75	1.07
2:B:149:CYS:C	2:B:242:TYR:OH	1.84	1.07
2:B:185:GLY:C	2:B:244:PRO:HB2	1.69	1.06
1:C:300:PHE:CE1	1:C:317:LEU:HB2	1.87	1.06
1:C:323:ALA:O	1:C:780:ILE:HD11	0.90	1.06
1:C:56:LEU:HB2	1:C:60:ARG:CD	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:HD13	1:A:310:TRP:CE3	1.90	1.06
1:C:807:THR:HB	1:C:954:GLU:HG3	1.38	1.05
2:D:80:ILE:HG13	2:D:81:PRO:HD3	1.38	1.05
1:A:99:ILE:HG22	1:A:103:LEU:CD1	1.84	1.05
1:A:96:LEU:HD12	1:A:285:ILE:HD13	1.35	1.05
1:A:312:GLU:HG3	1:A:315:ILE:HG21	1.35	1.03
1:C:64:ILE:HA	1:C:67:ARG:HD2	1.36	1.03
1:C:292:ALA:HB1	1:C:324:ASN:ND2	1.73	1.03
2:B:186:PHE:CA	2:B:244:PRO:HB3	1.88	1.03
1:A:143:GLN:HE22	1:A:338:THR:CG2	1.70	1.03
1:A:312:GLU:CD	1:A:315:ILE:HD13	1.79	1.02
1:A:120:ASN:HA	1:A:124:TYR:CE2	1.93	1.02
2:B:185:GLY:O	2:B:244:PRO:CG	2.06	1.02
1:C:370:LYS:HE2	1:C:612:ASP:OD2	1.59	1.02
1:C:64:ILE:HG23	1:C:67:ARG:HD3	1.03	1.02
1:A:864:VAL:HG22	2:B:57:MET:HG3	1.42	1.02
1:C:111:GLN:NE2	1:C:116:GLU:OE2	1.90	1.01
1:C:327:GLU:HB2	1:C:804:ASP:HB3	1.42	1.01
1:C:937:VAL:O	1:C:941:GLY:N	1.92	1.01
1:A:56:LEU:HD21	1:A:60:ARG:CG	1.89	1.01
1:A:143:GLN:HE22	1:A:338:THR:HG23	1.21	1.01
1:A:312:GLU:OE1	1:A:315:ILE:HD13	1.59	1.01
1:A:56:LEU:HD21	1:A:60:ARG:HG3	1.06	1.00
2:D:102:VAL:CG1	2:D:169:TYR:HE2	1.44	1.00
1:C:295:LEU:HB3	1:C:299:PHE:CE2	1.97	1.00
1:A:56:LEU:HD11	1:A:60:ARG:HG2	1.01	1.00
1:C:302:LEU:HA	1:C:305:ILE:HG22	1.03	1.00
1:C:795:LEU:HD13	1:C:915:PHE:HB3	1.43	1.00
1:C:212:THR:O	1:C:611:GLY:HA3	1.62	0.99
1:C:151:MET:SD	1:C:350:LEU:CD2	2.51	0.99
2:B:170:LYS:HB2	2:B:174:PRO:HA	1.44	0.98
1:C:35:ASP:OD2	1:C:229:PRO:HB3	1.62	0.98
1:A:312:GLU:HG3	1:A:315:ILE:CG2	1.93	0.98
1:A:136:THR:HG21	1:A:330:LEU:HD11	1.42	0.97
1:C:638:ALA:HA	1:C:643:ILE:CG2	1.94	0.97
1:C:300:PHE:CD2	1:C:317:LEU:HD22	2.00	0.97
1:C:302:LEU:CA	1:C:305:ILE:CG2	2.27	0.97
1:C:324:ASN:OD1	1:C:780:ILE:HD13	1.65	0.97
1:A:96:LEU:HD11	1:A:285:ILE:HD13	0.97	0.96
2:D:102:VAL:CG2	2:D:169:TYR:HD2	1.78	0.96
1:A:136:THR:HG21	1:A:330:LEU:HG	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:THR:HG22	1:C:725:VAL:HB	1.46	0.96
2:D:102:VAL:CG1	2:D:169:TYR:HD2	1.78	0.96
1:C:1011:GLU:HG3	1:C:1015:TYR:HB2	1.46	0.95
1:C:164:VAL:HG22	1:C:184:VAL:HG22	1.44	0.95
1:A:101:ALA:HA	1:A:129:LEU:HD13	1.48	0.94
1:A:56:LEU:CD2	1:A:60:ARG:HG3	1.97	0.94
1:C:151:MET:HE1	1:C:742:ILE:HG13	1.48	0.94
1:C:612:ASP:OD1	1:C:613:HIS:N	1.99	0.94
1:C:797:THR:HG23	1:C:800:ILE:HD12	1.49	0.94
1:A:120:ASN:HA	1:A:124:TYR:HE2	1.23	0.94
1:A:783:PHE:CZ	1:A:800:ILE:CD1	2.50	0.94
1:C:64:ILE:C	1:C:67:ARG:HG2	1.88	0.93
1:A:96:LEU:HD11	1:A:285:ILE:CD1	1.88	0.93
1:A:288:ILE:HG23	1:A:289:THR:H	1.32	0.93
1:C:302:LEU:O	1:C:305:ILE:HG22	1.65	0.93
1:A:317:LEU:HD12	1:A:321:ILE:HG12	1.49	0.93
1:A:285:ILE:HA	1:A:288:ILE:CG2	1.98	0.93
1:A:899:TRP:CH2	2:B:72:VAL:CG2	2.50	0.93
1:C:183:LEU:HD11	1:C:248:ARG:HB3	1.51	0.93
1:C:184:VAL:HG11	1:C:193:PRO:HG2	1.49	0.93
1:C:151:MET:HE2	1:C:742:ILE:HG13	1.49	0.93
1:C:64:ILE:CG2	1:C:67:ARG:CD	2.36	0.92
1:C:136:THR:HG21	1:C:330:LEU:HD21	1.51	0.92
1:A:807:THR:HB	1:A:954:GLU:HG3	1.52	0.92
1:A:297:VAL:O	1:A:300:PHE:CE2	2.23	0.91
1:A:1000:LEU:HD13	1:A:1003:ARG:HH22	1.33	0.91
1:C:35:ASP:OD2	1:C:229:PRO:CB	2.19	0.90
1:C:56:LEU:HD13	1:C:60:ARG:HB3	1.49	0.90
2:D:136:ARG:O	2:D:146:ARG:NH1	2.03	0.90
1:A:890:ASP:OD1	2:B:181:ASN:OD1	1.89	0.90
1:A:320:ILE:CD1	1:A:787:ILE:HD11	1.99	0.90
1:A:1000:LEU:HD13	1:A:1003:ARG:NH2	1.87	0.90
2:B:186:PHE:O	2:B:244:PRO:HB3	1.70	0.90
2:B:22:LYS:O	2:B:24:PHE:HD2	1.55	0.90
1:A:104:CYS:SG	1:A:129:LEU:HD11	2.12	0.89
1:A:120:ASN:CA	1:A:124:TYR:HE2	1.86	0.89
2:B:91:ARG:HD2	2:B:94:ASP:H	1.37	0.89
1:A:505:GLU:OE2	1:A:532:GLN:NE2	2.05	0.89
1:C:94:SER:HB3	1:C:133:VAL:HG13	1.55	0.89
1:C:164:VAL:HG11	1:C:166:ARG:NH2	1.87	0.89
1:A:98:TRP:CH2	1:A:102:ILE:CD1	2.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:MET:HE2	1:A:712:VAL:CG2	2.02	0.89
1:A:317:LEU:HD11	1:A:321:ILE:HG13	1.54	0.89
2:B:150:ARG:N	2:B:242:TYR:OH	2.05	0.89
2:D:158:ASN:HA	2:D:165:GLU:HG3	1.53	0.89
2:B:94:ASP:OD1	2:B:95:PRO:HD2	1.73	0.88
1:C:292:ALA:HA	1:C:295:LEU:HD12	1.55	0.88
1:A:96:LEU:HD13	1:A:285:ILE:CB	2.04	0.88
1:A:783:PHE:CZ	1:A:800:ILE:HD12	2.09	0.88
1:A:312:GLU:O	1:A:315:ILE:HG22	1.73	0.88
1:A:297:VAL:HG13	1:A:300:PHE:CZ	2.08	0.87
1:C:64:ILE:O	1:C:67:ARG:CG	2.22	0.87
1:C:1011:GLU:OE2	1:C:1015:TYR:HD2	1.57	0.87
1:A:312:GLU:CG	1:A:315:ILE:HG21	2.05	0.87
1:C:345:ALA:O	1:C:348:ASN:N	2.05	0.87
1:A:206:VAL:HG23	1:A:242:CYS:HA	1.56	0.87
2:D:136:ARG:HB3	2:D:146:ARG:HH11	1.40	0.87
2:D:102:VAL:HG11	2:D:169:TYR:HE2	1.18	0.86
1:A:278:ALA:HA	1:A:281:ILE:HD12	1.57	0.86
1:C:1011:GLU:HG3	1:C:1015:TYR:CB	2.05	0.86
1:C:1008:GLY:C	1:C:1012:LYS:HG2	1.95	0.86
2:B:80:ILE:HG13	2:B:81:PRO:HD3	1.57	0.86
1:C:64:ILE:HA	1:C:67:ARG:CD	2.04	0.86
1:C:166:ARG:NH2	1:C:182:ASP:OD2	2.08	0.86
2:D:25:LEU:HD21	2:D:29:GLY:HA3	1.58	0.85
1:A:99:ILE:CG2	1:A:103:LEU:HD11	2.05	0.85
1:A:783:PHE:CE2	1:A:800:ILE:HD12	2.10	0.85
1:A:508:LEU:HD11	1:A:528:LYS:HE2	1.58	0.85
1:A:136:THR:CG2	1:A:330:LEU:HD11	2.07	0.85
1:A:136:THR:CG2	1:A:330:LEU:HG	2.06	0.85
1:A:292:ALA:HA	1:A:324:ASN:ND2	1.92	0.85
1:C:768:SER:HA	1:C:815:LEU:CD1	2.06	0.85
1:A:297:VAL:HA	1:A:300:PHE:CD2	2.11	0.84
1:C:56:LEU:HB2	1:C:60:ARG:HD2	0.89	0.84
1:C:64:ILE:CA	1:C:67:ARG:HD2	2.07	0.84
1:A:98:TRP:CZ2	1:A:102:ILE:HD11	2.12	0.84
1:C:605:LYS:HE3	1:C:607:ILE:HD11	1.58	0.84
1:A:297:VAL:HA	1:A:300:PHE:HE2	0.75	0.84
1:A:312:GLU:CD	1:A:315:ILE:CD1	2.45	0.84
2:B:158:ASN:C	2:B:166:THR:HG22	1.98	0.83
1:C:811:PRO:HB3	1:C:927:LEU:HD22	1.58	0.83
1:A:512:SER:HA	1:A:523:LEU:HD23	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:TYR:HD1	1:C:118:PRO:HB2	1.43	0.83
1:C:638:ALA:O	1:C:643:ILE:HG22	1.78	0.83
2:B:186:PHE:N	2:B:244:PRO:HB2	1.83	0.83
1:A:98:TRP:CH2	1:A:102:ILE:HD11	2.13	0.83
1:C:292:ALA:HB1	1:C:324:ASN:HD22	1.44	0.83
2:B:88:ILE:HG21	2:B:170:LYS:NZ	1.94	0.82
2:B:153:LEU:H	2:B:153:LEU:HD12	1.44	0.82
1:C:863:PHE:HD2	1:C:873:PRO:HB3	1.42	0.82
1:A:669:GLU:HA	1:A:672:ASP:HB2	1.61	0.82
1:A:285:ILE:HA	1:A:288:ILE:HG22	1.61	0.82
1:A:488:ASN:ND2	1:A:493:GLU:O	2.11	0.82
1:C:1008:GLY:O	1:C:1012:LYS:CB	2.26	0.82
2:B:136:ARG:O	2:B:146:ARG:NH1	2.13	0.82
1:A:871:PHE:HB3	1:A:876:LEU:HD21	1.61	0.82
2:B:185:GLY:C	2:B:244:PRO:CG	2.45	0.82
1:A:288:ILE:HG23	1:A:289:THR:N	1.94	0.82
1:A:1009:TRP:CD1	1:A:1010:VAL:N	2.45	0.82
2:B:129:VAL:O	2:B:241:GLN:NE2	2.13	0.82
1:A:1009:TRP:CG	1:A:1010:VAL:N	2.47	0.82
2:B:185:GLY:CA	2:B:244:PRO:HB2	2.10	0.82
1:C:609:VAL:CG1	1:C:691:LYS:HE2	2.10	0.82
1:A:568:ASP:OD1	1:A:569:VAL:N	2.12	0.81
2:B:158:ASN:O	2:B:166:THR:HG22	1.80	0.81
1:C:316:PHE:CE1	1:C:786:PHE:HE1	1.96	0.81
1:C:94:SER:O	1:C:98:TRP:N	2.11	0.81
1:A:260:MET:HE2	1:A:712:VAL:HG21	1.61	0.81
1:C:56:LEU:HD13	1:C:60:ARG:CB	2.10	0.81
1:C:931:LYS:HE3	1:C:942:MET:SD	2.20	0.81
1:A:92:GLY:O	1:A:96:LEU:HD12	1.80	0.81
2:B:88:ILE:HG21	2:B:170:LYS:HZ2	1.44	0.81
1:A:317:LEU:CD1	1:A:321:ILE:HG13	2.10	0.81
1:A:783:PHE:HE2	1:A:800:ILE:HD11	0.67	0.81
1:C:524:ASP:O	1:C:526:GLU:N	2.14	0.81
1:A:591:ALA:HB1	1:A:749:ALA:HB2	1.61	0.80
2:B:80:ILE:CG2	2:B:177:ILE:HB	2.10	0.80
1:C:44:LEU:HD22	1:C:197:ARG:HD2	1.63	0.80
1:C:638:ALA:HA	1:C:643:ILE:HG22	1.62	0.80
1:A:263:ILE:HD13	1:A:688:PRO:HG2	1.63	0.80
1:A:796:GLY:O	1:A:799:THR:OG1	1.98	0.80
2:B:80:ILE:CG1	2:B:81:PRO:HD3	2.11	0.80
1:C:205:LYS:HG2	1:C:219:THR:HG22	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:ALA:O	1:C:780:ILE:CG1	2.29	0.80
1:C:300:PHE:HE1	1:C:313:ALA:C	1.84	0.80
1:A:899:TRP:CZ3	2:B:72:VAL:CG2	2.64	0.80
1:A:317:LEU:CD1	1:A:321:ILE:CG1	2.60	0.79
1:A:136:THR:HG21	1:A:330:LEU:CD2	2.12	0.79
1:A:803:ILE:O	1:A:808:ASP:HB2	1.82	0.79
1:A:898:GLN:NE2	2:B:181:ASN:HA	1.96	0.79
1:C:164:VAL:HG21	1:C:178:VAL:CG1	2.13	0.79
1:C:291:VAL:CG1	1:C:295:LEU:HD11	2.13	0.79
1:A:143:GLN:NE2	1:A:338:THR:HG23	1.97	0.79
1:C:118:PRO:HB3	1:C:122:ASN:H	1.48	0.79
1:C:298:SER:HA	1:C:301:ILE:HD12	1.65	0.79
2:D:18:ASN:OD1	2:D:19:SER:N	2.15	0.79
1:A:596:VAL:HA	1:A:599:CYS:SG	2.23	0.79
2:B:221:LYS:HB2	2:B:223:LYS:HG3	1.65	0.79
1:A:317:LEU:HD12	1:A:321:ILE:CG1	2.12	0.79
1:C:131:ALA:O	1:C:135:ILE:N	2.15	0.79
1:A:324:ASN:HA	1:A:780:ILE:HD11	1.66	0.78
2:B:186:PHE:C	2:B:244:PRO:CB	2.48	0.78
1:A:120:ASN:CB	1:A:124:TYR:HE2	1.96	0.78
1:A:136:THR:CG2	1:A:330:LEU:CG	2.57	0.78
1:C:166:ARG:HH22	1:C:178:VAL:HA	1.48	0.78
1:A:92:GLY:O	1:A:96:LEU:HD11	1.83	0.78
1:A:895:TYR:OH	2:B:62:SER:O	2.02	0.78
1:C:108:TYR:CD1	1:C:118:PRO:HB2	2.19	0.78
1:C:768:SER:HA	1:C:815:LEU:HD12	1.64	0.78
1:C:164:VAL:HG11	1:C:166:ARG:CZ	2.13	0.78
2:D:91:ARG:HD2	2:D:94:ASP:H	1.49	0.78
1:A:96:LEU:CD1	1:A:285:ILE:CG1	2.62	0.77
1:C:185:GLU:HB2	1:C:248:ARG:HD3	1.65	0.77
1:A:288:ILE:HG23	1:A:289:THR:HG23	1.64	0.77
1:C:34:MET:O	1:C:35:ASP:OD1	2.02	0.77
1:C:385:TRP:HB3	1:C:581:LEU:H	1.47	0.77
1:A:302:LEU:HA	1:A:305:ILE:HB	1.65	0.77
1:C:488:ASN:HD22	1:C:494:PRO:HA	1.46	0.77
1:C:641:LEU:O	1:C:642:ASN:HB3	1.84	0.77
1:C:300:PHE:CE2	1:C:317:LEU:CD2	2.67	0.77
2:D:102:VAL:HG11	2:D:169:TYR:CD2	2.00	0.77
1:A:297:VAL:CG1	1:A:300:PHE:CZ	2.68	0.77
2:D:91:ARG:HG2	2:D:93:ASN:H	1.50	0.77
1:A:285:ILE:HA	1:A:288:ILE:HG21	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:VAL:HG21	1:C:178:VAL:HG12	1.67	0.76
1:C:284:PHE:CD2	1:C:285:ILE:HG13	2.20	0.76
1:C:111:GLN:HE21	1:C:116:GLU:CD	1.89	0.76
1:C:961:LEU:HB3	1:C:973:MET:SD	2.26	0.76
1:A:183:LEU:HD21	1:A:248:ARG:HD2	1.66	0.76
2:B:22:LYS:O	2:B:24:PHE:CD2	2.38	0.76
1:C:795:LEU:HD13	1:C:915:PHE:CB	2.16	0.76
1:A:297:VAL:C	1:A:300:PHE:CE2	2.59	0.76
2:B:72:VAL:O	2:B:72:VAL:HG12	1.85	0.76
2:D:170:LYS:HB2	2:D:174:PRO:HA	1.68	0.76
1:C:118:PRO:HA	1:C:121:ASP:HB2	1.68	0.76
2:B:160:SER:O	2:B:160:SER:OG	2.03	0.75
1:C:95:MET:O	1:C:99:ILE:HG23	1.86	0.75
1:C:293:VAL:HG22	1:C:321:ILE:CD1	2.16	0.75
1:A:918:THR:HG23	1:A:984:ALA:HB2	1.68	0.75
2:B:108:PHE:HD1	2:B:109:LEU:HD12	1.48	0.75
2:D:119:ASP:HB2	2:D:122:ILE:HG12	1.65	0.75
1:C:56:LEU:HD12	1:C:57:THR:O	1.86	0.75
1:C:147:SER:O	1:C:151:MET:HG2	1.87	0.75
1:C:638:ALA:O	1:C:643:ILE:N	2.20	0.75
1:A:108:TYR:HD1	1:A:122:ASN:HB3	1.51	0.75
1:A:136:THR:CG2	1:A:330:LEU:CD1	2.61	0.75
1:C:326:PRO:HB2	1:C:329:LEU:HB2	1.68	0.75
1:C:963:TYR:CD2	3:E:30:GLY:HA3	2.21	0.75
1:A:98:TRP:CZ3	1:A:102:ILE:HD12	2.22	0.75
2:D:32:TRP:CE2	2:D:36:LEU:HD11	2.22	0.74
2:D:216:LYS:HB2	2:D:221:LYS:HG2	1.69	0.74
1:C:888:ILE:O	1:C:904:ARG:NH2	2.19	0.74
1:C:994:TYR:O	1:C:997:VAL:HG22	1.86	0.74
1:C:41:LEU:HA	1:C:44:LEU:HB3	1.69	0.74
1:C:164:VAL:HG12	1:C:166:ARG:NE	2.02	0.74
1:C:913:THR:HG23	1:C:973:MET:HG3	1.69	0.74
1:C:196:LEU:HD13	1:C:249:GLY:HA3	1.69	0.74
1:C:872:LEU:HD23	1:C:894:SER:HB2	1.69	0.74
1:A:90:PHE:O	1:A:94:SER:OG	2.05	0.74
1:A:285:ILE:CA	1:A:288:ILE:HG22	2.18	0.74
2:B:167:TYR:C	2:B:169:TYR:H	1.91	0.74
1:A:312:GLU:OE2	1:A:315:ILE:HD12	1.88	0.74
1:A:88:GLN:OE1	1:A:140:SER:OG	2.02	0.73
1:C:45:HIS:ND1	1:C:52:LEU:HD21	2.03	0.73
1:C:204:CYS:SG	1:C:220:ARG:HB2	2.27	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:136:ARG:HB3	2:D:146:ARG:NH1	2.03	0.73
2:B:186:PHE:O	2:B:244:PRO:CB	2.35	0.73
1:C:64:ILE:HG23	1:C:67:ARG:HD2	1.68	0.73
1:C:164:VAL:CG1	1:C:166:ARG:NE	2.51	0.73
1:C:327:GLU:HB2	1:C:804:ASP:CB	2.18	0.73
2:B:94:ASP:OD1	2:B:95:PRO:CD	2.36	0.73
2:B:216:LYS:HB2	2:B:221:LYS:HG2	1.69	0.73
2:D:102:VAL:HG22	2:D:169:TYR:HD2	1.52	0.73
1:C:890:ASP:OD1	1:C:890:ASP:O	2.06	0.73
1:A:260:MET:HE2	1:A:712:VAL:CG1	2.18	0.73
2:B:80:ILE:HG21	2:B:177:ILE:HB	1.68	0.73
1:A:293:VAL:HG13	1:A:297:VAL:HG21	1.69	0.73
1:C:293:VAL:HA	1:C:321:ILE:HD11	1.70	0.73
2:D:72:VAL:O	2:D:72:VAL:HG12	1.88	0.73
1:A:412:LEU:O	1:A:415:SER:OG	2.06	0.73
1:A:288:ILE:CG2	1:A:289:THR:H	2.00	0.73
1:A:304:LEU:CD1	1:A:310:TRP:CE3	2.71	0.73
1:A:96:LEU:CD1	1:A:285:ILE:CG2	2.36	0.72
1:C:376:GLN:HG2	1:C:589:ARG:HG2	1.69	0.72
1:C:913:THR:HG23	1:C:973:MET:CG	2.20	0.72
1:A:164:VAL:HG21	1:A:166:ARG:NH2	2.04	0.72
1:C:205:LYS:HB2	1:C:244:GLU:HG2	1.71	0.72
1:A:183:LEU:HD12	1:A:249:GLY:O	1.90	0.72
1:A:304:LEU:HD22	1:A:310:TRP:HA	1.72	0.72
1:C:844:SER:O	1:C:849:GLN:NE2	2.21	0.72
1:A:120:ASN:CB	1:A:124:TYR:CE2	2.73	0.72
1:C:640:ARG:HH11	1:C:641:LEU:CD1	2.02	0.72
1:A:430:GLN:HG3	1:A:438:ARG:HB2	1.72	0.72
1:C:302:LEU:O	1:C:305:ILE:CG2	2.36	0.72
1:C:781:THR:HG22	1:C:784:LEU:HD12	1.70	0.72
1:A:96:LEU:HD12	1:A:285:ILE:CD1	2.02	0.72
1:A:297:VAL:HG13	1:A:300:PHE:HZ	1.53	0.72
1:A:324:ASN:HA	1:A:780:ILE:CD1	2.20	0.72
1:A:329:LEU:CD2	1:A:772:THR:CB	2.61	0.72
1:A:899:TRP:CZ3	2:B:72:VAL:HG22	2.24	0.72
1:A:783:PHE:CZ	1:A:800:ILE:HD11	2.11	0.71
1:A:844:SER:O	1:A:849:GLN:NE2	2.23	0.71
1:C:260:MET:HG3	1:C:712:VAL:HG21	1.72	0.71
1:C:383:HIS:CD2	1:C:392:GLU:HB3	2.26	0.71
1:A:260:MET:CE	1:A:712:VAL:HG21	2.20	0.71
1:A:329:LEU:HD21	1:A:772:THR:OG1	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:TRP:CZ2	2:D:36:LEU:HD11	2.25	0.71
2:D:222:GLU:OE1	2:D:222:GLU:N	2.16	0.71
1:A:122:ASN:O	1:A:122:ASN:OD1	2.09	0.71
1:A:126:GLY:HA2	1:A:129:LEU:HD12	1.73	0.71
1:A:297:VAL:HG13	1:A:300:PHE:CE2	2.25	0.71
2:B:80:ILE:HD12	2:B:105:ILE:HG23	1.72	0.71
1:C:64:ILE:HD13	1:C:67:ARG:HH11	1.56	0.71
1:A:120:ASN:CA	1:A:124:TYR:CE2	2.68	0.71
1:A:899:TRP:CZ2	2:B:72:VAL:CG2	2.74	0.70
1:A:627:ILE:HG12	1:A:680:GLU:HB3	1.73	0.70
1:C:210:SER:O	1:C:713:ASN:ND2	2.24	0.70
1:A:278:ALA:O	1:A:281:ILE:HB	1.91	0.70
1:A:297:VAL:O	1:A:300:PHE:CD2	2.44	0.70
1:A:104:CYS:SG	1:A:125:LEU:HD21	2.31	0.70
1:A:282:GLU:HA	1:A:285:ILE:HD12	1.74	0.70
1:C:993:VAL:O	1:C:997:VAL:HG13	1.91	0.70
1:C:125:LEU:CD1	1:C:801:LEU:HD21	2.21	0.70
1:A:600:ARG:NH2	1:A:626:ILE:O	2.25	0.70
1:C:326:PRO:HB2	1:C:329:LEU:CB	2.22	0.70
1:C:733:ASP:HA	1:C:736:LYS:HB3	1.72	0.70
1:C:964:CYS:HB3	1:C:967:MET:HG2	1.74	0.70
1:C:64:ILE:HG22	1:C:67:ARG:HD3	1.73	0.70
2:B:80:ILE:HG13	2:B:81:PRO:CD	2.20	0.70
1:C:111:GLN:NE2	1:C:315:ILE:HG22	2.07	0.70
1:A:909:PHE:CD2	1:A:972:ARG:HB3	2.27	0.69
1:C:781:THR:HA	1:C:784:LEU:HB2	1.74	0.69
1:A:296:GLY:CA	1:A:321:ILE:HD12	2.22	0.69
1:A:649:ASN:HD21	1:A:651:ARG:HD2	1.56	0.69
1:A:164:VAL:HG21	1:A:166:ARG:CZ	2.22	0.69
1:A:286:HIS:O	1:A:290:GLY:HA3	1.92	0.69
1:A:296:GLY:HA3	1:A:321:ILE:HD12	1.74	0.69
1:C:94:SER:HB3	1:C:133:VAL:CG1	2.23	0.69
1:A:306:LEU:O	1:A:307:GLU:HG3	1.92	0.69
1:C:64:ILE:CA	1:C:67:ARG:CD	2.68	0.69
1:A:326:PRO:HB2	1:A:329:LEU:HD12	1.75	0.69
1:A:632:GLU:OE1	1:A:640:ARG:NH1	2.25	0.69
1:C:424:ALA:HA	1:C:441:ALA:O	1.92	0.69
1:C:436:LEU:HD21	1:C:455:LEU:HD22	1.75	0.69
2:D:230:PHE:HB2	2:D:260:ALA:HB3	1.73	0.69
1:A:796:GLY:O	1:A:800:ILE:HG13	1.93	0.69
1:C:64:ILE:HD13	1:C:67:ARG:NH1	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ALA:O	1:C:135:ILE:HG13	1.91	0.68
1:A:183:LEU:HD11	1:A:248:ARG:HB3	1.76	0.68
1:A:287:ILE:O	1:A:291:VAL:HG22	1.92	0.68
1:A:211:LEU:HD13	1:A:237:PHE:HB3	1.75	0.68
1:A:312:GLU:OE2	1:A:315:ILE:CD1	2.41	0.68
1:A:96:LEU:CG	1:A:285:ILE:HG21	2.23	0.68
1:A:318:ILE:HD12	1:A:318:ILE:O	1.94	0.68
1:C:107:ALA:HB2	1:C:318:ILE:HG21	1.74	0.68
1:A:239:SER:OG	1:A:260:MET:CE	2.42	0.68
1:C:638:ALA:CA	1:C:643:ILE:HG22	2.23	0.68
1:A:56:LEU:HD11	1:A:60:ARG:CB	2.23	0.68
2:B:185:GLY:O	2:B:244:PRO:CB	2.36	0.68
1:C:361:GLY:HA2	1:C:755:VAL:HG23	1.75	0.68
1:C:483:LEU:HD13	1:C:498:LEU:HD11	1.76	0.68
1:C:325:VAL:CG1	1:C:326:PRO:HD2	2.24	0.68
1:A:143:GLN:HE22	1:A:338:THR:HG21	1.57	0.67
1:C:239:SER:OG	1:C:260:MET:SD	2.49	0.67
2:D:224:VAL:HG23	2:D:272:ILE:HD13	1.75	0.67
1:C:284:PHE:HD2	1:C:285:ILE:HG13	1.58	0.67
2:D:64:PHE:CZ	2:D:141:ASN:HB2	2.28	0.67
1:A:299:PHE:HA	1:A:302:LEU:HG	1.76	0.67
1:A:915:PHE:O	1:A:919:ILE:HG12	1.95	0.67
2:D:102:VAL:CG2	2:D:169:TYR:CD2	2.70	0.67
2:D:222:GLU:O	2:D:224:VAL:HG22	1.93	0.67
1:A:39:LEU:HD22	1:A:43:GLU:HG2	1.76	0.67
1:A:201:ALA:HA	1:A:247:ALA:HA	1.77	0.67
1:A:899:TRP:CZ3	2:B:72:VAL:HG23	2.25	0.67
2:B:168:GLY:O	2:B:170:LYS:N	2.27	0.67
1:C:300:PHE:HE1	1:C:313:ALA:O	1.77	0.67
1:C:317:LEU:HA	1:C:320:ILE:HD12	1.77	0.67
2:D:209:LEU:HD21	2:D:283:ILE:HD11	1.76	0.67
1:A:293:VAL:HA	1:A:297:VAL:HG23	1.77	0.67
1:A:851:GLY:HA2	1:A:854:GLN:HB2	1.76	0.67
1:C:293:VAL:CG2	1:C:321:ILE:CD1	2.73	0.67
2:D:75:PRO:HB2	2:D:180:LEU:HD11	1.76	0.67
1:A:837:LEU:HG	1:A:838:VAL:HG23	1.77	0.67
2:B:103:VAL:O	2:B:107:ARG:HG3	1.94	0.67
1:C:90:PHE:HA	1:C:94:SER:OG	1.94	0.67
1:C:296:GLY:HA2	1:C:320:ILE:HD13	1.75	0.67
1:A:197:ARG:N	1:A:250:ILE:O	2.26	0.67
1:A:96:LEU:HD13	1:A:285:ILE:CG1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:CG1	1:A:300:PHE:CE2	2.76	0.67
2:B:124:GLU:HB2	2:B:147:LYS:HD3	1.77	0.67
2:B:155:TRP:CD2	2:B:232:LEU:HD22	2.29	0.67
1:C:473:ILE:HD12	1:C:483:LEU:HD21	1.76	0.66
1:A:320:ILE:HG23	1:A:783:PHE:HB3	1.77	0.66
1:A:844:SER:HG	2:B:39:TYR:HH	1.42	0.66
1:C:640:ARG:NH1	1:C:641:LEU:HD11	2.10	0.66
1:C:825:MET:HE2	1:C:825:MET:HA	1.77	0.66
1:A:631:ASN:CG	1:A:654:LYS:HB2	2.16	0.66
1:C:291:VAL:HG13	1:C:295:LEU:HD11	1.77	0.66
1:C:300:PHE:HD1	1:C:317:LEU:HB2	1.40	0.66
1:C:777:ILE:O	1:C:781:THR:OG1	2.12	0.66
2:D:62:SER:HB3	2:D:65:LYS:O	1.95	0.66
1:A:832:PRO:HG2	1:A:833:LYS:HD2	1.77	0.66
1:A:849:GLN:OE1	1:A:994:TYR:OH	2.13	0.66
1:A:300:PHE:CE1	1:A:301:ILE:HD13	2.31	0.66
1:A:369:ASP:OD1	1:A:370:LYS:N	2.29	0.66
1:C:136:THR:CG2	1:C:330:LEU:HD21	2.26	0.66
1:C:412:LEU:O	1:C:415:SER:OG	2.14	0.66
1:C:873:PRO:HA	1:C:876:LEU:HD12	1.78	0.66
2:D:102:VAL:HG22	2:D:169:TYR:CD2	2.31	0.66
1:A:285:ILE:C	1:A:288:ILE:HG22	2.16	0.66
1:C:766:LYS:HG3	1:C:837:LEU:HD12	1.78	0.66
2:D:158:ASN:CA	2:D:165:GLU:HG3	2.25	0.66
1:A:284:PHE:CE2	1:A:288:ILE:HD12	2.30	0.66
2:B:91:ARG:HG2	2:B:93:ASN:H	1.61	0.66
1:C:324:ASN:OD1	1:C:780:ILE:CD1	2.44	0.66
2:B:161:GLY:H	2:B:166:THR:HG21	1.61	0.66
1:C:675:LEU:HD23	1:C:681:ILE:HD12	1.76	0.66
1:C:883:TRP:CH2	1:C:904:ARG:HB2	2.31	0.66
2:B:161:GLY:N	2:B:166:THR:HG21	2.10	0.65
1:C:151:MET:HE1	1:C:742:ILE:CG1	2.23	0.65
2:D:89:SER:HA	2:D:300:GLU:O	1.96	0.65
1:A:775:SER:OG	1:A:779:GLU:OE1	2.09	0.65
1:A:986:PRO:HA	1:A:989:LEU:HB3	1.78	0.65
1:C:160:GLN:O	1:C:175:ALA:HB2	1.96	0.65
1:A:479:ASN:HB3	1:A:510:ARG:HH22	1.61	0.65
1:A:785:ILE:O	1:A:788:ILE:N	2.29	0.65
2:B:160:SER:H	2:B:166:THR:HB	1.61	0.65
1:C:852:MET:HG2	2:D:43:TYR:CE1	2.31	0.65
1:A:260:MET:HE2	1:A:712:VAL:HG11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:VAL:HG12	1:C:295:LEU:HD11	1.76	0.65
1:C:899:TRP:CH2	2:D:72:VAL:HG23	2.32	0.65
1:A:96:LEU:HD13	1:A:285:ILE:HG21	0.69	0.65
1:A:164:VAL:HG22	1:A:171:MET:O	1.96	0.65
1:A:961:LEU:O	1:A:967:MET:HG3	1.97	0.65
1:C:94:SER:HB2	1:C:133:VAL:HG11	1.78	0.65
1:C:185:GLU:HG2	1:C:186:VAL:N	2.12	0.65
1:C:610:THR:HG23	1:C:612:ASP:H	1.61	0.65
1:A:327:GLU:O	1:A:804:ASP:HB3	1.96	0.65
1:A:898:GLN:HE22	2:B:179:LYS:HE3	1.62	0.65
1:A:1000:LEU:CD1	1:A:1003:ARG:NH2	2.58	0.65
2:B:167:TYR:C	2:B:169:TYR:N	2.49	0.65
2:B:177:ILE:HG21	2:B:258:LEU:HB3	1.79	0.65
1:C:93:PHE:CD2	1:C:330:LEU:HD13	2.31	0.65
2:D:80:ILE:HG12	2:D:177:ILE:HB	1.77	0.65
1:A:637:ILE:HG12	1:A:640:ARG:HH12	1.61	0.65
2:B:214:THR:O	2:B:274:ILE:HA	1.96	0.65
1:C:30:LYS:HE2	1:C:692:LEU:HD21	1.78	0.65
1:C:183:LEU:HD21	1:C:248:ARG:HD2	1.79	0.65
1:C:768:SER:HA	1:C:815:LEU:HD13	1.79	0.65
1:A:785:ILE:HA	1:A:788:ILE:HG12	1.79	0.65
1:A:192:ILE:HD11	1:A:242:CYS:HB2	1.77	0.64
2:D:83:SER:OG	2:D:87:GLU:O	2.05	0.64
2:D:216:LYS:H	2:D:221:LYS:HD2	1.61	0.64
1:A:329:LEU:HD21	1:A:772:THR:CG2	2.27	0.64
1:C:899:TRP:CZ3	2:D:72:VAL:HG23	2.33	0.64
1:C:29:LYS:HE3	1:C:266:LEU:HB2	1.78	0.64
1:C:64:ILE:CB	1:C:67:ARG:HD2	2.28	0.64
1:C:473:ILE:HB	1:C:483:LEU:HG	1.79	0.64
1:A:277:ILE:HG21	1:A:355:GLU:HB2	1.80	0.64
1:A:775:SER:O	1:A:779:GLU:HG3	1.97	0.64
1:A:899:TRP:CE3	2:B:72:VAL:HG22	2.32	0.64
1:C:300:PHE:CZ	1:C:317:LEU:CD2	2.81	0.64
1:C:306:LEU:HB3	1:C:307:GLU:OE1	1.97	0.64
1:A:100:GLY:HA2	1:A:103:LEU:HD12	1.79	0.64
2:B:80:ILE:HG23	2:B:177:ILE:HB	1.78	0.64
1:C:312:GLU:N	1:C:312:GLU:OE2	2.31	0.64
1:C:325:VAL:HG13	1:C:326:PRO:HD2	1.78	0.64
2:D:216:LYS:NZ	2:D:222:GLU:OE1	2.28	0.64
1:A:334:THR:O	1:A:338:THR:OG1	2.13	0.64
1:C:936:SER:HB3	1:C:939:GLN:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:15:PHE:HD2	2:D:18:ASN:HD22	1.45	0.64
1:A:107:ALA:C	1:A:318:ILE:HD13	2.19	0.64
1:A:116:GLU:O	1:A:117:GLU:HG3	1.98	0.64
1:A:863:PHE:HB2	2:B:54:ILE:HD11	1.80	0.64
1:C:516:ILE:O	1:C:518:GLY:N	2.31	0.64
2:D:242:TYR:O	2:D:254:TYR:OH	2.10	0.64
2:B:277:LYS:HG3	2:B:294:ARG:HB3	1.79	0.64
1:C:284:PHE:HZ	1:C:326:PRO:HG2	1.63	0.64
1:A:204:CYS:O	1:A:220:ARG:N	2.29	0.63
1:C:766:LYS:HA	1:C:769:ILE:HD12	1.80	0.63
1:A:277:ILE:HG23	1:A:278:ALA:H	1.63	0.63
1:C:300:PHE:CE1	1:C:313:ALA:CA	2.82	0.63
1:A:898:GLN:HE21	2:B:181:ASN:HA	1.62	0.63
2:B:159:CYS:CA	2:B:166:THR:HG22	2.27	0.63
1:A:136:THR:HG21	1:A:330:LEU:HD21	1.80	0.63
1:A:277:ILE:HG23	1:A:278:ALA:N	2.13	0.63
1:C:56:LEU:CD1	1:C:60:ARG:HB3	2.26	0.63
1:C:316:PHE:HE1	1:C:786:PHE:HE1	1.41	0.63
1:C:867:ALA:HB2	1:C:873:PRO:HD3	1.79	0.63
2:B:238:PHE:HB3	2:B:243:TYR:OH	1.99	0.63
1:C:291:VAL:HG12	1:C:295:LEU:CD1	2.28	0.63
1:A:207:ASP:O	1:A:240:THR:HB	1.98	0.63
1:A:893:ASP:OD1	1:A:896:GLY:N	2.32	0.63
1:A:239:SER:OG	1:A:260:MET:HE1	1.98	0.63
1:A:778:PRO:HG3	1:A:854:GLN:HB3	1.80	0.63
1:A:964:CYS:HB3	1:A:967:MET:HG2	1.79	0.63
2:B:188:PRO:HB2	2:B:209:LEU:HD22	1.81	0.63
1:C:852:MET:O	1:C:856:LEU:HG	1.98	0.63
1:C:901:TYR:HA	1:C:904:ARG:HE	1.64	0.63
1:A:669:GLU:CA	1:A:672:ASP:HB2	2.28	0.63
2:B:31:SER:HB2	2:B:34:LYS:HD2	1.81	0.63
2:D:80:ILE:HG12	2:D:177:ILE:H	1.64	0.63
1:C:94:SER:CB	1:C:133:VAL:CG1	2.76	0.63
1:C:369:ASP:HA	1:C:609:VAL:O	1.99	0.63
2:B:188:PRO:HD3	2:B:243:TYR:HB3	1.80	0.62
1:C:367:CYS:HB2	1:C:707:VAL:HG22	1.78	0.62
2:D:263:PHE:HB3	2:D:266:LEU:HD21	1.81	0.62
1:A:688:PRO:HB3	1:A:713:ASN:HA	1.81	0.62
1:C:323:ALA:HB1	1:C:779:GLU:HB3	1.81	0.62
1:A:285:ILE:O	1:A:288:ILE:HG22	1.99	0.62
1:C:370:LYS:CE	1:C:612:ASP:OD2	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:ILE:HD12	2:D:105:ILE:HG12	1.80	0.62
1:C:98:TRP:CZ3	1:C:130:SER:HA	2.35	0.62
1:C:98:TRP:HZ3	1:C:130:SER:HA	1.65	0.62
1:C:90:PHE:O	1:C:94:SER:OG	2.13	0.62
1:C:585:ILE:HG13	1:C:586:ASP:H	1.64	0.62
1:C:909:PHE:CG	1:C:972:ARG:HB3	2.35	0.62
1:C:37:HIS:HB3	1:C:235:ILE:HD11	1.81	0.62
1:A:108:TYR:N	1:A:122:ASN:ND2	2.48	0.62
1:C:64:ILE:HA	1:C:67:ARG:CG	2.30	0.62
1:C:640:ARG:HH11	1:C:641:LEU:HD11	1.61	0.62
2:B:83:SER:OG	2:B:84:GLN:N	2.31	0.62
1:C:94:SER:HB2	1:C:98:TRP:NE1	2.14	0.62
1:C:132:VAL:O	1:C:136:THR:HB	2.00	0.62
2:D:15:PHE:HB2	2:D:18:ASN:HB2	1.80	0.62
2:B:112:TYR:CE1	2:B:255:LEU:HB3	2.34	0.62
1:C:99:ILE:O	1:C:103:LEU:HB2	2.00	0.62
1:C:111:GLN:HG2	1:C:116:GLU:OE1	2.00	0.62
1:C:335:VAL:O	1:C:339:LEU:HG	1.98	0.62
1:A:108:TYR:CE1	1:A:123:LEU:HB2	2.35	0.61
1:A:314:VAL:O	1:A:314:VAL:HG22	2.00	0.61
1:A:514:ILE:HG22	1:A:515:LEU:H	1.63	0.61
1:C:853:ILE:HG12	2:D:46:LEU:HD21	1.82	0.61
1:C:917:VAL:O	1:C:921:VAL:HG23	2.00	0.61
1:A:98:TRP:CZ3	1:A:102:ILE:CD1	2.82	0.61
1:A:470:ILE:HB	1:A:485:ILE:HG23	1.82	0.61
1:A:512:SER:HB3	1:A:575:ASN:HA	1.82	0.61
2:D:238:PHE:HD1	2:D:257:PRO:HB2	1.65	0.61
1:C:83:VAL:C	1:C:85:PHE:H	2.04	0.61
1:C:136:THR:HG21	1:C:330:LEU:CD2	2.28	0.61
1:C:337:LEU:HD23	1:C:761:ILE:HD11	1.83	0.61
1:A:551:LEU:HD22	1:A:576:LEU:HD23	1.82	0.61
2:B:21:LYS:O	2:B:24:PHE:O	2.18	0.61
1:C:850:ILE:HG21	1:C:926:ASP:OD1	2.00	0.61
1:A:548:PHE:CE1	1:A:582:ILE:HD12	2.36	0.61
1:A:551:LEU:HD13	1:A:576:LEU:HA	1.83	0.61
1:C:151:MET:CE	1:C:742:ILE:CG1	2.62	0.61
1:A:93:PHE:HA	1:A:96:LEU:HB2	1.83	0.61
1:A:264:ALA:HA	1:A:734:VAL:HG11	1.83	0.61
2:B:160:SER:N	2:B:166:THR:CG2	2.64	0.61
1:C:1001:ILE:HG22	1:C:1010:VAL:HG21	1.82	0.61
3:E:40:VAL:O	3:E:44:ILE:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:ND2	1:A:318:ILE:HD13	2.15	0.61
2:B:108:PHE:CD1	2:B:109:LEU:HD12	2.33	0.61
1:C:64:ILE:CG2	1:C:67:ARG:HD2	2.27	0.61
1:C:164:VAL:HG11	1:C:166:ARG:HH21	1.64	0.61
1:C:296:GLY:HA3	1:C:320:ILE:HG21	1.82	0.61
1:A:621:ALA:HA	1:A:624:VAL:HG22	1.81	0.61
1:A:849:GLN:O	1:A:853:ILE:HG13	2.01	0.61
1:A:852:MET:HG2	2:B:43:TYR:CE1	2.35	0.61
1:A:957:LEU:O	1:A:961:LEU:HG	2.01	0.61
2:B:245:TYR:OH	2:B:248:LYS:HA	2.00	0.61
1:C:151:MET:SD	1:C:350:LEU:HD21	2.40	0.61
1:C:443:ASP:OD1	1:C:444:ALA:N	2.30	0.61
1:A:312:GLU:HG3	1:A:312:GLU:O	2.00	0.60
1:A:476:ASN:HD21	1:A:481:TYR:H	1.48	0.60
1:C:93:PHE:O	1:C:97:LEU:HG	2.01	0.60
1:C:638:ALA:C	1:C:643:ILE:HG22	2.20	0.60
1:A:995:ASP:OD1	1:A:998:ARG:HD3	2.00	0.60
1:A:772:THR:O	1:A:775:SER:OG	2.20	0.60
2:B:188:PRO:HA	2:B:282:ASN:HD22	1.64	0.60
1:C:42:ASP:HA	1:C:45:HIS:CE1	2.36	0.60
1:C:638:ALA:CA	1:C:643:ILE:CG2	2.77	0.60
1:A:297:VAL:CB	1:A:300:PHE:HE2	2.14	0.60
1:C:295:LEU:HB3	1:C:299:PHE:HE2	1.64	0.60
1:C:503:ALA:HB3	1:C:506:ARG:HG3	1.82	0.60
1:C:516:ILE:C	1:C:518:GLY:H	2.05	0.60
2:D:98:TYR:OH	2:D:171:ASP:OD1	2.15	0.60
1:C:811:PRO:HB3	1:C:927:LEU:CD2	2.30	0.60
2:D:205:ASN:OD1	2:D:206:PRO:HD3	2.02	0.60
1:A:263:ILE:CD1	1:A:688:PRO:HG2	2.32	0.60
1:A:899:TRP:CZ2	2:B:72:VAL:HG23	2.32	0.60
1:C:300:PHE:CE1	1:C:313:ALA:C	2.73	0.60
1:C:302:LEU:O	1:C:306:LEU:HG	2.02	0.60
1:C:914:PRO:O	1:C:918:THR:N	2.22	0.60
1:C:51:ASP:HB3	1:C:55:GLY:O	2.02	0.60
1:C:545:VAL:HG11	1:C:581:LEU:HD13	1.83	0.60
1:A:605:LYS:NZ	1:A:675:LEU:O	2.34	0.60
2:B:213:CYS:HB2	2:B:227:MET:SD	2.41	0.60
2:B:213:CYS:HB3	2:B:274:ILE:HG23	1.84	0.60
1:C:1011:GLU:CG	1:C:1015:TYR:CB	2.79	0.60
2:B:186:PHE:O	2:B:244:PRO:CA	2.50	0.60
2:B:186:PHE:CE2	2:B:188:PRO:HB3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ILE:HG23	1:C:67:ARG:HH11	1.67	0.60
1:C:164:VAL:CG1	1:C:166:ARG:HE	2.14	0.60
1:C:723:ILE:HG13	1:C:740:ASP:HB2	1.84	0.60
1:A:607:ILE:HG23	1:A:681:ILE:HB	1.84	0.59
1:C:308:TYR:HD2	1:C:312:GLU:HG2	1.67	0.59
1:C:445:SER:HB3	1:C:544:ARG:HH21	1.67	0.59
2:D:279:TYR:HA	2:D:285:TYR:OH	2.02	0.59
1:A:898:GLN:HG3	2:B:182:ARG:HB2	1.83	0.59
1:C:638:ALA:HA	1:C:643:ILE:HG23	1.82	0.59
1:C:797:THR:CG2	1:C:800:ILE:HD12	2.29	0.59
2:D:102:VAL:CB	2:D:169:TYR:HD2	2.15	0.59
1:C:295:LEU:HB3	1:C:299:PHE:CZ	2.37	0.59
1:C:795:LEU:HD13	1:C:915:PHE:CG	2.38	0.59
1:A:56:LEU:CD2	1:A:60:ARG:CG	2.69	0.59
2:B:245:TYR:CE2	2:B:247:GLY:CA	2.85	0.59
1:C:426:PHE:CE1	1:C:438:ARG:HD2	2.37	0.59
2:D:143:ARG:HH11	2:D:146:ARG:NH1	2.00	0.59
1:A:900:THR:O	1:A:904:ARG:NH1	2.36	0.59
1:C:132:VAL:O	1:C:136:THR:N	2.24	0.59
1:C:300:PHE:CZ	1:C:317:LEU:HD22	2.37	0.59
1:C:466:ARG:NH1	1:C:467:TYR:OH	2.35	0.59
1:C:594:ASP:O	1:C:598:LYS:HG2	2.01	0.59
1:A:267:ALA:CB	1:A:715:SER:HB3	2.33	0.59
1:A:277:ILE:CG2	1:A:355:GLU:HB2	2.33	0.59
1:A:1009:TRP:CZ3	2:B:34:LYS:HB3	2.37	0.59
1:C:776:ASN:HA	1:C:779:GLU:HB2	1.85	0.59
2:D:41:ILE:O	2:D:45:CYS:N	2.34	0.59
1:C:64:ILE:CD1	1:C:67:ARG:HH11	2.15	0.59
1:C:179:VAL:HG22	1:C:182:ASP:HB3	1.85	0.59
1:C:858:GLY:HA2	1:C:918:THR:HG21	1.83	0.59
1:C:898:GLN:NE2	2:D:181:ASN:HA	2.17	0.59
1:C:1011:GLU:OE2	1:C:1015:TYR:CE2	2.54	0.59
1:A:56:LEU:CD1	1:A:60:ARG:CG	2.57	0.59
1:C:60:ARG:O	1:C:60:ARG:HG2	2.03	0.59
1:C:337:LEU:HD23	1:C:761:ILE:CD1	2.32	0.59
1:C:840:GLU:N	1:C:840:GLU:OE2	2.36	0.59
1:C:943:LYS:O	1:C:945:LYS:N	2.36	0.59
1:A:790:ASN:O	1:A:879:LEU:N	2.36	0.58
1:C:39:LEU:HD13	1:C:43:GLU:O	2.02	0.58
1:C:523:LEU:HB2	1:C:528:LYS:HG3	1.84	0.58
1:A:909:PHE:O	1:A:912:HIS:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:SER:N	2:B:166:THR:HG21	2.18	0.58
1:A:329:LEU:CD2	1:A:772:THR:OG1	2.51	0.58
1:A:914:PRO:HA	1:A:917:VAL:HB	1.85	0.58
2:B:75:PRO:HB2	2:B:180:LEU:HD11	1.84	0.58
1:C:154:PHE:HD2	1:C:736:LYS:HZ2	1.51	0.58
1:C:200:SER:HA	1:C:222:PRO:HG3	1.85	0.58
1:C:551:LEU:HD22	1:C:576:LEU:HD23	1.84	0.58
1:A:558:PHE:HB3	1:A:564:PHE:HZ	1.68	0.58
1:A:921:VAL:HG12	1:A:988:SER:OG	2.04	0.58
1:C:284:PHE:CE1	1:C:288:ILE:HG13	2.39	0.58
1:C:913:THR:O	1:C:916:PHE:HB3	2.03	0.58
1:A:979:THR:O	1:A:979:THR:HG22	2.03	0.58
1:C:348:ASN:HB2	1:C:745:ASP:OD2	2.03	0.58
1:C:323:ALA:HB1	1:C:779:GLU:OE2	2.03	0.58
2:D:79:GLN:HB3	2:D:295:PHE:HZ	1.69	0.58
1:A:143:GLN:NE2	1:A:338:THR:CG2	2.55	0.58
1:A:220:ARG:NH1	1:A:235:ILE:O	2.37	0.58
1:C:93:PHE:CB	1:C:330:LEU:HD13	2.33	0.58
1:A:337:LEU:HD22	1:A:357:VAL:CG1	2.34	0.58
1:A:337:LEU:HD22	1:A:357:VAL:HG11	1.85	0.58
2:B:113:LYS:HA	2:B:153:LEU:HD11	1.85	0.58
1:C:795:LEU:HD22	1:C:915:PHE:CD1	2.39	0.58
1:C:999:LYS:O	1:C:1003:ARG:NH2	2.35	0.58
2:D:31:SER:HB2	2:D:34:LYS:HD2	1.84	0.58
2:D:75:PRO:HG2	2:D:186:PHE:CE2	2.38	0.58
1:C:488:ASN:ND2	1:C:493:GLU:O	2.37	0.57
1:C:531:PHE:CE2	1:C:581:LEU:HG	2.39	0.57
2:D:80:ILE:CG1	2:D:177:ILE:H	2.17	0.57
1:A:120:ASN:HB2	1:A:124:TYR:HE2	1.69	0.57
1:A:336:CYS:HA	1:A:339:LEU:HD21	1.86	0.57
1:A:343:ARG:HG2	1:A:346:ARG:NH1	2.19	0.57
2:B:120:ASP:OD1	2:B:150:ARG:NH2	2.32	0.57
1:C:863:PHE:CD2	1:C:873:PRO:HB3	2.33	0.57
1:A:206:VAL:HG23	1:A:242:CYS:CA	2.31	0.57
1:A:691:LYS:O	1:A:695:VAL:HG23	2.03	0.57
1:C:111:GLN:HG2	1:C:116:GLU:CD	2.25	0.57
1:C:117:GLU:O	1:C:119:GLN:N	2.38	0.57
1:A:120:ASN:HA	1:A:124:TYR:CD2	2.39	0.57
1:C:293:VAL:HG23	1:C:321:ILE:HD13	1.86	0.57
1:A:479:ASN:CG	1:A:510:ARG:HH12	2.07	0.57
1:C:293:VAL:HG22	1:C:321:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:PHE:CE1	1:C:786:PHE:CE1	2.87	0.57
1:C:383:HIS:NE2	1:C:392:GLU:HB3	2.19	0.57
1:C:385:TRP:O	1:C:580:GLY:HA3	2.05	0.57
1:C:919:ILE:HA	1:C:922:VAL:HG22	1.86	0.57
1:C:942:MET:HE3	1:C:947:LEU:HB3	1.87	0.57
1:C:93:PHE:CD1	1:C:330:LEU:HD13	2.38	0.57
1:C:987:TYR:O	1:C:991:ILE:HG13	2.05	0.57
2:D:32:TRP:CE2	2:D:36:LEU:CD1	2.87	0.57
1:C:350:LEU:O	1:C:741:MET:HG3	2.05	0.57
1:C:708:THR:HA	1:C:725:VAL:O	2.03	0.57
1:A:589:ARG:HB2	1:A:592:VAL:HG23	1.87	0.57
1:A:637:ILE:HG12	1:A:640:ARG:NH1	2.19	0.57
2:B:18:ASN:O	2:B:26:GLY:HA2	2.04	0.57
1:C:295:LEU:O	1:C:299:PHE:CD2	2.58	0.57
1:C:797:THR:HA	1:C:800:ILE:HG13	1.87	0.57
1:C:999:LYS:O	1:C:1003:ARG:NE	2.38	0.57
1:A:780:ILE:HG22	1:A:784:LEU:HD21	1.87	0.57
1:A:853:ILE:HG12	2:B:46:LEU:HD11	1.86	0.57
2:B:168:GLY:C	2:B:170:LYS:H	2.07	0.57
1:C:164:VAL:CG1	1:C:166:ARG:CZ	2.83	0.57
1:C:229:PRO:O	1:C:237:PHE:HZ	1.88	0.57
1:C:321:ILE:O	1:C:321:ILE:HG22	2.05	0.57
1:A:120:ASN:HB2	1:A:124:TYR:CE2	2.40	0.56
2:B:245:TYR:CE2	2:B:247:GLY:C	2.79	0.56
2:D:245:TYR:OH	2:D:248:LYS:N	2.38	0.56
1:A:199:ILE:HG21	1:A:250:ILE:HD13	1.87	0.56
1:A:297:VAL:CG1	1:A:300:PHE:HZ	2.11	0.56
1:A:548:PHE:CD1	1:A:582:ILE:HD12	2.40	0.56
1:A:964:CYS:HB3	1:A:967:MET:CG	2.33	0.56
1:C:23:ARG:NH2	1:C:27:GLU:OE2	2.38	0.56
1:C:90:PHE:CA	1:C:94:SER:OG	2.52	0.56
1:C:220:ARG:NH1	1:C:235:ILE:O	2.31	0.56
1:C:362:SER:OG	1:C:830:ARG:HD3	2.06	0.56
2:D:92:PRO:HG2	2:D:303:SER:HB2	1.87	0.56
1:A:288:ILE:CG2	1:A:289:THR:N	2.63	0.56
1:C:430:GLN:HG3	1:C:438:ARG:HB2	1.86	0.56
1:C:712:VAL:C	1:C:714:ASP:H	2.08	0.56
1:A:108:TYR:CD1	1:A:122:ASN:HB3	2.37	0.56
2:B:150:ARG:N	2:B:242:TYR:HH	2.03	0.56
1:C:764:ASN:HA	1:C:767:LYS:HD2	1.87	0.56
1:C:781:THR:HA	1:C:784:LEU:CG	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:936:SER:HB2	1:C:1003:ARG:CZ	2.35	0.56
2:D:92:PRO:HG3	2:D:301:VAL:HG12	1.87	0.56
1:C:164:VAL:HG21	1:C:178:VAL:HG11	1.87	0.56
2:D:102:VAL:HG12	2:D:169:TYR:HE2	1.61	0.56
1:A:663:LEU:HD13	1:A:663:LEU:C	2.26	0.56
1:A:529:ASP:HA	1:A:532:GLN:HB2	1.87	0.56
1:C:73:LEU:HD21	1:C:261:GLY:HA2	1.88	0.56
1:C:771:TYR:HD2	1:C:812:ALA:HB2	1.70	0.56
1:C:883:TRP:CZ2	1:C:904:ARG:HB2	2.40	0.56
1:C:929:ILE:O	1:C:999:LYS:NZ	2.20	0.56
1:C:284:PHE:CZ	1:C:288:ILE:HG13	2.41	0.55
2:D:79:GLN:HB2	2:D:81:PRO:HD2	1.88	0.55
2:D:208:VAL:HG21	2:D:235:TYR:HB3	1.88	0.55
1:A:199:ILE:H	1:A:249:GLY:HA2	1.70	0.55
1:A:300:PHE:CE1	1:A:301:ILE:CD1	2.89	0.55
1:A:292:ALA:HA	1:A:324:ASN:HD22	1.67	0.55
2:D:108:PHE:CD1	2:D:109:LEU:HD12	2.41	0.55
1:A:37:HIS:HB3	1:A:235:ILE:HD11	1.88	0.55
1:A:93:PHE:HA	1:A:96:LEU:HD12	1.88	0.55
2:B:73:ALA:HB3	2:B:74:PRO:HD3	1.88	0.55
2:B:96:GLN:OE1	2:B:99:GLU:HG3	2.07	0.55
1:C:94:SER:CB	1:C:133:VAL:HG13	2.30	0.55
1:C:945:LYS:HA	1:C:948:ILE:HG12	1.89	0.55
1:A:105:PHE:HA	1:A:108:TYR:HB3	1.87	0.55
1:A:995:ASP:OD1	1:A:998:ARG:NH1	2.39	0.55
2:B:189:LYS:H	2:B:282:ASN:ND2	2.05	0.55
1:C:44:LEU:HD21	1:C:250:ILE:HG13	1.88	0.55
1:C:50:THR:HG23	1:C:56:LEU:HB3	1.89	0.55
1:C:197:ARG:HB2	1:C:252:VAL:HG23	1.87	0.55
1:C:640:ARG:NH1	1:C:641:LEU:CD1	2.69	0.55
2:D:211:VAL:HG22	2:D:278:ALA:HB2	1.89	0.55
1:A:476:ASN:HD21	1:A:481:TYR:N	2.05	0.55
1:C:40:SER:O	1:C:44:LEU:N	2.39	0.55
1:C:296:GLY:CA	1:C:320:ILE:HG21	2.36	0.55
1:C:871:PHE:CZ	1:C:893:ASP:HB3	2.40	0.55
1:C:926:ASP:HA	1:C:929:ILE:HG12	1.89	0.55
1:A:777:ILE:O	1:A:781:THR:OG1	2.15	0.55
1:C:108:TYR:CG	1:C:123:LEU:HG	2.42	0.55
1:C:641:LEU:O	1:C:642:ASN:CB	2.49	0.55
1:C:101:ALA:HB2	1:C:129:LEU:HB3	1.89	0.55
2:B:193:ASN:OD1	2:B:205:ASN:ND2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:ASN:HB3	2:B:155:TRP:CH2	2.42	0.54
1:C:35:ASP:OD2	1:C:229:PRO:HB2	2.03	0.54
1:C:64:ILE:CG2	1:C:67:ARG:HH11	2.19	0.54
1:C:163:LEU:O	1:C:184:VAL:HG13	2.07	0.54
1:A:872:LEU:HD23	1:A:894:SER:HB2	1.88	0.54
1:C:568:ASP:OD1	1:C:569:VAL:N	2.36	0.54
2:B:81:PRO:HG3	2:B:176:VAL:HG22	1.90	0.54
2:B:91:ARG:HD2	2:B:94:ASP:N	2.16	0.54
2:B:189:LYS:H	2:B:282:ASN:CB	2.21	0.54
1:C:197:ARG:N	1:C:250:ILE:O	2.25	0.54
1:C:762:PHE:CE2	1:C:830:ARG:HD2	2.43	0.54
1:A:70:PRO:O	1:A:72:ALA:N	2.40	0.54
1:C:94:SER:O	1:C:98:TRP:CB	2.55	0.54
1:C:94:SER:HB2	1:C:98:TRP:CD1	2.43	0.54
1:C:98:TRP:HA	1:C:98:TRP:CE3	2.42	0.54
1:C:111:GLN:NE2	1:C:116:GLU:CD	2.54	0.54
1:C:944:ASN:CG	1:C:947:LEU:HB2	2.28	0.54
2:D:102:VAL:CB	2:D:169:TYR:CD2	2.87	0.54
1:A:51:ASP:HB3	1:A:55:GLY:H	1.72	0.54
1:A:669:GLU:C	1:A:672:ASP:HB2	2.28	0.54
1:C:774:THR:O	1:C:778:PRO:HD2	2.08	0.54
1:C:913:THR:CG2	1:C:973:MET:HG3	2.36	0.54
1:C:182:ASP:O	1:C:251:VAL:HG23	2.08	0.54
1:C:379:MET:CE	1:C:585:ILE:HA	2.38	0.54
1:C:515:LEU:HD23	1:C:579:VAL:HG13	1.90	0.54
1:C:756:GLU:HA	1:C:825:MET:HE3	1.88	0.54
1:A:780:ILE:O	1:A:783:PHE:N	2.41	0.54
1:C:420:LEU:O	1:C:464:ARG:NH1	2.40	0.54
1:C:445:SER:HB3	1:C:544:ARG:NH2	2.23	0.54
1:C:853:ILE:HG12	2:D:46:LEU:HD11	1.90	0.53
1:C:867:ALA:HA	1:C:871:PHE:O	2.07	0.53
2:D:271:GLU:HB2	2:D:300:GLU:HB2	1.90	0.53
1:A:57:THR:HG22	1:A:167:ASN:OD1	2.07	0.53
1:A:515:LEU:HB2	1:A:577:CYS:SG	2.48	0.53
1:C:118:PRO:HB3	1:C:122:ASN:HB2	1.89	0.53
1:C:689:GLN:OE1	1:C:689:GLN:N	2.28	0.53
1:A:289:THR:HA	1:A:292:ALA:HB3	1.91	0.53
2:B:222:GLU:OE1	2:B:222:GLU:N	2.41	0.53
1:C:94:SER:CB	1:C:133:VAL:HG11	2.38	0.53
1:C:111:GLN:NE2	1:C:315:ILE:CG2	2.70	0.53
1:C:903:GLN:NE2	2:D:72:VAL:HA	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ILE:CG2	2:B:170:LYS:HZ1	2.22	0.53
1:C:184:VAL:HG11	1:C:193:PRO:CG	2.31	0.53
2:B:178:ILE:N	2:B:259:MET:O	2.40	0.53
1:C:56:LEU:HD13	1:C:60:ARG:CG	2.38	0.53
1:C:795:LEU:HD22	1:C:915:PHE:CE1	2.43	0.53
2:D:227:MET:HG2	2:D:263:PHE:CE1	2.44	0.53
1:A:352:LYS:NZ	1:A:737:GLN:HA	2.24	0.53
1:C:487:LYS:HZ2	1:C:560:GLU:HA	1.73	0.53
1:C:728:GLY:N	1:C:743:LEU:O	2.42	0.53
2:D:195:SER:O	2:D:197:GLU:N	2.41	0.53
1:A:688:PRO:O	1:A:691:LYS:HG3	2.09	0.53
1:C:39:LEU:HD22	1:C:43:GLU:HG2	1.91	0.53
1:A:505:GLU:CD	1:A:532:GLN:HE22	2.07	0.53
1:A:851:GLY:CA	1:A:854:GLN:HB2	2.39	0.53
2:B:88:ILE:CG2	2:B:170:LYS:NZ	2.69	0.53
2:B:245:TYR:CZ	2:B:247:GLY:C	2.83	0.53
1:C:864:VAL:HG12	1:C:980:TRP:CZ3	2.43	0.53
1:A:964:CYS:O	1:A:967:MET:HG2	2.08	0.53
2:B:173:LYS:HB3	2:B:264:THR:HA	1.91	0.53
2:B:221:LYS:HE3	2:B:223:LYS:HD3	1.90	0.53
1:C:771:TYR:CD2	1:C:812:ALA:HB2	2.43	0.53
1:C:795:LEU:CD1	1:C:915:PHE:HB3	2.26	0.53
1:C:1000:LEU:HD23	1:C:1003:ARG:CZ	2.38	0.53
2:D:22:LYS:HG2	2:D:22:LYS:O	2.08	0.53
2:D:167:TYR:O	2:D:169:TYR:CD1	2.62	0.53
1:A:302:LEU:HD23	1:A:305:ILE:HD12	1.91	0.53
2:B:169:TYR:O	2:B:170:LYS:HB3	2.08	0.53
2:D:76:GLY:O	2:D:180:LEU:HA	2.08	0.53
2:D:94:ASP:OD2	2:D:97:SER:N	2.42	0.53
1:A:342:LYS:HB3	1:A:346:ARG:HH21	1.73	0.52
1:A:360:LEU:HD22	1:A:360:LEU:H	1.74	0.52
1:A:669:GLU:O	1:A:672:ASP:HB2	2.08	0.52
1:C:762:PHE:HE1	1:C:837:LEU:HB2	1.73	0.52
1:A:564:PHE:CD2	1:A:570:ASN:HB3	2.44	0.52
2:B:238:PHE:CZ	2:B:259:MET:HE2	2.44	0.52
1:C:64:ILE:CB	1:C:67:ARG:CD	2.87	0.52
2:B:245:TYR:CZ	2:B:247:GLY:O	2.62	0.52
1:C:417:ILE:HG21	1:C:548:PHE:HB3	1.91	0.52
1:C:797:THR:HA	1:C:800:ILE:CG1	2.39	0.52
1:A:104:CYS:SG	1:A:129:LEU:CD1	2.94	0.52
1:A:632:GLU:CD	1:A:636:ASP:HB3	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:VAL:HA	2:B:57:MET:SD	2.48	0.52
1:C:316:PHE:HA	1:C:783:PHE:CZ	2.44	0.52
1:A:343:ARG:HA	1:A:346:ARG:HD2	1.90	0.52
1:A:553:LEU:HD21	1:A:571:PHE:HB2	1.92	0.52
2:B:80:ILE:HG12	2:B:81:PRO:HD3	1.88	0.52
1:C:151:MET:HE2	1:C:742:ILE:CG1	2.32	0.52
1:C:300:PHE:CZ	1:C:313:ALA:HB3	2.40	0.52
1:C:535:TYR:HB2	1:C:581:LEU:HD11	1.91	0.52
1:C:805:LEU:HA	1:C:809:MET:SD	2.49	0.52
2:D:205:ASN:N	2:D:206:PRO:HD2	2.25	0.52
2:B:129:VAL:HG22	2:B:130:PRO:HD2	1.91	0.52
1:C:45:HIS:CG	1:C:52:LEU:HD21	2.45	0.52
1:C:196:LEU:HD23	1:C:251:VAL:HG22	1.90	0.52
2:D:79:GLN:HB3	2:D:295:PHE:CZ	2.45	0.52
2:D:85:LYS:O	2:D:86:THR:OG1	2.22	0.52
2:D:224:VAL:HG21	2:D:267:THR:OG1	2.09	0.52
1:A:670:GLN:O	1:A:673:ASP:N	2.42	0.52
1:A:691:LYS:HB2	1:A:717:ALA:HB2	1.91	0.52
1:C:770:ALA:HB2	1:C:842:LEU:HD11	1.91	0.52
1:A:371:THR:C	1:A:373:THR:H	2.12	0.52
1:A:487:LYS:NZ	1:A:560:GLU:HG3	2.25	0.52
1:C:957:LEU:O	1:C:960:PHE:N	2.43	0.52
2:D:246:TYR:HB2	2:D:251:GLN:CD	2.30	0.52
1:A:414:LEU:CD1	1:A:548:PHE:HB2	2.40	0.52
1:A:791:ILE:O	1:A:880:ARG:HB3	2.08	0.52
2:B:79:GLN:HB2	2:B:81:PRO:HD2	1.91	0.52
1:C:417:ILE:HG22	1:C:548:PHE:HD2	1.74	0.52
3:E:45:ILE:HD12	3:E:46:LEU:HG	1.91	0.52
1:A:841:GLN:HB3	1:A:1014:THR:O	2.10	0.52
1:C:281:ILE:O	1:C:284:PHE:HB3	2.10	0.52
1:C:373:THR:O	1:C:589:ARG:NH1	2.43	0.52
2:D:230:PHE:N	2:D:260:ALA:O	2.38	0.52
1:A:411:TRP:CZ2	1:A:457:CYS:HB2	2.45	0.51
2:B:186:PHE:CD2	2:B:188:PRO:HG3	2.45	0.51
1:C:94:SER:O	1:C:98:TRP:HB2	2.10	0.51
1:C:1001:ILE:CG2	1:C:1010:VAL:HG21	2.39	0.51
2:D:186:PHE:O	2:D:188:PRO:HD3	2.10	0.51
1:A:143:GLN:O	1:A:145:ALA:N	2.43	0.51
1:A:239:SER:CB	1:A:260:MET:SD	2.98	0.51
1:A:267:ALA:HB2	1:A:715:SER:HB3	1.92	0.51
1:C:484:SER:O	1:C:498:LEU:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:908:GLU:HG2	1:C:912:HIS:CE1	2.45	0.51
1:A:105:PHE:O	1:A:108:TYR:HB3	2.10	0.51
1:A:284:PHE:CZ	1:A:288:ILE:HD12	2.45	0.51
1:A:891:VAL:H	1:A:899:TRP:H	1.58	0.51
1:A:995:ASP:HA	1:A:998:ARG:HB3	1.93	0.51
1:C:300:PHE:HE1	1:C:313:ALA:CA	2.21	0.51
1:C:753:THR:HA	1:C:756:GLU:HB3	1.92	0.51
1:A:96:LEU:CD1	1:A:285:ILE:CB	2.82	0.51
1:A:358:GLU:OE2	1:A:362:SER:OG	2.25	0.51
2:B:29:GLY:HA2	2:B:32:TRP:CD1	2.46	0.51
2:B:91:ARG:CD	2:B:94:ASP:H	2.15	0.51
1:C:397:GLU:O	1:C:436:LEU:HD12	2.11	0.51
1:A:108:TYR:CA	1:A:122:ASN:ND2	2.74	0.51
1:A:714:ASP:O	1:A:718:SER:N	2.33	0.51
1:A:1002:ILE:O	1:A:1006:PRO:HG3	2.10	0.51
2:B:213:CYS:HA	2:B:275:GLU:O	2.09	0.51
1:C:853:ILE:HG22	1:C:987:TYR:HD1	1.74	0.51
1:C:921:VAL:HG12	1:C:988:SER:OG	2.10	0.51
2:D:246:TYR:O	2:D:250:LEU:HB2	2.11	0.51
2:D:263:PHE:HB2	2:D:266:LEU:HD11	1.92	0.51
1:A:278:ALA:HA	1:A:281:ILE:CD1	2.37	0.51
1:A:649:ASN:ND2	1:A:651:ARG:HB2	2.25	0.51
1:A:707:VAL:O	1:A:725:VAL:N	2.42	0.51
1:A:758:GLY:HA2	1:A:761:ILE:HG22	1.92	0.51
2:B:112:TYR:CD1	2:B:151:PHE:HD2	2.29	0.51
1:C:214:GLU:OE1	1:C:218:GLN:HG3	2.11	0.51
1:C:364:SER:OG	1:C:703:ALA:HB1	2.10	0.51
1:C:430:GLN:HB3	1:C:438:ARG:HD3	1.92	0.51
1:C:794:PRO:HA	1:C:862:TYR:CE1	2.46	0.51
1:C:845:MET:HA	1:C:849:GLN:NE2	2.25	0.51
1:C:1002:ILE:HG23	1:C:1011:GLU:OE1	2.11	0.51
1:A:976:LEU:HB3	1:A:980:TRP:HD1	1.76	0.51
2:B:209:LEU:HD21	2:B:283:ILE:HD11	1.92	0.51
1:C:295:LEU:O	1:C:299:PHE:CG	2.63	0.51
1:C:933:ARG:HB3	1:C:1015:TYR:HE1	1.75	0.51
1:C:962:SER:OG	1:C:975:PRO:HA	2.10	0.51
1:A:534:ALA:HA	1:A:537:GLU:HB3	1.93	0.51
2:B:54:ILE:HG13	2:B:57:MET:HE3	1.93	0.51
1:C:610:THR:OG1	4:C:1101:BEF:F2	2.09	0.51
1:C:633:THR:H	1:C:636:ASP:HB2	1.75	0.51
1:C:651:ARG:N	1:C:651:ARG:HH11	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:781:THR:HA	1:C:784:LEU:CB	2.39	0.51
1:A:606:VAL:O	1:A:626:ILE:HG23	2.11	0.51
1:A:933:ARG:HG2	1:A:1016:TYR:CZ	2.45	0.51
3:G:40:VAL:O	3:G:44:ILE:HG12	2.11	0.51
1:C:488:ASN:ND2	1:C:494:PRO:HA	2.22	0.51
1:A:29:LYS:HE3	1:A:266:LEU:HB2	1.92	0.50
1:A:104:CYS:O	1:A:108:TYR:N	2.45	0.50
2:B:79:GLN:HB3	2:B:295:PHE:CZ	2.46	0.50
2:B:212:HIS:O	2:B:276:CYS:HA	2.11	0.50
1:C:375:THR:HA	1:C:588:PRO:HA	1.93	0.50
1:A:385:TRP:HB2	1:A:581:LEU:HB2	1.94	0.50
1:A:765:LEU:HA	1:A:768:SER:OG	2.11	0.50
1:A:920:VAL:HA	1:A:923:GLN:HB2	1.93	0.50
2:B:109:LEU:HA	2:B:112:TYR:HD2	1.77	0.50
2:B:128:ASN:HB3	2:B:155:TRP:HH2	1.76	0.50
1:C:25:MET:O	1:C:29:LYS:HG3	2.10	0.50
1:C:36:ASP:OD1	1:C:48:TYR:OH	2.27	0.50
1:C:592:VAL:O	1:C:596:VAL:HG23	2.11	0.50
1:C:957:LEU:O	1:C:961:LEU:HD13	2.11	0.50
2:D:286:SER:HB3	2:D:292:GLN:HB3	1.93	0.50
1:A:129:LEU:HD21	1:A:327:GLU:OE2	2.11	0.50
1:C:238:PHE:O	1:C:239:SER:OG	2.30	0.50
1:C:735:SER:HA	1:C:738:ALA:HB3	1.93	0.50
1:A:254:THR:O	1:A:257:ARG:HB2	2.11	0.50
1:A:558:PHE:HB3	1:A:564:PHE:CZ	2.46	0.50
1:C:184:VAL:HB	1:C:196:LEU:HD21	1.93	0.50
1:C:635:GLU:CD	1:C:635:GLU:H	2.15	0.50
2:D:186:PHE:CD2	2:D:188:PRO:HG3	2.46	0.50
2:D:238:PHE:CD1	2:D:257:PRO:HB2	2.46	0.50
1:A:25:MET:O	1:A:29:LYS:HG3	2.12	0.50
1:A:312:GLU:O	1:A:315:ILE:CG2	2.55	0.50
1:A:801:LEU:O	1:A:805:LEU:HB2	2.11	0.50
2:B:159:CYS:N	2:B:166:THR:HG22	2.27	0.50
2:B:212:HIS:HA	2:B:229:TYR:OH	2.12	0.50
1:A:108:TYR:HB2	1:A:122:ASN:OD1	2.12	0.50
1:A:790:ASN:HB2	1:A:878:GLY:HA2	1.94	0.50
1:C:164:VAL:HG12	1:C:166:ARG:HE	1.71	0.50
1:C:300:PHE:O	1:C:303:SER:OG	2.19	0.50
1:C:321:ILE:HG23	1:C:324:ASN:HB2	1.94	0.50
1:C:323:ALA:CB	1:C:779:GLU:HB3	2.41	0.50
1:A:300:PHE:CD1	1:A:301:ILE:HD13	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:SER:O	2:B:26:GLY:N	2.44	0.50
2:B:205:ASN:N	2:B:206:PRO:HD2	2.26	0.50
1:C:64:ILE:HG23	1:C:67:ARG:NH1	2.27	0.50
1:A:108:TYR:HD1	1:A:122:ASN:CB	2.22	0.50
1:A:151:MET:HE1	1:A:742:ILE:HG21	1.92	0.50
1:A:239:SER:HB3	1:A:260:MET:SD	2.52	0.50
1:A:533:ASN:O	1:A:537:GLU:HB2	2.12	0.50
1:C:385:TRP:HB3	1:C:581:LEU:N	2.22	0.50
1:C:791:ILE:HG22	1:C:877:LEU:HA	1.94	0.50
2:D:88:ILE:O	2:D:299:ILE:HD12	2.12	0.50
1:C:151:MET:SD	1:C:742:ILE:HG13	2.51	0.50
1:C:819:GLN:HG2	1:C:820:ALA:H	1.76	0.50
2:D:108:PHE:HD1	2:D:109:LEU:HD12	1.77	0.50
1:A:105:PHE:CE1	1:A:126:GLY:HA3	2.47	0.49
1:A:329:LEU:CD2	1:A:772:THR:HG21	2.41	0.49
1:A:360:LEU:HD11	1:A:723:ILE:HD13	1.94	0.49
1:A:524:ASP:OD2	1:A:527:LEU:HD13	2.12	0.49
1:C:315:ILE:HG13	1:C:316:PHE:N	2.27	0.49
1:C:780:ILE:HG22	1:C:784:LEU:HG	1.93	0.49
1:A:495:ARG:HG2	1:A:555:ASP:CG	2.33	0.49
1:A:696:GLU:CG	1:A:720:LYS:HE2	2.42	0.49
1:A:977:LYS:HB2	1:A:980:TRP:NE1	2.26	0.49
2:B:88:ILE:HB	2:B:299:ILE:HD12	1.94	0.49
1:C:49:GLY:O	1:C:50:THR:OG1	2.24	0.49
2:B:186:PHE:O	2:B:188:PRO:HD3	2.13	0.49
1:C:712:VAL:O	1:C:714:ASP:N	2.46	0.49
1:C:927:LEU:HD23	1:C:951:LEU:HD21	1.93	0.49
1:A:166:ARG:HH12	1:A:173:ILE:CD1	2.25	0.49
1:C:56:LEU:HD12	1:C:56:LEU:C	2.33	0.49
1:C:713:ASN:ND2	1:C:713:ASN:H	2.10	0.49
1:C:818:GLU:OE2	1:C:931:LYS:HE2	2.13	0.49
1:C:371:THR:O	1:C:373:THR:N	2.37	0.49
1:C:842:LEU:HB2	1:C:1016:TYR:HB2	1.94	0.49
1:A:281:ILE:O	1:A:285:ILE:HG13	2.12	0.49
1:A:297:VAL:O	1:A:300:PHE:CZ	2.65	0.49
1:A:1009:TRP:HD1	1:A:1010:VAL:HG13	1.77	0.49
2:B:81:PRO:O	2:B:83:SER:N	2.45	0.49
2:B:214:THR:C	2:B:274:ILE:HD13	2.33	0.49
1:C:300:PHE:CZ	1:C:317:LEU:HD23	2.48	0.49
2:D:113:LYS:HA	2:D:153:LEU:HD11	1.95	0.49
2:D:211:VAL:HA	2:D:277:LYS:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TYR:HB2	1:A:122:ASN:CG	2.33	0.49
1:A:315:ILE:HG23	1:A:316:PHE:CD2	2.46	0.49
2:B:211:VAL:HG11	2:B:259:MET:HE1	1.93	0.49
1:C:125:LEU:HD13	1:C:801:LEU:HD11	1.95	0.49
1:C:845:MET:HA	1:C:849:GLN:HE21	1.78	0.49
2:D:31:SER:HB2	2:D:34:LYS:CD	2.42	0.49
1:A:155:LYS:HG3	1:A:733:ASP:OD1	2.12	0.49
1:A:163:LEU:HD12	1:A:172:SER:HB3	1.94	0.49
1:A:921:VAL:O	1:A:924:TRP:HB2	2.13	0.49
2:B:177:ILE:CG2	2:B:258:LEU:HB3	2.43	0.49
1:C:798:VAL:O	1:C:801:LEU:HB2	2.13	0.49
1:C:839:ASN:OD1	1:C:839:ASN:N	2.43	0.49
2:D:247:GLY:O	2:D:251:GLN:N	2.43	0.49
1:A:691:LYS:HA	1:A:694:ILE:HD12	1.95	0.49
1:A:982:PHE:HD1	1:A:985:PHE:CZ	2.31	0.49
2:B:242:TYR:HB3	2:B:254:TYR:OH	2.13	0.49
1:C:41:LEU:O	1:C:45:HIS:ND1	2.45	0.49
1:C:293:VAL:CG2	1:C:321:ILE:HD13	2.41	0.49
1:C:807:THR:O	1:C:811:PRO:HD2	2.13	0.49
1:A:637:ILE:HG22	1:A:648:VAL:HG11	1.94	0.49
1:A:843:ILE:HG23	1:A:847:TYR:CD2	2.48	0.49
1:C:71:ASN:OD1	1:C:254:THR:OG1	2.27	0.49
1:C:861:THR:HG23	1:C:983:CYS:HB2	1.95	0.49
1:C:873:PRO:HA	1:C:876:LEU:CD1	2.42	0.49
1:A:108:TYR:HA	1:A:122:ASN:ND2	2.27	0.48
2:B:23:GLU:O	2:B:24:PHE:CG	2.66	0.48
2:B:170:LYS:CB	2:B:175:CYS:H	2.26	0.48
1:C:263:ILE:HD13	1:C:688:PRO:HG2	1.95	0.48
2:D:117:GLN:HA	2:D:123:PHE:CE2	2.48	0.48
1:A:471:VAL:HG11	1:A:566:THR:HB	1.95	0.48
2:B:167:TYR:O	2:B:169:TYR:CD2	2.66	0.48
1:C:638:ALA:HB1	1:C:643:ILE:O	2.12	0.48
2:D:91:ARG:HA	2:D:302:LYS:O	2.13	0.48
1:A:360:LEU:O	1:A:755:VAL:HG23	2.14	0.48
1:A:495:ARG:HA	1:A:555:ASP:HB3	1.95	0.48
1:A:982:PHE:CD1	1:A:985:PHE:CZ	3.00	0.48
1:C:70:PRO:O	1:C:72:ALA:N	2.46	0.48
2:D:170:LYS:CB	2:D:174:PRO:HA	2.39	0.48
1:A:183:LEU:HD21	1:A:248:ARG:HH21	1.79	0.48
1:A:291:VAL:HB	1:A:295:LEU:CD1	2.43	0.48
1:A:785:ILE:HG13	1:A:786:PHE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:TRP:CZ2	2:B:72:VAL:HG21	2.48	0.48
2:B:284:GLY:O	2:B:293:GLY:HA3	2.13	0.48
1:C:229:PRO:O	1:C:232:THR:HG22	2.12	0.48
1:C:732:SER:O	1:C:736:LYS:HB2	2.13	0.48
1:C:770:ALA:CB	1:C:842:LEU:HD11	2.43	0.48
2:D:277:LYS:HG3	2:D:294:ARG:HB3	1.94	0.48
1:A:56:LEU:CG	1:A:60:ARG:CG	2.91	0.48
1:A:917:VAL:O	1:A:921:VAL:HG23	2.14	0.48
2:B:92:PRO:HD2	2:B:303:SER:HB2	1.94	0.48
1:C:50:THR:HG21	1:C:181:GLY:O	2.13	0.48
1:C:63:GLU:C	1:C:65:LEU:H	2.17	0.48
1:C:845:MET:SD	1:C:849:GLN:NE2	2.86	0.48
2:D:166:THR:O	2:D:167:TYR:CG	2.66	0.48
1:A:286:HIS:O	1:A:290:GLY:CA	2.59	0.48
1:A:708:THR:HA	1:A:725:VAL:HB	1.94	0.48
1:C:98:TRP:CE2	1:C:133:VAL:HG11	2.49	0.48
1:C:185:GLU:CB	1:C:248:ARG:HD3	2.41	0.48
1:C:476:ASN:HB2	1:C:481:TYR:CE1	2.48	0.48
1:C:778:PRO:HA	1:C:855:ALA:HB2	1.96	0.48
1:A:342:LYS:O	1:A:346:ARG:NE	2.47	0.48
1:A:378:ARG:NH1	1:A:380:THR:OG1	2.47	0.48
1:A:710:ASP:O	1:A:731:GLY:HA2	2.13	0.48
1:C:766:LYS:HG2	1:C:837:LEU:O	2.13	0.48
1:C:807:THR:HG22	1:C:957:LEU:HD23	1.95	0.48
1:C:220:ARG:HD3	1:C:233:ARG:O	2.13	0.48
1:A:385:TRP:O	1:A:580:GLY:HA3	2.13	0.48
1:A:866:LEU:O	1:A:871:PHE:N	2.34	0.48
1:C:89:LEU:O	1:C:94:SER:CB	2.62	0.48
1:C:325:VAL:HA	1:C:326:PRO:HD3	1.65	0.48
1:C:903:GLN:O	1:C:907:VAL:HG23	2.14	0.48
1:A:315:ILE:HG23	1:A:316:PHE:CE2	2.49	0.48
1:A:411:TRP:CH2	1:A:456:CYS:HB2	2.49	0.48
1:A:496:HIS:HB2	1:A:553:LEU:HB2	1.96	0.48
1:A:693:ILE:HA	1:A:696:GLU:HB2	1.96	0.48
1:C:380:THR:HA	1:C:448:ALA:HB1	1.95	0.48
1:C:764:ASN:O	1:C:767:LYS:HB2	2.14	0.48
1:C:790:ASN:HB2	1:C:878:GLY:HA2	1.94	0.48
1:A:122:ASN:HD22	1:A:318:ILE:HD13	1.78	0.47
1:A:143:GLN:C	1:A:145:ALA:H	2.17	0.47
2:B:39:TYR:O	2:B:43:TYR:HD2	1.96	0.47
2:B:69:GLN:HB2	3:G:19:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:VAL:O	2:B:72:VAL:CG1	2.55	0.47
2:B:80:ILE:HD12	2:B:105:ILE:HG12	1.96	0.47
1:C:183:LEU:HA	1:C:249:GLY:O	2.14	0.47
1:C:300:PHE:CD1	1:C:317:LEU:CA	2.93	0.47
1:C:495:ARG:HD3	1:C:552:PHE:HB3	1.94	0.47
1:C:987:TYR:HA	1:C:990:LEU:HB3	1.96	0.47
1:A:798:VAL:HG23	1:A:799:THR:H	1.79	0.47
1:A:921:VAL:HG11	1:A:984:ALA:HB3	1.96	0.47
2:B:185:GLY:C	2:B:244:PRO:HB3	1.98	0.47
1:C:196:LEU:HD13	1:C:249:GLY:CA	2.43	0.47
2:D:130:PRO:HA	2:D:239:PRO:HB3	1.96	0.47
1:A:196:LEU:HD23	1:A:251:VAL:HG22	1.96	0.47
1:A:264:ALA:HA	1:A:734:VAL:CG1	2.44	0.47
1:A:434:PRO:HG2	1:A:437:LYS:HB2	1.95	0.47
2:B:181:ASN:O	2:B:183:VAL:HG23	2.14	0.47
2:B:189:LYS:H	2:B:282:ASN:CG	2.18	0.47
1:C:369:ASP:OD1	1:C:370:LYS:N	2.47	0.47
1:C:764:ASN:ND2	1:C:816:ALA:O	2.46	0.47
1:C:781:THR:HA	1:C:784:LEU:HG	1.96	0.47
1:A:64:ILE:HG22	1:A:179:VAL:HB	1.97	0.47
1:A:538:LEU:HD23	1:A:538:LEU:HA	1.67	0.47
1:A:641:LEU:HD23	1:A:643:ILE:HD13	1.95	0.47
2:B:25:LEU:HD11	2:B:32:TRP:CZ2	2.50	0.47
1:C:371:THR:C	1:C:373:THR:H	2.16	0.47
1:C:790:ASN:CB	1:C:878:GLY:HA2	2.44	0.47
1:A:260:MET:CE	1:A:712:VAL:HG11	2.45	0.47
1:A:430:GLN:O	1:A:438:ARG:NH1	2.48	0.47
2:B:114:ASP:N	2:B:114:ASP:OD1	2.45	0.47
1:C:96:LEU:O	1:C:99:ILE:HG12	2.15	0.47
1:C:321:ILE:HA	1:C:324:ASN:HB2	1.96	0.47
1:C:715:SER:OG	1:C:734:VAL:HG12	2.14	0.47
1:C:824:ILE:C	1:C:826:LYS:N	2.68	0.47
2:D:148:VAL:HG11	2:D:254:TYR:HA	1.96	0.47
1:A:476:ASN:ND2	1:A:481:TYR:O	2.47	0.47
1:A:811:PRO:HB3	1:A:927:LEU:HD22	1.95	0.47
1:C:64:ILE:CA	1:C:67:ARG:CG	2.92	0.47
1:C:86:CYS:HA	1:C:89:LEU:HB2	1.95	0.47
1:C:361:GLY:HA2	1:C:755:VAL:CG2	2.45	0.47
1:C:797:THR:HG23	1:C:800:ILE:CD1	2.34	0.47
1:A:23:ARG:NH1	1:A:26:ASP:OD2	2.47	0.47
1:A:143:GLN:O	1:A:146:LYS:N	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:VAL:N	1:A:254:THR:HG21	2.29	0.47
1:A:564:PHE:HD2	1:A:570:ASN:HB3	1.80	0.47
1:A:689:GLN:OE1	1:A:689:GLN:N	2.31	0.47
2:B:91:ARG:HD3	2:B:93:ASN:HB2	1.95	0.47
1:C:44:LEU:O	1:C:44:LEU:HG	2.07	0.47
1:C:64:ILE:CG1	1:C:67:ARG:HH11	2.28	0.47
1:C:103:LEU:HD23	1:C:106:LEU:HD23	1.95	0.47
1:C:107:ALA:HB2	1:C:318:ILE:CG2	2.44	0.47
1:C:253:TYR:CD1	1:C:257:ARG:HD3	2.49	0.47
1:C:514:ILE:HD11	1:C:521:GLN:HB2	1.96	0.47
1:C:799:THR:O	1:C:802:CYS:N	2.48	0.47
1:C:821:GLU:OE1	1:C:933:ARG:HB2	2.14	0.47
1:C:854:GLN:HG2	1:C:922:VAL:HB	1.96	0.47
1:C:870:GLY:HA2	1:C:895:TYR:CE2	2.50	0.47
2:D:80:ILE:HG13	2:D:81:PRO:CD	2.27	0.47
2:D:81:PRO:HG3	2:D:176:VAL:HG22	1.97	0.47
2:D:157:GLY:O	2:D:159:CYS:N	2.47	0.47
1:A:205:LYS:HA	1:A:219:THR:HA	1.97	0.47
1:A:260:MET:CE	1:A:712:VAL:CG2	2.82	0.47
1:A:288:ILE:HD11	1:A:326:PRO:HD2	1.97	0.47
1:A:416:ARG:HA	1:A:463:MET:CE	2.45	0.47
1:A:777:ILE:HB	1:A:851:GLY:HA3	1.97	0.47
1:A:853:ILE:HG12	2:B:46:LEU:HD21	1.96	0.47
2:B:115:LEU:HD23	2:B:115:LEU:HA	1.68	0.47
1:C:86:CYS:HA	1:C:89:LEU:HD22	1.95	0.47
1:C:292:ALA:HB1	1:C:324:ASN:CG	2.30	0.47
1:C:316:PHE:CD2	1:C:787:ILE:HD13	2.50	0.47
1:C:688:PRO:O	1:C:691:LYS:HB2	2.15	0.47
2:D:77:LEU:HB2	2:D:294:ARG:O	2.15	0.47
1:A:306:LEU:O	1:A:307:GLU:CG	2.62	0.47
1:A:473:ILE:HD12	1:A:483:LEU:HD21	1.96	0.47
2:B:80:ILE:HG13	2:B:81:PRO:N	2.30	0.47
1:C:191:ARG:NH2	1:C:239:SER:HA	2.29	0.47
1:C:696:GLU:HG2	1:C:720:LYS:HE2	1.96	0.47
1:C:907:VAL:HA	1:C:910:THR:HG22	1.96	0.47
2:D:167:TYR:C	2:D:169:TYR:H	2.17	0.47
2:D:189:LYS:H	2:D:282:ASN:HB2	1.79	0.47
1:A:925:ALA:O	1:A:929:ILE:HG12	2.14	0.47
2:B:188:PRO:CB	2:B:209:LEU:HD22	2.45	0.47
1:C:64:ILE:CA	1:C:67:ARG:HG2	2.45	0.47
1:C:165:ILE:O	1:C:166:ARG:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:VAL:HG22	1:C:247:ALA:O	2.15	0.47
1:C:221:SER:O	1:C:234:ASN:HA	2.15	0.47
1:C:257:ARG:O	1:C:257:ARG:HG2	2.15	0.47
1:C:308:TYR:HB3	1:C:312:GLU:CB	2.45	0.47
1:C:308:TYR:HB3	1:C:312:GLU:HB2	1.96	0.47
1:C:316:PHE:CE2	1:C:787:ILE:HG23	2.51	0.47
1:C:831:ASN:HB3	1:C:834:THR:HB	1.97	0.47
1:A:297:VAL:CB	1:A:300:PHE:CE2	2.95	0.46
1:A:859:PHE:HA	1:A:862:TYR:HB3	1.96	0.46
2:B:71:ARG:HD3	2:B:71:ARG:HA	1.62	0.46
1:C:608:MET:HB2	1:C:626:ILE:CD1	2.45	0.46
1:A:92:GLY:C	1:A:96:LEU:CD1	2.74	0.46
1:A:100:GLY:CA	1:A:103:LEU:HD12	2.45	0.46
2:B:158:ASN:O	2:B:166:THR:CG2	2.57	0.46
1:C:64:ILE:CD1	1:C:67:ARG:NH1	2.77	0.46
2:D:174:PRO:O	2:D:262:GLN:HG3	2.16	0.46
1:A:92:GLY:C	1:A:96:LEU:HD12	2.33	0.46
1:A:312:GLU:CD	1:A:315:ILE:HG21	2.35	0.46
1:A:774:THR:HG22	1:A:854:GLN:CD	2.36	0.46
1:A:880:ARG:HA	1:A:883:TRP:HB3	1.97	0.46
1:A:892:GLU:HG2	1:A:893:ASP:O	2.15	0.46
2:B:245:TYR:OH	2:B:247:GLY:O	2.30	0.46
1:C:164:VAL:HG11	1:C:166:ARG:NE	2.24	0.46
2:D:160:SER:O	2:D:160:SER:OG	2.33	0.46
2:D:205:ASN:OD1	2:D:206:PRO:CD	2.63	0.46
1:A:94:SER:O	1:A:98:TRP:N	2.48	0.46
1:A:192:ILE:HG12	1:A:240:THR:O	2.16	0.46
2:B:41:ILE:O	2:B:45:CYS:N	2.47	0.46
1:C:178:VAL:HB	1:C:182:ASP:OD2	2.15	0.46
1:C:614:PRO:HG2	1:C:659:HIS:CE1	2.51	0.46
1:C:914:PRO:O	1:C:915:PHE:C	2.52	0.46
2:D:153:LEU:HD23	2:D:160:SER:O	2.15	0.46
1:A:99:ILE:HG22	1:A:103:LEU:CG	2.43	0.46
1:A:197:ARG:NE	1:A:234:ASN:OD1	2.49	0.46
1:A:963:TYR:HD1	1:A:975:PRO:HB3	1.80	0.46
2:B:183:VAL:HB	2:B:186:PHE:HB2	1.98	0.46
1:C:908:GLU:O	1:C:911:CYS:HB2	2.16	0.46
1:C:963:TYR:CE1	3:E:26:VAL:HG12	2.50	0.46
2:D:199:TYR:O	2:D:200:PRO:C	2.54	0.46
1:A:414:LEU:HG	1:A:582:ILE:HD11	1.98	0.46
1:A:476:ASN:ND2	1:A:481:TYR:H	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:CYS:HA	2:B:166:THR:HG22	1.96	0.46
1:C:45:HIS:HB3	1:C:52:LEU:HD11	1.97	0.46
2:D:174:PRO:HD2	2:D:263:PHE:O	2.16	0.46
1:A:392:GLU:O	1:A:392:GLU:HG3	2.15	0.46
1:A:513:SER:HA	1:A:521:GLN:O	2.15	0.46
1:A:780:ILE:O	1:A:784:LEU:HG	2.14	0.46
1:A:1004:ARG:HG2	1:A:1005:ARG:HG3	1.98	0.46
1:C:163:LEU:HB3	1:C:185:GLU:O	2.15	0.46
1:C:292:ALA:CB	1:C:324:ASN:HB3	2.46	0.46
1:A:48:TYR:OH	1:A:252:VAL:HG13	2.16	0.46
1:A:883:TRP:CZ2	1:A:904:ARG:HB2	2.51	0.46
2:D:158:ASN:HA	2:D:165:GLU:CG	2.37	0.46
2:D:238:PHE:CE2	2:D:259:MET:SD	3.09	0.46
1:A:105:PHE:HE1	1:A:123:LEU:HA	1.80	0.46
3:G:18:PRO:HG2	3:G:19:PHE:CE2	2.50	0.46
1:A:64:ILE:CG2	1:A:179:VAL:HB	2.46	0.46
1:A:105:PHE:HA	1:A:108:TYR:CB	2.45	0.46
1:A:277:ILE:CG2	1:A:278:ALA:N	2.79	0.46
1:A:292:ALA:HA	1:A:324:ASN:HD21	1.78	0.46
1:A:551:LEU:CD2	1:A:572:PRO:HG2	2.46	0.46
1:A:770:ALA:O	1:A:774:THR:OG1	2.32	0.46
1:C:796:GLY:O	1:C:800:ILE:HG13	2.16	0.46
2:D:85:LYS:HG3	2:D:87:GLU:OE2	2.16	0.46
2:D:214:THR:HG22	2:D:215:GLY:H	1.81	0.46
1:C:453:ILE:HG22	1:C:460:VAL:HG22	1.97	0.45
1:C:470:ILE:HG22	1:C:471:VAL:HG23	1.98	0.45
2:D:50:PHE:O	2:D:54:ILE:HG12	2.15	0.45
1:A:762:PHE:CE2	1:A:830:ARG:HD2	2.50	0.45
2:B:160:SER:N	2:B:166:THR:HB	2.28	0.45
2:B:214:THR:O	2:B:274:ILE:HD13	2.16	0.45
1:C:85:PHE:O	1:C:89:LEU:HD13	2.16	0.45
1:C:317:LEU:HA	1:C:320:ILE:CD1	2.44	0.45
1:C:347:LYS:HE2	1:C:753:THR:HG21	1.98	0.45
3:E:45:ILE:H	3:E:45:ILE:HG13	1.46	0.45
1:A:905:LYS:O	1:A:908:GLU:HB3	2.16	0.45
1:A:942:MET:HB3	1:A:948:ILE:HD11	1.98	0.45
2:B:91:ARG:HD2	2:B:94:ASP:CB	2.47	0.45
2:B:282:ASN:C	2:B:283:ILE:HG13	2.36	0.45
1:C:281:ILE:O	1:C:285:ILE:HD12	2.16	0.45
1:C:766:LYS:CG	1:C:837:LEU:HD12	2.44	0.45
1:A:462:GLU:HA	1:A:465:GLU:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ILE:HG23	1:A:640:ARG:NH2	2.31	0.45
2:B:21:LYS:HB3	2:B:24:PHE:HB2	1.99	0.45
1:C:369:ASP:O	1:C:373:THR:HB	2.16	0.45
1:C:378:ARG:HD2	1:C:451:LYS:NZ	2.31	0.45
1:C:452:CYS:O	1:C:456:CYS:SG	2.74	0.45
1:C:814:SER:HB2	1:C:947:LEU:HA	1.99	0.45
1:C:924:TRP:CD1	1:C:951:LEU:HD22	2.51	0.45
2:D:32:TRP:NE1	2:D:36:LEU:CD2	2.80	0.45
1:A:107:ALA:O	1:A:318:ILE:HD13	2.16	0.45
1:A:229:PRO:O	1:A:232:THR:HG22	2.16	0.45
1:A:663:LEU:HD12	1:A:690:GLN:CD	2.37	0.45
1:A:856:LEU:HD11	2:B:46:LEU:HD13	1.99	0.45
1:C:600:ARG:NH2	1:C:680:GLU:OE2	2.50	0.45
2:D:85:LYS:HG3	2:D:87:GLU:CD	2.37	0.45
1:A:39:LEU:HB3	1:A:43:GLU:HB3	1.98	0.45
2:B:80:ILE:HD12	2:B:105:ILE:CG2	2.44	0.45
2:B:160:SER:HB2	2:B:169:TYR:HE1	1.81	0.45
1:A:280:GLU:HB3	1:A:837:LEU:HB3	1.98	0.45
1:A:781:THR:HA	1:A:784:LEU:HD12	1.99	0.45
2:B:245:TYR:CE2	2:B:247:GLY:HA2	2.52	0.45
1:C:96:LEU:HD21	1:C:325:VAL:CG2	2.47	0.45
1:C:824:ILE:C	1:C:826:LYS:H	2.17	0.45
2:D:46:LEU:HD23	2:D:46:LEU:HA	1.82	0.45
2:D:271:GLU:HA	2:D:299:ILE:O	2.16	0.45
1:A:710:ASP:CG	1:A:711:GLY:N	2.70	0.45
2:B:186:PHE:HZ	2:B:282:ASN:O	2.00	0.45
1:C:225:THR:HG21	1:C:233:ARG:HD2	1.99	0.45
1:C:260:MET:HE1	1:C:712:VAL:HB	1.99	0.45
1:C:295:LEU:CB	1:C:299:PHE:CE2	2.86	0.45
1:C:550:HIS:O	1:C:577:CYS:HB3	2.17	0.45
1:C:714:ASP:C	1:C:716:PRO:HD2	2.38	0.45
1:A:143:GLN:C	1:A:145:ALA:N	2.70	0.45
1:A:285:ILE:O	1:A:288:ILE:CG2	2.63	0.45
1:A:662:ASP:O	1:A:666:MET:HG3	2.16	0.45
1:A:909:PHE:CE2	1:A:972:ARG:HB3	2.51	0.45
1:A:944:ASN:O	1:A:948:ILE:HG12	2.17	0.45
2:B:76:GLY:O	2:B:180:LEU:HD12	2.17	0.45
1:C:73:LEU:CD2	1:C:261:GLY:HA2	2.47	0.45
1:C:316:PHE:CZ	1:C:786:PHE:HE1	2.33	0.45
1:C:367:CYS:O	1:C:707:VAL:HG13	2.16	0.45
1:C:443:ASP:HB3	1:C:446:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:202:MET:HG3	2:D:203:LYS:H	1.82	0.45
1:A:302:LEU:CA	1:A:305:ILE:HB	2.43	0.45
1:A:823:ASP:HB3	1:A:826:LYS:HB2	1.99	0.45
1:C:185:GLU:CG	1:C:186:VAL:N	2.79	0.45
1:C:460:VAL:HG12	1:C:464:ARG:HG2	1.98	0.45
1:C:936:SER:O	1:C:939:GLN:HB2	2.17	0.45
1:A:628:SER:O	1:A:630:GLY:N	2.50	0.44
1:A:843:ILE:HG23	1:A:847:TYR:HB2	1.98	0.44
1:A:946:ILE:O	1:A:950:GLY:N	2.48	0.44
2:B:62:SER:HB3	2:B:65:LYS:O	2.18	0.44
1:C:863:PHE:HD2	1:C:873:PRO:CB	2.22	0.44
1:C:958:ALA:HA	1:C:961:LEU:HD22	1.99	0.44
1:A:803:ILE:HG22	1:A:804:ASP:N	2.32	0.44
2:B:179:LYS:HG2	2:B:180:LEU:N	2.30	0.44
1:C:101:ALA:N	1:C:129:LEU:HD13	2.32	0.44
1:C:610:THR:HG23	1:C:612:ASP:N	2.30	0.44
1:C:913:THR:HB	1:C:914:PRO:HD3	1.99	0.44
2:D:92:PRO:HD2	2:D:303:SER:HB2	2.00	0.44
2:D:131:SER:OG	2:D:132:GLU:N	2.50	0.44
2:D:193:ASN:O	2:D:195:SER:N	2.46	0.44
2:B:155:TRP:CE3	2:B:232:LEU:HA	2.53	0.44
1:C:325:VAL:CG1	1:C:326:PRO:CD	2.94	0.44
1:C:325:VAL:HG12	1:C:326:PRO:HD2	1.99	0.44
1:C:337:LEU:HA	1:C:761:ILE:HD11	2.00	0.44
1:C:614:PRO:O	1:C:617:ALA:HB3	2.16	0.44
2:D:155:TRP:CD2	2:D:232:LEU:HD22	2.52	0.44
1:A:140:SER:HB3	1:A:334:THR:HG21	2.00	0.44
1:A:378:ARG:NH2	1:A:436:LEU:HD13	2.32	0.44
1:A:387:ASP:N	1:A:387:ASP:OD1	2.49	0.44
2:B:209:LEU:HD11	2:B:283:ILE:HD11	1.99	0.44
2:B:263:PHE:HZ	2:B:274:ILE:HG21	1.82	0.44
1:C:63:GLU:C	1:C:65:LEU:N	2.70	0.44
1:C:89:LEU:O	1:C:94:SER:OG	2.35	0.44
1:C:118:PRO:CA	1:C:121:ASP:HB2	2.44	0.44
1:C:147:SER:OG	1:C:351:VAL:O	2.33	0.44
1:C:591:ALA:HB1	1:C:749:ALA:HB2	2.00	0.44
1:C:784:LEU:O	1:C:788:ILE:HG12	2.18	0.44
1:A:329:LEU:CD2	1:A:772:THR:CG2	2.95	0.44
1:A:844:SER:OG	2:B:39:TYR:OH	2.14	0.44
2:B:186:PHE:CZ	2:B:282:ASN:HB3	2.52	0.44
1:C:83:VAL:C	1:C:85:PHE:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LEU:N	1:C:302:LEU:HD23	2.32	0.44
1:C:329:LEU:O	1:C:333:VAL:HG23	2.17	0.44
1:C:379:MET:HE3	1:C:585:ILE:HA	2.00	0.44
2:D:130:PRO:HA	2:D:241:GLN:NE2	2.33	0.44
1:A:136:THR:CB	1:A:330:LEU:HD21	2.47	0.44
1:A:885:ASP:OD1	1:A:888:ILE:HG13	2.17	0.44
1:C:143:GLN:HE22	1:C:146:LYS:NZ	2.16	0.44
1:C:1008:GLY:O	1:C:1012:LYS:N	2.50	0.44
2:D:64:PHE:HZ	2:D:141:ASN:HB2	1.78	0.44
2:D:227:MET:HG2	2:D:263:PHE:CD1	2.51	0.44
1:A:160:GLN:NE2	1:A:191:ARG:H	2.16	0.44
1:A:631:ASN:ND2	1:A:654:LYS:HB2	2.33	0.44
1:A:866:LEU:HA	1:A:866:LEU:HD23	1.36	0.44
1:C:427:GLN:HB2	1:C:430:GLN:OE1	2.17	0.44
1:C:564:PHE:CD2	1:C:571:PHE:HZ	2.36	0.44
1:C:803:ILE:HD13	1:C:803:ILE:HA	1.69	0.44
1:C:814:SER:OG	1:C:947:LEU:HG	2.18	0.44
1:A:759:ARG:O	1:A:762:PHE:HB3	2.18	0.44
1:A:1000:LEU:HD12	1:A:1003:ARG:CZ	2.47	0.44
2:B:98:TYR:OH	2:B:171:ASP:OD2	2.36	0.44
1:C:342:LYS:HE2	1:C:346:ARG:HH21	1.82	0.44
2:D:157:GLY:C	2:D:159:CYS:H	2.21	0.44
2:D:180:LEU:HG	2:D:181:ASN:N	2.32	0.44
1:A:136:THR:CG2	1:A:330:LEU:HD21	2.46	0.44
1:A:289:THR:HA	1:A:292:ALA:CB	2.47	0.44
1:A:295:LEU:HB3	1:A:299:PHE:CE2	2.53	0.44
1:A:416:ARG:HA	1:A:463:MET:HE1	2.00	0.44
1:A:836:LYS:HB2	1:A:839:ASN:HB3	1.99	0.44
1:A:913:THR:HG23	1:A:973:MET:SD	2.57	0.44
1:C:479:ASN:HB3	1:C:481:TYR:HD1	1.83	0.44
1:C:651:ARG:HA	1:C:651:ARG:HD3	1.84	0.44
1:C:684:ALA:O	1:C:686:THR:HG23	2.17	0.44
2:D:166:THR:O	2:D:167:TYR:CD2	2.70	0.44
1:A:249:GLY:C	1:A:250:ILE:HD12	2.37	0.43
1:A:364:SER:OG	1:A:703:ALA:HB1	2.17	0.43
1:A:663:LEU:O	1:A:663:LEU:HD22	2.17	0.43
1:A:982:PHE:HD1	1:A:985:PHE:CE1	2.36	0.43
2:B:108:PHE:O	2:B:111:LYS:HE3	2.18	0.43
1:C:83:VAL:O	1:C:85:PHE:N	2.51	0.43
1:C:612:ASP:CG	1:C:613:HIS:N	2.65	0.43
1:C:733:ASP:O	1:C:737:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:777:ILE:HG23	1:C:777:ILE:HD12	1.71	0.43
1:C:958:ALA:O	1:C:961:LEU:HB2	2.18	0.43
2:D:70:ASP:OD1	2:D:70:ASP:N	2.50	0.43
1:A:108:TYR:CD1	1:A:122:ASN:C	2.92	0.43
1:A:116:GLU:O	1:A:117:GLU:CG	2.64	0.43
1:A:297:VAL:HG12	1:A:300:PHE:CZ	2.51	0.43
1:A:708:THR:HG22	1:A:725:VAL:HB	2.00	0.43
1:A:769:ILE:CD1	1:A:837:LEU:HD11	2.48	0.43
1:A:791:ILE:C	1:A:880:ARG:HB3	2.39	0.43
1:A:929:ILE:HG21	1:A:992:PHE:HA	2.00	0.43
2:B:170:LYS:HB2	2:B:175:CYS:H	1.82	0.43
1:C:354:LEU:HD12	1:C:354:LEU:HA	1.79	0.43
1:C:883:TRP:HA	1:C:904:ARG:NH1	2.34	0.43
1:C:891:VAL:HG21	1:C:904:ARG:NH1	2.33	0.43
1:C:897:GLN:OE1	2:D:184:LEU:N	2.44	0.43
2:D:115:LEU:HA	2:D:115:LEU:HD13	1.77	0.43
3:E:28:ASN:O	3:E:31:LEU:HB2	2.18	0.43
1:A:120:ASN:OD1	1:A:124:TYR:CD2	2.70	0.43
1:A:196:LEU:CD2	1:A:251:VAL:HG22	2.48	0.43
1:A:293:VAL:HG13	1:A:297:VAL:CG2	2.44	0.43
1:A:531:PHE:CE1	1:A:578:PHE:CZ	3.07	0.43
1:A:803:ILE:HD13	1:A:807:THR:OG1	2.17	0.43
1:C:316:PHE:CE2	1:C:787:ILE:HG12	2.53	0.43
2:D:32:TRP:HE1	2:D:36:LEU:HD21	1.83	0.43
1:A:51:ASP:HB3	1:A:55:GLY:N	2.32	0.43
1:A:74:THR:HG23	1:A:256:ASP:OD2	2.17	0.43
1:A:112:ALA:HA	1:A:118:PRO:HG3	2.00	0.43
1:A:199:ILE:N	1:A:249:GLY:HA2	2.34	0.43
1:A:382:ALA:HB2	1:A:585:ILE:HG22	2.00	0.43
1:A:808:ASP:OD2	1:A:923:GLN:NE2	2.50	0.43
1:A:949:PHE:HB2	3:G:45:ILE:HG23	1.99	0.43
1:C:93:PHE:CE2	1:C:281:ILE:HD13	2.53	0.43
1:C:551:LEU:HG	1:C:552:PHE:O	2.18	0.43
1:C:640:ARG:HH11	1:C:641:LEU:HD12	1.83	0.43
1:C:756:GLU:HA	1:C:825:MET:CE	2.48	0.43
1:C:865:ILE:HG12	1:C:980:TRP:CE2	2.52	0.43
2:D:153:LEU:H	2:D:153:LEU:HD12	1.84	0.43
2:D:263:PHE:CB	2:D:266:LEU:HD11	2.48	0.43
1:A:165:ILE:HG23	1:A:168:GLY:O	2.19	0.43
2:B:155:TRP:CE2	2:B:232:LEU:HD22	2.53	0.43
1:C:61:ALA:C	1:C:63:GLU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:ILE:HG13	1:C:515:LEU:N	2.34	0.43
1:C:895:TYR:OH	2:D:62:SER:O	2.24	0.43
2:D:232:LEU:HB3	2:D:239:PRO:HG3	2.00	0.43
1:A:365:THR:HG22	1:A:605:LYS:HB3	2.01	0.43
1:A:411:TRP:HH2	1:A:456:CYS:HB2	1.82	0.43
1:A:464:ARG:HG2	1:A:464:ARG:O	2.18	0.43
1:A:513:SER:HA	1:A:522:PRO:HA	1.99	0.43
1:A:674:ILE:HG22	1:A:675:LEU:N	2.34	0.43
1:C:98:TRP:HA	1:C:98:TRP:HE3	1.83	0.43
1:C:126:GLY:HA2	1:C:129:LEU:HB2	2.01	0.43
1:C:299:PHE:N	1:C:299:PHE:CD1	2.81	0.43
1:C:322:VAL:HG11	1:C:797:THR:CG2	2.48	0.43
1:C:363:THR:HG21	1:C:706:ALA:CB	2.48	0.43
1:C:781:THR:O	1:C:784:LEU:HB2	2.18	0.43
2:D:284:GLY:O	2:D:293:GLY:HA3	2.18	0.43
1:A:761:ILE:O	1:A:765:LEU:HD12	2.19	0.43
1:A:803:ILE:C	1:A:805:LEU:N	2.71	0.43
2:B:92:PRO:HB3	2:B:171:ASP:O	2.19	0.43
2:B:186:PHE:HZ	2:B:282:ASN:HB3	1.83	0.43
2:B:207:TYR:O	2:B:208:VAL:HB	2.18	0.43
2:B:240:LEU:C	2:B:242:TYR:H	2.21	0.43
3:G:41:GLY:O	3:G:45:ILE:HG12	2.18	0.43
1:C:73:LEU:H	1:C:73:LEU:HD12	1.84	0.43
1:C:487:LYS:HZ2	1:C:560:GLU:CA	2.32	0.43
1:C:855:ALA:O	1:C:859:PHE:N	2.41	0.43
1:C:915:PHE:HE1	1:C:919:ILE:HD11	1.84	0.43
1:A:126:GLY:CA	1:A:129:LEU:HD12	2.47	0.43
1:A:883:TRP:O	1:A:883:TRP:CD1	2.72	0.43
1:C:41:LEU:H	1:C:41:LEU:HD12	1.83	0.43
1:C:64:ILE:C	1:C:67:ARG:CG	2.75	0.43
1:C:93:PHE:CD2	1:C:330:LEU:CD1	3.00	0.43
1:C:238:PHE:CD1	1:C:239:SER:N	2.86	0.43
1:C:668:SER:HA	1:C:700:ARG:NH2	2.34	0.43
1:C:909:PHE:HD1	1:C:912:HIS:HD2	1.66	0.43
1:A:300:PHE:CD2	1:A:317:LEU:HD13	2.54	0.43
1:A:304:LEU:CD2	1:A:310:TRP:HA	2.45	0.43
1:A:818:GLU:CD	1:A:931:LYS:HG3	2.39	0.43
1:A:851:GLY:C	1:A:854:GLN:HB2	2.38	0.43
1:A:892:GLU:HG3	1:A:896:GLY:HA2	2.00	0.43
2:B:168:GLY:C	2:B:170:LYS:N	2.72	0.43
1:C:42:ASP:O	1:C:46:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LYS:HA	1:C:219:THR:HA	2.01	0.43
1:C:299:PHE:HA	1:C:302:LEU:HG	1.99	0.43
2:D:130:PRO:HA	2:D:241:GLN:HE21	1.84	0.43
1:A:86:CYS:HA	1:A:89:LEU:HB2	1.99	0.43
1:A:374:LEU:O	1:A:592:VAL:HG21	2.19	0.43
1:A:1012:LYS:HD3	1:A:1012:LYS:HA	1.83	0.43
1:C:925:ALA:HB1	1:C:992:PHE:HB2	2.00	0.43
2:D:167:TYR:C	2:D:169:TYR:N	2.71	0.43
3:E:41:GLY:O	3:E:44:ILE:HB	2.19	0.43
1:A:853:ILE:O	1:A:856:LEU:HB2	2.19	0.42
2:B:112:TYR:CE1	2:B:151:PHE:HD2	2.36	0.42
2:B:185:GLY:N	2:B:244:PRO:HB2	2.34	0.42
1:C:44:LEU:CD2	1:C:250:ILE:HG13	2.49	0.42
1:C:723:ILE:HG12	1:C:724:GLY:N	2.34	0.42
1:C:825:MET:HE2	1:C:825:MET:CA	2.48	0.42
1:C:883:TRP:HA	1:C:904:ARG:HH11	1.84	0.42
2:D:23:GLU:O	2:D:24:PHE:CG	2.72	0.42
2:D:119:ASP:HB2	2:D:122:ILE:CG1	2.41	0.42
2:D:146:ARG:HD3	2:D:146:ARG:HA	1.63	0.42
2:D:183:VAL:HB	2:D:186:PHE:HB2	2.01	0.42
1:A:312:GLU:HG3	1:A:315:ILE:HG22	1.92	0.42
1:A:372:GLY:C	1:A:710:ASP:HB3	2.39	0.42
1:A:473:ILE:HB	1:A:483:LEU:HG	2.01	0.42
1:A:671:LEU:HD12	1:A:671:LEU:HA	1.75	0.42
1:A:851:GLY:O	1:A:854:GLN:HB2	2.20	0.42
2:B:130:PRO:HB2	2:B:204:TYR:OH	2.19	0.42
1:C:123:LEU:HA	1:C:123:LEU:HD23	1.40	0.42
1:C:300:PHE:HZ	1:C:313:ALA:CB	2.12	0.42
1:C:516:ILE:C	1:C:518:GLY:N	2.71	0.42
1:C:733:ASP:O	1:C:737:GLN:N	2.46	0.42
1:C:821:GLU:C	1:C:935:ASN:HD21	2.22	0.42
1:C:865:ILE:HG12	1:C:980:TRP:CZ2	2.54	0.42
2:D:156:LEU:HD22	2:D:260:ALA:CB	2.50	0.42
1:A:378:ARG:HD2	1:A:451:LYS:NZ	2.34	0.42
1:A:618:LYS:NZ	1:A:636:ASP:OD1	2.50	0.42
1:A:893:ASP:OD1	1:A:893:ASP:C	2.57	0.42
2:B:204:TYR:C	2:B:206:PRO:HD2	2.40	0.42
2:B:213:CYS:HB3	2:B:274:ILE:CG2	2.49	0.42
3:G:35:ALA:O	3:G:39:ILE:N	2.51	0.42
1:C:105:PHE:CZ	1:C:126:GLY:C	2.92	0.42
1:C:197:ARG:O	1:C:199:ILE:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:PHE:CG	1:C:787:ILE:CD1	3.02	0.42
1:C:564:PHE:CD2	1:C:571:PHE:CZ	3.07	0.42
1:C:913:THR:O	1:C:916:PHE:HD2	2.02	0.42
2:D:72:VAL:O	2:D:72:VAL:CG1	2.61	0.42
2:D:249:LEU:HD12	2:D:249:LEU:H	1.84	0.42
1:A:120:ASN:CG	1:A:124:TYR:CE2	2.93	0.42
2:B:152:ARG:C	2:B:154:GLU:N	2.71	0.42
1:C:58:PRO:HD3	1:C:167:ASN:HB2	2.00	0.42
1:C:586:ASP:OD1	1:C:586:ASP:N	2.50	0.42
1:C:843:ILE:N	1:C:843:ILE:HD13	2.33	0.42
1:C:977:LYS:HB2	1:C:980:TRP:NE1	2.35	0.42
2:D:80:ILE:HG22	2:D:108:PHE:CG	2.54	0.42
1:A:373:THR:HG21	1:A:708:THR:O	2.18	0.42
1:A:778:PRO:HB3	1:A:855:ALA:HA	2.02	0.42
2:B:179:LYS:HB3	2:B:179:LYS:HE2	1.45	0.42
1:C:712:VAL:C	1:C:714:ASP:N	2.71	0.42
1:C:998:ARG:NH2	1:C:1016:TYR:CE1	2.88	0.42
2:D:222:GLU:HG2	2:D:272:ILE:HB	2.01	0.42
1:A:107:ALA:O	1:A:318:ILE:CD1	2.68	0.42
1:A:116:GLU:C	1:A:117:GLU:HG3	2.39	0.42
1:A:207:ASP:HB2	1:A:243:VAL:CG2	2.50	0.42
1:A:211:LEU:HA	1:A:712:VAL:HG22	2.01	0.42
1:A:551:LEU:HD21	1:A:572:PRO:HG2	2.00	0.42
1:A:815:LEU:HD12	1:A:815:LEU:HA	1.77	0.42
1:A:922:VAL:CG1	1:A:991:ILE:HD12	2.50	0.42
1:A:974:TYR:HB3	1:A:975:PRO:HD2	2.02	0.42
1:A:1013:GLU:OE2	2:B:35:ILE:HG12	2.20	0.42
2:B:85:LYS:HG3	2:B:87:GLU:HG2	2.01	0.42
1:C:470:ILE:HG21	1:C:564:PHE:HD1	1.84	0.42
1:C:483:LEU:CD1	1:C:498:LEU:HD11	2.47	0.42
1:C:649:ASN:O	1:C:652:ASP:N	2.45	0.42
1:A:166:ARG:NH1	1:A:173:ILE:CD1	2.83	0.42
1:A:264:ALA:O	1:A:267:ALA:HB3	2.20	0.42
1:A:550:HIS:O	1:A:577:CYS:HB3	2.19	0.42
1:A:845:MET:SD	1:A:849:GLN:NE2	2.93	0.42
2:B:130:PRO:HB2	2:B:207:TYR:O	2.20	0.42
1:C:64:ILE:HD13	1:C:64:ILE:HG21	1.85	0.42
1:C:340:THR:OG1	1:C:761:ILE:HD12	2.20	0.42
1:C:842:LEU:HD13	1:C:1016:TYR:CD2	2.55	0.42
1:C:883:TRP:HZ2	1:C:904:ARG:O	2.03	0.42
1:C:920:VAL:HA	1:C:923:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:SER:O	1:A:308:TYR:HD2	2.03	0.42
1:A:325:VAL:HA	1:A:326:PRO:HD3	1.75	0.42
1:A:378:ARG:HH22	1:A:436:LEU:HD13	1.84	0.42
1:A:427:GLN:HB2	1:A:430:GLN:OE1	2.20	0.42
1:A:487:LYS:HD2	1:A:487:LYS:HA	1.94	0.42
2:B:152:ARG:O	2:B:154:GLU:N	2.53	0.42
2:B:216:LYS:HD2	2:B:221:LYS:HA	2.01	0.42
1:C:166:ARG:HH11	1:C:166:ARG:HD3	1.69	0.42
1:C:316:PHE:O	1:C:320:ILE:N	2.53	0.42
1:C:323:ALA:HB3	1:C:780:ILE:CG1	2.49	0.42
1:C:608:MET:HB2	1:C:626:ILE:HD13	2.01	0.42
1:C:747:ASN:HD21	1:C:749:ALA:HB3	1.85	0.42
1:C:777:ILE:HG12	1:C:847:TYR:CD2	2.55	0.42
1:C:779:GLU:OE2	1:C:804:ASP:OD2	2.37	0.42
1:A:277:ILE:CG2	1:A:278:ALA:H	2.28	0.42
1:A:484:SER:O	1:A:498:LEU:HD12	2.20	0.42
1:A:691:LYS:NZ	4:A:1101:BEF:F1	2.43	0.42
2:B:160:SER:CA	2:B:166:THR:HG21	2.50	0.42
1:C:372:GLY:H	1:C:377:ASN:HB2	1.85	0.42
1:C:475:PHE:HA	1:C:481:TYR:O	2.20	0.42
1:C:626:ILE:O	1:C:680:GLU:HB3	2.20	0.42
1:A:284:PHE:HD1	1:A:838:VAL:HG21	1.85	0.42
1:A:320:ILE:HG23	1:A:783:PHE:CB	2.48	0.42
2:B:128:ASN:N	2:B:128:ASN:HD22	2.18	0.42
2:B:245:TYR:CE1	2:B:251:GLN:HB2	2.55	0.42
1:C:263:ILE:CD1	1:C:688:PRO:HG2	2.50	0.42
1:C:899:TRP:CE3	2:D:72:VAL:CG2	3.03	0.42
2:D:173:LYS:HB3	2:D:264:THR:HA	2.01	0.42
1:A:914:PRO:HB3	1:A:976:LEU:HD13	2.02	0.41
1:A:946:ILE:HD13	3:G:45:ILE:HG22	2.00	0.41
1:A:977:LYS:HB2	1:A:980:TRP:CE2	2.54	0.41
2:B:205:ASN:N	2:B:206:PRO:CD	2.83	0.41
2:B:302:LYS:HB2	2:B:302:LYS:HE3	1.83	0.41
1:C:206:VAL:HG12	1:C:218:GLN:O	2.20	0.41
1:C:753:THR:HG22	1:C:757:GLU:HG2	2.02	0.41
1:C:913:THR:HG21	1:C:974:TYR:O	2.20	0.41
2:D:216:LYS:HB2	2:D:221:LYS:CG	2.46	0.41
1:A:277:ILE:HG21	1:A:355:GLU:CB	2.48	0.41
1:A:336:CYS:HA	1:A:339:LEU:CD2	2.49	0.41
2:B:131:SER:HB3	2:B:241:GLN:HB3	2.01	0.41
1:C:296:GLY:CA	1:C:320:ILE:HD13	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:414:LEU:O	1:C:417:ILE:HB	2.20	0.41
1:C:487:LYS:NZ	1:C:560:GLU:HA	2.34	0.41
1:C:609:VAL:HG11	1:C:691:LYS:HG2	2.02	0.41
1:C:879:LEU:HD21	1:C:883:TRP:HE3	1.85	0.41
1:C:998:ARG:C	1:C:1000:LEU:H	2.23	0.41
1:A:105:PHE:CZ	1:A:126:GLY:HA3	2.54	0.41
1:A:384:MET:HE3	1:A:411:TRP:HZ3	1.85	0.41
1:A:649:ASN:OD1	1:A:651:ARG:HG3	2.20	0.41
1:A:842:LEU:O	1:A:846:ALA:N	2.39	0.41
2:B:42:PHE:O	2:B:46:LEU:N	2.38	0.41
2:B:79:GLN:HB3	2:B:295:PHE:HZ	1.84	0.41
2:B:82:GLN:H	2:B:82:GLN:HG2	1.68	0.41
2:B:240:LEU:O	2:B:242:TYR:N	2.52	0.41
1:C:216:GLU:H	1:C:216:GLU:HG2	1.65	0.41
1:C:316:PHE:O	1:C:320:ILE:HG13	2.21	0.41
1:C:889:ASN:OD1	1:C:900:THR:HB	2.19	0.41
1:C:1011:GLU:CG	1:C:1015:TYR:HB3	2.49	0.41
1:A:120:ASN:OD1	1:A:124:TYR:CE2	2.73	0.41
1:A:430:GLN:HB3	1:A:438:ARG:HD3	2.01	0.41
1:A:512:SER:O	1:A:523:LEU:N	2.54	0.41
1:A:654:LYS:HE2	1:A:654:LYS:HB3	1.79	0.41
2:B:189:LYS:H	2:B:282:ASN:HB2	1.85	0.41
1:C:534:ALA:O	1:C:538:LEU:HB2	2.20	0.41
1:C:775:SER:O	1:C:779:GLU:HG3	2.20	0.41
1:C:777:ILE:N	1:C:778:PRO:HD2	2.36	0.41
1:C:943:LYS:H	1:C:943:LYS:HG3	1.55	0.41
1:A:545:VAL:HG12	1:A:583:SER:OG	2.21	0.41
2:B:189:LYS:O	2:B:282:ASN:HB2	2.20	0.41
1:C:651:ARG:HH11	1:C:651:ARG:CA	2.34	0.41
1:C:776:ASN:O	1:C:780:ILE:HD12	2.20	0.41
1:C:985:PHE:N	1:C:986:PRO:HD2	2.36	0.41
1:C:999:LYS:O	1:C:1003:ARG:CZ	2.68	0.41
1:A:111:GLN:OE1	1:A:122:ASN:HB3	2.19	0.41
1:A:945:LYS:H	1:A:945:LYS:HG2	1.52	0.41
2:B:187:LYS:HA	2:B:244:PRO:HD3	2.02	0.41
1:C:257:ARG:O	1:C:257:ARG:CG	2.68	0.41
1:C:675:LEU:HD23	1:C:681:ILE:CD1	2.49	0.41
2:D:167:TYR:O	2:D:169:TYR:CE1	2.74	0.41
2:D:216:LYS:HD2	2:D:220:ASP:O	2.21	0.41
2:D:222:GLU:H	2:D:222:GLU:CD	2.12	0.41
3:E:21:TYR:HB3	3:E:23:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ILE:HG22	1:A:103:LEU:HD12	1.91	0.41
1:A:478:THR:O	1:A:479:ASN:HB2	2.21	0.41
1:A:565:ASP:HB3	1:A:566:THR:H	1.46	0.41
1:A:745:ASP:OD2	1:A:747:ASN:HB3	2.21	0.41
2:B:15:PHE:HB3	2:B:16:ILE:H	1.49	0.41
2:B:42:PHE:CE1	2:B:46:LEU:HG	2.56	0.41
2:B:170:LYS:HB2	2:B:174:PRO:CA	2.31	0.41
1:C:312:GLU:O	1:C:315:ILE:HG12	2.21	0.41
1:C:797:THR:O	1:C:800:ILE:HB	2.21	0.41
1:C:953:GLU:HG3	3:E:38:PHE:CE1	2.55	0.41
1:C:1014:THR:O	1:C:1016:TYR:N	2.54	0.41
2:D:112:TYR:CE2	2:D:255:LEU:HB3	2.55	0.41
2:D:203:LYS:C	2:D:205:ASN:H	2.24	0.41
1:A:30:LYS:HD3	1:A:692:LEU:HD21	2.03	0.41
1:A:57:THR:HA	1:A:58:PRO:HD3	1.83	0.41
1:A:332:THR:HA	1:A:813:ILE:HD11	2.03	0.41
1:A:719:LYS:HB2	1:A:738:ALA:HB1	2.02	0.41
1:A:774:THR:O	1:A:778:PRO:HD2	2.20	0.41
1:A:798:VAL:HG23	1:A:799:THR:N	2.36	0.41
2:B:98:TYR:HH	2:B:171:ASP:CG	2.23	0.41
2:B:170:LYS:HB2	2:B:175:CYS:N	2.35	0.41
1:C:102:ILE:C	1:C:104:CYS:H	2.24	0.41
1:C:538:LEU:HA	1:C:538:LEU:HD23	1.81	0.41
1:C:607:ILE:HG23	1:C:681:ILE:HB	2.02	0.41
1:C:743:LEU:HD23	1:C:743:LEU:HA	1.82	0.41
1:C:943:LYS:O	1:C:945:LYS:HG3	2.20	0.41
2:D:268:MET:HE3	2:D:303:SER:HB3	2.01	0.41
1:A:166:ARG:NH2	1:A:178:VAL:HG13	2.36	0.41
1:A:187:LYS:HG2	1:A:188:GLY:H	1.85	0.41
1:A:278:ALA:HB2	1:A:355:GLU:OE1	2.20	0.41
1:A:299:PHE:N	1:A:299:PHE:CD1	2.87	0.41
1:A:541:LEU:HD23	1:A:543:GLU:OE1	2.20	0.41
1:A:576:LEU:H	1:A:576:LEU:HG	1.65	0.41
1:A:600:ARG:O	1:A:603:GLY:N	2.38	0.41
1:A:920:VAL:HG22	1:A:954:GLU:OE2	2.20	0.41
2:B:69:GLN:HB2	3:G:19:PHE:CD1	2.55	0.41
2:B:229:TYR:CD1	2:B:261:VAL:HG22	2.56	0.41
2:B:273:ARG:HG2	2:B:298:LYS:HG2	2.03	0.41
3:G:18:PRO:HG2	3:G:19:PHE:CZ	2.56	0.41
3:G:41:GLY:HA2	3:G:44:ILE:HB	2.02	0.41
1:C:136:THR:CB	1:C:330:LEU:HD21	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLN:HB2	1:C:173:ILE:O	2.21	0.41
1:C:211:LEU:HA	1:C:712:VAL:CG1	2.51	0.41
1:C:316:PHE:CZ	1:C:786:PHE:CE1	3.09	0.41
1:C:381:VAL:CG2	1:C:449:LEU:HD23	2.50	0.41
1:C:899:TRP:CZ3	2:D:72:VAL:CG2	3.04	0.41
1:A:174:ASN:C	1:A:176:GLU:H	2.23	0.41
1:A:326:PRO:HB2	1:A:329:LEU:CD1	2.48	0.41
1:A:553:LEU:CD2	1:A:572:PRO:HD2	2.51	0.41
1:A:608:MET:HB3	1:A:682:VAL:HG22	2.03	0.41
1:A:776:ASN:OD1	1:A:779:GLU:OE2	2.39	0.41
2:B:216:LYS:HB2	2:B:221:LYS:CG	2.43	0.41
1:C:745:ASP:OD1	1:C:745:ASP:N	2.44	0.41
1:C:803:ILE:HG22	1:C:804:ASP:N	2.36	0.41
1:C:857:GLY:HA2	1:C:987:TYR:CD2	2.56	0.41
2:D:71:ARG:HA	2:D:71:ARG:HD3	1.86	0.41
1:A:199:ILE:CG2	1:A:250:ILE:HD13	2.50	0.40
1:A:225:THR:OG1	1:A:226:ASN:N	2.53	0.40
1:A:275:THR:O	1:A:277:ILE:N	2.54	0.40
1:A:609:VAL:HG21	1:A:694:ILE:HG21	2.03	0.40
1:A:858:GLY:HA2	1:A:918:THR:HG21	2.03	0.40
1:A:898:GLN:HE22	2:B:179:LYS:CE	2.33	0.40
3:G:36:LEU:HA	3:G:39:ILE:HG12	2.02	0.40
1:C:365:THR:HG21	1:C:698:CYS:SG	2.62	0.40
1:A:65:LEU:HD11	1:A:177:GLU:HA	2.02	0.40
1:A:165:ILE:HD12	1:A:183:LEU:HD23	2.03	0.40
1:A:776:ASN:HA	1:A:779:GLU:HB2	2.03	0.40
1:A:856:LEU:HD11	2:B:46:LEU:HB3	2.02	0.40
1:A:1000:LEU:CD1	1:A:1003:ARG:CZ	2.98	0.40
1:C:197:ARG:HB3	1:C:250:ILE:HB	2.04	0.40
1:C:948:ILE:HB	3:E:44:ILE:HG21	2.04	0.40
1:A:197:ARG:C	1:A:197:ARG:HD3	2.42	0.40
1:A:328:GLY:HA2	1:A:805:LEU:CD2	2.51	0.40
1:A:883:TRP:NE1	1:A:908:GLU:OE1	2.52	0.40
3:G:36:LEU:O	3:G:40:VAL:HG23	2.22	0.40
1:C:94:SER:O	1:C:98:TRP:CG	2.74	0.40
1:C:125:LEU:HD11	1:C:801:LEU:HD21	2.00	0.40
1:C:286:HIS:O	1:C:290:GLY:N	2.50	0.40
1:C:332:THR:HA	1:C:813:ILE:HD11	2.03	0.40
1:C:360:LEU:H	1:C:360:LEU:HD22	1.86	0.40
1:C:369:ASP:HB3	1:C:373:THR:OG1	2.21	0.40
1:C:630:GLY:O	1:C:632:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:MET:SD	1:A:712:VAL:HG11	2.62	0.40
1:A:306:LEU:C	1:A:307:GLU:HG3	2.41	0.40
2:B:25:LEU:CD2	2:B:29:GLY:HA3	2.51	0.40
2:B:217:ARG:CZ	2:B:294:ARG:HH12	2.34	0.40
1:C:483:LEU:HB3	1:C:500:MET:HB2	2.04	0.40
1:C:793:LEU:O	1:C:912:HIS:HE1	2.04	0.40
1:C:866:LEU:HD23	1:C:866:LEU:HA	1.79	0.40
1:C:970:ALA:O	1:C:971:LEU:HD23	2.21	0.40
2:D:15:PHE:HB2	2:D:18:ASN:CB	2.50	0.40
2:D:31:SER:HB2	2:D:34:LYS:CG	2.52	0.40
2:D:178:ILE:HD11	2:D:276:CYS:SG	2.62	0.40
2:D:179:LYS:HD2	2:D:256:GLN:CD	2.41	0.40
1:A:184:VAL:HG11	1:A:193:PRO:HG2	2.04	0.40
1:A:581:LEU:C	1:A:582:ILE:HG13	2.41	0.40
1:A:734:VAL:O	1:A:734:VAL:HG12	2.21	0.40
1:A:786:PHE:CD1	1:A:793:LEU:HA	2.56	0.40
1:A:975:PRO:HG3	3:G:27:ARG:HH21	1.86	0.40
2:B:87:GLU:HA	2:B:298:LYS:O	2.22	0.40
1:C:51:ASP:OD1	1:C:52:LEU:N	2.55	0.40
1:C:323:ALA:O	1:C:780:ILE:HG13	2.19	0.40
1:C:335:VAL:O	1:C:338:THR:HB	2.21	0.40
1:C:624:VAL:HG23	1:C:626:ILE:HG13	2.02	0.40
3:E:35:ALA:O	3:E:39:ILE:HG23	2.21	0.40

There are no symmetry-related clashes.

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	994/1020 (98%)	825 (83%)	144 (14%)	25 (2%)	5 32
1	C	994/1020 (98%)	822 (83%)	137 (14%)	35 (4%)	3 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	287/302 (95%)	217 (76%)	56 (20%)	14 (5%)	2 20
2	D	287/302 (95%)	231 (80%)	43 (15%)	13 (4%)	2 22
3	E	30/64 (47%)	26 (87%)	3 (10%)	1 (3%)	4 26
3	G	30/64 (47%)	26 (87%)	4 (13%)	0	100 100
All	All	2622/2772 (95%)	2147 (82%)	387 (15%)	88 (3%)	3 26

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	115	GLU
1	A	1010	VAL
2	B	160	SER
2	B	169	TYR
2	B	170	LYS
1	C	193	PRO
1	C	517	HIS
1	C	525	GLU
1	C	585	ILE
1	C	944	ASN
2	D	158	ASN
2	D	165	GLU
2	D	194	GLU
2	D	200	PRO
1	A	82	TRP
1	A	144	GLU
1	A	170	LYS
1	A	522	PRO
1	A	692	LEU
1	A	982	PHE
2	B	82	GLN
2	B	158	ASN
1	C	64	ILE
1	C	71	ASN
1	C	84	LYS
1	C	310	TRP
1	C	314	VAL
1	C	563	GLN
1	C	640	ARG
1	C	931	LYS
1	C	1015	TYR

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Mol	Chain	Res	Type
2	D	167	TYR
2	D	196	LEU
1	A	113	ALA
1	A	307	GLU
1	A	348	ASN
1	A	739	ALA
1	A	880	ARG
1	A	900	THR
2	B	19	SER
2	B	29	GLY
1	C	198	ILE
1	C	461	LYS
1	C	492	ALA
1	C	561	GLY
1	C	562	PHE
1	C	771	TYR
1	C	981	TRP
2	D	197	GLU
2	D	223	LYS
1	A	121	ASP
1	A	372	GLY
1	A	629	GLU
2	B	167	TYR
2	B	199	TYR
2	B	208	VAL
1	C	118	PRO
1	C	327	GLU
1	C	399	GLN
1	C	479	ASN
2	D	199	TYR
1	A	227	GLU
1	C	291	VAL
1	C	306	LEU
1	C	373	THR
1	C	767	LYS
1	C	864	VAL
1	C	900	THR
2	D	19	SER
2	D	74	PRO
2	D	259	MET
3	E	27	ARG
1	A	168	GLY

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Mol	Chain	Res	Type
1	A	776	ASN
1	A	793	LEU
2	B	74	PRO
1	C	642	ASN
1	C	939	GLN
2	D	81	PRO
1	C	32	VAL
1	A	318	ILE
1	A	222	PRO
1	A	870	GLY
2	B	206	PRO
2	B	16	ILE
2	B	49	ILE
1	C	769	ILE

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	847/864 (98%)	831 (98%)	16 (2%)	57	75
1	C	847/864 (98%)	823 (97%)	24 (3%)	43	65
2	B	259/268 (97%)	250 (96%)	9 (4%)	36	59
2	D	259/268 (97%)	248 (96%)	11 (4%)	30	54
3	E	26/51 (51%)	26 (100%)	0	100	100
3	G	26/51 (51%)	26 (100%)	0	100	100
All	All	2264/2366 (96%)	2204 (97%)	60 (3%)	44	65

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	79	THR
1	A	154	PHE
1	A	164	VAL

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Mol	Chain	Res	Type
1	A	173	ILE
1	A	197	ARG
1	A	224	PHE
1	A	241	ASN
1	A	430	GLN
1	A	681	ILE
1	A	768	SER
1	A	781	THR
1	A	814	SER
1	A	917	VAL
1	A	991	ILE
1	A	1010	VAL
2	B	25	LEU
2	B	32	TRP
2	B	111	LYS
2	B	120	ASP
2	B	128	ASN
2	B	133	LEU
2	B	151	PHE
2	B	154	GLU
2	B	211	VAL
1	C	78	THR
1	C	136	THR
1	C	166	ARG
1	C	204	CYS
1	C	294	PHE
1	C	299	PHE
1	C	312	GLU
1	C	327	GLU
1	C	373	THR
1	C	610	THR
1	C	698	CYS
1	C	713	ASN
1	C	746	ASP
1	C	777	ILE
1	C	781	THR
1	C	824	ILE
1	C	830	ARG
1	C	835	ASP
1	C	839	ASN
1	C	906	ILE
1	C	918	THR

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Mol	Chain	Res	Type
1	C	947	LEU
1	C	988	SER
1	C	1010	VAL
2	D	25	LEU
2	D	80	ILE
2	D	85	LYS
2	D	120	ASP
2	D	151	PHE
2	D	159	CYS
2	D	163	ASN
2	D	170	LYS
2	D	175	CYS
2	D	204	TYR
2	D	273	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	ASN
1	A	143	GLN
1	A	160	GLN
1	A	324	ASN
1	A	476	ASN
1	A	488	ASN
2	B	282	ASN
1	C	111	GLN
1	C	122	ASN
1	C	143	GLN
1	C	399	GLN
1	C	482	GLN
1	C	488	ASN
1	C	613	HIS
1	C	713	ASN
1	C	903	GLN
1	C	912	HIS
2	D	256	GLN

5.3.3 RNA

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	BEF	C	1101	1	0,3,3	-	-	-		
4	BEF	A	1101	1	0,3,3	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

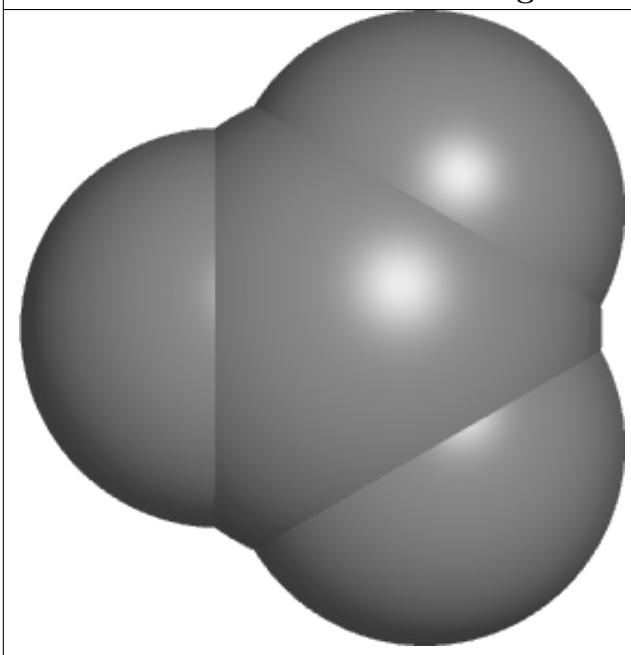
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1101	BEF	1	0
4	A	1101	BEF	1	0

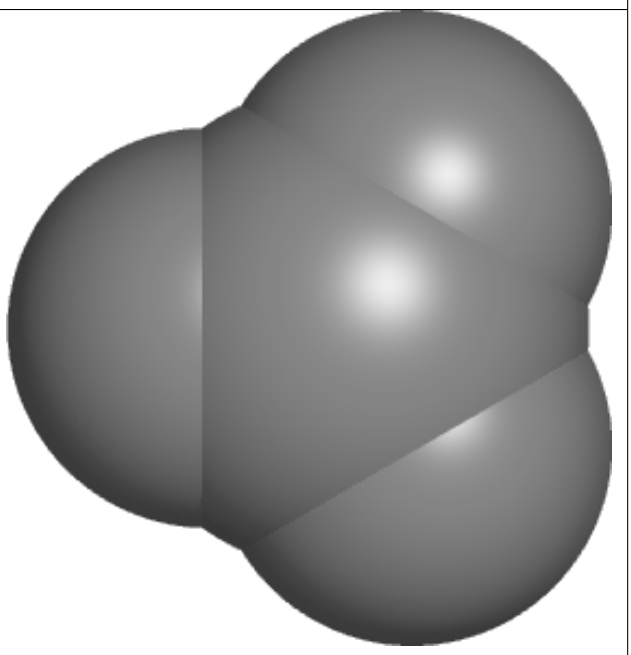
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

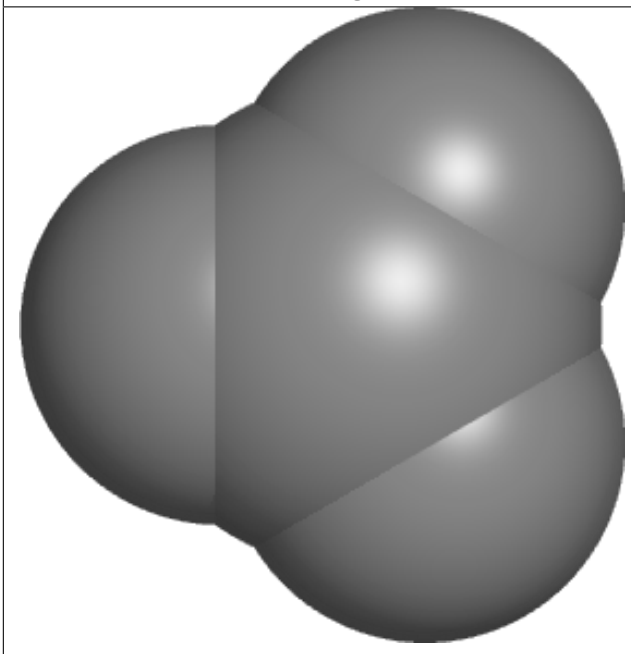
Ligand BEF C 1101



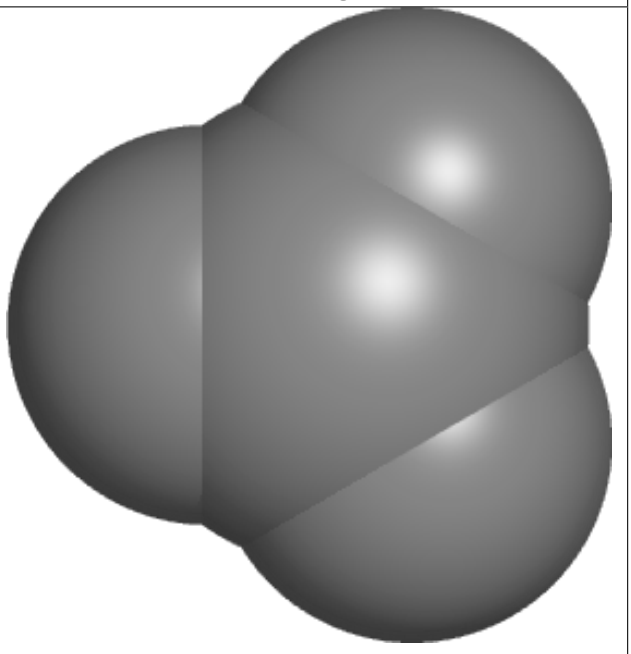
Bond lengths



Bond angles

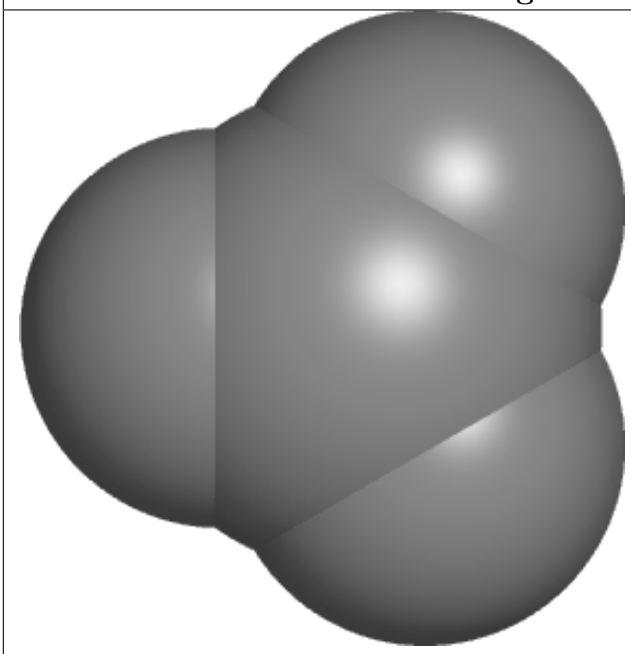


Torsions

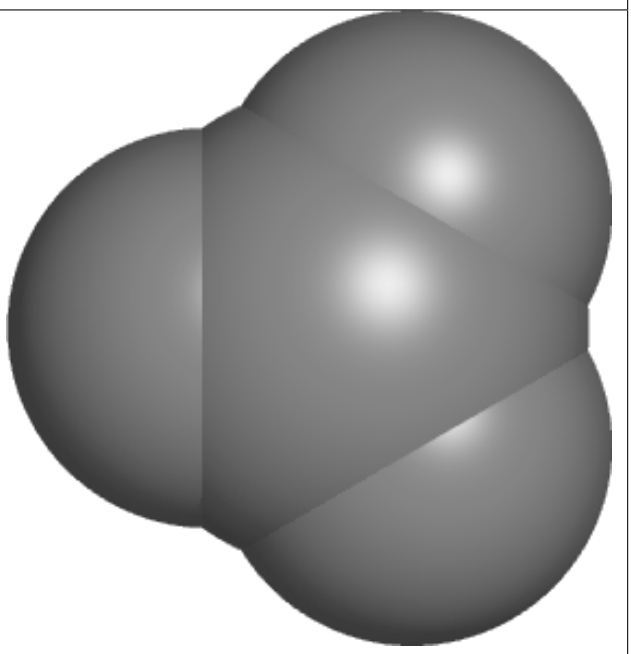


Rings

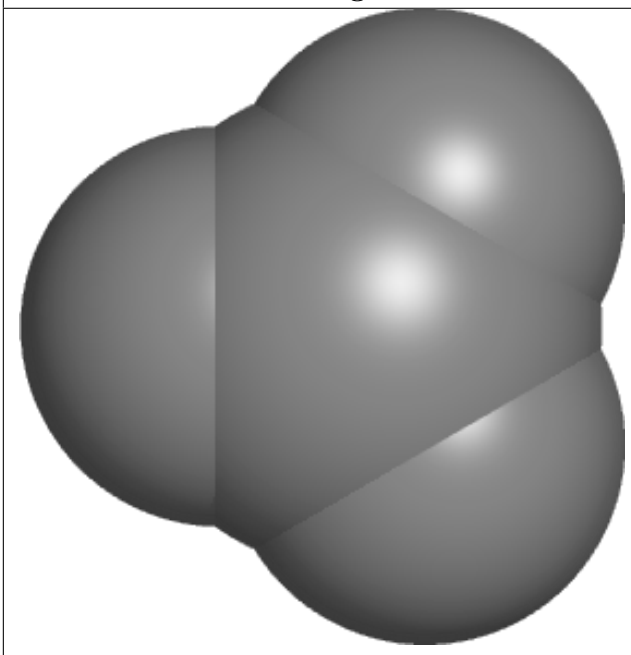
Ligand BEF A 1101



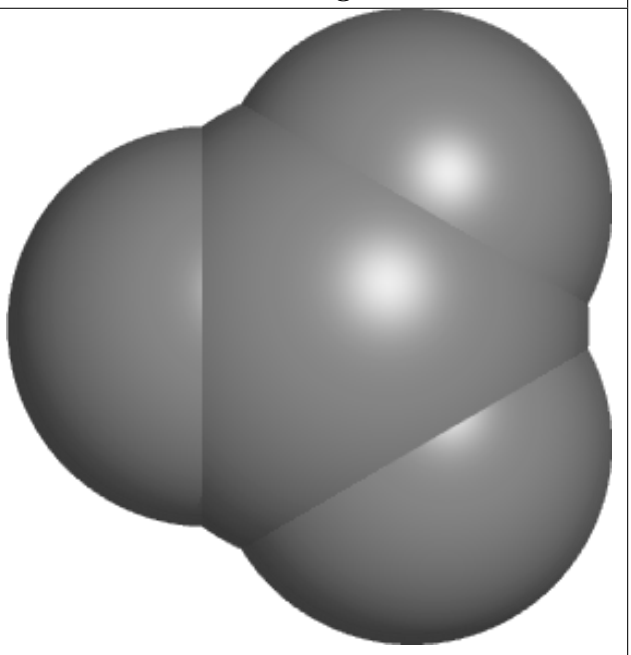
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

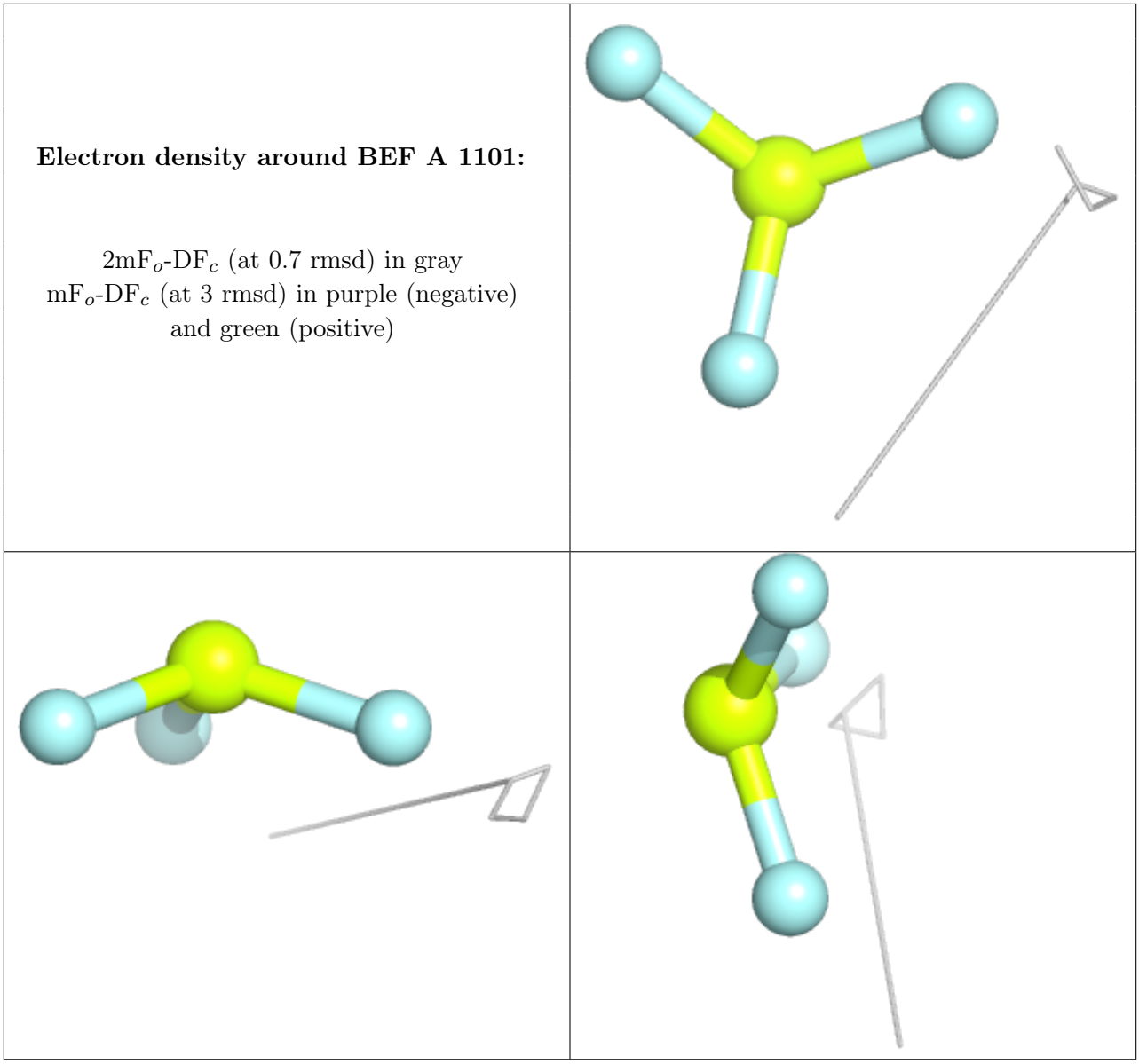
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

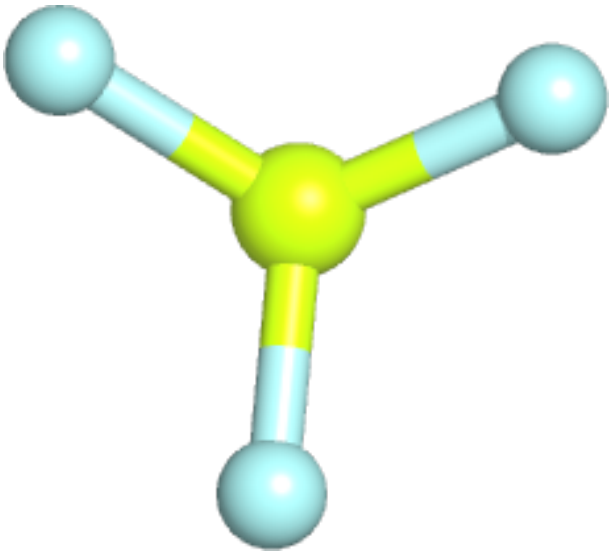
Electron density around BEF A 1101:

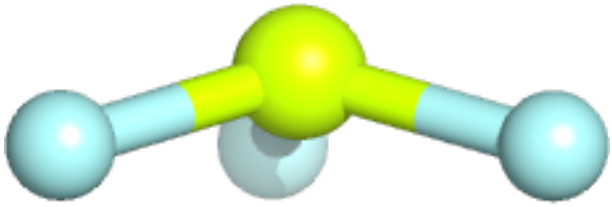
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around BEF C 1101:

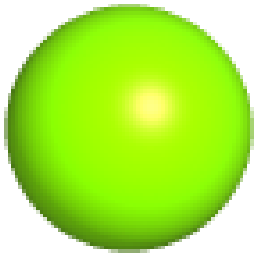
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

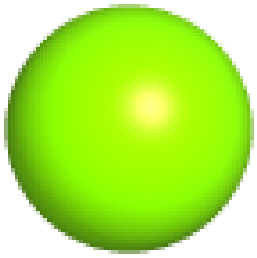


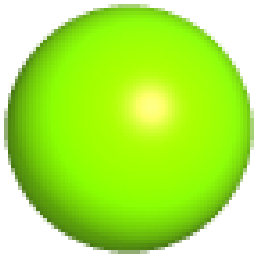


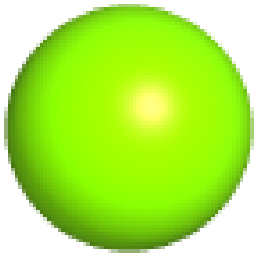
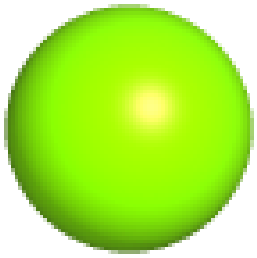
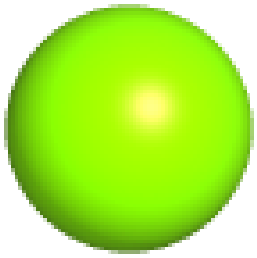
Electron density around MG A 1102:

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







Electron density around MG C 1102: $2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.