



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:21 AM UTC

PDB ID : 2NYL / pdb\_00002nyl  
Title : Crystal structure of Protein Phosphatase 2A (PP2A) holoenzyme with the catalytic subunit carboxyl terminus truncated  
Authors : Xing, Y.; Xu, Y.; Chen, Y.; Chao, Y.; Lin, Z.; Shi, Y.  
Deposited on : 2006-11-20  
Resolution : 3.80 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

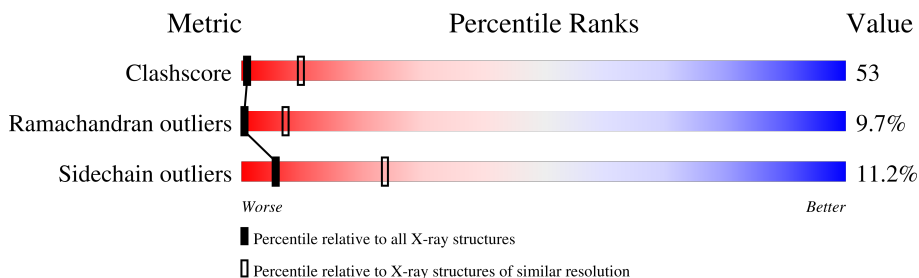
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	582	30% 53% 15% .
1	D	582	32% 50% 16% .
2	B	388	25% 56% 17% .
2	E	388	25% 53% 20% .
3	C	293	29% 59% 12%
3	F	293	32% 58% 10% .
4	G	7	43% 14% 43%
4	H	7	29% 57% 14%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 20212 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 Protein phosphatase 2, regulatory subunit A (PR 65), alpha isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	582	Total	C	N	O	S	Se	0	0	0
			4535	2881	764	863	14	13			
1	D	582	Total	C	N	O	S	Se	0	0	0
			4535	2881	764	863	14	13			

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	388	Total	C	N	O	S	Se	0	0	0
			3131	2043	513	561	3	11			
2	E	388	Total	C	N	O	S	Se	0	0	0
			3131	2043	513	561	3	11			

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	293	Total	C	N	O	S	0	0	0
			2367	1497	405	450	15			
3	F	293	Total	C	N	O	S	0	0	0
			2367	1497	405	450	15			

- Molecule 4 is a protein called microcystin LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	G	7	Total	C	N	O	0	0	0
			71	49	10	12			
4	H	7	Total	C	N	O	0	0	0
			71	49	10	12			

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total 2	Mn 2	0	0
5	F	2	Total 2	Mn 2	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

Note EDS was not executed.

- Molecule 1: Protein phosphatase 2, regulatory subunit A (PR 65), alpha isoform



- Molecule 1: Protein phosphatase 2, regulatory subunit A (PR 65), alpha isoform

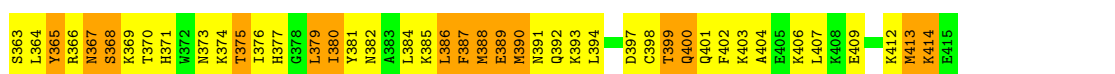
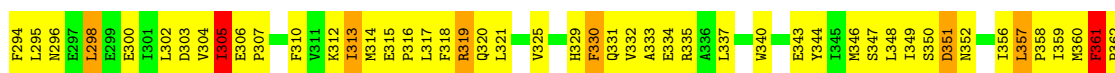






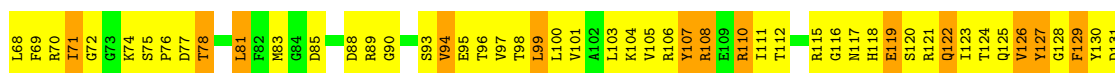
- Molecule 2: Serine/threonine-protein phosphatase 2A 56 kDa regulatory subunit gamma isoform

Chain E: 25% 53% 20%



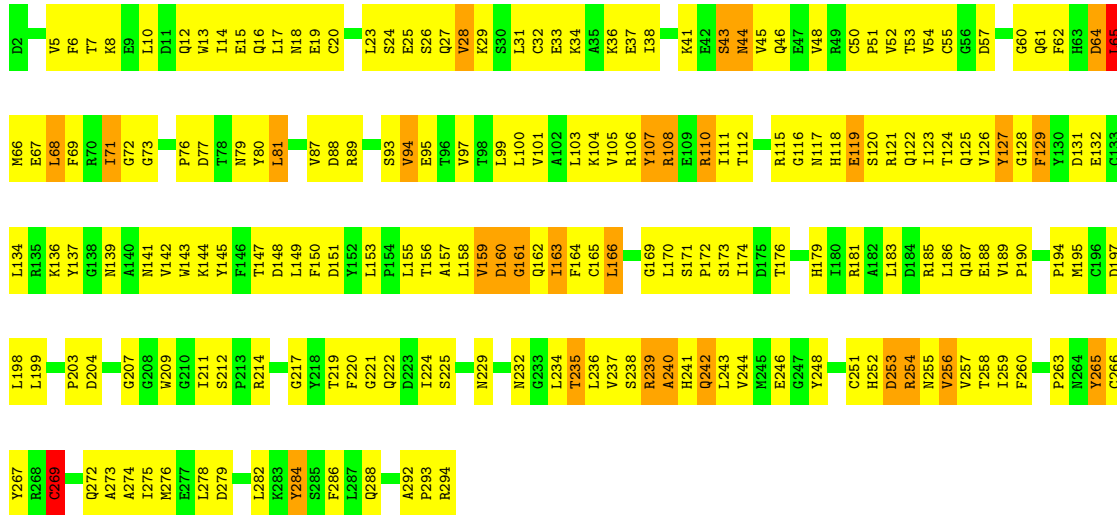
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain C: 29% 59% 12%



- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain F: 32% 58% 10%



• Molecule 4: microcystin LR



• Molecule 4: microcystin LR



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.48Å 159.85Å 270.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 3.80	Depositor
% Data completeness (in resolution range)	99.6 (100.00-3.80)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.282 , 0.335	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	20212	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MN, ACB, DAL, FGA, 1ZN, DAM

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	0.60	0/4596	1.11	38/6218 (0.6%)
1	D	0.77	0/4596	1.13	36/6218 (0.6%)
2	B	0.62	0/3202	1.11	28/4326 (0.6%)
2	E	0.70	1/3202 (0.0%)	1.11	30/4326 (0.7%)
3	C	0.59	0/2424	1.04	11/3285 (0.3%)
3	F	0.61	0/2424	1.06	12/3285 (0.4%)
4	G	0.32	0/17	0.90	0/19
4	H	0.35	0/17	0.96	0/19
All	All	0.66	1/20478 (0.0%)	1.10	155/27696 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	3
4	H	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	252	VAL	CA-CB	-5.48	1.49	1.55

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	220	VAL	N-CA-C	-14.09	100.28	112.12
1	A	38	ILE	N-CA-C	-11.54	102.42	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	ILE	N-CA-C	-11.22	102.54	113.53
2	B	144	ILE	N-CA-C	-11.20	99.92	112.80
1	A	220	VAL	N-CA-C	-10.42	101.68	111.48
2	B	162	ASP	N-CA-C	9.78	129.35	113.89
2	E	162	ASP	N-CA-C	9.64	129.12	113.89
3	F	127	TYR	N-CA-C	8.66	123.90	113.16
1	A	436	VAL	N-CA-C	8.26	120.03	110.62
2	B	92	ASN	N-CA-C	-8.13	103.88	113.88
2	E	163	SER	N-CA-C	7.96	127.77	110.80
1	D	564	LEU	N-CA-C	-7.94	104.56	112.97
3	F	44	ASN	N-CA-C	-7.89	104.17	113.88
1	D	39	ALA	N-CA-C	-7.82	103.73	113.28
1	D	384	ILE	N-CA-C	-7.71	105.66	111.90
2	B	163	SER	N-CA-C	7.63	127.06	110.80
1	D	91	PRO	N-CA-C	7.61	119.99	110.70
1	A	80	VAL	N-CA-C	-7.53	104.14	112.80
2	E	91	VAL	N-CA-C	-7.49	106.01	113.20
3	C	127	TYR	N-CA-C	7.46	122.40	113.16
2	E	283	TRP	CA-C-N	7.43	129.13	119.84
2	E	283	TRP	C-N-CA	7.43	129.13	119.84
3	C	269	CYS	N-CA-C	7.30	123.45	113.37
2	E	37	ARG	N-CA-C	-7.18	105.04	114.31
2	B	270	THR	N-CA-C	-7.12	101.79	112.04
3	C	44	ASN	N-CA-C	-7.11	104.87	113.97
3	C	65	LEU	N-CA-C	-7.04	103.54	111.14
2	E	252	VAL	N-CA-C	7.01	117.59	111.56
2	B	283	TRP	CA-C-N	6.95	128.53	119.84
2	B	283	TRP	C-N-CA	6.95	128.53	119.84
2	B	356	ILE	N-CA-C	6.92	117.03	110.74
2	B	37	ARG	N-CA-C	-6.84	105.56	114.04
3	F	126	VAL	N-CA-C	6.82	116.96	110.42
1	A	386	SER	N-CA-C	6.71	120.93	113.21
2	E	132	LEU	N-CA-C	-6.63	102.61	111.96
2	E	92	ASN	N-CA-C	-6.58	105.78	113.88
1	A	126	ALA	N-CA-C	6.51	121.49	112.45
1	A	565	GLU	N-CA-C	-6.48	105.26	113.43
3	F	269	CYS	N-CA-C	6.48	124.61	110.80
1	D	336	ASP	N-CA-C	-6.45	100.92	110.46
1	A	398	ARG	N-CA-C	-6.41	102.97	111.24
2	B	365	TYR	N-CA-C	-6.38	105.13	113.17
1	D	216	GLU	N-CA-C	-6.38	104.41	111.36
1	D	224	ALA	N-CA-C	-6.37	105.67	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	136	GLU	N-CA-C	-6.37	105.34	113.23
2	B	241	LEU	N-CA-C	6.32	117.86	110.97
2	E	49	PRO	N-CA-CB	6.31	109.88	103.25
2	E	219	GLY	N-CA-C	-6.30	98.24	113.18
1	D	80	VAL	N-CA-C	-6.29	104.51	113.07
2	E	270	THR	N-CA-C	-6.27	103.15	111.24
2	B	137	SER	CA-C-N	6.27	126.24	120.03
2	B	137	SER	C-N-CA	6.27	126.24	120.03
2	E	148	TYR	N-CA-C	-6.26	105.42	114.12
1	A	216	GLU	N-CA-C	-6.25	104.56	111.82
2	B	319	ARG	N-CA-C	-6.24	104.47	111.28
2	E	399	THR	N-CA-C	-6.24	103.62	111.11
1	D	417	TRP	N-CA-C	6.24	119.73	111.75
2	B	49	PRO	N-CA-CB	6.23	109.79	103.25
1	D	153	VAL	N-CA-C	6.19	121.55	113.07
3	F	65	LEU	N-CA-C	-6.16	104.25	110.97
3	C	122	GLN	N-CA-C	6.15	118.49	111.11
1	D	126	ALA	N-CA-C	6.10	121.00	113.50
3	C	246	GLU	N-CA-C	6.10	120.42	112.92
1	A	91	PRO	N-CA-C	6.09	118.13	110.70
1	A	9	SER	N-CA-C	6.08	118.02	108.96
2	B	252	VAL	CB-CA-C	-6.06	105.69	111.44
1	A	564	LEU	N-CA-C	-6.05	106.56	112.97
3	F	163	ILE	N-CA-C	5.95	116.50	108.17
2	B	148	TYR	N-CA-C	-5.93	106.01	113.72
1	D	383	ASN	CA-C-N	-5.92	116.92	122.66
1	D	383	ASN	C-N-CA	-5.92	116.92	122.66
2	B	252	VAL	N-CA-C	5.90	116.63	111.56
1	D	326	ILE	N-CA-C	5.88	115.95	110.42
1	D	364	HIS	N-CA-C	5.85	120.71	112.93
1	D	163	LYS	N-CA-C	-5.85	104.81	111.07
1	A	138	GLY	N-CA-C	5.84	118.75	112.33
2	B	327	SER	N-CA-C	-5.82	103.43	110.13
1	A	389	ASP	N-CA-C	-5.82	104.78	112.34
3	C	272	GLN	N-CA-C	-5.79	101.44	110.42
1	A	288	GLN	N-CA-C	-5.79	104.66	110.97
2	E	162	ASP	CA-C-N	-5.78	110.49	121.54
2	E	162	ASP	C-N-CA	-5.78	110.49	121.54
1	D	82	GLY	CA-C-N	5.68	126.95	119.84
1	D	82	GLY	C-N-CA	5.68	126.95	119.84
1	D	391	VAL	CB-CA-C	-5.68	101.97	111.29
1	D	545	GLN	N-CA-C	-5.63	105.90	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	388	MSE	N-CA-C	-5.60	104.87	110.97
3	F	272	GLN	N-CA-C	-5.59	102.24	110.52
1	D	270	LEU	N-CA-C	-5.59	104.82	111.03
1	A	79	LEU	N-CA-C	5.58	119.56	112.87
3	C	163	ILE	N-CA-C	5.55	115.88	108.11
1	D	565	GLU	N-CA-C	-5.54	105.81	113.18
1	D	463	THR	N-CA-C	-5.52	104.95	110.97
1	A	39	ALA	N-CA-C	-5.51	106.53	113.20
2	B	121	TRP	N-CA-C	-5.51	104.68	112.17
2	E	41	VAL	N-CA-C	-5.50	105.25	110.42
1	A	44	VAL	N-CA-C	5.49	120.76	109.34
3	C	156	THR	N-CA-C	5.49	117.31	109.14
1	A	417	TRP	N-CA-C	5.48	117.26	111.28
3	C	141	ASN	N-CA-C	-5.47	106.66	113.55
3	F	126	VAL	CB-CA-C	-5.46	104.98	111.97
1	D	419	VAL	N-CA-C	-5.45	105.54	110.82
1	A	82	GLY	CA-C-N	5.41	126.60	119.84
1	A	82	GLY	C-N-CA	5.41	126.60	119.84
1	A	193	ALA	N-CA-C	-5.40	105.47	111.36
1	A	49	SER	N-CA-C	5.40	119.97	113.17
3	C	126	VAL	N-CA-C	5.40	115.84	110.23
1	A	540	VAL	N-CA-C	-5.39	105.12	110.62
1	D	9	SER	N-CA-C	5.38	117.37	109.24
2	B	372	TRP	N-CA-C	-5.34	106.82	113.55
1	A	163	LYS	N-CA-C	-5.33	105.47	111.28
1	D	173	LEU	N-CA-C	-5.33	106.48	112.87
1	A	24	ASP	N-CA-C	-5.32	102.21	109.71
2	B	120	ALA	N-CA-C	-5.32	106.16	113.56
2	E	239	LYS	N-CA-C	5.32	119.76	113.16
1	D	583	LEU	N-CA-C	-5.32	105.86	112.93
2	E	97	LEU	CA-C-N	5.31	125.85	120.38
2	E	97	LEU	C-N-CA	5.31	125.85	120.38
3	F	64	ASP	N-CA-C	-5.30	106.08	112.54
2	E	109	ASP	CA-C-N	5.29	125.35	119.32
2	E	109	ASP	C-N-CA	5.29	125.35	119.32
3	F	246	GLU	N-CA-C	5.29	119.42	112.92
1	A	249	ARG	N-CA-C	-5.27	105.45	111.14
1	D	90	LEU	CA-C-N	5.24	125.78	120.38
1	D	90	LEU	C-N-CA	5.24	125.78	120.38
2	B	221	ILE	N-CA-C	5.24	115.86	110.36
1	A	90	LEU	CA-C-N	5.22	125.76	120.38
1	A	90	LEU	C-N-CA	5.22	125.76	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	316	ASP	N-CA-C	5.21	117.93	110.68
1	D	385	ILE	CB-CA-C	-5.21	104.44	112.05
3	F	73	GLY	N-CA-C	-5.21	104.88	112.17
1	A	364	HIS	N-CA-C	5.20	119.09	112.12
1	A	492	ASP	CA-C-N	5.20	124.64	119.24
1	A	492	ASP	C-N-CA	5.20	124.64	119.24
2	B	216	GLU	N-CA-C	-5.19	105.51	111.07
2	B	34	GLN	N-CA-C	-5.19	106.11	112.90
2	E	365	TYR	N-CA-C	-5.19	106.95	113.28
1	D	436	VAL	N-CA-C	5.18	115.62	110.23
1	A	316	ASP	N-CA-C	5.18	117.88	110.68
1	D	228	CYS	N-CA-C	-5.16	105.73	112.23
2	E	144	ILE	N-CA-C	-5.16	98.62	109.34
1	A	153	VAL	N-CA-C	5.15	119.56	113.22
2	E	319	ARG	N-CA-C	-5.14	105.75	111.36
1	D	579	ALA	N-CA-C	-5.13	105.60	111.14
2	B	366	ARG	N-CA-C	-5.11	102.96	110.42
2	E	361	PHE	N-CA-C	5.11	121.10	109.81
2	B	238	LEU	N-CA-C	5.11	116.85	111.28
2	E	252	VAL	CB-CA-C	-5.11	106.59	111.44
1	A	381	ARG	N-CA-C	-5.10	105.37	111.03
2	B	229	LEU	N-CA-C	5.09	121.65	110.80
1	A	16	LEU	N-CA-C	-5.08	105.87	111.71
1	A	18	ASP	N-CA-C	-5.08	107.75	114.04
1	A	322	ILE	N-CA-C	-5.05	105.62	110.72
2	E	34	GLN	N-CA-C	-5.04	107.26	113.41
3	F	19	GLU	N-CA-C	-5.03	106.83	113.17

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	4	ARG	Peptide
4	G	5	1ZN	Peptide,Mainchain
4	H	4	ARG	Peptide
4	H	5	1ZN	Peptide,Mainchain

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4535	0	4637	491	0
1	D	4535	0	4637	469	0
2	B	3131	0	3050	359	0
2	E	3131	0	3050	381	0
3	C	2367	0	2268	234	0
3	F	2367	0	2268	234	0
4	G	71	0	61	1	0
4	H	71	0	61	3	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	20212	0	20032	2146	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 53.

All (2146) 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:D:278:ILE:H	1:D:278:ILE:HD12	1.10	1.12
2:E:325:VAL:HG13	2:E:337:LEU:HD11	1.29	1.11
3:C:276:MET:HE3	3:C:278:LEU:HD21	1.33	1.10
1:D:350:MSE:HE1	1:D:391:VAL:HG13	1.24	1.10
2:B:277:MSE:HE1	2:B:316:PRO:HG3	1.35	1.08
2:E:340:TRP:HA	2:E:346:MSE:HE3	1.34	1.06
1:A:288:GLN:HA	1:A:291:MSE:HE3	1.34	1.06
2:E:146:LYS:HE3	2:E:147:LYS:HE3	1.35	1.05
1:A:278:ILE:H	1:A:278:ILE:HD12	1.18	1.02
1:D:500:THR:HA	1:D:503:PHE:HD1	1.25	1.01
3:C:13:TRP:HE1	3:C:27:GLN:NE2	1.58	1.00
1:D:416:LYS:O	1:D:419:VAL:HG23	1.61	1.00
1:A:535:ASN:HA	1:A:538:PHE:CE2	1.95	0.99
1:A:38:ILE:O	1:A:42:LEU:HB2	1.61	0.99
1:A:25:VAL:HG22	1:A:28:ARG:HH21	1.28	0.99
1:A:502:LEU:HD11	1:A:540:VAL:HG23	1.45	0.98
2:B:208:HIS:HD2	2:B:209:ASN:H	1.15	0.95
1:A:392:ASN:HB3	1:A:400:LEU:HD22	1.47	0.94
3:C:239:ARG:HH12	3:C:242:GLN:HG3	1.32	0.94
1:A:350:MSE:HE1	1:A:391:VAL:HG22	1.48	0.93
1:D:427:MSE:HA	1:D:427:MSE:HE3	1.47	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:MSE:HA	1:A:427:MSE:HE3	1.49	0.93
1:D:535:ASN:HA	1:D:538:PHE:CE2	2.05	0.92
3:F:276:MET:HE3	3:F:278:LEU:HD21	1.50	0.92
2:B:160:LEU:O	2:B:162:ASP:N	2.02	0.92
2:E:318:PHE:HD2	2:E:360:MSE:HE2	1.35	0.91
3:F:237:VAL:HB	3:F:256:VAL:HG23	1.49	0.91
1:A:526:LEU:HD22	1:A:563:ILE:HG21	1.51	0.91
1:D:77:THR:HG21	1:D:118:GLU:HG3	1.53	0.91
1:D:338:ASN:HD22	1:D:341:VAL:HG23	1.36	0.91
3:F:159:VAL:HG23	3:F:163:ILE:HB	1.52	0.91
1:A:385:ILE:HD11	1:A:411:LEU:HG	1.52	0.90
1:D:392:ASN:HD21	1:D:433:GLN:HE22	1.18	0.90
1:D:448:MSE:HE2	1:D:448:MSE:HA	1.54	0.90
2:E:164:GLU:O	2:E:165:ASP:O	1.90	0.90
1:A:270:LEU:O	1:A:274:VAL:HG23	1.71	0.89
2:E:318:PHE:CD2	2:E:360:MSE:HE2	2.07	0.89
1:A:452:VAL:HG13	1:A:497:HIS:CD2	2.07	0.89
3:F:240:ALA:HA	3:F:258:THR:HG23	1.54	0.89
2:B:80:PRO:HG2	2:B:82:TYR:CE2	2.08	0.89
1:D:38:ILE:O	1:D:42:LEU:HB2	1.73	0.88
2:E:208:HIS:HD2	2:E:209:ASN:H	1.20	0.88
1:A:227:ALA:O	1:A:231:ILE:HG13	1.72	0.88
1:A:343:SER:CA	1:A:380:VAL:HG22	2.04	0.88
2:E:218:LEU:HD23	2:E:221:ILE:HD12	1.55	0.88
3:C:123:ILE:HG23	3:C:127:TYR:HD2	1.37	0.88
3:F:190:PRO:HD3	3:F:195:MET:HE2	1.56	0.88
1:A:225:VAL:HG11	1:A:262:MSE:HB3	1.57	0.87
2:B:340:TRP:HA	2:B:346:MSE:HE3	1.55	0.87
1:D:180:MSE:HE3	1:D:180:MSE:H	1.40	0.87
2:E:128:TYR:HB3	2:E:171:PHE:CD2	2.08	0.87
1:D:278:ILE:H	1:D:278:ILE:CD1	1.88	0.87
1:D:409:VAL:HG13	1:D:446:LEU:HD21	1.56	0.87
2:B:251:SER:HA	2:B:293:MSE:HE1	1.55	0.86
1:A:362:ILE:HD13	1:A:399:GLN:HG3	1.56	0.86
3:F:239:ARG:HH12	3:F:242:GLN:HG3	1.39	0.86
1:A:300:ALA:HB2	1:A:341:VAL:HG22	1.56	0.86
2:B:318:PHE:HD2	2:B:360:MSE:HE2	1.41	0.86
1:D:77:THR:CG2	1:D:118:GLU:HG3	2.05	0.86
2:B:146:LYS:HE3	2:B:147:LYS:HE3	1.57	0.86
2:B:313:ILE:O	2:B:316:PRO:HD2	1.75	0.86
1:D:35:LEU:HD21	1:D:55:LEU:HD11	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.58	0.86
3:C:203:PRO:HD2	3:C:242:GLN:OE1	1.74	0.86
2:E:202:ILE:HD11	2:E:244:LEU:HG	1.58	0.85
1:A:25:VAL:HG22	1:A:28:ARG:NH2	1.91	0.85
1:A:405:LEU:O	1:A:409:VAL:HG23	1.76	0.85
2:B:78:THR:C	2:B:80:PRO:HD2	2.01	0.85
2:E:277:MSE:HE1	2:E:316:PRO:HG3	1.57	0.85
1:A:477:TRP:CH2	1:A:482:ILE:HD11	2.11	0.84
2:B:329:HIS:CD2	2:B:331:GLN:HB2	2.12	0.84
1:D:392:ASN:ND2	1:D:433:GLN:HE22	1.73	0.84
2:B:318:PHE:CD2	2:B:360:MSE:HE2	2.12	0.84
2:B:388:MSE:HE2	2:B:392:GLN:HE22	1.41	0.84
1:A:352:LEU:HA	1:A:355:ILE:HD12	1.58	0.84
1:D:79:LEU:H	1:D:79:LEU:HD12	1.42	0.84
2:E:160:LEU:O	2:E:162:ASP:N	2.10	0.84
1:D:561:LYS:O	1:D:565:GLU:HG2	1.77	0.84
2:B:83:PRO:HB3	2:B:148:TYR:CD1	2.13	0.83
1:D:35:LEU:HD11	1:D:51:LEU:HD11	1.61	0.83
1:A:71:GLU:HG3	1:A:107:LYS:HE3	1.59	0.83
2:E:88:MSE:HE2	2:E:92:ASN:ND2	1.93	0.83
1:A:564:LEU:HD22	1:A:583:LEU:HD21	1.59	0.83
2:B:373:ASN:ND2	2:B:376:ILE:HG23	1.94	0.82
3:C:115:ARG:NH1	3:C:151:ASP:HA	1.93	0.82
2:E:164:GLU:O	2:E:165:ASP:C	2.22	0.82
1:D:22:ASN:ND2	1:D:27:LEU:HD12	1.95	0.82
1:A:482:ILE:C	1:A:484:PRO:HD2	2.05	0.82
1:D:310:CYS:HA	1:D:313:LEU:HD12	1.61	0.82
2:B:208:HIS:HD2	2:B:209:ASN:N	1.78	0.82
1:D:407:ALA:O	1:D:411:LEU:HD22	1.79	0.81
2:E:251:SER:HA	2:E:293:MSE:HE1	1.61	0.81
3:F:123:ILE:HG23	3:F:127:TYR:HD2	1.44	0.81
2:E:78:THR:C	2:E:80:PRO:HD2	2.06	0.81
1:A:452:VAL:HG13	1:A:497:HIS:NE2	1.97	0.80
1:D:261:TYR:HA	1:D:298:VAL:HG22	1.62	0.80
1:D:405:LEU:O	1:D:409:VAL:HG23	1.82	0.80
1:D:390:CYS:O	1:D:392:ASN:N	2.15	0.80
3:F:239:ARG:HH12	3:F:242:GLN:CG	1.94	0.80
1:D:502:LEU:HD11	1:D:540:VAL:HG23	1.61	0.80
2:B:202:ILE:HD11	2:B:244:LEU:HG	1.60	0.80
3:C:159:VAL:HG23	3:C:163:ILE:HB	1.64	0.80
1:A:205:ILE:HA	1:A:208:MSE:HE3	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASN:HD22	1:A:341:VAL:HG23	1.47	0.79
1:A:347:SER:HB3	1:A:383:ASN:HD22	1.47	0.79
1:D:452:VAL:HG13	1:D:497:HIS:CD2	2.18	0.79
1:D:564:LEU:HD22	1:D:583:LEU:HD21	1.64	0.79
1:A:343:SER:HA	1:A:380:VAL:HG22	1.63	0.79
1:D:490:SER:HB2	1:D:528:MSE:HE3	1.64	0.79
3:C:237:VAL:HB	3:C:256:VAL:HG23	1.65	0.79
1:A:409:VAL:HG13	1:A:446:LEU:HD21	1.65	0.79
1:D:79:LEU:HD12	1:D:79:LEU:N	1.98	0.79
2:E:373:ASN:ND2	2:E:376:ILE:HG23	1.98	0.79
3:F:209:TRP:N	3:F:224:ILE:HD11	1.99	0.78
2:E:88:MSE:HE2	2:E:92:ASN:HD22	1.47	0.78
2:E:85:VAL:HG11	2:E:134:PHE:CD1	2.19	0.78
3:F:52:VAL:HG12	3:F:79:ASN:HB3	1.65	0.78
2:E:330:PHE:CE1	2:E:331:GLN:HG2	2.19	0.78
1:A:401:SER:HB3	1:A:434:LEU:HD21	1.66	0.77
1:D:427:MSE:HA	1:D:427:MSE:CE	2.15	0.77
3:C:50:CYS:HB2	3:C:51:PRO:HA	1.67	0.77
3:C:68:LEU:HD23	3:C:68:LEU:C	2.08	0.77
1:A:564:LEU:O	1:A:564:LEU:HD23	1.83	0.77
3:C:209:TRP:N	3:C:224:ILE:HD11	1.99	0.77
1:D:197:GLU:H	1:D:197:GLU:CD	1.89	0.77
2:E:59:LYS:HD3	2:E:123:HIS:NE2	2.00	0.77
3:F:50:CYS:HB2	3:F:51:PRO:HA	1.64	0.77
1:D:427:MSE:HE1	1:D:430:LEU:HD12	1.64	0.77
1:A:90:LEU:HB2	1:A:91:PRO:HD3	1.66	0.77
1:A:495:TYR:O	1:A:499:MSE:HG3	1.85	0.77
2:B:164:GLU:HB3	2:B:168:GLU:HB2	1.67	0.77
3:C:214:ARG:HG2	3:C:214:ARG:HH11	1.50	0.77
1:A:500:THR:HA	1:A:503:PHE:HD1	1.48	0.77
2:B:128:TYR:HB3	2:B:171:PHE:CD2	2.20	0.77
1:A:416:LYS:O	1:A:419:VAL:HG23	1.85	0.77
2:B:164:GLU:O	2:B:165:ASP:O	2.02	0.77
1:A:278:ILE:H	1:A:278:ILE:CD1	1.93	0.77
2:E:223:ASN:HD22	2:E:263:GLN:HE21	1.33	0.77
1:D:25:VAL:HG22	1:D:28:ARG:NH2	1.99	0.77
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.15	0.76
2:B:190:ILE:O	2:B:194:ILE:HG13	1.83	0.76
3:F:203:PRO:HD2	3:F:242:GLN:OE1	1.85	0.76
1:A:561:LYS:O	1:A:565:GLU:HG2	1.86	0.76
2:B:208:HIS:CD2	2:B:209:ASN:H	2.02	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:PRO:HG2	2:B:82:TYR:HE2	1.50	0.76
2:B:222:ILE:HD13	2:B:264:PHE:HD1	1.50	0.76
1:D:564:LEU:HD22	1:D:583:LEU:CD2	2.16	0.76
1:A:180:MSE:HE2	1:A:183:ARG:HH22	1.50	0.76
3:C:62:PHE:HD2	3:C:63:HIS:HD2	1.34	0.76
1:D:278:ILE:HD12	1:D:278:ILE:N	1.94	0.76
1:D:429:LEU:O	1:D:433:GLN:HG3	1.85	0.75
2:E:83:PRO:HB3	2:E:148:TYR:CD1	2.21	0.75
2:E:388:MSE:HE2	2:E:392:GLN:HE22	1.51	0.75
3:F:28:VAL:HG11	3:F:142:VAL:HG13	1.69	0.75
1:A:102:THR:HG22	1:A:105:ARG:NH2	2.00	0.75
2:E:85:VAL:HG11	2:E:134:PHE:HD1	1.52	0.75
1:A:237:GLN:NE2	1:A:278:ILE:HD11	2.02	0.75
1:D:500:THR:HA	1:D:503:PHE:CD1	2.17	0.75
2:B:165:ASP:O	2:B:167:ARG:N	2.20	0.74
1:D:428:PRO:HD3	1:D:465:ASN:HD21	1.52	0.74
2:E:325:VAL:CG1	2:E:337:LEU:HD11	2.14	0.74
2:B:242:LEU:HD13	2:B:278:ALA:CB	2.17	0.74
2:B:218:LEU:HD23	2:B:221:ILE:HD12	1.70	0.74
3:F:89:ARG:HD2	3:F:266:CYS:SG	2.28	0.74
3:F:104:LYS:N	3:F:111:ILE:HD11	2.01	0.74
2:E:134:PHE:CD2	2:E:135:LEU:N	2.56	0.74
2:B:118:GLU:HB3	2:B:164:GLU:CG	2.18	0.74
2:E:166:PRO:O	2:E:167:ARG:C	2.30	0.74
3:F:67:GLU:HB2	3:F:292:ALA:HB2	1.68	0.74
2:B:325:VAL:HG13	2:B:337:LEU:HD11	1.69	0.74
2:B:133:ARG:HA	2:B:136:GLU:OE2	1.88	0.74
1:D:44:VAL:HG22	1:D:45:GLU:N	2.02	0.74
2:E:43:PHE:O	2:E:45:PHE:N	2.20	0.74
3:F:243:LEU:HD22	4:H:7:DAM:HM3	1.70	0.74
2:B:164:GLU:O	2:B:165:ASP:C	2.30	0.73
1:A:366:LEU:O	1:A:370:LEU:HD23	1.88	0.73
2:B:121:TRP:N	2:B:122:PRO:HD2	2.03	0.73
3:C:170:LEU:H	3:C:220:PHE:HE2	1.34	0.73
2:E:364:LEU:HB2	2:E:384:LEU:HD21	1.68	0.73
1:D:79:LEU:H	1:D:79:LEU:CD1	2.01	0.73
2:E:223:ASN:ND2	2:E:263:GLN:HE21	1.86	0.73
1:D:401:SER:HB3	1:D:434:LEU:HD21	1.70	0.73
1:D:556:LEU:O	1:D:560:VAL:HB	1.88	0.73
2:E:391:ASN:ND2	2:E:394:LEU:HD12	2.03	0.73
1:A:564:LEU:HD22	1:A:583:LEU:CD2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LEU:O	1:A:560:VAL:HB	1.89	0.73
3:C:229:ASN:HA	3:C:234:LEU:HB2	1.71	0.73
2:E:80:PRO:HG2	2:E:82:TYR:CE2	2.24	0.73
1:A:278:ILE:HD12	1:A:278:ILE:N	2.00	0.73
2:E:208:HIS:HD2	2:E:209:ASN:N	1.87	0.73
2:E:242:LEU:HD13	2:E:278:ALA:CB	2.18	0.73
1:A:179:PRO:HB2	1:A:180:MSE:HE3	1.71	0.73
2:B:208:HIS:CD2	2:B:209:ASN:N	2.56	0.73
2:E:145:ALA:O	2:E:147:LYS:N	2.21	0.73
2:E:71:THR:HG21	2:E:133:ARG:HH11	1.53	0.72
3:F:214:ARG:HG2	3:F:214:ARG:HH11	1.54	0.72
3:F:139:ASN:CG	3:F:141:ASN:HD22	1.97	0.72
1:A:155:TYR:CZ	1:A:163:LYS:HB3	2.24	0.72
1:D:495:TYR:HE2	1:D:535:ASN:HD22	1.36	0.72
2:B:166:PRO:O	2:B:167:ARG:C	2.33	0.72
2:E:371:HIS:CD2	2:E:376:ILE:HD11	2.25	0.72
3:F:143:TRP:CE2	3:F:147:THR:HG21	2.23	0.72
2:B:371:HIS:CD2	2:B:376:ILE:HD11	2.24	0.72
1:A:427:MSE:HA	1:A:427:MSE:CE	2.19	0.72
1:D:369:PHE:O	1:D:373:LEU:HB2	1.88	0.72
1:A:452:VAL:O	1:A:452:VAL:HG12	1.90	0.72
1:D:183:ARG:NH2	2:E:200:ARG:HD2	2.04	0.72
1:D:524:THR:O	1:D:528:MSE:HG3	1.90	0.72
2:E:208:HIS:CD2	2:E:209:ASN:H	2.07	0.72
1:D:109:VAL:HG13	1:D:150:LEU:HD21	1.71	0.72
2:E:313:ILE:HD12	2:E:313:ILE:N	2.05	0.72
2:B:118:GLU:HB3	2:B:164:GLU:HG2	1.72	0.71
2:E:313:ILE:HD12	2:E:313:ILE:H	1.55	0.71
2:E:121:TRP:N	2:E:122:PRO:HD2	2.05	0.71
2:E:190:ILE:O	2:E:194:ILE:HG13	1.90	0.71
1:D:104:VAL:HG12	1:D:105:ARG:N	2.05	0.71
2:E:391:ASN:OD1	2:E:394:LEU:HB2	1.91	0.71
2:E:406:LYS:O	2:E:406:LYS:HD3	1.89	0.71
1:A:362:ILE:CD1	1:A:399:GLN:HG3	2.21	0.71
2:B:313:ILE:H	2:B:313:ILE:HD12	1.55	0.71
3:C:220:PHE:HA	3:C:224:ILE:HD12	1.72	0.71
2:E:186:LEU:HB3	2:E:190:ILE:CD1	2.20	0.71
1:A:448:MSE:HA	1:A:448:MSE:HE2	1.72	0.71
1:A:261:TYR:HA	1:A:298:VAL:HG22	1.70	0.71
3:F:17:LEU:HD21	3:F:23:LEU:HG	1.72	0.70
2:B:240:VAL:O	2:B:243:PRO:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:68:LEU:HD23	3:F:68:LEU:C	2.16	0.70
3:F:197:ASP:OD1	3:F:217:GLY:HA2	1.89	0.70
1:A:35:LEU:HB3	1:A:72:GLN:HG2	1.71	0.70
2:B:132:LEU:C	2:B:134:PHE:H	1.97	0.70
2:E:208:HIS:CD2	2:E:209:ASN:N	2.60	0.70
2:E:151:GLN:HB3	2:E:189:TYR:CE2	2.25	0.70
2:E:165:ASP:O	2:E:167:ARG:N	2.25	0.70
2:E:376:ILE:HA	2:E:379:LEU:HB2	1.73	0.70
1:A:104:VAL:HG12	1:A:105:ARG:N	2.05	0.70
3:C:157:ALA:HB3	3:C:165:CYS:HB2	1.74	0.70
1:A:258:ARG:HH11	1:A:258:ARG:HG3	1.55	0.70
2:E:366:ARG:O	2:E:368:SER:N	2.24	0.70
1:A:407:ALA:O	1:A:411:LEU:HD22	1.92	0.69
1:D:66:LEU:HD22	1:D:96:LEU:HD23	1.75	0.69
2:E:167:ARG:CB	2:E:167:ARG:HH11	2.05	0.69
2:B:247:VAL:HG12	2:B:249:SER:H	1.57	0.69
3:C:89:ARG:HD2	3:C:266:CYS:SG	2.32	0.69
1:D:161:ALA:O	1:D:165:GLU:HG3	1.92	0.69
2:E:288:SER:HB2	2:E:289:PRO:HD3	1.74	0.69
3:F:160:ASP:O	3:F:162:GLN:N	2.25	0.69
1:A:35:LEU:HD11	1:A:51:LEU:HD11	1.73	0.69
3:F:137:TYR:CD2	3:F:142:VAL:HG21	2.28	0.69
2:B:310:PHE:O	2:B:314:MSE:HB2	1.93	0.69
1:D:452:VAL:O	1:D:452:VAL:HG12	1.92	0.69
1:A:193:ALA:HA	1:A:196:LEU:HD12	1.75	0.69
1:A:492:ASP:OD2	1:A:493:PRO:HD2	1.91	0.69
1:A:66:LEU:HD22	1:A:96:LEU:HD23	1.75	0.69
1:A:369:PHE:O	1:A:373:LEU:HB2	1.93	0.69
2:B:43:PHE:O	2:B:45:PHE:N	2.26	0.69
2:B:88:MSE:HE2	2:B:92:ASN:HD22	1.56	0.69
1:D:90:LEU:HB2	1:D:91:PRO:HD3	1.74	0.69
1:D:260:ARG:HH11	1:D:260:ARG:HG3	1.57	0.69
2:E:71:THR:HG21	2:E:133:ARG:NH1	2.08	0.69
3:F:13:TRP:HE1	3:F:27:GLN:NE2	1.90	0.69
2:E:169:ARG:HB3	2:E:213:GLU:HG2	1.75	0.69
3:F:165:CYS:SG	3:F:238:SER:HB3	2.33	0.69
2:E:356:ILE:C	2:E:358:PRO:HD2	2.17	0.69
1:A:286:ALA:O	1:A:289:ASN:HB2	1.94	0.68
2:B:305:ILE:HD13	2:B:306:GLU:H	1.56	0.68
3:C:194:PRO:HG2	3:C:195:MET:H	1.58	0.68
1:D:131:LEU:HD23	1:D:131:LEU:C	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:119:GLU:HG3	3:F:150:PHE:CD1	2.28	0.68
2:B:366:ARG:O	2:B:368:SER:N	2.27	0.68
1:D:288:GLN:HA	1:D:291:MSE:HE3	1.75	0.68
1:A:509:SER:OG	1:A:547:ILE:HG22	1.94	0.68
2:B:164:GLU:CB	2:B:168:GLU:HB2	2.23	0.68
1:D:428:PRO:HD3	1:D:465:ASN:ND2	2.08	0.68
1:A:428:PRO:HD3	1:A:465:ASN:ND2	2.08	0.68
1:D:499:MSE:HE1	3:F:77:ASP:O	1.94	0.68
1:D:20:LEU:HD23	1:D:31:SER:CB	2.24	0.68
1:A:528:MSE:C	1:A:530:GLY:H	2.01	0.68
2:B:162:ASP:O	2:B:163:SER:HB2	1.94	0.68
2:E:176:LEU:HG	2:E:176:LEU:O	1.94	0.68
2:E:118:GLU:HB3	2:E:164:GLU:HG2	1.75	0.67
2:E:313:ILE:HG22	2:E:317:LEU:HB2	1.76	0.67
1:A:204:GLU:O	1:A:207:PRO:HD2	1.94	0.67
1:D:388:LEU:HD12	1:D:408:ILE:HD11	1.77	0.67
1:A:44:VAL:HG22	1:A:45:GLU:N	2.09	0.67
1:A:358:LYS:O	1:A:362:ILE:HG13	1.94	0.67
3:C:170:LEU:HB2	3:C:220:PHE:CD2	2.29	0.67
1:D:362:ILE:HD13	1:D:399:GLN:HG3	1.76	0.67
2:E:73:ASN:C	2:E:75:ASN:H	2.01	0.67
1:A:100:GLU:O	1:A:105:ARG:NH1	2.26	0.67
1:D:350:MSE:HE1	1:D:391:VAL:CG1	2.14	0.67
2:B:154:VAL:O	2:B:157:LEU:HB3	1.93	0.67
1:D:556:LEU:CD2	1:D:588:LEU:HD11	2.24	0.67
1:A:219:SER:HA	1:A:222:LEU:HD22	1.75	0.67
1:D:182:ARG:HH11	1:D:182:ARG:HG3	1.59	0.67
2:E:166:PRO:O	2:E:169:ARG:N	2.28	0.67
3:F:165:CYS:HA	3:F:238:SER:O	1.94	0.67
1:A:388:LEU:HD13	1:A:408:ILE:HD11	1.77	0.67
2:B:345:ILE:O	2:B:349:ILE:HG13	1.95	0.67
1:D:71:GLU:HG3	1:D:107:LYS:HE3	1.75	0.67
1:D:264:ALA:O	1:D:267:PHE:HB2	1.94	0.67
1:D:392:ASN:ND2	1:D:433:GLN:NE2	2.42	0.67
1:D:528:MSE:C	1:D:530:GLY:H	2.01	0.67
2:E:59:LYS:HA	2:E:62:ALA:HB3	1.77	0.67
2:B:286:THR:HG22	3:C:134:LEU:HB3	1.77	0.67
3:C:25:GLU:CD	3:C:139:ASN:HD21	2.03	0.67
1:D:509:SER:HA	1:D:521:MSE:HE1	1.77	0.67
3:F:54:VAL:HG21	3:F:276:MET:HE2	1.76	0.67
1:A:524:THR:O	1:A:528:MSE:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:313:ILE:HD12	2:B:313:ILE:N	2.09	0.67
2:E:93:MSE:HE2	2:E:128:TYR:OH	1.94	0.67
1:A:411:LEU:O	1:A:413:GLU:N	2.28	0.66
1:A:489:MSE:O	1:A:491:GLY:N	2.28	0.66
3:C:121:ARG:HH11	3:C:121:ARG:HG3	1.60	0.66
2:E:236:PHE:O	2:E:240:VAL:HB	1.95	0.66
3:C:94:VAL:HG23	3:C:132:GLU:OE2	1.95	0.66
1:D:180:MSE:H	1:D:180:MSE:CE	2.07	0.66
2:E:391:ASN:CG	2:E:394:LEU:HD12	2.21	0.66
3:F:71:ILE:HG22	3:F:72:GLY:N	2.09	0.66
1:A:180:MSE:HE2	1:A:183:ARG:NH2	2.10	0.66
1:A:467:LYS:O	1:A:471:GLU:HG3	1.96	0.66
3:F:124:THR:HB	3:F:129:PHE:HB3	1.77	0.66
2:B:243:PRO:O	2:B:246:LYS:HB2	1.94	0.66
3:C:104:LYS:N	3:C:111:ILE:HD11	2.11	0.66
3:C:190:PRO:HD3	3:C:195:MET:HE2	1.78	0.66
1:A:282:ASP:O	1:A:285:PRO:HD2	1.96	0.66
1:A:438:PHE:O	1:A:438:PHE:HD1	1.78	0.66
2:E:93:MSE:O	2:E:95:ARG:HG3	1.96	0.66
2:E:165:ASP:OD2	2:E:166:PRO:HD2	1.96	0.66
1:A:364:HIS:O	1:A:367:PRO:HD2	1.96	0.66
2:B:134:PHE:CD2	2:B:135:LEU:N	2.64	0.66
1:D:388:LEU:CD1	1:D:408:ILE:HD11	2.26	0.66
1:D:427:MSE:CE	1:D:430:LEU:HD12	2.26	0.66
2:E:381:TYR:CE2	2:E:385:LYS:HD2	2.30	0.66
1:A:482:ILE:C	1:A:484:PRO:CD	2.68	0.65
1:D:35:LEU:HG	1:D:35:LEU:O	1.96	0.65
1:D:115:ILE:HG13	1:D:115:ILE:O	1.92	0.65
2:B:194:ILE:HG21	2:B:218:LEU:HD11	1.79	0.65
3:C:54:VAL:HG22	3:C:81:LEU:HD22	1.78	0.65
1:D:52:LEU:HB2	1:D:53:PRO:HD3	1.76	0.65
3:F:229:ASN:HA	3:F:234:LEU:HB2	1.78	0.65
1:A:24:ASP:O	1:A:26:GLN:N	2.29	0.65
1:A:427:MSE:HE1	1:A:430:LEU:HD12	1.79	0.65
3:C:17:LEU:HD11	3:C:98:THR:HG22	1.77	0.65
2:E:132:LEU:C	2:E:134:PHE:H	2.05	0.65
2:E:340:TRP:CH2	2:E:360:MSE:HE3	2.30	0.65
2:E:344:TYR:O	2:E:347:SER:HB3	1.97	0.65
1:A:411:LEU:HD22	1:A:411:LEU:H	1.62	0.65
1:D:100:GLU:O	1:D:105:ARG:NH1	2.29	0.65
2:B:85:VAL:HG13	2:B:130:PHE:CE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:78:THR:HB	1:D:79:LEU:HD12	1.77	0.65
1:D:490:SER:CB	1:D:528:MSE:HE3	2.26	0.65
3:F:240:ALA:HB2	3:F:259:ILE:H	1.62	0.65
2:B:167:ARG:CB	2:B:167:ARG:HH11	2.10	0.65
2:B:200:ARG:HA	2:B:204:GLU:HG3	1.78	0.65
3:C:42:GLU:HB3	3:C:46:GLN:OE1	1.97	0.65
3:F:141:ASN:HB3	3:F:145:TYR:CE1	2.32	0.65
1:A:22:ASN:ND2	1:A:24:ASP:HB3	2.12	0.65
2:E:97:LEU:H	2:E:97:LEU:HD12	1.62	0.65
2:E:329:HIS:CD2	2:E:331:GLN:HB2	2.31	0.65
3:F:157:ALA:HB3	3:F:165:CYS:HB2	1.79	0.65
3:F:174:ILE:HD11	3:F:194:PRO:HB2	1.79	0.65
2:B:218:LEU:O	2:B:222:ILE:HG13	1.97	0.65
2:B:367:ASN:O	2:B:369:LYS:N	2.23	0.65
1:D:408:ILE:HD13	1:D:426:TYR:HE2	1.61	0.65
3:F:143:TRP:O	3:F:147:THR:HG23	1.96	0.65
1:A:388:LEU:CD1	1:A:408:ILE:HD11	2.26	0.65
2:B:157:LEU:O	2:B:160:LEU:HB2	1.96	0.65
2:E:128:TYR:HB3	2:E:171:PHE:HD2	1.58	0.65
3:F:159:VAL:CG2	3:F:163:ILE:HB	2.25	0.65
1:A:427:MSE:HB3	1:A:428:PRO:CD	2.27	0.64
2:B:60:ARG:C	2:B:60:ARG:HD3	2.22	0.64
2:B:288:SER:HB2	2:B:289:PRO:HD3	1.78	0.64
1:A:325:GLN:O	1:A:328:PRO:HD2	1.96	0.64
1:A:345:LEU:HD23	1:A:346:ALA:N	2.12	0.64
2:B:330:PHE:CE2	3:C:122:GLN:HG3	2.31	0.64
1:D:470:VAL:HG11	1:D:511:VAL:HG23	1.79	0.64
2:E:42:LEU:O	2:E:59:LYS:HE3	1.97	0.64
2:E:165:ASP:CG	2:E:166:PRO:HD2	2.22	0.64
3:C:76:PRO:HB3	3:C:107:TYR:CD1	2.32	0.64
3:C:119:GLU:HG3	3:C:150:PHE:CD1	2.32	0.64
3:F:97:VAL:O	3:F:101:VAL:HG23	1.98	0.64
2:B:59:LYS:HD3	2:B:123:HIS:NE2	2.13	0.64
1:A:211:ASN:HD22	1:A:211:ASN:N	1.95	0.64
1:D:517:THR:HA	1:D:521:MSE:HE2	1.78	0.64
1:A:44:VAL:HG13	1:A:45:GLU:H	1.62	0.64
2:B:391:ASN:ND2	2:B:394:LEU:HD12	2.12	0.64
2:E:240:VAL:O	2:E:243:PRO:HG2	1.98	0.64
1:D:113:ARG:O	1:D:116:SER:HB3	1.98	0.64
1:D:535:ASN:HA	1:D:538:PHE:HE2	1.61	0.64
3:F:115:ARG:HH12	3:F:151:ASP:HA	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:PRO:HD3	1:A:465:ASN:HD21	1.63	0.64
2:B:85:VAL:HG11	2:B:134:PHE:CD1	2.33	0.64
3:C:71:ILE:HG22	3:C:72:GLY:N	2.13	0.64
3:C:155:LEU:HD21	3:C:185:ARG:HB2	1.80	0.64
3:C:274:ALA:HB2	3:C:288:GLN:HA	1.80	0.64
1:D:556:LEU:HD22	1:D:588:LEU:HD11	1.80	0.64
2:E:149:ILE:HG22	2:E:149:ILE:O	1.96	0.64
1:A:158:VAL:HG23	1:A:163:LYS:HG3	1.80	0.63
2:E:375:THR:HG22	2:E:379:LEU:HD12	1.80	0.63
3:F:170:LEU:H	3:F:220:PHE:HE2	1.44	0.63
3:C:137:TYR:CD2	3:C:142:VAL:HG21	2.33	0.63
1:A:113:ARG:O	1:A:116:SER:HB3	1.98	0.63
1:A:270:LEU:C	1:A:274:VAL:HG23	2.24	0.63
1:A:346:ALA:HB2	1:A:380:VAL:HG13	1.80	0.63
1:A:427:MSE:CE	1:A:430:LEU:HD12	2.28	0.63
2:B:88:MSE:HE2	2:B:92:ASN:ND2	2.13	0.63
2:E:186:LEU:HB3	2:E:190:ILE:HD12	1.80	0.63
1:D:35:LEU:HD21	1:D:55:LEU:CD1	2.27	0.63
2:E:364:LEU:CB	2:E:384:LEU:HD21	2.29	0.63
2:B:166:PRO:O	2:B:169:ARG:N	2.32	0.63
3:C:158:LEU:CD2	3:C:161:GLY:HA2	2.28	0.63
1:D:35:LEU:HB3	1:D:72:GLN:HG2	1.81	0.63
2:E:60:ARG:C	2:E:60:ARG:HD3	2.23	0.63
2:E:83:PRO:C	2:E:85:VAL:H	2.07	0.63
3:F:194:PRO:HG2	3:F:195:MET:H	1.62	0.63
3:C:203:PRO:HA	3:C:220:PHE:CE1	2.34	0.63
1:A:556:LEU:CD2	1:A:588:LEU:HD11	2.29	0.62
2:B:151:GLN:HB3	2:B:189:TYR:CE2	2.34	0.62
2:E:329:HIS:CE1	3:F:125:GLN:HB3	2.34	0.62
2:E:373:ASN:C	2:E:375:THR:H	2.06	0.62
1:A:438:PHE:HD1	1:A:438:PHE:C	2.07	0.62
2:B:244:LEU:HD22	2:B:253:TYR:CE1	2.34	0.62
2:B:364:LEU:HB2	2:B:384:LEU:HD21	1.81	0.62
3:C:159:VAL:CG2	3:C:163:ILE:HB	2.28	0.62
2:E:169:ARG:O	2:E:170:ASP:C	2.42	0.62
2:E:330:PHE:O	2:E:334:GLU:HB2	1.99	0.62
2:B:236:PHE:O	2:B:240:VAL:HB	1.99	0.62
3:C:239:ARG:NH1	3:C:242:GLN:HG3	2.11	0.62
1:D:237:GLN:NE2	1:D:278:ILE:HD11	2.15	0.62
2:E:389:GLU:O	2:E:390:MSE:HB2	1.99	0.62
1:A:349:ILE:HG23	1:A:350:MSE:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:GLU:C	2:B:67:VAL:H	2.06	0.62
2:B:169:ARG:O	2:B:172:LEU:N	2.33	0.62
1:D:300:ALA:HB2	1:D:341:VAL:HG22	1.80	0.62
2:E:209:ASN:N	2:E:209:ASN:ND2	2.47	0.62
2:E:134:PHE:HD2	2:E:134:PHE:C	2.07	0.62
2:E:313:ILE:CG2	2:E:317:LEU:HB2	2.28	0.62
3:F:115:ARG:NH1	3:F:151:ASP:HA	2.14	0.62
1:A:495:TYR:CD2	1:A:533:VAL:HG11	2.34	0.62
1:D:11:TYR:N	1:D:12:PRO:HD2	2.15	0.62
3:F:158:LEU:HD12	3:F:163:ILE:O	2.00	0.62
1:A:497:HIS:O	1:A:500:THR:HB	1.99	0.62
2:E:144:ILE:O	2:E:144:ILE:HG22	2.00	0.62
1:A:25:VAL:CG2	1:A:28:ARG:HH21	2.09	0.62
1:D:20:LEU:HD23	1:D:31:SER:HB2	1.80	0.62
2:E:133:ARG:HG2	2:E:136:GLU:OE2	2.00	0.62
2:E:170:ASP:O	2:E:173:LYS:HB3	2.00	0.62
1:A:382:LEU:HD12	1:A:419:VAL:HG22	1.81	0.62
2:B:233:HIS:O	2:B:236:PHE:HB3	2.00	0.62
1:D:297:GLU:O	1:D:298:VAL:C	2.42	0.62
2:E:110:PRO:HG3	2:E:249:SER:HB2	1.81	0.62
3:F:209:TRP:H	3:F:224:ILE:HD11	1.65	0.62
3:C:13:TRP:HE1	3:C:27:GLN:HE21	1.45	0.62
3:C:55:CYS:SG	3:C:68:LEU:HD11	2.39	0.62
1:D:261:TYR:C	1:D:261:TYR:CD2	2.77	0.62
3:F:62:PHE:O	3:F:65:LEU:HB3	1.99	0.62
1:A:502:LEU:HD22	1:A:543:SER:OG	1.99	0.61
3:C:160:ASP:C	3:C:162:GLN:H	2.08	0.61
1:D:438:PHE:CD1	1:D:438:PHE:C	2.77	0.61
1:D:455:VAL:HG23	3:F:71:ILE:HG13	1.82	0.61
2:E:406:LYS:HD3	2:E:406:LYS:C	2.25	0.61
2:E:180:TYR:CE1	2:E:187:ARG:HA	2.35	0.61
3:F:183:LEU:HD21	3:F:194:PRO:HG3	1.82	0.61
3:F:236:LEU:HD11	3:F:257:VAL:HG12	1.81	0.61
1:D:561:LYS:HB3	1:D:562:PRO:HD3	1.81	0.61
2:E:180:TYR:HE1	2:E:187:ARG:HA	1.65	0.61
2:E:80:PRO:HG2	2:E:82:TYR:CD2	2.36	0.61
2:E:134:PHE:CD2	2:E:134:PHE:C	2.78	0.61
1:A:245:MSE:O	1:A:249:ARG:HG3	1.99	0.61
2:B:118:GLU:H	2:B:164:GLU:HG2	1.65	0.61
2:B:329:HIS:CE1	3:C:125:GLN:HB3	2.35	0.61
3:C:13:TRP:NE1	3:C:27:GLN:NE2	2.39	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LYS:O	1:D:36:SER:N	2.33	0.61
1:D:398:ARG:HB3	1:D:398:ARG:HH11	1.65	0.61
1:D:401:SER:HB3	1:D:434:LEU:CD2	2.31	0.61
1:D:427:MSE:O	1:D:429:LEU:N	2.34	0.61
1:D:258:ARG:HG3	1:D:258:ARG:HH11	1.66	0.61
3:F:155:LEU:HD21	3:F:185:ARG:HB2	1.83	0.61
2:B:222:ILE:HD13	2:B:264:PHE:CD1	2.35	0.61
1:D:538:PHE:HB3	1:D:575:VAL:HA	1.83	0.61
2:E:72:HIS:O	2:E:74:ARG:N	2.34	0.61
1:A:489:MSE:C	1:A:491:GLY:H	2.09	0.61
1:D:66:LEU:HD22	1:D:96:LEU:CD2	2.31	0.61
2:E:255:PRO:HG2	2:E:256:GLN:CD	2.25	0.61
1:A:77:THR:HG21	1:A:118:GLU:HG3	1.83	0.61
3:C:33:GLU:O	3:C:36:LYS:HB2	2.01	0.61
2:E:164:GLU:OE2	2:E:164:GLU:C	2.43	0.61
2:E:373:ASN:O	2:E:375:THR:N	2.32	0.61
3:F:103:LEU:HB3	3:F:111:ILE:HD13	1.82	0.61
1:A:24:ASP:O	1:A:25:VAL:C	2.42	0.61
1:A:35:LEU:HD21	1:A:55:LEU:HD11	1.81	0.61
1:A:39:ALA:HB1	1:A:47:THR:HG21	1.83	0.61
1:A:66:LEU:HB3	1:A:104:VAL:HG21	1.83	0.61
1:A:180:MSE:CE	1:A:183:ARG:HH22	2.13	0.61
1:A:237:GLN:O	1:A:238:GLU:C	2.43	0.61
1:A:346:ALA:CB	1:A:380:VAL:HG13	2.31	0.61
1:A:438:PHE:C	1:A:438:PHE:CD1	2.77	0.61
1:A:438:PHE:HE1	1:A:442:LYS:HB2	1.66	0.61
1:D:385:ILE:HD11	1:D:411:LEU:HG	1.83	0.61
1:A:171:ARG:HG3	1:A:208:MSE:SE	2.50	0.60
2:B:97:LEU:H	2:B:97:LEU:HD12	1.66	0.60
2:B:321:LEU:HB3	2:B:360:MSE:HE1	1.83	0.60
2:E:361:PHE:O	2:E:363:SER:N	2.34	0.60
1:A:258:ARG:HG3	1:A:258:ARG:NH1	2.15	0.60
2:B:364:LEU:CB	2:B:384:LEU:HD21	2.32	0.60
3:C:83:MET:HE3	3:C:240:ALA:HB3	1.82	0.60
3:C:97:VAL:HG13	3:C:98:THR:N	2.16	0.60
1:D:526:LEU:HD22	1:D:563:ILE:HG21	1.83	0.60
1:A:424:ILE:HG12	1:A:450:TRP:CE3	2.36	0.60
1:A:477:TRP:CH2	1:A:482:ILE:CD1	2.83	0.60
2:B:35:LYS:C	2:B:37:ARG:H	2.08	0.60
1:D:427:MSE:HE2	1:D:430:LEU:HB2	1.84	0.60
1:D:467:LYS:HB2	1:D:507:VAL:CG1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:GLY:O	1:D:492:ASP:C	2.44	0.60
2:E:325:VAL:HG22	2:E:337:LEU:HD12	1.84	0.60
1:A:79:LEU:HD12	1:A:79:LEU:N	2.17	0.60
3:C:139:ASN:CG	3:C:141:ASN:HD22	2.08	0.60
1:D:205:ILE:HA	1:D:208:MSE:HE3	1.83	0.60
1:D:438:PHE:C	1:D:438:PHE:HD1	2.09	0.60
2:E:54:LYS:O	2:E:56:LYS:N	2.29	0.60
2:E:313:ILE:O	2:E:316:PRO:HD2	2.01	0.60
2:E:375:THR:CG2	2:E:379:LEU:HD12	2.32	0.60
1:A:52:LEU:HB2	1:A:53:PRO:HD3	1.82	0.60
2:B:376:ILE:HA	2:B:379:LEU:HB2	1.83	0.60
1:D:411:LEU:O	1:D:413:GLU:N	2.34	0.60
1:D:436:VAL:HG13	1:D:437:GLU:H	1.65	0.60
3:F:166:LEU:O	3:F:239:ARG:HA	2.02	0.60
1:A:388:LEU:HA	1:A:391:VAL:CG2	2.31	0.60
2:B:217:ILE:O	2:B:221:ILE:HG13	2.02	0.60
1:D:564:LEU:O	1:D:564:LEU:HD23	2.02	0.60
2:E:329:HIS:HB3	2:E:332:VAL:HG23	1.83	0.60
1:A:180:MSE:HE3	1:A:180:MSE:H	1.67	0.60
1:A:284:VAL:HB	1:A:285:PRO:HD3	1.83	0.60
2:B:373:ASN:HD22	2:B:376:ILE:HG23	1.67	0.60
2:B:412:LYS:O	2:B:414:LYS:N	2.34	0.60
2:E:141:GLN:HB3	2:E:142:PRO:HD2	1.84	0.60
3:F:214:ARG:HG2	3:F:214:ARG:NH1	2.15	0.60
3:F:220:PHE:HA	3:F:224:ILE:HD12	1.84	0.60
1:A:509:SER:HA	1:A:521:MSE:HE1	1.83	0.60
1:D:85:TYR:O	1:D:87:HIS:N	2.35	0.60
2:E:79:GLU:N	2:E:80:PRO:CD	2.64	0.60
2:B:357:LEU:N	2:B:358:PRO:HD2	2.17	0.60
2:B:361:PHE:O	2:B:363:SER:N	2.35	0.60
3:C:14:ILE:O	3:C:18:ASN:HB2	2.01	0.60
1:D:24:ASP:O	1:D:26:GLN:N	2.35	0.60
1:D:25:VAL:CG2	1:D:28:ARG:HH21	2.14	0.60
1:D:268:THR:HG23	1:D:305:LYS:HD2	1.84	0.60
2:B:222:ILE:HG21	2:B:264:PHE:CD1	2.37	0.59
1:A:197:GLU:H	1:A:197:GLU:CD	2.09	0.59
1:A:579:ALA:O	1:A:582:ALA:HB3	2.02	0.59
3:C:141:ASN:HB3	3:C:145:TYR:CE1	2.38	0.59
1:D:270:LEU:O	1:D:274:VAL:HG23	2.02	0.59
1:D:448:MSE:HA	1:D:448:MSE:CE	2.31	0.59
2:E:325:VAL:HG22	2:E:337:LEU:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:CYS:O	1:A:158:VAL:HG13	2.02	0.59
2:B:31:LEU:C	2:B:33:ILE:H	2.10	0.59
1:D:179:PRO:HB2	1:D:180:MSE:HE3	1.83	0.59
3:C:253:ASP:O	3:C:254:ARG:C	2.45	0.59
2:E:189:TYR:O	2:E:190:ILE:C	2.45	0.59
2:E:253:TYR:H	2:E:253:TYR:HD2	1.48	0.59
3:F:80:TYR:HB2	3:F:111:ILE:HG22	1.83	0.59
1:A:470:VAL:HG22	1:A:478:ALA:HB2	1.84	0.59
1:D:261:TYR:CA	1:D:298:VAL:HG22	2.33	0.59
2:E:134:PHE:HD2	2:E:135:LEU:N	1.99	0.59
2:B:43:PHE:C	2:B:45:PHE:H	2.09	0.59
2:B:93:MSE:O	2:B:95:ARG:HG3	2.02	0.59
2:B:110:PRO:HA	2:B:113:ASP:OD2	2.03	0.59
2:B:248:LYS:HD3	2:B:290:LYS:HZ2	1.67	0.59
2:B:251:SER:HA	2:B:293:MSE:CE	2.31	0.59
3:C:166:LEU:O	3:C:239:ARG:HA	2.03	0.59
1:D:25:VAL:CG2	1:D:28:ARG:NH2	2.66	0.59
1:D:274:VAL:HG12	1:D:278:ILE:HB	1.85	0.59
3:F:160:ASP:C	3:F:162:GLN:H	2.11	0.59
1:A:381:ARG:HH12	1:A:414:ASP:CG	2.11	0.59
2:B:73:ASN:C	2:B:75:ASN:H	2.10	0.59
2:B:356:ILE:C	2:B:358:PRO:HD2	2.28	0.59
1:D:455:VAL:HG23	3:F:71:ILE:HA	1.85	0.59
1:D:528:MSE:O	1:D:530:GLY:N	2.36	0.59
2:E:169:ARG:O	2:E:172:LEU:N	2.36	0.59
3:F:190:PRO:CD	3:F:195:MET:HE2	2.31	0.59
3:F:240:ALA:CB	3:F:259:ILE:H	2.16	0.59
3:C:160:ASP:O	3:C:162:GLN:N	2.36	0.59
3:C:214:ARG:HG2	3:C:214:ARG:NH1	2.18	0.59
1:D:24:ASP:O	1:D:25:VAL:C	2.46	0.59
2:E:276:VAL:HG11	2:E:313:ILE:HG21	1.85	0.59
2:B:158:LEU:O	2:B:159:GLU:C	2.44	0.58
3:C:57:ASP:O	3:C:261:SER:HB2	2.03	0.58
2:E:79:GLU:N	2:E:80:PRO:HD2	2.17	0.58
2:B:373:ASN:C	2:B:375:THR:H	2.11	0.58
3:C:284:TYR:N	3:C:284:TYR:CD2	2.68	0.58
1:D:22:ASN:ND2	1:D:24:ASP:HB3	2.17	0.58
2:E:183:PHE:N	2:E:183:PHE:CD1	2.71	0.58
1:A:247:THR:O	1:A:250:GLN:HB3	2.03	0.58
1:D:262:MSE:O	1:D:263:VAL:C	2.47	0.58
1:D:350:MSE:HE2	1:D:369:PHE:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:186:LEU:O	2:E:190:ILE:HD12	2.02	0.58
2:B:176:LEU:HD11	2:B:190:ILE:HG12	1.86	0.58
3:C:261:SER:O	3:C:263:PRO:HD3	2.03	0.58
1:D:144:ARG:HH21	1:D:176:ASP:CG	2.12	0.58
1:D:570:ASP:OD2	1:D:571:GLN:N	2.36	0.58
1:D:588:LEU:O	1:D:589:ALA:HB2	2.03	0.58
3:F:29:LYS:HD2	3:F:145:TYR:CE2	2.38	0.58
1:A:36:SER:C	1:A:38:ILE:H	2.11	0.58
1:A:572:ASP:OD2	3:C:110:ARG:NH2	2.36	0.58
2:B:164:GLU:HB3	2:B:168:GLU:CB	2.34	0.58
2:B:253:TYR:H	2:B:253:TYR:HD2	1.52	0.58
2:B:313:ILE:O	2:B:315:GLU:N	2.36	0.58
2:E:35:LYS:C	2:E:37:ARG:H	2.11	0.58
2:E:165:ASP:O	2:E:166:PRO:C	2.45	0.58
1:A:79:LEU:HD12	1:A:79:LEU:H	1.68	0.58
2:B:183:PHE:N	2:B:183:PHE:CD1	2.71	0.58
3:C:45:VAL:HG22	3:C:156:THR:OG1	2.04	0.58
1:D:109:VAL:O	1:D:113:ARG:HG3	2.02	0.58
2:E:71:THR:O	2:E:73:ASN:N	2.34	0.58
3:F:147:THR:HA	3:F:150:PHE:CD2	2.38	0.58
2:B:128:TYR:O	2:B:132:LEU:HB2	2.03	0.58
2:B:165:ASP:O	2:B:166:PRO:C	2.46	0.58
3:C:103:LEU:HB3	3:C:111:ILE:HD13	1.85	0.58
1:A:464:SER:O	1:A:466:LEU:N	2.37	0.58
1:A:588:LEU:O	1:A:589:ALA:HB2	2.04	0.58
3:C:243:LEU:HD11	3:C:271:ASN:CG	2.29	0.58
1:D:227:ALA:O	1:D:231:ILE:HG13	2.04	0.58
3:F:46:GLN:O	3:F:157:ALA:HA	2.02	0.58
1:A:325:GLN:C	1:A:328:PRO:HD2	2.29	0.58
3:F:170:LEU:HB2	3:F:220:PHE:CD2	2.39	0.58
1:A:34:LYS:O	1:A:36:SER:N	2.37	0.58
1:A:77:THR:CG2	1:A:118:GLU:HG3	2.33	0.58
2:B:242:LEU:N	2:B:243:PRO:HD2	2.19	0.58
1:D:219:SER:HA	1:D:222:LEU:HD22	1.86	0.58
1:A:88:CYS:C	1:A:90:LEU:H	2.11	0.57
2:E:333:ALA:O	2:E:337:LEU:HD13	2.04	0.57
3:C:117:ASN:ND2	3:C:241:HIS:HE1	2.01	0.57
2:E:119:ALA:O	2:E:120:ALA:HB3	2.04	0.57
2:E:316:PRO:HG2	2:E:317:LEU:H	1.69	0.57
2:E:330:PHE:CE2	3:F:122:GLN:HG3	2.38	0.57
2:E:337:LEU:HD21	2:E:380:ILE:HG13	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LEU:HD23	1:A:31:SER:CB	2.34	0.57
1:A:491:GLY:O	1:A:492:ASP:C	2.47	0.57
2:B:380:ILE:O	2:B:381:TYR:C	2.48	0.57
1:D:60:TYR:CD2	1:D:65:VAL:HG11	2.39	0.57
1:D:262:MSE:O	1:D:264:ALA:N	2.38	0.57
1:D:390:CYS:O	1:D:391:VAL:C	2.47	0.57
1:D:528:MSE:C	1:D:530:GLY:N	2.61	0.57
2:E:83:PRO:C	2:E:85:VAL:N	2.57	0.57
2:E:244:LEU:HD22	2:E:253:TYR:HE1	1.69	0.57
2:E:365:TYR:O	2:E:366:ARG:C	2.47	0.57
1:A:163:LYS:O	1:A:167:ARG:HG3	2.04	0.57
1:A:509:SER:CA	1:A:521:MSE:HE1	2.34	0.57
3:C:115:ARG:HG3	3:C:119:GLU:HB2	1.84	0.57
1:D:509:SER:CA	1:D:521:MSE:HE1	2.35	0.57
1:D:533:VAL:HG12	1:D:535:ASN:HB2	1.86	0.57
2:E:209:ASN:H	2:E:209:ASN:HD22	1.50	0.57
3:F:253:ASP:O	3:F:254:ARG:C	2.46	0.57
1:A:129:VAL:HB	1:A:130:PRO:HD3	1.85	0.57
1:A:483:ILE:N	1:A:484:PRO:CD	2.68	0.57
1:A:529:ALA:HB2	1:A:540:VAL:HG11	1.85	0.57
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.86	0.57
3:C:197:ASP:OD1	3:C:217:GLY:HA2	2.05	0.57
1:A:427:MSE:HE2	1:A:430:LEU:HB2	1.85	0.57
1:A:489:MSE:C	1:A:491:GLY:N	2.61	0.57
2:B:289:PRO:O	2:B:293:MSE:HG3	2.04	0.57
1:D:72:GLN:O	1:D:74:GLY:N	2.37	0.57
3:F:106:ARG:O	3:F:108:ARG:N	2.36	0.57
1:A:22:ASN:O	1:A:23:GLU:CB	2.52	0.57
3:C:143:TRP:O	3:C:147:THR:HG23	2.04	0.57
3:C:240:ALA:HA	3:C:258:THR:HG23	1.87	0.57
3:C:244:VAL:HG23	3:C:244:VAL:O	2.05	0.57
1:D:479:HIS:ND1	1:D:479:HIS:O	2.34	0.57
2:E:43:PHE:C	2:E:45:PHE:H	2.12	0.57
1:A:88:CYS:O	1:A:91:PRO:HD2	2.05	0.57
3:F:117:ASN:ND2	3:F:241:HIS:HE1	2.03	0.57
1:A:217:GLN:O	1:A:220:VAL:HB	2.05	0.57
2:B:384:LEU:O	2:B:387:PHE:N	2.35	0.57
3:C:29:LYS:HD2	3:C:145:TYR:CE2	2.40	0.57
2:E:118:GLU:HB3	2:E:164:GLU:CG	2.35	0.57
2:E:218:LEU:O	2:E:222:ILE:HG13	2.03	0.57
2:E:315:GLU:HB3	2:E:319:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:PRO:HG2	2:B:82:TYR:CD2	2.39	0.57
3:C:128:GLY:O	3:C:129:PHE:C	2.46	0.57
1:D:179:PRO:HG3	1:D:182:ARG:HH22	1.70	0.57
2:E:340:TRP:HH2	2:E:360:MSE:HE3	1.69	0.57
3:F:176:THR:HA	3:F:232:ASN:OD1	2.05	0.57
1:A:390:CYS:O	1:A:392:ASN:N	2.37	0.56
2:B:79:GLU:N	2:B:80:PRO:CD	2.67	0.56
2:B:340:TRP:HH2	2:B:360:MSE:HE3	1.70	0.56
3:C:5:VAL:O	3:C:5:VAL:HG12	2.04	0.56
3:C:62:PHE:O	3:C:65:LEU:HB3	2.05	0.56
2:E:73:ASN:C	2:E:75:ASN:N	2.63	0.56
3:F:189:VAL:HA	3:F:195:MET:HE2	1.86	0.56
1:A:343:SER:N	1:A:380:VAL:HG22	2.19	0.56
1:A:535:ASN:HA	1:A:538:PHE:HE2	1.61	0.56
2:B:302:LEU:HD11	2:B:317:LEU:HD21	1.87	0.56
1:D:102:THR:HG22	1:D:105:ARG:NH2	2.20	0.56
1:D:409:VAL:O	1:D:409:VAL:HG12	2.04	0.56
2:E:124:LEU:O	2:E:126:LEU:N	2.38	0.56
2:E:305:ILE:HD13	2:E:306:GLU:H	1.69	0.56
1:A:322:ILE:HG21	1:A:356:LEU:HD21	1.87	0.56
1:A:336:ASP:OD1	1:A:337:ALA:N	2.38	0.56
1:A:352:LEU:HD23	1:A:355:ILE:HD12	1.88	0.56
2:B:118:GLU:HB3	2:B:164:GLU:HG3	1.86	0.56
2:B:134:PHE:C	2:B:136:GLU:H	2.13	0.56
2:B:340:TRP:CH2	2:B:360:MSE:HE3	2.40	0.56
3:C:100:LEU:HA	3:C:103:LEU:HD12	1.86	0.56
3:C:189:VAL:HA	3:C:195:MET:HE2	1.87	0.56
1:D:115:ILE:O	1:D:119:HIS:CD2	2.58	0.56
1:D:427:MSE:HB3	1:D:428:PRO:CD	2.36	0.56
1:D:533:VAL:CG1	1:D:535:ASN:HB2	2.35	0.56
2:E:162:ASP:O	2:E:163:SER:HB2	2.05	0.56
2:E:250:LEU:C	2:E:252:VAL:H	2.11	0.56
2:E:262:VAL:O	2:E:265:LEU:N	2.38	0.56
3:F:266:CYS:SG	4:H:2:LEU:HD12	2.45	0.56
1:A:201:VAL:O	1:A:205:ILE:HB	2.05	0.56
1:A:342:LYS:O	1:A:346:ALA:HB2	2.05	0.56
1:A:395:ILE:HD11	1:A:400:LEU:CA	2.35	0.56
2:E:256:GLN:CD	2:E:256:GLN:H	2.13	0.56
3:F:265:TYR:HB3	3:F:269:CYS:HB2	1.86	0.56
3:C:276:MET:HB2	3:C:286:PHE:CE1	2.40	0.56
1:D:128:PHE:O	1:D:129:VAL:C	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:GLU:O	1:D:411:LEU:C	2.47	0.56
3:F:101:VAL:O	3:F:105:VAL:HG23	2.05	0.56
3:F:240:ALA:HB1	3:F:259:ILE:O	2.05	0.56
2:B:189:TYR:O	2:B:190:ILE:C	2.48	0.56
3:F:284:TYR:N	3:F:284:TYR:CD2	2.72	0.56
2:B:121:TRP:CZ2	2:B:167:ARG:HB3	2.40	0.56
1:D:206:ILE:HB	1:D:207:PRO:HD3	1.88	0.56
1:D:277:GLU:C	1:D:279:THR:N	2.60	0.56
2:B:180:TYR:CE1	2:B:187:ARG:HA	2.41	0.56
3:C:68:LEU:C	3:C:68:LEU:CD2	2.79	0.56
3:F:45:VAL:HA	3:F:156:THR:OG1	2.06	0.56
1:A:409:VAL:O	1:A:409:VAL:HG12	2.06	0.56
1:D:145:THR:HG22	1:D:146:SER:N	2.21	0.56
2:E:254:HIS:N	2:E:255:PRO:HD2	2.21	0.56
3:F:53:THR:HG21	3:F:275:ILE:HD12	1.87	0.56
1:A:526:LEU:CD2	1:A:563:ILE:HG21	2.32	0.56
2:B:257:LEU:O	2:B:258:ALA:C	2.49	0.56
3:C:253:ASP:O	3:C:255:ASN:N	2.39	0.56
2:E:412:LYS:O	2:E:414:LYS:N	2.39	0.56
3:F:176:THR:HG23	3:F:179:HIS:HD2	1.69	0.56
1:A:261:TYR:CA	1:A:298:VAL:HG22	2.36	0.55
1:A:350:MSE:HE3	1:A:391:VAL:HG13	1.88	0.55
2:B:119:ALA:O	2:B:120:ALA:HB3	2.05	0.55
2:B:134:PHE:CD2	2:B:134:PHE:C	2.83	0.55
3:C:240:ALA:HB1	3:C:259:ILE:O	2.05	0.55
2:E:218:LEU:CD2	2:E:221:ILE:HD12	2.32	0.55
1:D:436:VAL:HG13	1:D:437:GLU:N	2.20	0.55
1:A:310:CYS:HA	1:A:313:LEU:HD12	1.87	0.55
1:A:578:PHE:O	1:A:582:ALA:HB2	2.06	0.55
2:E:373:ASN:ND2	2:E:376:ILE:H	2.05	0.55
1:A:561:LYS:HB3	1:A:562:PRO:HD3	1.87	0.55
3:C:115:ARG:HH12	3:C:151:ASP:HA	1.67	0.55
1:D:424:ILE:HG12	1:D:450:TRP:CE3	2.41	0.55
2:E:79:GLU:O	2:E:80:PRO:C	2.50	0.55
3:F:76:PRO:HB3	3:F:107:TYR:CD1	2.41	0.55
2:B:333:ALA:O	2:B:337:LEU:HD13	2.06	0.55
1:D:66:LEU:HB3	1:D:104:VAL:HG21	1.88	0.55
2:E:65:GLU:C	2:E:67:VAL:H	2.13	0.55
3:F:162:GLN:HB3	3:F:235:THR:CG2	2.36	0.55
2:B:134:PHE:O	2:B:136:GLU:N	2.39	0.55
1:D:412:ALA:O	1:D:413:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:257:LEU:O	2:E:258:ALA:C	2.50	0.55
1:A:282:ASP:C	1:A:285:PRO:HD2	2.32	0.55
1:A:556:LEU:HD22	1:A:588:LEU:HD11	1.89	0.55
2:B:310:PHE:CD1	2:B:348:LEU:HD13	2.42	0.55
1:D:12:PRO:O	1:D:15:VAL:HG12	2.07	0.55
2:E:183:PHE:C	2:E:185:GLY:N	2.63	0.55
2:E:380:ILE:O	2:E:381:TYR:C	2.46	0.55
1:D:154:CYS:O	1:D:158:VAL:HG13	2.07	0.55
1:D:427:MSE:O	1:D:428:PRO:C	2.49	0.55
2:E:332:VAL:O	2:E:333:ALA:C	2.48	0.55
2:E:357:LEU:N	2:E:358:PRO:HD2	2.22	0.55
3:F:244:VAL:O	3:F:244:VAL:HG23	2.07	0.55
1:A:29:LEU:HA	1:A:65:VAL:HG22	1.89	0.55
1:A:360:ASN:O	1:A:364:HIS:N	2.38	0.55
1:A:364:HIS:C	1:A:367:PRO:HD2	2.31	0.55
1:A:456:TYR:CD1	1:A:456:TYR:C	2.84	0.55
2:B:134:PHE:C	2:B:134:PHE:HD2	2.15	0.55
1:D:559:GLU:O	1:D:563:ILE:HG22	2.07	0.55
1:A:182:ARG:HH11	1:A:182:ARG:HG3	1.70	0.55
1:A:517:THR:HA	1:A:521:MSE:HE2	1.88	0.55
1:D:470:VAL:HG22	1:D:478:ALA:HB2	1.88	0.55
2:E:400:GLN:O	2:E:401:GLN:C	2.49	0.55
2:B:330:PHE:O	2:B:334:GLU:HB2	2.06	0.54
2:B:406:LYS:O	2:B:406:LYS:HD3	2.06	0.54
3:C:101:VAL:O	3:C:105:VAL:HG23	2.07	0.54
1:D:260:ARG:HG3	1:D:260:ARG:NH1	2.22	0.54
2:E:83:PRO:O	2:E:85:VAL:N	2.40	0.54
3:F:265:TYR:CD2	3:F:266:CYS:N	2.74	0.54
1:A:127:HIS:C	1:A:130:PRO:HD2	2.32	0.54
2:B:158:LEU:O	2:B:161:PHE:HD1	1.90	0.54
2:B:409:GLU:O	2:B:413:MSE:HB2	2.08	0.54
3:C:51:PRO:HB3	3:C:279:ASP:C	2.31	0.54
2:E:255:PRO:HG2	2:E:256:GLN:NE2	2.22	0.54
3:F:28:VAL:O	3:F:31:LEU:N	2.41	0.54
3:F:203:PRO:HA	3:F:220:PHE:CE1	2.42	0.54
1:A:438:PHE:CE1	1:A:442:LYS:HB2	2.42	0.54
3:C:10:LEU:HD13	3:C:106:ARG:HB2	1.90	0.54
3:C:65:LEU:O	3:C:68:LEU:HB3	2.08	0.54
3:C:170:LEU:HD12	3:C:220:PHE:CD2	2.43	0.54
3:C:248:TYR:CE2	3:C:286:PHE:CD2	2.95	0.54
2:E:244:LEU:HD22	2:E:253:TYR:CE1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:350:SER:O	2:E:352:ASN:N	2.39	0.54
1:A:367:PRO:O	1:A:370:LEU:HB2	2.07	0.54
1:D:477:TRP:CH2	1:D:482:ILE:HD11	2.42	0.54
3:F:76:PRO:HG3	3:F:107:TYR:CE1	2.43	0.54
2:B:310:PHE:CG	2:B:348:LEU:HD13	2.42	0.54
1:D:91:PRO:HB2	1:D:92:PRO:HD3	1.89	0.54
3:F:239:ARG:C	3:F:239:ARG:HD3	2.32	0.54
1:A:204:GLU:C	1:A:207:PRO:HD2	2.32	0.54
1:A:366:LEU:N	1:A:367:PRO:CD	2.70	0.54
2:B:250:LEU:HA	2:B:253:TYR:CE2	2.42	0.54
1:D:131:LEU:HD23	1:D:132:VAL:N	2.23	0.54
1:D:381:ARG:O	1:D:385:ILE:HG12	2.07	0.54
2:E:152:LYS:O	2:E:156:GLN:HG3	2.08	0.54
2:B:67:VAL:C	2:B:69:TYR:H	2.15	0.54
1:D:120:SER:O	1:D:121:PRO:C	2.49	0.54
1:D:452:VAL:HG13	1:D:497:HIS:HD2	1.72	0.54
1:D:489:MSE:C	1:D:491:GLY:H	2.16	0.54
2:E:121:TRP:C	2:E:123:HIS:N	2.66	0.54
3:C:97:VAL:O	3:C:101:VAL:HG23	2.08	0.54
1:D:317:CYS:O	1:D:320:ASN:N	2.38	0.54
2:E:316:PRO:HG2	2:E:317:LEU:N	2.23	0.54
2:E:332:VAL:O	2:E:335:ARG:N	2.40	0.54
1:A:270:LEU:O	1:A:271:GLN:C	2.51	0.54
2:B:65:GLU:C	2:B:67:VAL:N	2.64	0.54
1:D:348:VAL:O	1:D:350:MSE:N	2.41	0.54
2:E:262:VAL:O	2:E:263:GLN:C	2.51	0.54
2:E:381:TYR:HE2	2:E:385:LYS:HD2	1.71	0.54
2:B:380:ILE:HG22	2:B:381:TYR:N	2.22	0.54
1:D:158:VAL:HG23	1:D:163:LYS:HG3	1.90	0.54
1:D:375:ASP:OD2	1:D:376:GLU:N	2.41	0.54
1:D:408:ILE:CD1	1:D:426:TYR:HE2	2.20	0.54
2:E:138:PRO:O	2:E:140:PHE:CD1	2.61	0.54
2:E:211:ILE:HG21	2:E:253:TYR:CD1	2.43	0.54
3:F:276:MET:HE3	3:F:278:LEU:CD2	2.33	0.54
1:A:411:LEU:C	1:A:413:GLU:N	2.66	0.53
2:B:79:GLU:N	2:B:80:PRO:HD2	2.22	0.53
2:B:121:TRP:H	2:B:122:PRO:HD2	1.72	0.53
3:C:62:PHE:HD2	3:C:63:HIS:CD2	2.23	0.53
1:A:570:ASP:OD2	1:A:571:GLN:N	2.41	0.53
1:D:211:ASN:HD22	1:D:211:ASN:N	2.04	0.53
2:E:86:VAL:O	2:E:87:HIS:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:ILE:O	1:A:426:TYR:N	2.36	0.53
2:B:141:GLN:HB3	2:B:142:PRO:HD2	1.91	0.53
1:D:47:THR:HG23	1:D:51:LEU:HD23	1.90	0.53
1:D:405:LEU:C	1:D:405:LEU:HD13	2.33	0.53
2:E:183:PHE:C	2:E:185:GLY:H	2.15	0.53
2:B:89:PHE:CE2	2:B:93:MSE:HG3	2.44	0.53
1:D:171:ARG:HG3	1:D:208:MSE:SE	2.58	0.53
3:F:10:LEU:HD23	3:F:13:TRP:CE3	2.43	0.53
1:A:178:THR:HB	1:A:180:MSE:HG2	1.89	0.53
1:A:326:ILE:N	1:A:326:ILE:HD12	2.24	0.53
1:A:479:HIS:O	1:A:479:HIS:ND1	2.39	0.53
2:B:389:GLU:O	2:B:390:MSE:HB2	2.09	0.53
1:D:79:LEU:N	1:D:79:LEU:CD1	2.65	0.53
1:A:429:LEU:O	1:A:433:GLN:HG3	2.09	0.53
1:A:455:VAL:HG23	3:C:71:ILE:HA	1.90	0.53
2:B:149:ILE:O	2:B:149:ILE:HG22	2.08	0.53
2:B:250:LEU:C	2:B:252:VAL:H	2.16	0.53
1:D:86:VAL:C	1:D:88:CYS:H	2.17	0.53
1:D:245:MSE:O	1:D:246:PRO:C	2.48	0.53
1:D:284:VAL:HB	1:D:285:PRO:HD3	1.90	0.53
1:D:310:CYS:HB3	1:D:322:ILE:HD11	1.90	0.53
2:E:121:TRP:C	2:E:123:HIS:H	2.16	0.53
1:A:116:SER:HB2	1:A:128:PHE:CE1	2.44	0.53
1:A:277:GLU:C	1:A:279:THR:N	2.67	0.53
1:A:352:LEU:HA	1:A:355:ILE:CD1	2.36	0.53
2:B:124:LEU:O	2:B:126:LEU:N	2.42	0.53
3:C:36:LYS:O	3:C:39:LEU:N	2.40	0.53
1:D:489:MSE:O	1:D:491:GLY:N	2.41	0.53
2:E:197:ILE:HD13	2:E:208:HIS:HE1	1.74	0.53
3:F:185:ARG:O	3:F:187:GLN:N	2.37	0.53
1:A:313:LEU:HD13	1:A:321:VAL:CG2	2.39	0.53
2:B:132:LEU:C	2:B:134:PHE:N	2.66	0.53
2:B:393:LYS:HG2	2:B:397:ASP:OD2	2.08	0.53
1:D:12:PRO:O	1:D:13:ILE:C	2.52	0.53
1:D:405:LEU:HB3	1:D:406:PRO:HD3	1.91	0.53
1:D:586:LEU:O	1:D:587:SER:HB2	2.09	0.53
1:A:390:CYS:SG	1:A:391:VAL:N	2.82	0.53
2:B:54:LYS:O	2:B:56:LYS:N	2.33	0.53
2:B:208:HIS:CD2	2:B:210:GLY:H	2.27	0.53
1:D:75:THR:C	1:D:77:THR:H	2.17	0.53
1:D:398:ARG:O	1:D:399:GLN:C	2.52	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:234:LYS:O	2:E:238:LEU:HD23	2.08	0.53
2:E:236:PHE:CD2	2:E:236:PHE:C	2.86	0.53
2:E:247:VAL:HG12	2:E:249:SER:H	1.73	0.53
2:E:287:HIS:O	2:E:288:SER:C	2.52	0.53
1:A:470:VAL:HG11	1:A:511:VAL:HG23	1.89	0.53
2:B:313:ILE:C	2:B:316:PRO:HD2	2.33	0.53
3:C:185:ARG:O	3:C:187:GLN:N	2.40	0.53
1:D:198:LEU:CD1	1:D:202:LYS:HE3	2.39	0.53
2:E:91:VAL:O	2:E:91:VAL:HG12	2.08	0.53
2:E:211:ILE:CG2	2:E:253:TYR:CD1	2.92	0.53
2:B:42:LEU:CB	2:B:63:LEU:HD21	2.39	0.52
2:B:108:PHE:HB3	3:C:268:ARG:NH2	2.24	0.52
2:B:391:ASN:CG	2:B:394:LEU:HD12	2.34	0.52
2:E:42:LEU:CB	2:E:63:LEU:HD21	2.39	0.52
1:A:105:ARG:HD2	1:A:146:SER:OG	2.09	0.52
1:A:350:MSE:HE1	1:A:391:VAL:CG2	2.33	0.52
1:A:405:LEU:N	1:A:406:PRO:CD	2.71	0.52
1:A:580:GLN:C	1:A:582:ALA:H	2.16	0.52
1:D:102:THR:O	1:D:103:VAL:C	2.52	0.52
2:E:87:HIS:O	2:E:91:VAL:HG23	2.09	0.52
3:F:68:LEU:C	3:F:68:LEU:CD2	2.81	0.52
3:F:162:GLN:OE1	3:F:235:THR:HG21	2.09	0.52
2:B:180:TYR:HE1	2:B:187:ARG:HA	1.73	0.52
2:B:254:HIS:O	2:B:257:LEU:HB3	2.10	0.52
2:B:400:GLN:O	2:B:401:GLN:C	2.53	0.52
1:D:43:GLY:O	1:D:44:VAL:C	2.52	0.52
1:D:448:MSE:HE1	1:D:466:LEU:HD21	1.92	0.52
1:A:29:LEU:HD12	1:A:65:VAL:HG22	1.90	0.52
1:A:35:LEU:HD21	1:A:55:LEU:CD1	2.40	0.52
1:A:77:THR:HG23	1:A:86:VAL:HG21	1.90	0.52
1:A:218:ASP:C	1:A:220:VAL:H	2.16	0.52
2:B:285:LYS:O	2:B:286:THR:HG23	2.09	0.52
2:B:365:TYR:O	2:B:366:ARG:C	2.52	0.52
2:B:407:LEU:HD23	2:B:407:LEU:C	2.34	0.52
1:A:77:THR:O	1:A:80:VAL:HG12	2.09	0.52
1:A:130:PRO:O	1:A:133:LYS:HB2	2.10	0.52
1:A:358:LYS:HA	1:A:394:VAL:HG12	1.92	0.52
2:B:85:VAL:HG11	2:B:134:PHE:HD1	1.74	0.52
3:C:166:LEU:HD11	3:C:169:GLY:C	2.34	0.52
1:D:119:HIS:CD2	1:D:119:HIS:H	2.27	0.52
1:D:155:TYR:N	1:D:156:PRO:CD	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:304:VAL:O	2:E:304:VAL:HG12	2.09	0.52
1:A:408:ILE:HD13	1:A:426:TYR:HE2	1.74	0.52
2:B:71:THR:HG21	2:B:133:ARG:HH11	1.74	0.52
1:D:506:ASN:HD21	1:D:543:SER:HA	1.75	0.52
1:D:560:VAL:HG12	1:D:561:LYS:N	2.25	0.52
2:E:42:LEU:O	2:E:43:PHE:O	2.27	0.52
2:E:262:VAL:HG12	2:E:263:GLN:N	2.23	0.52
1:A:141:PHE:CD1	1:A:141:PHE:C	2.87	0.52
1:A:506:ASN:HD21	1:A:543:SER:CB	2.23	0.52
3:C:17:LEU:HD21	3:C:23:LEU:HG	1.91	0.52
3:C:170:LEU:HD12	3:C:220:PHE:CG	2.45	0.52
3:C:252:HIS:O	3:C:253:ASP:O	2.28	0.52
3:C:252:HIS:O	3:C:255:ASN:HB2	2.10	0.52
1:D:40:LEU:C	1:D:42:LEU:N	2.67	0.52
1:D:345:LEU:HD23	1:D:346:ALA:N	2.25	0.52
2:E:250:LEU:O	2:E:252:VAL:N	2.43	0.52
3:F:137:TYR:CG	3:F:142:VAL:HG21	2.44	0.52
1:A:100:GLU:O	1:A:101:GLU:C	2.53	0.52
3:C:166:LEU:O	3:C:166:LEU:HD23	2.10	0.52
1:D:105:ARG:HD2	1:D:146:SER:OG	2.10	0.52
1:D:317:CYS:O	1:D:318:ARG:C	2.53	0.52
1:D:358:LYS:O	1:D:362:ILE:HG13	2.10	0.52
1:A:12:PRO:O	1:A:15:VAL:HG12	2.10	0.52
1:A:20:LEU:HD23	1:A:31:SER:HB2	1.90	0.52
1:A:500:THR:HA	1:A:503:PHE:CD1	2.36	0.52
2:B:88:MSE:HE1	2:B:127:VAL:HG22	1.92	0.52
2:B:254:HIS:CD2	2:B:293:MSE:HE2	2.44	0.52
3:C:166:LEU:CD2	3:C:239:ARG:HB3	2.40	0.52
1:D:141:PHE:CD1	1:D:142:THR:N	2.78	0.52
2:E:72:HIS:C	2:E:74:ARG:H	2.17	0.52
2:E:286:THR:HG22	3:F:134:LEU:HB3	1.91	0.52
2:E:310:PHE:O	2:E:314:MSE:HB2	2.09	0.52
2:B:169:ARG:O	2:B:170:ASP:C	2.53	0.52
3:C:209:TRP:H	3:C:224:ILE:HD11	1.73	0.52
1:D:20:LEU:HD21	1:D:31:SER:O	2.09	0.52
1:D:164:ALA:HA	1:D:167:ARG:NH1	2.25	0.52
1:D:349:ILE:HG23	1:D:350:MSE:N	2.25	0.52
3:F:166:LEU:HD12	3:F:198:LEU:HD22	1.92	0.52
1:A:89:LEU:N	1:A:89:LEU:CD1	2.72	0.51
1:A:586:LEU:O	1:A:587:SER:HB2	2.10	0.51
3:C:166:LEU:HD21	3:C:239:ARG:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:PHE:HD1	1:D:438:PHE:O	1.94	0.51
1:D:482:ILE:C	1:D:484:PRO:HD2	2.35	0.51
3:F:189:VAL:HA	3:F:195:MET:CE	2.40	0.51
1:A:29:LEU:HD12	1:A:65:VAL:CG2	2.40	0.51
1:A:90:LEU:CB	1:A:91:PRO:HD3	2.37	0.51
1:A:424:ILE:HA	1:A:450:TRP:CZ3	2.45	0.51
2:B:324:CYS:O	2:B:325:VAL:C	2.53	0.51
1:D:348:VAL:O	1:D:349:ILE:C	2.53	0.51
1:D:366:LEU:HB3	1:D:367:PRO:HD3	1.90	0.51
2:E:249:SER:O	2:E:252:VAL:HG23	2.10	0.51
2:E:373:ASN:HD21	2:E:376:ILE:HG23	1.75	0.51
3:F:13:TRP:NE1	3:F:27:GLN:NE2	2.57	0.51
3:F:121:ARG:HH11	3:F:121:ARG:HG3	1.75	0.51
1:A:17:ILE:HG12	1:A:38:ILE:HG23	1.92	0.51
2:B:35:LYS:C	2:B:37:ARG:N	2.68	0.51
2:B:72:HIS:O	2:B:74:ARG:N	2.44	0.51
2:B:87:HIS:O	2:B:91:VAL:HG23	2.11	0.51
2:B:363:SER:HA	2:B:366:ARG:HB2	1.92	0.51
2:B:373:ASN:ND2	2:B:376:ILE:H	2.09	0.51
3:C:118:HIS:ND1	3:C:123:ILE:HG21	2.24	0.51
1:D:155:TYR:CE2	1:D:196:LEU:HD23	2.45	0.51
2:E:134:PHE:CE2	2:E:135:LEU:HD22	2.45	0.51
2:E:136:GLU:OE1	2:E:178:ARG:NH1	2.40	0.51
2:B:121:TRP:N	2:B:122:PRO:CD	2.73	0.51
2:B:262:VAL:O	2:B:265:LEU:N	2.43	0.51
3:C:81:LEU:HD23	3:C:81:LEU:O	2.10	0.51
1:D:155:TYR:N	1:D:156:PRO:HD3	2.25	0.51
1:D:411:LEU:C	1:D:413:GLU:N	2.67	0.51
2:E:242:LEU:N	2:E:243:PRO:HD2	2.25	0.51
3:F:6:PHE:HE2	3:F:34:LYS:HG3	1.75	0.51
3:F:103:LEU:C	3:F:111:ILE:HD11	2.34	0.51
1:A:11:TYR:N	1:A:12:PRO:HD2	2.26	0.51
1:A:174:CYS:SG	1:A:185:ALA:HB1	2.50	0.51
1:A:215:ASP:O	1:A:221:ARG:NH1	2.42	0.51
2:B:145:ALA:O	2:B:147:LYS:N	2.44	0.51
2:B:346:MSE:CE	2:B:349:ILE:HD12	2.41	0.51
3:C:121:ARG:HG3	3:C:121:ARG:NH1	2.25	0.51
1:D:91:PRO:HB2	1:D:92:PRO:CD	2.41	0.51
2:E:65:GLU:C	2:E:67:VAL:N	2.67	0.51
2:E:271:LEU:O	2:E:274:PRO:HG2	2.10	0.51
1:A:515:ASP:O	1:A:518:THR:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:MSE:HE1	2:E:127:VAL:HG22	1.93	0.51
2:E:202:ILE:HD11	2:E:244:LEU:CG	2.36	0.51
1:D:414:ASP:OD2	1:D:415:ALA:N	2.44	0.51
1:D:419:VAL:O	1:D:422:ALA:HB3	2.10	0.51
2:E:145:ALA:O	2:E:146:LYS:C	2.54	0.51
2:E:167:ARG:HH11	2:E:167:ARG:CG	2.23	0.51
2:E:180:TYR:HE2	2:E:221:ILE:HG23	1.76	0.51
1:A:558:SER:O	1:A:562:PRO:HG2	2.10	0.51
1:D:580:GLN:C	1:D:582:ALA:H	2.19	0.51
3:F:95:GLU:OE1	3:F:95:GLU:N	2.38	0.51
3:C:142:VAL:HA	3:C:145:TYR:HD1	1.76	0.51
1:D:155:TYR:CZ	1:D:163:LYS:HB3	2.46	0.51
1:D:343:SER:HA	1:D:380:VAL:HG22	1.92	0.51
2:E:160:LEU:C	2:E:162:ASP:N	2.69	0.51
1:A:476:GLU:H	1:A:476:GLU:CD	2.18	0.51
3:C:36:LYS:O	3:C:37:GLU:C	2.53	0.51
3:C:258:THR:C	3:C:259:ILE:HG13	2.35	0.51
1:D:253:GLU:O	1:D:254:ASP:C	2.54	0.51
2:E:194:ILE:HG21	2:E:218:LEU:HD11	1.92	0.51
3:F:155:LEU:HD11	3:F:195:MET:HG3	1.93	0.51
1:A:161:ALA:O	1:A:164:ALA:HB3	2.11	0.50
1:A:168:GLN:NE2	1:A:171:ARG:HH12	2.09	0.50
3:C:162:GLN:OE1	3:C:235:THR:HG21	2.11	0.50
3:C:239:ARG:O	3:C:240:ALA:HB2	2.11	0.50
1:D:155:TYR:CE1	1:D:163:LYS:HB3	2.46	0.50
1:D:205:ILE:HD13	1:D:208:MSE:HE3	1.93	0.50
1:D:439:PHE:CD1	1:D:443:LEU:HB3	2.47	0.50
3:F:33:GLU:O	3:F:36:LYS:HB2	2.11	0.50
3:F:141:ASN:O	3:F:145:TYR:CD1	2.64	0.50
3:F:194:PRO:HG2	3:F:195:MET:N	2.26	0.50
3:F:274:ALA:HB2	3:F:288:GLN:HA	1.94	0.50
2:B:94:PHE:N	2:B:94:PHE:CD2	2.79	0.50
2:B:267:LYS:O	2:B:268:ASP:HB2	2.11	0.50
3:C:34:LYS:O	3:C:38:ILE:HG13	2.11	0.50
1:D:52:LEU:HD11	1:D:89:LEU:HD12	1.93	0.50
1:D:245:MSE:O	1:D:249:ARG:HG3	2.10	0.50
1:D:277:GLU:C	1:D:279:THR:H	2.19	0.50
1:D:338:ASN:ND2	1:D:341:VAL:HG23	2.17	0.50
1:D:378:PRO:O	1:D:379:GLU:C	2.54	0.50
1:D:502:LEU:HD21	1:D:540:VAL:HG22	1.93	0.50
1:D:518:THR:HG22	1:D:518:THR:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:PHE:CB	1:D:575:VAL:HA	2.41	0.50
2:E:310:PHE:CG	2:E:348:LEU:HD13	2.45	0.50
1:A:453:ASP:OD2	1:A:458:ILE:HG21	2.11	0.50
1:D:126:ALA:C	1:D:127:HIS:HD2	2.19	0.50
1:D:179:PRO:O	1:D:180:MSE:C	2.53	0.50
1:D:489:MSE:C	1:D:491:GLY:N	2.67	0.50
2:E:287:HIS:CE1	2:E:289:PRO:HB2	2.46	0.50
3:F:181:ARG:HH11	3:F:181:ARG:HG3	1.76	0.50
1:A:257:TRP:CH2	2:B:99:PRO:HB3	2.46	0.50
1:A:388:LEU:C	1:A:390:CYS:N	2.67	0.50
1:A:399:GLN:HE21	1:A:399:GLN:C	2.19	0.50
3:C:81:LEU:HA	3:C:112:THR:O	2.11	0.50
1:D:529:ALA:HB2	1:D:540:VAL:HG11	1.93	0.50
3:F:118:HIS:C	3:F:120:SER:H	2.20	0.50
1:A:502:LEU:HA	1:A:505:ILE:HD12	1.94	0.50
1:A:560:VAL:HG12	1:A:561:LYS:N	2.26	0.50
2:B:67:VAL:C	2:B:69:TYR:N	2.70	0.50
2:B:248:LYS:NZ	2:B:290:LYS:HZ2	2.09	0.50
1:D:146:SER:O	1:D:147:ALA:C	2.54	0.50
1:D:581:GLU:HG3	1:D:581:GLU:O	2.11	0.50
3:F:34:LYS:O	3:F:38:ILE:HG13	2.12	0.50
3:F:243:LEU:HD12	3:F:260:PHE:CE2	2.47	0.50
1:A:230:ASN:O	1:A:234:LEU:HG	2.11	0.50
1:A:390:CYS:O	1:A:391:VAL:C	2.54	0.50
2:B:144:ILE:HG22	2:B:144:ILE:O	2.11	0.50
3:C:74:LYS:O	3:C:78:THR:HG22	2.12	0.50
3:C:143:TRP:CE2	3:C:147:THR:HG21	2.45	0.50
1:D:489:MSE:HB3	1:D:501:THR:OG1	2.11	0.50
2:E:121:TRP:CZ2	2:E:167:ARG:HB3	2.46	0.50
1:A:372:GLN:O	1:A:374:LYS:N	2.45	0.50
2:B:167:ARG:O	2:B:168:GLU:C	2.54	0.50
3:C:225:SER:OG	3:C:252:HIS:ND1	2.33	0.50
1:D:180:MSE:HE2	1:D:183:ARG:NH2	2.27	0.50
1:D:397:ILE:O	1:D:397:ILE:HG13	2.11	0.50
1:D:410:GLU:C	1:D:412:ALA:N	2.69	0.50
2:E:294:PHE:O	2:E:295:LEU:C	2.53	0.50
2:E:397:ASP:O	2:E:400:GLN:HB3	2.11	0.50
1:A:377:CYS:SG	1:A:380:VAL:HG23	2.51	0.50
1:A:528:MSE:C	1:A:530:GLY:N	2.65	0.50
3:C:106:ARG:HG3	3:C:107:TYR:N	2.26	0.50
3:C:190:PRO:O	3:C:196:CYS:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:LEU:HD13	1:D:150:LEU:HD11	1.92	0.50
1:D:256:SER:OG	2:E:96:THR:HG21	2.11	0.50
1:D:295:GLU:O	1:D:296:ALA:C	2.54	0.50
2:E:88:MSE:HE1	2:E:127:VAL:HG13	1.94	0.50
3:F:100:LEU:HA	3:F:103:LEU:HD12	1.94	0.50
3:F:141:ASN:HB3	3:F:145:TYR:HE1	1.73	0.50
1:A:12:PRO:O	1:A:13:ILE:C	2.55	0.50
1:D:423:ILE:O	1:D:426:TYR:N	2.42	0.50
1:D:560:VAL:O	1:D:561:LYS:C	2.55	0.50
2:E:164:GLU:C	2:E:165:ASP:O	2.50	0.50
2:E:218:LEU:HD13	2:E:236:PHE:HZ	1.76	0.50
1:A:237:GLN:CD	1:A:278:ILE:HD11	2.36	0.49
1:D:20:LEU:HD23	1:D:31:SER:HB3	1.92	0.49
1:D:426:TYR:O	1:D:426:TYR:CG	2.65	0.49
2:E:35:LYS:O	2:E:38:GLN:N	2.44	0.49
2:E:402:PHE:O	2:E:403:LYS:C	2.55	0.49
2:B:63:LEU:C	2:B:65:GLU:N	2.68	0.49
1:D:16:LEU:HD23	1:D:16:LEU:N	2.27	0.49
1:D:322:ILE:HG21	1:D:356:LEU:HD21	1.93	0.49
1:D:412:ALA:O	1:D:413:GLU:CG	2.60	0.49
2:E:44:ASP:O	2:E:45:PHE:C	2.55	0.49
2:E:89:PHE:CE2	2:E:93:MSE:HG3	2.47	0.49
2:E:223:ASN:HD22	2:E:263:GLN:NE2	2.05	0.49
2:E:250:LEU:HA	2:E:253:TYR:CE2	2.47	0.49
3:F:183:LEU:HD21	3:F:194:PRO:CG	2.41	0.49
1:A:197:GLU:O	1:A:198:LEU:C	2.55	0.49
1:A:583:LEU:HD22	1:A:588:LEU:HB2	1.93	0.49
2:B:195:ASN:O	2:B:198:PHE:N	2.45	0.49
3:C:243:LEU:HD12	3:C:260:PHE:CD2	2.47	0.49
1:D:570:ASP:OD1	1:D:575:VAL:HG11	2.12	0.49
2:E:253:TYR:CD2	2:E:253:TYR:N	2.79	0.49
1:A:85:TYR:O	1:A:87:HIS:N	2.45	0.49
1:A:155:TYR:OH	1:A:167:ARG:HD3	2.11	0.49
1:A:313:LEU:HD13	1:A:321:VAL:HG21	1.94	0.49
3:C:93:SER:O	3:C:94:VAL:C	2.55	0.49
3:C:162:GLN:HB3	3:C:235:THR:CG2	2.42	0.49
1:D:34:LYS:C	1:D:36:SER:H	2.20	0.49
2:E:65:GLU:O	2:E:67:VAL:N	2.44	0.49
2:E:97:LEU:HD22	2:E:162:ASP:CB	2.42	0.49
2:E:183:PHE:O	2:E:185:GLY:N	2.46	0.49
3:F:276:MET:HB2	3:F:286:PHE:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:THR:HG23	1:A:86:VAL:CG2	2.43	0.49
1:A:129:VAL:CB	1:A:130:PRO:HD3	2.42	0.49
1:A:297:GLU:O	1:A:298:VAL:C	2.56	0.49
2:B:314:MSE:O	2:B:315:GLU:C	2.56	0.49
1:D:342:LYS:O	1:D:346:ALA:HB2	2.12	0.49
2:E:250:LEU:C	2:E:252:VAL:N	2.71	0.49
2:E:350:SER:C	2:E:352:ASN:N	2.71	0.49
3:F:158:LEU:HA	3:F:163:ILE:O	2.12	0.49
3:F:251:CYS:SG	3:F:256:VAL:HG12	2.53	0.49
1:A:141:PHE:CD1	1:A:142:THR:N	2.80	0.49
1:A:399:GLN:NE2	1:A:403:SER:OG	2.46	0.49
1:A:559:GLU:O	1:A:563:ILE:HG22	2.13	0.49
2:B:88:MSE:SE	2:B:127:VAL:HG13	2.62	0.49
2:B:121:TRP:C	2:B:123:HIS:N	2.69	0.49
3:C:43:SER:OG	3:C:45:VAL:C	2.56	0.49
3:C:104:LYS:CA	3:C:111:ILE:HD11	2.41	0.49
3:C:118:HIS:C	3:C:120:SER:H	2.20	0.49
1:D:426:TYR:O	1:D:426:TYR:CD1	2.64	0.49
1:D:517:THR:HG23	1:D:521:MSE:HE3	1.95	0.49
2:E:31:LEU:C	2:E:33:ILE:H	2.19	0.49
2:E:175:THR:O	2:E:179:ILE:HG13	2.13	0.49
1:A:112:LEU:HD13	1:A:150:LEU:HD11	1.94	0.49
1:A:552:ASP:OD1	1:A:554:SER:HB3	2.12	0.49
2:B:64:SER:O	2:B:68:GLU:HG3	2.13	0.49
3:C:209:TRP:CD2	3:C:224:ILE:HD13	2.48	0.49
1:D:179:PRO:HG3	1:D:182:ARG:NH2	2.27	0.49
1:D:410:GLU:O	1:D:412:ALA:N	2.46	0.49
3:F:118:HIS:ND1	3:F:123:ILE:HG21	2.27	0.49
1:A:24:ASP:O	1:A:24:ASP:OD2	2.30	0.49
3:C:160:ASP:C	3:C:162:GLN:N	2.70	0.49
1:D:297:GLU:O	1:D:299:ARG:N	2.46	0.49
1:D:481:THR:O	1:D:481:THR:HG22	2.13	0.49
1:D:588:LEU:O	1:D:589:ALA:CB	2.60	0.49
2:E:43:PHE:C	2:E:45:PHE:N	2.70	0.49
2:E:167:ARG:HH11	2:E:167:ARG:HB3	1.78	0.49
3:F:153:LEU:O	3:F:185:ARG:HD2	2.12	0.49
3:F:166:LEU:CD2	3:F:239:ARG:HB3	2.42	0.49
1:A:29:LEU:HD12	1:A:65:VAL:HA	1.94	0.49
1:A:178:THR:OG1	1:A:181:VAL:HG23	2.12	0.49
1:A:283:LEU:O	1:A:287:PHE:N	2.42	0.49
1:A:305:LYS:O	1:A:309:PHE:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:C	1:A:367:PRO:HD2	2.37	0.49
2:B:118:GLU:H	2:B:164:GLU:CG	2.25	0.49
2:B:329:HIS:NE2	2:B:331:GLN:HB2	2.26	0.49
2:B:371:HIS:NE2	2:B:376:ILE:HD11	2.27	0.49
3:C:24:SER:OG	3:C:27:GLN:HG3	2.13	0.49
1:D:123:ASP:O	1:D:124:LEU:C	2.54	0.49
2:E:118:GLU:H	2:E:164:GLU:HG2	1.76	0.49
2:E:126:LEU:C	2:E:128:TYR:N	2.70	0.49
2:E:141:GLN:HB2	2:E:144:ILE:HG13	1.93	0.49
2:E:367:ASN:O	2:E:369:LYS:N	2.32	0.49
3:F:57:ASP:HB2	3:F:260:PHE:CE1	2.48	0.49
1:A:88:CYS:O	1:A:90:LEU:N	2.46	0.49
1:A:89:LEU:CD1	1:A:89:LEU:H	2.25	0.49
2:B:330:PHE:CE1	2:B:331:GLN:HG2	2.48	0.49
1:D:100:GLU:O	1:D:101:GLU:C	2.55	0.49
3:F:45:VAL:HG22	3:F:156:THR:OG1	2.12	0.49
3:F:181:ARG:HG3	3:F:181:ARG:NH1	2.27	0.49
3:F:244:VAL:O	3:F:244:VAL:CG2	2.61	0.49
1:A:155:TYR:HE1	1:A:167:ARG:HG2	1.78	0.48
1:A:347:SER:HB3	1:A:383:ASN:ND2	2.24	0.48
1:D:183:ARG:CZ	2:E:200:ARG:HD2	2.43	0.48
2:E:121:TRP:N	2:E:122:PRO:CD	2.75	0.48
1:A:66:LEU:HD22	1:A:96:LEU:CD2	2.42	0.48
1:A:179:PRO:HD2	2:B:196:ASN:ND2	2.27	0.48
1:A:261:TYR:C	1:A:261:TYR:CD2	2.91	0.48
2:B:63:LEU:O	2:B:67:VAL:HG23	2.13	0.48
2:B:337:LEU:HD21	2:B:380:ILE:HG13	1.94	0.48
3:C:46:GLN:O	3:C:157:ALA:HA	2.13	0.48
3:C:119:GLU:HG2	3:C:153:LEU:HD12	1.95	0.48
1:D:574:ASP:OD2	3:F:110:ARG:NE	2.46	0.48
2:E:373:ASN:C	2:E:375:THR:N	2.71	0.48
2:E:388:MSE:O	2:E:390:MSE:N	2.46	0.48
3:F:55:CYS:SG	3:F:68:LEU:HD11	2.53	0.48
3:F:237:VAL:CB	3:F:256:VAL:HG23	2.32	0.48
1:A:24:ASP:O	1:A:27:LEU:N	2.39	0.48
1:A:24:ASP:OD2	1:A:24:ASP:C	2.56	0.48
1:A:277:GLU:O	1:A:279:THR:N	2.47	0.48
2:B:236:PHE:C	2:B:236:PHE:CD2	2.91	0.48
3:C:58:VAL:O	3:C:61:GLN:HG3	2.14	0.48
3:C:115:ARG:HB2	3:C:153:LEU:HB2	1.95	0.48
3:C:239:ARG:HH12	3:C:242:GLN:CG	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:SER:C	1:D:38:ILE:H	2.22	0.48
1:D:67:LEU:HA	1:D:104:VAL:HG22	1.94	0.48
1:D:381:ARG:HH12	1:D:414:ASP:CG	2.21	0.48
1:D:567:LEU:C	1:D:569:GLN:N	2.70	0.48
2:E:124:LEU:O	2:E:125:GLN:C	2.55	0.48
2:E:217:ILE:O	2:E:221:ILE:HG13	2.13	0.48
2:B:68:GLU:HB3	2:B:72:HIS:HD2	1.79	0.48
3:C:176:THR:HA	3:C:232:ASN:OD1	2.13	0.48
1:D:260:ARG:NE	1:D:293:ASP:OD2	2.42	0.48
1:D:399:GLN:NE2	1:D:403:SER:OG	2.45	0.48
3:F:123:ILE:HG23	3:F:127:TYR:CD2	2.35	0.48
1:A:89:LEU:N	1:A:89:LEU:HD12	2.27	0.48
1:A:120:SER:O	1:A:121:PRO:C	2.56	0.48
1:D:94:GLU:HB2	1:D:131:LEU:CD1	2.44	0.48
1:D:353:SER:N	1:D:354:PRO:HD2	2.29	0.48
1:D:389:ASP:OD2	1:D:389:ASP:N	2.46	0.48
2:E:80:PRO:HG2	2:E:82:TYR:HE2	1.73	0.48
2:E:143:ASN:C	2:E:145:ALA:H	2.18	0.48
2:E:195:ASN:O	2:E:198:PHE:N	2.46	0.48
2:E:373:ASN:HD22	2:E:376:ILE:HG23	1.75	0.48
3:F:253:ASP:O	3:F:255:ASN:N	2.45	0.48
1:A:39:ALA:HB1	1:A:47:THR:CG2	2.44	0.48
1:A:277:GLU:C	1:A:279:THR:H	2.21	0.48
1:A:506:ASN:ND2	1:A:543:SER:HA	2.29	0.48
2:B:287:HIS:O	2:B:288:SER:C	2.56	0.48
2:B:344:TYR:O	2:B:347:SER:HB3	2.12	0.48
3:C:158:LEU:HD21	3:C:161:GLY:HA2	1.96	0.48
2:E:259:TYR:O	2:E:263:GLN:HB2	2.12	0.48
1:A:25:VAL:HG13	1:A:62:GLU:HG2	1.95	0.48
1:A:502:LEU:O	1:A:506:ASN:OD1	2.32	0.48
2:B:250:LEU:C	2:B:252:VAL:N	2.71	0.48
3:C:202:ASP:HA	3:C:239:ARG:NH2	2.29	0.48
3:C:237:VAL:CB	3:C:256:VAL:HG23	2.41	0.48
1:D:11:TYR:O	1:D:12:PRO:C	2.56	0.48
1:D:40:LEU:C	1:D:42:LEU:H	2.22	0.48
2:E:245:HIS:CE1	2:E:257:LEU:HD21	2.49	0.48
1:A:27:LEU:O	1:A:28:ARG:C	2.56	0.48
3:C:236:LEU:HD11	3:C:257:VAL:HG12	1.95	0.48
1:D:77:THR:O	1:D:80:VAL:HG12	2.13	0.48
2:E:296:ASN:O	2:E:300:GLU:HG3	2.13	0.48
2:B:79:GLU:O	2:B:80:PRO:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:PHE:C	2:B:185:GLY:H	2.22	0.48
2:B:325:VAL:HG22	2:B:337:LEU:HD12	1.96	0.48
2:B:325:VAL:HG22	2:B:337:LEU:CD1	2.44	0.48
1:D:198:LEU:HD12	1:D:202:LYS:HE3	1.96	0.48
1:D:270:LEU:O	1:D:271:GLN:C	2.56	0.48
2:E:121:TRP:O	2:E:123:HIS:N	2.47	0.48
3:F:142:VAL:HA	3:F:145:TYR:HD1	1.77	0.48
3:F:251:CYS:SG	3:F:256:VAL:CG1	3.02	0.48
1:A:52:LEU:HD11	1:A:89:LEU:HD12	1.95	0.48
1:A:136:ALA:C	1:A:138:GLY:H	2.22	0.48
1:A:253:GLU:O	1:A:254:ASP:C	2.56	0.48
2:B:42:LEU:O	2:B:59:LYS:HE3	2.14	0.48
2:B:315:GLU:HB2	2:B:316:PRO:HD3	1.96	0.48
3:C:176:THR:HG23	3:C:179:HIS:HD2	1.78	0.48
3:C:239:ARG:HD3	3:C:240:ALA:N	2.29	0.48
1:D:22:ASN:O	1:D:23:GLU:CB	2.61	0.48
1:D:141:PHE:CD1	1:D:141:PHE:C	2.92	0.48
1:D:482:ILE:O	1:D:486:VAL:HG23	2.14	0.48
2:E:356:ILE:O	2:E:359:ILE:N	2.46	0.48
3:F:65:LEU:O	3:F:66:MET:C	2.56	0.48
3:F:120:SER:O	3:F:124:THR:HG23	2.13	0.48
1:A:179:PRO:CB	1:A:183:ARG:NH1	2.76	0.47
1:A:375:ASP:OD2	1:A:376:GLU:N	2.47	0.47
1:A:455:VAL:HG13	1:A:458:ILE:HB	1.95	0.47
1:D:245:MSE:HA	1:D:245:MSE:HE3	1.96	0.47
2:E:67:VAL:C	2:E:69:TYR:H	2.22	0.47
2:E:255:PRO:HG2	2:E:256:GLN:H	1.79	0.47
2:E:256:GLN:CD	2:E:256:GLN:N	2.72	0.47
2:E:361:PHE:C	2:E:363:SER:H	2.22	0.47
1:A:155:TYR:HB3	1:A:156:PRO:HD3	1.94	0.47
1:A:327:LEU:O	1:A:331:LYS:HG3	2.13	0.47
1:A:499:MSE:O	1:A:500:THR:C	2.58	0.47
3:F:28:VAL:HG21	3:F:142:VAL:HG13	1.95	0.47
1:A:102:THR:HG22	1:A:105:ARG:HH22	1.77	0.47
1:A:466:LEU:O	1:A:469:LEU:N	2.43	0.47
1:A:509:SER:O	1:A:550:ILE:HD13	2.14	0.47
1:A:533:VAL:HG12	1:A:535:ASN:HB2	1.95	0.47
3:C:122:GLN:O	3:C:126:VAL:HG23	2.15	0.47
1:D:398:ARG:O	1:D:400:LEU:N	2.47	0.47
2:E:35:LYS:C	2:E:37:ARG:N	2.71	0.47
2:E:215:LEU:HD13	2:E:257:LEU:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:288:SER:HB2	2:E:289:PRO:CD	2.43	0.47
3:F:17:LEU:O	3:F:20:CYS:N	2.36	0.47
1:A:131:LEU:HD23	1:A:131:LEU:C	2.39	0.47
1:A:382:LEU:HD12	1:A:419:VAL:HG13	1.97	0.47
2:B:132:LEU:O	2:B:134:PHE:N	2.47	0.47
1:D:565:GLU:C	1:D:567:LEU:H	2.22	0.47
2:E:97:LEU:HB3	2:E:98:PRO:HD2	1.97	0.47
2:E:151:GLN:O	2:E:154:VAL:N	2.47	0.47
2:E:241:LEU:HA	2:E:241:LEU:HD23	1.66	0.47
2:E:409:GLU:O	2:E:413:MSE:HB2	2.13	0.47
3:F:51:PRO:HB3	3:F:279:ASP:C	2.38	0.47
3:F:119:GLU:HG3	3:F:150:PHE:CE1	2.49	0.47
1:A:115:ILE:O	1:A:119:HIS:CD2	2.67	0.47
1:A:377:CYS:SG	1:A:379:GLU:HB2	2.55	0.47
2:B:145:ALA:O	2:B:146:LYS:C	2.58	0.47
2:B:186:LEU:O	2:B:190:ILE:HD12	2.14	0.47
2:B:242:LEU:HD13	2:B:278:ALA:HB2	1.94	0.47
1:D:515:ASP:O	1:D:516:ILE:C	2.57	0.47
2:E:285:LYS:HE3	2:E:285:LYS:HB2	1.74	0.47
2:E:314:MSE:O	2:E:315:GLU:C	2.58	0.47
1:A:499:MSE:O	1:A:501:THR:N	2.47	0.47
2:B:73:ASN:C	2:B:75:ASN:N	2.71	0.47
1:D:587:SER:C	1:D:588:LEU:HD23	2.40	0.47
3:F:28:VAL:O	3:F:29:LYS:C	2.57	0.47
1:A:11:TYR:O	1:A:12:PRO:C	2.55	0.47
1:A:76:PHE:HB2	1:A:89:LEU:HD21	1.95	0.47
1:A:96:LEU:HA	1:A:99:VAL:HG23	1.96	0.47
2:B:59:LYS:HA	2:B:62:ALA:HB3	1.96	0.47
2:B:104:THR:OG1	2:B:105:GLY:N	2.46	0.47
2:B:118:GLU:CB	2:B:164:GLU:HG2	2.43	0.47
2:B:124:LEU:C	2:B:126:LEU:N	2.70	0.47
2:B:133:ARG:HA	2:B:136:GLU:CD	2.40	0.47
2:B:158:LEU:HD23	2:B:161:PHE:CE1	2.50	0.47
2:B:335:ARG:HH11	2:B:335:ARG:HG3	1.78	0.47
2:B:392:GLN:O	2:B:393:LYS:C	2.58	0.47
3:C:45:VAL:HA	3:C:156:THR:OG1	2.14	0.47
3:C:106:ARG:O	3:C:108:ARG:N	2.36	0.47
3:C:117:ASN:HB2	3:C:200:TRP:CZ2	2.49	0.47
3:C:119:GLU:HG3	3:C:150:PHE:CG	2.49	0.47
3:C:294:ARG:HG2	3:C:294:ARG:HH11	1.80	0.47
1:D:67:LEU:HD12	1:D:67:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:TYR:O	1:D:86:VAL:C	2.57	0.47
1:D:94:GLU:HB2	1:D:131:LEU:HD12	1.96	0.47
1:D:193:ALA:HB2	1:D:205:ILE:HG13	1.97	0.47
1:D:385:ILE:HD12	1:D:423:ILE:HD11	1.96	0.47
2:E:63:LEU:C	2:E:65:GLU:N	2.72	0.47
2:E:117:LEU:HD23	2:E:164:GLU:OE1	2.15	0.47
2:E:121:TRP:CG	2:E:167:ARG:HH12	2.32	0.47
2:E:124:LEU:C	2:E:126:LEU:N	2.72	0.47
1:A:177:ASP:OD1	1:A:177:ASP:N	2.48	0.47
1:A:288:GLN:CA	1:A:291:MSE:HE3	2.25	0.47
1:A:349:ILE:HG23	1:A:350:MSE:H	1.80	0.47
3:C:10:LEU:HD23	3:C:13:TRP:CE3	2.50	0.47
1:D:307:LYS:HD2	1:D:351:GLY:HA3	1.97	0.47
2:E:288:SER:O	2:E:289:PRO:C	2.57	0.47
3:F:248:TYR:CE2	3:F:286:PHE:CD2	3.03	0.47
1:A:76:PHE:CB	1:A:89:LEU:HD21	2.45	0.47
1:A:225:VAL:HG11	1:A:262:MSE:CB	2.37	0.47
1:A:349:ILE:CG2	1:A:350:MSE:N	2.78	0.47
1:A:560:VAL:O	1:A:561:LYS:C	2.56	0.47
2:B:169:ARG:HB3	2:B:213:GLU:HG2	1.97	0.47
2:B:250:LEU:O	2:B:252:VAL:N	2.48	0.47
2:B:402:PHE:O	2:B:403:LYS:C	2.56	0.47
3:C:94:VAL:O	3:C:97:VAL:HG12	2.15	0.47
3:C:220:PHE:CA	3:C:224:ILE:HD12	2.44	0.47
1:D:17:ILE:HG12	1:D:38:ILE:HG23	1.95	0.47
1:D:119:HIS:CD2	1:D:119:HIS:N	2.83	0.47
1:D:492:ASP:OD2	1:D:493:PRO:HD2	2.15	0.47
2:E:315:GLU:O	2:E:319:ARG:HB2	2.14	0.47
3:F:244:VAL:HG21	3:F:248:TYR:N	2.30	0.47
1:A:119:HIS:CD2	1:A:119:HIS:H	2.33	0.47
1:A:452:VAL:HG13	1:A:497:HIS:HE2	1.75	0.47
2:B:268:ASP:C	2:B:268:ASP:OD1	2.58	0.47
2:B:305:ILE:HD13	2:B:306:GLU:N	2.27	0.47
2:B:388:MSE:HE2	2:B:392:GLN:NE2	2.19	0.47
1:D:352:LEU:HD23	1:D:355:ILE:HD12	1.96	0.47
1:D:522:LEU:N	1:D:523:PRO:CD	2.77	0.47
2:E:72:HIS:C	2:E:74:ARG:N	2.71	0.47
2:E:251:SER:HA	2:E:293:MSE:CE	2.41	0.47
3:F:87:VAL:O	3:F:88:ASP:HB2	2.14	0.47
3:F:88:ASP:O	3:F:89:ARG:HB2	2.15	0.47
3:F:171:SER:HB2	3:F:197:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:HIS:O	1:A:344:ALA:HB2	2.15	0.46
1:A:353:SER:N	1:A:354:PRO:HD2	2.30	0.46
1:A:399:GLN:HE21	1:A:399:GLN:CA	2.27	0.46
2:B:222:ILE:O	2:B:224:GLY:N	2.47	0.46
3:C:39:LEU:O	3:C:40:THR:C	2.58	0.46
1:D:350:MSE:CE	1:D:391:VAL:HG13	2.18	0.46
1:D:535:ASN:HA	1:D:538:PHE:CD2	2.49	0.46
2:E:313:ILE:HG22	2:E:314:MSE:N	2.30	0.46
3:F:5:VAL:O	3:F:5:VAL:HG12	2.14	0.46
3:F:131:ASP:O	3:F:132:GLU:C	2.57	0.46
1:A:245:MSE:O	1:A:246:PRO:C	2.56	0.46
2:B:241:LEU:HA	2:B:241:LEU:HD23	1.61	0.46
2:B:335:ARG:HG3	2:B:335:ARG:NH1	2.30	0.46
1:D:61:ASP:N	1:D:62:GLU:OE2	2.47	0.46
1:D:215:ASP:O	1:D:221:ARG:NH1	2.49	0.46
1:D:495:TYR:O	1:D:499:MSE:HG3	2.14	0.46
2:E:61:ALA:O	2:E:63:LEU:N	2.48	0.46
1:A:85:TYR:O	1:A:86:VAL:C	2.58	0.46
2:B:186:LEU:HB3	2:B:190:ILE:CD1	2.45	0.46
2:B:329:HIS:HD2	2:B:332:VAL:HG23	1.80	0.46
3:C:97:VAL:HG13	3:C:98:THR:H	1.79	0.46
1:D:182:ARG:HG3	1:D:182:ARG:NH1	2.29	0.46
1:D:567:LEU:C	1:D:569:GLN:H	2.22	0.46
2:E:258:ALA:O	2:E:259:TYR:C	2.59	0.46
3:F:106:ARG:HG3	3:F:107:TYR:N	2.30	0.46
1:A:40:LEU:C	1:A:42:LEU:H	2.23	0.46
1:A:80:VAL:HG22	1:A:80:VAL:O	2.16	0.46
2:B:83:PRO:HD3	2:B:148:TYR:CE1	2.50	0.46
3:C:59:HIS:HE1	3:C:118:HIS:CD2	2.34	0.46
3:C:174:ILE:HD11	3:C:194:PRO:HB2	1.98	0.46
1:D:349:ILE:HD11	1:D:368:LEU:HD12	1.97	0.46
1:D:384:ILE:CG2	1:D:385:ILE:N	2.78	0.46
1:D:388:LEU:HA	1:D:391:VAL:HG22	1.97	0.46
2:E:45:PHE:CB	2:E:59:LYS:HD2	2.46	0.46
2:E:97:LEU:HD22	2:E:162:ASP:HB3	1.97	0.46
3:F:236:LEU:HD11	3:F:257:VAL:CG1	2.45	0.46
3:F:265:TYR:HD2	3:F:266:CYS:H	1.63	0.46
1:A:22:ASN:O	1:A:23:GLU:HB2	2.16	0.46
1:A:79:LEU:H	1:A:79:LEU:CD1	2.27	0.46
1:A:179:PRO:HB3	1:A:183:ARG:NH1	2.31	0.46
1:A:182:ARG:HG3	1:A:182:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HD23	1:A:223:LEU:N	2.30	0.46
1:A:295:GLU:O	1:A:296:ALA:C	2.58	0.46
2:B:215:LEU:HD13	2:B:257:LEU:HA	1.97	0.46
2:B:406:LYS:HD3	2:B:406:LYS:C	2.40	0.46
3:C:50:CYS:HB2	3:C:51:PRO:CA	2.43	0.46
1:D:388:LEU:HA	1:D:391:VAL:CG2	2.46	0.46
1:D:495:TYR:CD2	1:D:533:VAL:HG11	2.50	0.46
2:E:133:ARG:HA	2:E:136:GLU:OE2	2.15	0.46
2:E:313:ILE:C	2:E:316:PRO:HD2	2.40	0.46
3:F:76:PRO:HB3	3:F:107:TYR:CG	2.51	0.46
3:F:171:SER:HB2	3:F:197:ASP:CB	2.45	0.46
1:A:316:ASP:O	1:A:317:CYS:HB3	2.15	0.46
1:A:470:VAL:HG11	1:A:511:VAL:CG2	2.45	0.46
2:B:350:SER:C	2:B:352:ASN:N	2.73	0.46
1:D:104:VAL:CG1	1:D:105:ARG:N	2.72	0.46
1:D:338:ASN:HD21	1:D:340:HIS:HB2	1.81	0.46
1:D:579:ALA:O	1:D:582:ALA:HB3	2.16	0.46
2:E:67:VAL:C	2:E:69:TYR:N	2.71	0.46
3:F:158:LEU:CD2	3:F:161:GLY:HA2	2.45	0.46
3:F:172:PRO:C	3:F:174:ILE:H	2.23	0.46
1:A:141:PHE:HE2	2:B:199:TYR:CD2	2.34	0.46
1:A:211:ASN:N	1:A:211:ASN:ND2	2.62	0.46
1:A:229:VAL:O	1:A:233:GLN:HG3	2.16	0.46
1:A:339:GLN:HE21	1:A:377:CYS:HB2	1.79	0.46
1:A:377:CYS:O	1:A:378:PRO:C	2.59	0.46
1:A:522:LEU:N	1:A:523:PRO:CD	2.79	0.46
2:B:83:PRO:C	2:B:85:VAL:H	2.22	0.46
2:B:121:TRP:O	2:B:123:HIS:N	2.48	0.46
2:B:186:LEU:HB3	2:B:190:ILE:HD12	1.97	0.46
3:C:141:ASN:O	3:C:145:TYR:CD1	2.68	0.46
3:C:272:GLN:OE1	3:C:288:GLN:NE2	2.48	0.46
1:D:504:CYS:HB3	1:D:508:LEU:HD23	1.96	0.46
3:F:162:GLN:HB3	3:F:235:THR:HG21	1.98	0.46
1:A:218:ASP:C	1:A:220:VAL:N	2.74	0.46
1:A:564:LEU:O	1:A:564:LEU:CD2	2.60	0.46
2:B:83:PRO:C	2:B:85:VAL:N	2.74	0.46
3:C:144:LYS:O	3:C:145:TYR:C	2.56	0.46
1:D:482:ILE:C	1:D:484:PRO:CD	2.89	0.46
1:D:503:PHE:O	1:D:504:CYS:C	2.59	0.46
2:E:107:GLU:H	2:E:107:GLU:HG2	1.55	0.46
1:A:40:LEU:C	1:A:42:LEU:N	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LEU:C	1:A:413:GLU:H	2.23	0.46
2:B:313:ILE:CG2	2:B:317:LEU:HB2	2.46	0.46
1:D:506:ASN:HD21	1:D:543:SER:CB	2.29	0.46
2:E:35:LYS:O	2:E:37:ARG:N	2.48	0.46
2:E:137:SER:O	2:E:140:PHE:HD1	1.99	0.46
3:F:12:GLN:HE22	3:F:16:GLN:HB2	1.81	0.46
1:A:67:LEU:HD11	1:A:107:LYS:HG3	1.97	0.46
2:B:86:VAL:O	2:B:87:HIS:C	2.58	0.46
2:B:218:LEU:HD23	2:B:218:LEU:HA	1.80	0.46
2:B:313:ILE:HG22	2:B:314:MSE:N	2.31	0.46
2:B:313:ILE:HG22	2:B:317:LEU:HB2	1.98	0.46
3:C:12:GLN:O	3:C:12:GLN:NE2	2.49	0.46
3:C:183:LEU:HD21	3:C:194:PRO:HG3	1.97	0.46
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.97	0.46
1:D:326:ILE:HG22	1:D:327:LEU:N	2.31	0.46
2:E:248:LYS:C	2:E:250:LEU:H	2.23	0.46
2:E:330:PHE:CD1	2:E:331:GLN:N	2.84	0.46
2:B:150:ASP:O	2:B:151:GLN:C	2.59	0.45
2:B:237:LEU:HD12	2:B:241:LEU:HD12	1.98	0.45
2:B:305:ILE:HD12	2:B:310:PHE:N	2.31	0.45
3:C:76:PRO:HB3	3:C:107:TYR:CG	2.51	0.45
1:D:455:VAL:O	1:D:455:VAL:HG13	2.16	0.45
1:D:525:VAL:HG11	1:D:544:LEU:CD2	2.46	0.45
2:E:80:PRO:O	2:E:81:ILE:C	2.59	0.45
2:E:407:LEU:HD23	2:E:407:LEU:C	2.40	0.45
3:F:99:LEU:O	3:F:100:LEU:C	2.57	0.45
3:F:166:LEU:HD23	3:F:239:ARG:HB3	1.97	0.45
2:B:257:LEU:O	2:B:260:CYS:N	2.49	0.45
2:B:407:LEU:HD23	2:B:407:LEU:O	2.16	0.45
3:C:67:GLU:HA	3:C:70:ARG:NH1	2.31	0.45
1:D:98:THR:O	1:D:99:VAL:C	2.58	0.45
1:D:401:SER:HA	1:D:405:LEU:HB2	1.98	0.45
1:D:405:LEU:HD13	1:D:409:VAL:CG2	2.46	0.45
2:E:150:ASP:O	2:E:151:GLN:C	2.58	0.45
2:E:242:LEU:HD13	2:E:278:ALA:HB2	1.96	0.45
3:F:103:LEU:CB	3:F:111:ILE:HD13	2.46	0.45
3:F:115:ARG:HG3	3:F:119:GLU:HB2	1.98	0.45
1:A:77:THR:HA	1:A:86:VAL:HG23	1.97	0.45
1:A:395:ILE:HD11	1:A:400:LEU:HA	1.97	0.45
1:A:528:MSE:O	1:A:530:GLY:N	2.49	0.45
1:A:572:ASP:CG	3:C:110:ARG:HH21	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:LEU:HD22	2:B:162:ASP:CB	2.47	0.45
2:B:184:LEU:HA	2:B:187:ARG:HG3	1.97	0.45
3:C:119:GLU:HB3	3:C:150:PHE:HB3	1.98	0.45
1:D:270:LEU:C	1:D:274:VAL:HG23	2.41	0.45
1:D:348:VAL:CG2	1:D:349:ILE:N	2.78	0.45
1:D:370:LEU:HD13	1:D:370:LEU:HA	1.76	0.45
2:E:69:TYR:CZ	2:E:75:ASN:ND2	2.85	0.45
2:E:103:PRO:HG3	2:E:108:PHE:CD2	2.51	0.45
2:E:132:LEU:C	2:E:134:PHE:N	2.71	0.45
1:A:398:ARG:O	1:A:399:GLN:C	2.58	0.45
1:A:400:LEU:HD12	1:A:404:LEU:HD23	1.98	0.45
1:A:408:ILE:HA	1:A:411:LEU:HD23	1.98	0.45
2:B:43:PHE:C	2:B:45:PHE:N	2.72	0.45
2:B:164:GLU:HB2	2:B:168:GLU:HB2	1.99	0.45
2:B:183:PHE:HB2	2:B:186:LEU:HD22	1.97	0.45
2:B:265:LEU:HD21	2:B:272:THR:HA	1.98	0.45
2:B:320:GLN:O	2:B:321:LEU:C	2.58	0.45
3:C:165:CYS:HA	3:C:238:SER:O	2.16	0.45
3:C:265:TYR:HB3	3:C:269:CYS:HB2	1.98	0.45
1:D:42:LEU:HD23	1:D:47:THR:HA	1.99	0.45
1:D:495:TYR:CD2	1:D:499:MSE:HE2	2.51	0.45
2:E:273:GLU:OE1	2:E:312:LYS:HD3	2.16	0.45
1:A:490:SER:HB2	1:A:528:MSE:HE3	1.99	0.45
1:A:552:ASP:O	1:A:554:SER:N	2.50	0.45
2:B:65:GLU:O	2:B:67:VAL:N	2.49	0.45
2:B:72:HIS:C	2:B:74:ARG:H	2.24	0.45
2:B:298:LEU:HA	2:B:298:LEU:HD12	1.45	0.45
3:C:294:ARG:HG2	3:C:294:ARG:NH1	2.32	0.45
1:D:327:LEU:O	1:D:327:LEU:HG	2.16	0.45
2:E:361:PHE:C	2:E:363:SER:N	2.73	0.45
3:F:43:SER:OG	3:F:45:VAL:C	2.60	0.45
3:F:93:SER:O	3:F:94:VAL:C	2.58	0.45
3:F:95:GLU:OE1	3:F:136:LYS:NZ	2.49	0.45
3:F:176:THR:HG23	3:F:179:HIS:CD2	2.49	0.45
3:F:252:HIS:O	3:F:253:ASP:O	2.34	0.45
1:A:52:LEU:HD12	1:A:88:CYS:HB3	1.98	0.45
1:A:86:VAL:C	1:A:88:CYS:H	2.24	0.45
1:A:179:PRO:CB	1:A:183:ARG:HH12	2.29	0.45
1:A:343:SER:CB	1:A:380:VAL:HG22	2.46	0.45
1:A:410:GLU:O	1:A:411:LEU:C	2.59	0.45
2:B:242:LEU:HD11	2:B:275:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:SER:O	3:C:124:THR:HG23	2.15	0.45
2:E:118:GLU:HG3	2:E:119:ALA:O	2.16	0.45
3:F:24:SER:OG	3:F:27:GLN:HG3	2.17	0.45
1:A:34:LYS:C	1:A:36:SER:H	2.24	0.45
1:A:327:LEU:N	1:A:328:PRO:CD	2.78	0.45
1:A:400:LEU:HD12	1:A:404:LEU:CD2	2.45	0.45
1:A:587:SER:C	1:A:588:LEU:HD23	2.41	0.45
2:B:182:LYS:HB2	2:B:183:PHE:CD1	2.52	0.45
2:B:306:GLU:O	2:B:307:PRO:C	2.59	0.45
3:C:137:TYR:CG	3:C:142:VAL:HG21	2.51	0.45
1:D:22:ASN:HD21	1:D:24:ASP:HB3	1.82	0.45
1:D:25:VAL:O	1:D:26:GLN:C	2.60	0.45
1:D:35:LEU:O	1:D:76:PHE:HZ	1.99	0.45
1:D:262:MSE:O	1:D:265:ASP:N	2.49	0.45
1:D:521:MSE:C	1:D:523:PRO:CD	2.89	0.45
3:F:12:GLN:O	3:F:15:GLU:HB3	2.16	0.45
3:F:194:PRO:CG	3:F:195:MET:H	2.30	0.45
1:A:384:ILE:HG22	1:A:385:ILE:N	2.31	0.45
1:A:581:GLU:O	1:A:581:GLU:HG3	2.17	0.45
3:C:172:PRO:HG3	3:C:209:TRP:CD2	2.51	0.45
3:C:203:PRO:HB3	3:C:220:PHE:HE1	1.82	0.45
1:D:38:ILE:HD12	1:D:38:ILE:N	2.32	0.45
1:D:257:TRP:CZ2	2:E:99:PRO:HD3	2.52	0.45
1:D:405:LEU:HD13	1:D:409:VAL:HG23	1.99	0.45
2:E:85:VAL:HG11	2:E:134:PHE:CE1	2.52	0.45
2:E:121:TRP:CE2	2:E:167:ARG:NH1	2.85	0.45
3:F:14:ILE:O	3:F:18:ASN:HB2	2.17	0.45
3:F:134:LEU:HD12	3:F:134:LEU:N	2.32	0.45
1:A:88:CYS:C	1:A:90:LEU:N	2.70	0.45
2:B:152:LYS:O	2:B:156:GLN:HG3	2.17	0.45
2:B:237:LEU:HA	2:B:241:LEU:HB2	1.98	0.45
2:B:258:ALA:O	2:B:259:TYR:C	2.58	0.45
1:D:120:SER:O	1:D:123:ASP:N	2.50	0.45
1:D:211:ASN:N	1:D:211:ASN:ND2	2.65	0.45
1:D:287:PHE:CD2	1:D:291:MSE:HE2	2.52	0.45
1:D:451:LEU:HD12	1:D:451:LEU:HA	1.64	0.45
1:D:525:VAL:CG1	1:D:544:LEU:HD21	2.47	0.45
2:E:162:ASP:O	2:E:163:SER:CB	2.62	0.45
2:E:182:LYS:HB2	2:E:183:PHE:CE1	2.51	0.45
2:E:398:CYS:O	2:E:399:THR:C	2.58	0.45
1:A:333:LEU:O	1:A:335:SER:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:PHE:CD2	1:A:369:PHE:N	2.83	0.45
2:B:71:THR:HG21	2:B:133:ARG:NH1	2.31	0.45
3:C:121:ARG:HG2	3:C:147:THR:HB	1.98	0.45
3:C:203:PRO:CA	3:C:220:PHE:CE1	2.99	0.45
1:D:90:LEU:HB2	1:D:91:PRO:CD	2.45	0.45
3:F:61:GLN:NE2	3:F:64:ASP:OD2	2.50	0.45
1:A:221:ARG:O	1:A:224:ALA:HB3	2.17	0.44
1:A:384:ILE:CG2	1:A:385:ILE:N	2.80	0.44
1:A:515:ASP:O	1:A:517:THR:N	2.50	0.44
3:C:166:LEU:HD11	3:C:169:GLY:CA	2.47	0.44
1:D:146:SER:O	1:D:148:CYS:N	2.49	0.44
1:D:205:ILE:HG22	1:D:206:ILE:N	2.32	0.44
1:D:307:LYS:O	1:D:311:GLU:HG3	2.17	0.44
2:E:43:PHE:HA	2:E:88:MSE:HG2	1.98	0.44
2:E:93:MSE:HE2	2:E:128:TYR:CZ	2.52	0.44
1:A:115:ILE:O	1:A:115:ILE:HG13	2.14	0.44
1:A:229:VAL:HG22	1:A:270:LEU:CD2	2.46	0.44
1:A:588:LEU:O	1:A:589:ALA:CB	2.64	0.44
2:B:71:THR:O	2:B:73:ASN:N	2.42	0.44
2:B:89:PHE:C	2:B:91:VAL:H	2.25	0.44
2:B:209:ASN:N	2:B:209:ASN:ND2	2.65	0.44
2:B:244:LEU:HD22	2:B:253:TYR:HE1	1.78	0.44
2:B:405:GLU:O	2:B:406:LYS:C	2.59	0.44
1:D:44:VAL:HG13	1:D:45:GLU:H	1.82	0.44
1:D:499:MSE:O	1:D:502:LEU:N	2.50	0.44
2:E:61:ALA:C	2:E:63:LEU:N	2.72	0.44
3:F:119:GLU:HG2	3:F:153:LEU:HD12	1.99	0.44
3:F:293:PRO:O	3:F:293:PRO:HG2	2.17	0.44
1:A:271:GLN:HA	1:A:283:LEU:CD1	2.48	0.44
1:A:288:GLN:O	1:A:291:MSE:N	2.50	0.44
1:A:333:LEU:O	1:A:334:VAL:C	2.57	0.44
1:A:521:MSE:C	1:A:523:PRO:CD	2.90	0.44
1:A:560:VAL:O	1:A:563:ILE:HG22	2.17	0.44
1:A:567:LEU:C	1:A:569:GLN:N	2.74	0.44
2:B:183:PHE:C	2:B:185:GLY:N	2.74	0.44
2:B:315:GLU:HB2	2:B:316:PRO:CD	2.47	0.44
3:C:94:VAL:O	3:C:95:GLU:C	2.59	0.44
3:C:118:HIS:CE1	3:C:123:ILE:HG21	2.51	0.44
1:D:218:ASP:HB3	1:D:221:ARG:NH2	2.33	0.44
1:D:439:PHE:CE1	1:D:443:LEU:HB3	2.52	0.44
2:E:289:PRO:O	2:E:293:MSE:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:344:TYR:HE1	2:E:348:LEU:HD11	1.83	0.44
3:F:12:GLN:NE2	3:F:16:GLN:HB2	2.33	0.44
1:A:198:LEU:O	1:A:199:ASP:C	2.61	0.44
1:A:326:ILE:C	1:A:328:PRO:HD2	2.43	0.44
1:A:436:VAL:HG22	1:A:440:ASP:OD2	2.17	0.44
2:B:271:LEU:C	2:B:274:PRO:HD2	2.41	0.44
3:C:185:ARG:HG2	3:C:185:ARG:HH11	1.83	0.44
1:D:87:HIS:C	1:D:87:HIS:ND1	2.75	0.44
1:D:141:PHE:O	1:D:142:THR:C	2.60	0.44
1:D:427:MSE:C	1:D:429:LEU:N	2.75	0.44
2:E:182:LYS:HB2	2:E:183:PHE:CD1	2.52	0.44
2:E:348:LEU:O	2:E:349:ILE:C	2.60	0.44
3:F:156:THR:HG22	3:F:166:LEU:HB3	1.98	0.44
1:A:236:PRO:O	1:A:237:GLN:C	2.60	0.44
1:A:515:ASP:O	1:A:516:ILE:C	2.60	0.44
2:B:93:MSE:HA	2:B:93:MSE:HE3	1.99	0.44
2:B:121:TRP:HB3	2:B:122:PRO:CD	2.48	0.44
2:B:242:LEU:HA	2:B:242:LEU:HD23	1.62	0.44
3:C:123:ILE:HG23	3:C:127:TYR:CD2	2.29	0.44
1:D:39:ALA:HB3	1:D:79:LEU:HD23	1.99	0.44
1:D:178:THR:O	1:D:179:PRO:C	2.61	0.44
1:D:206:ILE:O	1:D:209:PHE:HB3	2.17	0.44
1:D:370:LEU:O	1:D:371:ALA:C	2.60	0.44
1:D:497:HIS:O	1:D:500:THR:HB	2.18	0.44
3:F:115:ARG:HB2	3:F:153:LEU:HB2	1.98	0.44
1:A:22:ASN:ND2	1:A:27:LEU:HD12	2.33	0.44
1:A:92:PRO:O	1:A:93:LEU:C	2.61	0.44
2:B:365:TYR:HD2	2:B:402:PHE:HE2	1.66	0.44
2:B:397:ASP:O	2:B:400:GLN:HB3	2.18	0.44
1:D:587:SER:O	1:D:588:LEU:HD23	2.18	0.44
2:E:247:VAL:HG12	2:E:248:LYS:N	2.33	0.44
3:F:7:THR:O	3:F:7:THR:HG22	2.18	0.44
3:F:87:VAL:HG23	3:F:88:ASP:OD2	2.17	0.44
3:F:199:LEU:N	3:F:199:LEU:CD1	2.80	0.44
3:F:239:ARG:HD3	3:F:240:ALA:N	2.33	0.44
1:A:61:ASP:N	1:A:62:GLU:OE2	2.50	0.44
1:A:98:THR:O	1:A:99:VAL:C	2.61	0.44
1:A:350:MSE:C	1:A:352:LEU:H	2.25	0.44
1:A:450:TRP:HB3	1:A:462:ALA:HB2	2.00	0.44
1:A:469:LEU:O	1:A:470:VAL:C	2.60	0.44
1:A:498:ARG:NH2	3:C:280:ASP:OD1	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ASN:HD21	1:A:543:SER:HA	1.82	0.44
2:B:302:LEU:HA	2:B:305:ILE:HB	1.99	0.44
1:D:80:VAL:HG21	1:D:88:CYS:HB2	1.99	0.44
2:E:121:TRP:H	2:E:122:PRO:HD2	1.82	0.44
2:E:236:PHE:CE2	2:E:241:LEU:HG	2.52	0.44
3:F:265:TYR:C	3:F:267:TYR:H	2.25	0.44
1:A:277:GLU:O	1:A:280:LYS:N	2.51	0.44
2:B:85:VAL:HG13	2:B:130:PHE:CZ	2.52	0.44
2:B:97:LEU:HD22	2:B:162:ASP:HB3	1.98	0.44
2:B:117:LEU:HA	2:B:164:GLU:OE1	2.18	0.44
3:C:12:GLN:NE2	3:C:16:GLN:HB2	2.33	0.44
1:D:61:ASP:O	1:D:62:GLU:C	2.60	0.44
1:D:213:ALA:O	1:D:221:ARG:HG2	2.17	0.44
1:D:265:ASP:O	1:D:305:LYS:HE3	2.18	0.44
1:D:405:LEU:N	1:D:406:PRO:CD	2.81	0.44
1:D:509:SER:OG	1:D:547:ILE:HG22	2.17	0.44
2:E:94:PHE:CD2	2:E:94:PHE:N	2.84	0.44
2:E:151:GLN:O	2:E:152:LYS:C	2.61	0.44
2:E:186:LEU:O	2:E:190:ILE:CD1	2.65	0.44
2:E:382:ASN:OD1	2:E:386:LEU:CD1	2.66	0.44
2:B:78:THR:C	2:B:80:PRO:CD	2.84	0.44
2:B:302:LEU:HA	2:B:302:LEU:HD23	1.85	0.44
1:D:221:ARG:NE	1:D:254:ASP:OD2	2.51	0.44
1:D:237:GLN:O	1:D:238:GLU:C	2.61	0.44
1:D:259:VAL:O	1:D:260:ARG:C	2.60	0.44
1:D:448:MSE:CE	1:D:466:LEU:HD21	2.47	0.44
2:E:313:ILE:N	2:E:313:ILE:CD1	2.77	0.44
1:A:61:ASP:O	1:A:62:GLU:C	2.61	0.43
1:A:144:ARG:HH21	1:A:176:ASP:CG	2.26	0.43
2:B:326:SER:OG	2:B:363:SER:HB3	2.18	0.43
2:B:373:ASN:O	2:B:375:THR:N	2.47	0.43
3:C:68:LEU:O	3:C:71:ILE:HB	2.18	0.43
1:A:128:PHE:C	1:A:128:PHE:CD2	2.96	0.43
1:A:169:TYR:HA	1:A:172:ASN:HD22	1.83	0.43
1:A:467:LYS:HB2	1:A:507:VAL:HG13	1.96	0.43
1:A:502:LEU:HD21	1:A:540:VAL:HG22	2.00	0.43
2:B:248:LYS:CD	2:B:290:LYS:HZ2	2.30	0.43
3:C:51:PRO:HB3	3:C:279:ASP:O	2.18	0.43
1:D:438:PHE:CD1	1:D:438:PHE:O	2.71	0.43
2:E:85:VAL:HG13	2:E:130:PHE:CE2	2.53	0.43
2:E:134:PHE:C	2:E:136:GLU:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:330:PHE:CD1	2:E:330:PHE:C	2.96	0.43
3:F:81:LEU:HD23	3:F:81:LEU:O	2.18	0.43
3:F:118:HIS:ND1	3:F:123:ILE:CG2	2.80	0.43
3:F:221:GLY:O	3:F:222:GLN:C	2.61	0.43
1:A:262:MSE:O	1:A:263:VAL:C	2.59	0.43
2:B:164:GLU:C	2:B:165:ASP:O	2.58	0.43
2:B:309:GLU:C	2:B:311:VAL:N	2.75	0.43
3:C:125:GLN:HA	3:C:130:TYR:HB2	1.99	0.43
1:D:475:LYS:HB2	1:D:516:ILE:CD1	2.47	0.43
1:D:483:ILE:N	1:D:484:PRO:CD	2.81	0.43
2:E:245:HIS:HD1	2:E:245:HIS:H	1.66	0.43
2:E:283:TRP:HA	2:E:284:PRO:HD3	1.76	0.43
2:E:392:GLN:O	2:E:393:LYS:C	2.61	0.43
3:F:43:SER:OG	3:F:44:ASN:N	2.50	0.43
3:F:48:VAL:O	3:F:159:VAL:HA	2.18	0.43
1:A:144:ARG:O	1:A:145:THR:C	2.61	0.43
1:A:250:GLN:NE2	1:A:250:GLN:O	2.52	0.43
1:A:313:LEU:O	1:A:314:SER:C	2.61	0.43
2:B:280:LEU:HD11	2:B:317:LEU:HA	2.01	0.43
3:C:212:SER:C	3:C:214:ARG:H	2.25	0.43
1:D:500:THR:O	1:D:503:PHE:HB2	2.18	0.43
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.83	0.43
1:A:322:ILE:CD1	1:A:355:ILE:HG21	2.49	0.43
1:A:570:ASP:OD1	1:A:575:VAL:HG11	2.17	0.43
2:B:89:PHE:CZ	2:B:93:MSE:HG3	2.54	0.43
2:B:138:PRO:O	2:B:140:PHE:CD1	2.72	0.43
2:B:202:ILE:HD11	2:B:244:LEU:CG	2.41	0.43
3:C:76:PRO:HG3	3:C:107:TYR:CE1	2.53	0.43
3:C:117:ASN:H	3:C:167:HIS:CD2	2.36	0.43
3:C:187:GLN:HE21	3:C:187:GLN:HB2	1.66	0.43
1:D:109:VAL:O	1:D:110:GLU:C	2.62	0.43
1:D:189:LEU:HD11	1:D:205:ILE:HD12	1.99	0.43
1:D:368:LEU:O	1:D:369:PHE:C	2.62	0.43
1:D:411:LEU:O	1:D:412:ALA:C	2.61	0.43
2:E:78:THR:O	2:E:78:THR:HG22	2.17	0.43
2:E:222:ILE:HD13	2:E:264:PHE:HD1	1.83	0.43
2:E:242:LEU:HD11	2:E:275:VAL:HA	2.00	0.43
2:E:387:PHE:HD1	2:E:387:PHE:HA	1.68	0.43
3:F:36:LYS:O	3:F:37:GLU:C	2.62	0.43
3:F:123:ILE:N	3:F:123:ILE:HD12	2.34	0.43
1:A:36:SER:C	1:A:38:ILE:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:SER:C	1:A:118:GLU:H	2.26	0.43
1:A:180:MSE:CE	1:A:180:MSE:H	2.29	0.43
1:A:206:ILE:HB	1:A:207:PRO:HD3	2.00	0.43
2:B:254:HIS:N	2:B:255:PRO:HD2	2.33	0.43
2:B:271:LEU:O	2:B:274:PRO:HD2	2.19	0.43
2:B:373:ASN:C	2:B:375:THR:N	2.76	0.43
1:D:40:LEU:O	1:D:42:LEU:N	2.51	0.43
1:D:408:ILE:HD13	1:D:426:TYR:CE2	2.48	0.43
1:D:506:ASN:ND2	1:D:543:SER:HA	2.34	0.43
2:E:167:ARG:O	2:E:168:GLU:C	2.61	0.43
2:E:313:ILE:HG22	2:E:317:LEU:CB	2.46	0.43
1:A:78:THR:HB	1:A:79:LEU:HD12	2.00	0.43
1:A:128:PHE:O	1:A:129:VAL:C	2.61	0.43
1:A:155:TYR:CE1	1:A:167:ARG:HG2	2.54	0.43
1:A:535:ASN:HA	1:A:538:PHE:CD2	2.50	0.43
2:B:176:LEU:O	2:B:176:LEU:HG	2.19	0.43
2:B:332:VAL:O	2:B:335:ARG:N	2.52	0.43
3:C:25:GLU:O	3:C:26:SER:C	2.61	0.43
3:C:131:ASP:O	3:C:132:GLU:C	2.61	0.43
1:D:142:THR:OG1	1:D:143:SER:N	2.51	0.43
1:D:239:ASP:O	1:D:240:LEU:C	2.60	0.43
2:E:316:PRO:CG	2:E:317:LEU:N	2.82	0.43
1:A:24:ASP:OD2	1:A:26:GLN:HB3	2.19	0.43
2:B:88:MSE:HE1	2:B:127:VAL:HG13	2.00	0.43
2:B:384:LEU:O	2:B:385:LYS:C	2.59	0.43
3:C:24:SER:O	3:C:25:GLU:C	2.61	0.43
3:C:24:SER:O	3:C:27:GLN:HB2	2.18	0.43
3:C:48:VAL:O	3:C:159:VAL:HA	2.18	0.43
3:C:274:ALA:CB	3:C:288:GLN:HA	2.46	0.43
1:D:578:PHE:O	1:D:582:ALA:HB2	2.18	0.43
2:E:356:ILE:O	2:E:357:LEU:C	2.61	0.43
1:A:9:SER:OG	1:A:10:LEU:N	2.51	0.43
1:A:179:PRO:HB2	1:A:183:ARG:HH12	1.84	0.43
2:B:254:HIS:CD2	2:B:293:MSE:HB3	2.54	0.43
2:B:361:PHE:N	2:B:362:PRO:HD2	2.33	0.43
3:C:162:GLN:HB3	3:C:235:THR:HG21	2.00	0.43
1:D:145:THR:CG2	1:D:146:SER:N	2.78	0.43
1:D:353:SER:HB3	1:D:394:VAL:HG21	2.01	0.43
1:D:522:LEU:O	1:D:522:LEU:HD12	2.19	0.43
3:F:17:LEU:CD1	3:F:99:LEU:HA	2.48	0.43
1:A:423:ILE:O	1:A:424:ILE:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ILE:C	1:A:507:VAL:N	2.76	0.43
2:B:35:LYS:O	2:B:38:GLN:N	2.52	0.43
2:E:222:ILE:O	2:E:224:GLY:N	2.52	0.43
2:E:242:LEU:HA	2:E:242:LEU:HD23	1.75	0.43
2:E:302:LEU:HD11	2:E:317:LEU:HD21	1.99	0.43
3:F:94:VAL:O	3:F:95:GLU:C	2.62	0.43
1:A:11:TYR:HD2	1:A:11:TYR:HA	1.69	0.42
1:A:317:CYS:O	1:A:321:VAL:HG13	2.19	0.42
1:A:326:ILE:C	1:A:328:PRO:CD	2.92	0.42
3:C:28:VAL:O	3:C:29:LYS:C	2.62	0.42
1:D:506:ASN:HD21	1:D:543:SER:CA	2.32	0.42
2:E:393:LYS:HG2	2:E:397:ASP:OD2	2.18	0.42
1:A:16:LEU:C	1:A:18:ASP:H	2.27	0.42
1:A:506:ASN:HD21	1:A:543:SER:CA	2.32	0.42
3:C:17:LEU:O	3:C:20:CYS:N	2.42	0.42
3:C:279:ASP:OD1	3:C:283:LYS:N	2.51	0.42
1:D:179:PRO:O	1:D:182:ARG:N	2.52	0.42
1:D:350:MSE:HG3	1:D:387:ASN:HB3	2.01	0.42
1:D:507:VAL:HA	1:D:510:GLU:OE1	2.19	0.42
1:D:509:SER:CB	1:D:547:ILE:HG22	2.50	0.42
2:E:332:VAL:C	2:E:334:GLU:N	2.77	0.42
1:A:38:ILE:N	1:A:38:ILE:HD12	2.34	0.42
1:A:262:MSE:C	1:A:264:ALA:N	2.76	0.42
1:A:438:PHE:O	1:A:438:PHE:CD1	2.66	0.42
1:A:482:ILE:O	1:A:483:ILE:C	2.62	0.42
1:A:517:THR:HG23	1:A:521:MSE:HE3	2.00	0.42
1:A:538:PHE:HB3	1:A:575:VAL:HA	2.01	0.42
1:A:563:ILE:C	1:A:565:GLU:H	2.27	0.42
2:B:304:VAL:O	2:B:305:ILE:C	2.62	0.42
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.82	0.42
3:C:85:ASP:OD1	3:C:117:ASN:OD1	2.37	0.42
1:D:90:LEU:HD23	1:D:90:LEU:HA	1.76	0.42
1:D:260:ARG:NH1	1:D:260:ARG:CG	2.82	0.42
1:D:275:GLY:HA3	1:D:278:ILE:HD13	2.01	0.42
2:E:76:VAL:O	2:E:76:VAL:HG12	2.19	0.42
2:E:350:SER:C	2:E:352:ASN:H	2.27	0.42
3:F:68:LEU:O	3:F:71:ILE:N	2.47	0.42
3:F:240:ALA:HA	3:F:258:THR:CG2	2.38	0.42
1:A:251:ALA:C	1:A:253:GLU:H	2.28	0.42
1:A:388:LEU:HA	1:A:391:VAL:HG22	2.01	0.42
1:A:482:ILE:O	1:A:484:PRO:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:LEU:O	2:B:65:GLU:N	2.53	0.42
2:B:97:LEU:HD12	2:B:97:LEU:N	2.32	0.42
2:B:393:LYS:O	2:B:394:LEU:C	2.62	0.42
1:D:141:PHE:HA	1:D:144:ARG:HD3	2.01	0.42
1:D:205:ILE:HA	1:D:205:ILE:HD13	1.79	0.42
1:D:222:LEU:HG	1:D:223:LEU:HD23	2.00	0.42
1:D:537:ARG:HG3	1:D:537:ARG:HH11	1.84	0.42
2:E:176:LEU:O	2:E:176:LEU:CG	2.64	0.42
2:E:202:ILE:HG22	2:E:203:TYR:CD2	2.55	0.42
1:A:326:ILE:N	1:A:326:ILE:CD1	2.82	0.42
2:B:85:VAL:O	2:B:88:MSE:HB3	2.19	0.42
2:B:254:HIS:CG	2:B:293:MSE:HE2	2.55	0.42
2:B:306:GLU:O	2:B:309:GLU:N	2.47	0.42
3:C:97:VAL:CG1	3:C:98:THR:N	2.83	0.42
3:C:124:THR:HB	3:C:129:PHE:HB3	2.00	0.42
3:C:125:GLN:HA	3:C:130:TYR:CB	2.50	0.42
3:C:155:LEU:CD1	3:C:195:MET:HG3	2.50	0.42
1:D:65:VAL:O	1:D:68:ALA:HB3	2.18	0.42
1:D:205:ILE:O	1:D:206:ILE:C	2.61	0.42
3:F:166:LEU:O	3:F:166:LEU:HD23	2.20	0.42
3:F:187:GLN:HE21	3:F:187:GLN:HB2	1.68	0.42
3:F:204:ASP:HB2	3:F:219:THR:HB	2.01	0.42
3:F:263:PRO:N	3:F:273:ALA:HB2	2.35	0.42
2:B:287:HIS:O	2:B:287:HIS:ND1	2.53	0.42
2:B:329:HIS:CD2	2:B:332:VAL:HG23	2.55	0.42
2:B:329:HIS:O	2:B:330:PHE:C	2.61	0.42
2:B:337:LEU:HD12	2:B:337:LEU:N	2.34	0.42
2:B:407:LEU:C	2:B:407:LEU:CD2	2.92	0.42
3:C:99:LEU:O	3:C:100:LEU:C	2.61	0.42
3:C:274:ALA:HB1	3:C:287:LEU:O	2.20	0.42
1:D:180:MSE:HE2	1:D:183:ARG:HH22	1.84	0.42
2:E:69:TYR:O	2:E:74:ARG:HB2	2.19	0.42
2:E:222:ILE:HD13	2:E:264:PHE:CD1	2.54	0.42
2:E:313:ILE:H	2:E:313:ILE:CD1	2.27	0.42
2:E:335:ARG:O	2:E:335:ARG:HG3	2.18	0.42
3:F:120:SER:O	3:F:121:ARG:C	2.61	0.42
3:F:148:ASP:O	3:F:149:LEU:C	2.62	0.42
1:A:22:ASN:HD22	1:A:24:ASP:HB3	1.80	0.42
1:A:161:ALA:O	1:A:165:GLU:HG3	2.18	0.42
1:A:275:GLY:HA3	1:A:278:ILE:HD13	2.00	0.42
1:A:500:THR:O	1:A:503:PHE:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:ASP:OD1	1:A:552:ASP:O	2.38	0.42
2:B:71:THR:CG2	2:B:133:ARG:HH11	2.32	0.42
2:B:121:TRP:C	2:B:123:HIS:H	2.28	0.42
2:B:164:GLU:CB	2:B:168:GLU:CB	2.95	0.42
2:B:325:VAL:HG11	2:B:364:LEU:CD2	2.50	0.42
3:C:135:ARG:HG2	3:C:135:ARG:HH11	1.83	0.42
3:C:156:THR:HG22	3:C:166:LEU:HB3	2.02	0.42
1:D:497:HIS:O	1:D:498:ARG:C	2.63	0.42
2:E:119:ALA:O	2:E:120:ALA:CB	2.68	0.42
2:E:134:PHE:HE2	2:E:135:LEU:HD22	1.84	0.42
3:F:131:ASP:O	3:F:134:LEU:N	2.53	0.42
4:G:6:FGA:HG3	4:G:7:DAM:HM1	1.79	0.42
1:A:178:THR:OG1	1:A:181:VAL:CG2	2.67	0.42
1:A:362:ILE:HD13	1:A:399:GLN:CG	2.39	0.42
1:A:368:LEU:O	1:A:371:ALA:HB3	2.19	0.42
2:B:157:LEU:HD11	2:B:172:LEU:HD23	2.02	0.42
3:C:61:GLN:HA	3:C:267:TYR:OH	2.20	0.42
3:C:239:ARG:HD3	3:C:239:ARG:C	2.45	0.42
1:D:76:PHE:O	1:D:80:VAL:HG12	2.19	0.42
1:D:213:ALA:C	1:D:221:ARG:HG2	2.45	0.42
1:D:572:ASP:OD2	3:F:110:ARG:NH2	2.52	0.42
2:E:132:LEU:O	2:E:134:PHE:N	2.52	0.42
3:F:17:LEU:HD12	3:F:99:LEU:HA	2.01	0.42
3:F:66:MET:O	3:F:69:PHE:HB2	2.19	0.42
1:A:343:SER:OG	1:A:379:GLU:HB3	2.19	0.42
1:A:372:GLN:C	1:A:374:LYS:N	2.76	0.42
2:B:72:HIS:C	2:B:74:ARG:N	2.78	0.42
2:B:276:VAL:HG11	2:B:313:ILE:HG21	2.02	0.42
2:B:295:LEU:HA	2:B:295:LEU:HD23	1.79	0.42
2:B:346:MSE:O	2:B:347:SER:C	2.62	0.42
1:D:197:GLU:O	1:D:201:VAL:HG23	2.19	0.42
3:F:164:PHE:HB2	3:F:234:LEU:HD13	2.01	0.42
3:F:185:ARG:HG2	3:F:185:ARG:HH11	1.85	0.42
1:A:20:LEU:HD23	1:A:31:SER:HB3	2.01	0.42
1:A:348:VAL:O	1:A:349:ILE:C	2.63	0.42
1:A:368:LEU:O	1:A:371:ALA:N	2.53	0.42
1:A:464:SER:C	1:A:466:LEU:N	2.77	0.42
2:B:31:LEU:C	2:B:33:ILE:N	2.76	0.42
1:D:27:LEU:C	1:D:29:LEU:N	2.77	0.42
1:D:180:MSE:HE3	1:D:180:MSE:N	2.21	0.42
1:D:277:GLU:O	1:D:279:THR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:63:LEU:O	2:E:64:SER:C	2.62	0.42
2:E:134:PHE:O	2:E:136:GLU:N	2.53	0.42
1:A:257:TRP:CZ2	2:B:99:PRO:HD3	2.55	0.41
2:B:59:LYS:O	2:B:60:ARG:C	2.63	0.41
2:B:202:ILE:HG22	2:B:203:TYR:CG	2.55	0.41
2:B:235:ILE:O	2:B:236:PHE:C	2.63	0.41
1:D:44:VAL:O	1:D:46:ARG:N	2.53	0.41
1:D:105:ARG:O	1:D:109:VAL:HG23	2.20	0.41
1:D:334:VAL:O	1:D:334:VAL:HG12	2.20	0.41
1:D:377:CYS:O	1:D:378:PRO:C	2.64	0.41
1:D:505:ILE:C	1:D:507:VAL:H	2.28	0.41
2:E:368:SER:O	2:E:377:HIS:ND1	2.52	0.41
3:F:54:VAL:HB	3:F:276:MET:HB3	2.02	0.41
3:F:104:LYS:CA	3:F:111:ILE:HD11	2.50	0.41
4:H:2:LEU:H	4:H:7:DAM:C	2.33	0.41
1:A:90:LEU:HB2	1:A:91:PRO:CD	2.43	0.41
1:A:127:HIS:O	1:A:130:PRO:HD2	2.20	0.41
2:B:241:LEU:HD22	2:B:257:LEU:CD1	2.50	0.41
3:C:12:GLN:O	3:C:13:TRP:C	2.61	0.41
3:C:94:VAL:HB	3:C:95:GLU:OE1	2.20	0.41
3:C:134:LEU:O	3:C:136:LYS:N	2.54	0.41
3:C:203:PRO:HA	3:C:220:PHE:CD1	2.55	0.41
3:C:228:PHE:O	3:C:231:ALA:HB3	2.20	0.41
1:D:24:ASP:O	1:D:24:ASP:CG	2.62	0.41
1:D:128:PHE:O	1:D:131:LEU:N	2.52	0.41
1:D:258:ARG:HG3	1:D:258:ARG:NH1	2.32	0.41
1:D:373:LEU:HD11	1:D:385:ILE:HD13	2.02	0.41
2:E:306:GLU:O	2:E:307:PRO:C	2.63	0.41
3:F:107:TYR:HB3	3:F:110:ARG:HG3	2.02	0.41
1:A:151:PHE:O	1:A:153:VAL:N	2.54	0.41
1:A:515:ASP:C	1:A:517:THR:N	2.77	0.41
2:B:69:TYR:CZ	2:B:75:ASN:ND2	2.87	0.41
2:B:76:VAL:O	2:B:76:VAL:HG12	2.20	0.41
2:B:160:LEU:C	2:B:162:ASP:N	2.72	0.41
3:C:59:HIS:CE1	3:C:85:ASP:HB3	2.55	0.41
1:D:343:SER:O	1:D:346:ALA:HB3	2.20	0.41
2:E:219:GLY:O	2:E:220:SER:C	2.64	0.41
2:E:278:ALA:O	2:E:279:LEU:C	2.63	0.41
2:E:305:ILE:CG2	2:E:348:LEU:HD11	2.50	0.41
3:F:118:HIS:C	3:F:120:SER:N	2.77	0.41
3:F:144:LYS:O	3:F:145:TYR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:203:PRO:HB3	3:F:220:PHE:HE1	1.85	0.41
1:A:429:LEU:O	1:A:430:LEU:C	2.64	0.41
1:A:456:TYR:O	1:A:457:ALA:C	2.64	0.41
2:B:78:THR:O	2:B:78:THR:HG22	2.21	0.41
2:B:183:PHE:CB	2:B:186:LEU:HD22	2.51	0.41
3:C:6:PHE:O	3:C:9:GLU:N	2.53	0.41
3:C:279:ASP:CG	3:C:280:ASP:N	2.77	0.41
3:C:286:PHE:O	3:C:287:LEU:HD23	2.20	0.41
1:D:219:SER:HA	1:D:222:LEU:CD2	2.50	0.41
1:D:245:MSE:HE3	1:D:245:MSE:CA	2.50	0.41
1:D:273:ALA:O	1:D:274:VAL:C	2.63	0.41
2:E:184:LEU:HA	2:E:187:ARG:HG3	2.01	0.41
2:E:295:LEU:HA	2:E:295:LEU:HD23	1.77	0.41
3:F:65:LEU:HD12	3:F:65:LEU:C	2.46	0.41
3:F:194:PRO:O	3:F:195:MET:C	2.64	0.41
3:F:211:ILE:HD12	3:F:212:SER:H	1.85	0.41
1:A:73:LEU:HB2	1:A:93:LEU:HD21	2.03	0.41
1:A:119:HIS:CD2	1:A:119:HIS:N	2.89	0.41
1:A:359:ASP:O	1:A:360:ASN:C	2.63	0.41
1:A:509:SER:N	1:A:521:MSE:HE1	2.36	0.41
2:B:357:LEU:HD12	2:B:361:PHE:CE1	2.56	0.41
3:C:134:LEU:C	3:C:136:LYS:N	2.77	0.41
1:D:378:PRO:O	1:D:381:ARG:N	2.53	0.41
1:D:515:ASP:O	1:D:518:THR:N	2.52	0.41
1:D:522:LEU:O	1:D:526:LEU:HG	2.20	0.41
2:E:121:TRP:CD1	2:E:167:ARG:NH1	2.89	0.41
2:E:329:HIS:O	2:E:330:PHE:C	2.63	0.41
3:F:76:PRO:HD3	3:F:107:TYR:CZ	2.55	0.41
3:F:121:ARG:N	3:F:188:GLU:OE2	2.54	0.41
3:F:169:GLY:HA3	3:F:220:PHE:HE2	1.85	0.41
1:A:90:LEU:CB	1:A:91:PRO:CD	2.97	0.41
1:A:196:LEU:CD1	1:A:205:ILE:HD11	2.51	0.41
1:A:378:PRO:O	1:A:379:GLU:C	2.64	0.41
1:A:423:ILE:HD13	1:A:423:ILE:HA	1.81	0.41
2:B:165:ASP:CG	2:B:166:PRO:HD2	2.45	0.41
2:B:316:PRO:HG2	2:B:317:LEU:N	2.36	0.41
2:B:344:TYR:CD1	2:B:344:TYR:C	2.98	0.41
2:B:365:TYR:CD2	2:B:402:PHE:HE2	2.37	0.41
2:B:387:PHE:HD1	2:B:387:PHE:HA	1.76	0.41
3:C:96:THR:O	3:C:99:LEU:HB3	2.20	0.41
3:C:100:LEU:HA	3:C:100:LEU:HD23	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:170:LEU:HB2	3:C:220:PHE:HD2	1.80	0.41
1:D:285:PRO:HA	1:D:288:GLN:OE1	2.20	0.41
1:D:345:LEU:HD23	1:D:345:LEU:C	2.45	0.41
1:D:475:LYS:HB2	1:D:516:ILE:HD11	2.01	0.41
2:E:145:ALA:O	2:E:148:TYR:N	2.31	0.41
1:A:205:ILE:HD13	1:A:208:MSE:HE3	2.03	0.41
1:A:426:TYR:CD1	1:A:426:TYR:O	2.73	0.41
2:B:124:LEU:O	2:B:127:VAL:N	2.54	0.41
2:B:134:PHE:CE2	2:B:135:LEU:HD22	2.56	0.41
2:B:285:LYS:HB2	2:B:285:LYS:HE3	1.87	0.41
3:C:118:HIS:ND1	3:C:123:ILE:CG2	2.83	0.41
1:D:52:LEU:CB	1:D:53:PRO:HD3	2.48	0.41
1:D:86:VAL:C	1:D:88:CYS:N	2.79	0.41
1:D:90:LEU:CB	1:D:91:PRO:HD3	2.47	0.41
1:D:107:LYS:HZ2	1:D:110:GLU:CD	2.28	0.41
1:D:398:ARG:HH11	1:D:398:ARG:CB	2.32	0.41
1:D:415:ALA:O	1:D:416:LYS:C	2.63	0.41
1:D:427:MSE:CE	1:D:430:LEU:HB2	2.50	0.41
1:D:563:ILE:O	1:D:563:ILE:HG12	2.20	0.41
2:E:184:LEU:HD23	2:E:187:ARG:CZ	2.51	0.41
2:E:320:GLN:O	2:E:321:LEU:C	2.61	0.41
2:E:346:MSE:CE	2:E:349:ILE:HD12	2.51	0.41
3:F:116:GLY:C	3:F:118:HIS:N	2.77	0.41
3:F:128:GLY:O	3:F:129:PHE:C	2.63	0.41
3:F:194:PRO:CG	3:F:195:MET:N	2.84	0.41
1:A:155:TYR:CE2	1:A:163:LYS:HD3	2.56	0.41
1:A:174:CYS:O	1:A:212:LEU:HD21	2.21	0.41
1:A:237:GLN:O	1:A:240:LEU:HB2	2.20	0.41
1:A:259:VAL:O	1:A:262:MSE:HB2	2.20	0.41
1:A:264:ALA:O	1:A:267:PHE:HB2	2.21	0.41
1:A:274:VAL:HG12	1:A:278:ILE:HB	2.02	0.41
1:A:388:LEU:C	1:A:390:CYS:H	2.29	0.41
1:A:400:LEU:CD1	1:A:404:LEU:HD23	2.50	0.41
1:A:419:VAL:O	1:A:420:ARG:C	2.64	0.41
2:B:271:LEU:O	2:B:274:PRO:HG2	2.21	0.41
3:C:68:LEU:HD23	3:C:69:PHE:N	2.35	0.41
3:C:153:LEU:HA	3:C:154:PRO:HD2	1.90	0.41
3:C:154:PRO:HA	3:C:185:ARG:NE	2.35	0.41
1:D:101:GLU:C	1:D:101:GLU:OE1	2.63	0.41
1:D:316:ASP:O	1:D:317:CYS:HB3	2.21	0.41
1:D:411:LEU:C	1:D:413:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:126:LEU:O	2:E:127:VAL:C	2.62	0.41
2:E:180:TYR:CE2	2:E:221:ILE:HG23	2.54	0.41
2:E:344:TYR:CD1	2:E:344:TYR:C	2.99	0.41
1:A:365:LEU:C	1:A:367:PRO:CD	2.93	0.41
1:A:424:ILE:HG12	1:A:450:TRP:CD2	2.55	0.41
1:A:455:VAL:HG13	1:A:455:VAL:O	2.20	0.41
2:B:61:ALA:C	2:B:63:LEU:N	2.79	0.41
2:B:68:GLU:HG3	2:B:68:GLU:H	1.72	0.41
2:B:109:ASP:HA	2:B:110:PRO:HD2	1.87	0.41
3:C:43:SER:OG	3:C:45:VAL:O	2.35	0.41
3:C:76:PRO:O	3:C:77:ASP:C	2.62	0.41
3:C:163:ILE:HG23	3:C:236:LEU:O	2.20	0.41
3:C:199:LEU:HD12	3:C:199:LEU:N	2.36	0.41
3:C:221:GLY:O	3:C:222:GLN:C	2.63	0.41
3:C:264:ASN:O	3:C:265:TYR:O	2.39	0.41
1:D:75:THR:C	1:D:77:THR:N	2.79	0.41
1:D:136:ALA:O	1:D:144:ARG:HG2	2.20	0.41
1:D:172:ASN:C	1:D:174:CYS:N	2.77	0.41
1:D:176:ASP:OD1	1:D:177:ASP:N	2.54	0.41
1:D:189:LEU:HD11	1:D:205:ILE:CD1	2.51	0.41
1:D:436:VAL:HB	1:D:473:PHE:CE1	2.55	0.41
1:D:505:ILE:C	1:D:507:VAL:N	2.77	0.41
1:D:521:MSE:C	1:D:523:PRO:HD2	2.45	0.41
1:D:564:LEU:O	1:D:564:LEU:CD2	2.67	0.41
2:E:75:ASN:OD1	2:E:78:THR:OG1	2.38	0.41
2:E:97:LEU:HD12	2:E:97:LEU:N	2.31	0.41
2:E:316:PRO:CG	2:E:317:LEU:H	2.32	0.41
2:E:350:SER:O	2:E:351:ASP:C	2.63	0.41
2:E:356:ILE:C	2:E:358:PRO:CD	2.90	0.41
2:E:401:GLN:O	2:E:404:ALA:HB3	2.21	0.41
3:F:24:SER:HG	3:F:27:GLN:HG3	1.85	0.41
3:F:25:GLU:O	3:F:26:SER:C	2.62	0.41
3:F:190:PRO:HD3	3:F:195:MET:CE	2.38	0.41
3:F:204:ASP:N	3:F:220:PHE:O	2.51	0.41
3:F:244:VAL:HG21	3:F:248:TYR:CA	2.51	0.41
1:A:24:ASP:O	1:A:24:ASP:CG	2.63	0.41
1:A:192:PHE:O	1:A:195:VAL:HG22	2.21	0.41
2:B:361:PHE:C	2:B:363:SER:N	2.79	0.41
1:D:126:ALA:C	1:D:127:HIS:CD2	2.99	0.41
1:D:423:ILE:O	1:D:424:ILE:C	2.61	0.41
2:E:63:LEU:O	2:E:67:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:159:GLU:O	2:E:161:PHE:N	2.53	0.41
3:F:6:PHE:C	3:F:8:LYS:N	2.78	0.41
3:F:32:CYS:O	3:F:33:GLU:C	2.64	0.41
1:A:67:LEU:HA	1:A:104:VAL:HG22	2.02	0.40
1:A:79:LEU:N	1:A:79:LEU:CD1	2.84	0.40
1:A:464:SER:O	1:A:465:ASN:C	2.63	0.40
2:B:158:LEU:O	2:B:161:PHE:CD1	2.74	0.40
2:B:202:ILE:HG22	2:B:203:TYR:CD1	2.57	0.40
2:B:216:GLU:O	2:B:219:GLY:N	2.49	0.40
2:B:301:ILE:O	2:B:302:LEU:C	2.62	0.40
1:D:262:MSE:C	1:D:264:ALA:N	2.78	0.40
1:D:297:GLU:C	1:D:299:ARG:N	2.79	0.40
1:D:366:LEU:N	1:D:367:PRO:CD	2.83	0.40
1:D:384:ILE:HG22	1:D:385:ILE:N	2.36	0.40
1:D:414:ASP:OD2	1:D:414:ASP:C	2.64	0.40
1:D:455:VAL:HG13	1:D:458:ILE:HB	2.02	0.40
3:F:265:TYR:C	3:F:267:TYR:N	2.78	0.40
1:A:131:LEU:HD23	1:A:135:LEU:HD12	2.03	0.40
1:A:151:PHE:C	1:A:153:VAL:N	2.79	0.40
1:A:353:SER:HB3	1:A:394:VAL:HG21	2.03	0.40
1:A:379:GLU:O	1:A:383:ASN:HB2	2.21	0.40
2:B:121:TRP:O	2:B:122:PRO:C	2.65	0.40
2:B:372:TRP:O	2:B:374:LYS:N	2.54	0.40
3:C:56:GLY:N	3:C:261:SER:OG	2.49	0.40
3:C:116:GLY:C	3:C:118:HIS:N	2.78	0.40
1:D:94:GLU:O	1:D:94:GLU:HG2	2.21	0.40
1:D:121:PRO:O	1:D:122:SER:C	2.65	0.40
1:D:526:LEU:C	1:D:528:MSE:N	2.79	0.40
1:D:563:ILE:C	1:D:565:GLU:H	2.29	0.40
2:E:97:LEU:HD22	2:E:162:ASP:HB2	2.03	0.40
2:E:332:VAL:O	2:E:334:GLU:N	2.54	0.40
2:E:337:LEU:HD12	2:E:337:LEU:N	2.36	0.40
3:F:266:CYS:O	3:F:267:TYR:HB2	2.21	0.40
1:A:116:SER:C	1:A:118:GLU:N	2.79	0.40
1:A:120:SER:O	1:A:123:ASP:N	2.54	0.40
1:A:251:ALA:C	1:A:253:GLU:N	2.77	0.40
1:A:372:GLN:O	1:A:373:LEU:C	2.64	0.40
2:B:63:LEU:C	2:B:65:GLU:H	2.29	0.40
1:D:124:LEU:O	1:D:126:ALA:N	2.54	0.40
2:E:59:LYS:C	2:E:61:ALA:N	2.78	0.40
2:E:283:TRP:HZ3	2:E:298:LEU:CD2	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:50:CYS:HB2	3:F:51:PRO:CA	2.43	0.40
3:F:81:LEU:HA	3:F:112:THR:O	2.21	0.40
3:F:225:SER:OG	3:F:252:HIS:ND1	2.52	0.40
1:A:146:SER:O	1:A:147:ALA:C	2.64	0.40
1:A:353:SER:HB2	1:A:354:PRO:CD	2.52	0.40
1:A:395:ILE:HD11	1:A:400:LEU:HB2	2.04	0.40
1:A:427:MSE:N	1:A:428:PRO:HD2	2.36	0.40
2:B:126:LEU:C	2:B:128:TYR:N	2.79	0.40
2:B:262:VAL:O	2:B:263:GLN:C	2.63	0.40
3:C:155:LEU:HD11	3:C:195:MET:HG3	2.03	0.40
3:C:212:SER:OG	3:C:214:ARG:HB2	2.22	0.40
3:C:265:TYR:C	3:C:267:TYR:N	2.75	0.40
1:D:29:LEU:HD13	1:D:64:GLU:HG2	2.03	0.40
1:D:63:ASP:O	1:D:64:GLU:C	2.64	0.40
1:D:453:ASP:O	1:D:459:ARG:HD3	2.21	0.40
2:E:67:VAL:O	2:E:69:TYR:N	2.53	0.40
2:E:109:ASP:OD1	2:E:110:PRO:HD2	2.21	0.40
2:E:117:LEU:HA	2:E:164:GLU:OE1	2.21	0.40
3:F:121:ARG:HG3	3:F:121:ARG:NH1	2.35	0.40
3:F:162:GLN:O	3:F:235:THR:HG22	2.21	0.40
3:F:172:PRO:C	3:F:174:ILE:N	2.79	0.40
1:A:274:VAL:HG21	1:A:283:LEU:HD11	2.02	0.40
1:A:391:VAL:C	1:A:393:GLU:N	2.77	0.40
2:B:244:LEU:C	2:B:246:LYS:H	2.29	0.40
1:D:23:GLU:HG2	1:D:23:GLU:O	2.20	0.40
1:D:76:PHE:N	1:D:76:PHE:CD1	2.90	0.40
1:D:236:PRO:O	1:D:237:GLN:C	2.64	0.40
2:E:85:VAL:HB	2:E:134:PHE:HE1	1.86	0.40
2:E:121:TRP:HB3	2:E:122:PRO:CD	2.51	0.40
2:E:128:TYR:O	2:E:129:GLU:C	2.65	0.40
2:E:161:PHE:CD2	2:E:214:LEU:HG	2.56	0.40
2:E:208:HIS:HB3	2:E:211:ILE:HD13	2.03	0.40
3:F:51:PRO:O	3:F:52:VAL:HG13	2.22	0.40
3:F:209:TRP:CD2	3:F:224:ILE:HD13	2.57	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	580/582 (100%)	411 (71%)	124 (21%)	45 (8%)	1	11
1	D	580/582 (100%)	411 (71%)	119 (20%)	50 (9%)	0	9
2	B	386/388 (100%)	234 (61%)	97 (25%)	55 (14%)	0	3
2	E	386/388 (100%)	234 (61%)	95 (25%)	57 (15%)	0	2
3	C	291/293 (99%)	203 (70%)	69 (24%)	19 (6%)	1	14
3	F	291/293 (99%)	210 (72%)	63 (22%)	18 (6%)	1	14
4	G	1/7 (14%)	1 (100%)	0	0	100	100
4	H	1/7 (14%)	1 (100%)	0	0	100	100
All	All	2516/2540 (99%)	1705 (68%)	567 (22%)	244 (10%)	0	7

All (244) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	35	LEU
1	A	44	VAL
1	A	317	CYS
1	A	391	VAL
1	A	412	ALA
1	A	560	VAL
2	B	33	ILE
2	B	43	PHE
2	B	44	ASP
2	B	46	VAL
2	B	55	TRP
2	B	57	GLU
2	B	73	ASN
2	B	81	ILE
2	B	103	PRO
2	B	104	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	146	LYS
2	B	161	PHE
2	B	165	ASP
2	B	166	PRO
2	B	167	ARG
2	B	229	LEU
2	B	268	ASP
2	B	367	ASN
2	B	368	SER
2	B	390	MSE
2	B	413	MSE
3	C	94	VAL
3	C	254	ARG
3	C	265	TYR
1	D	25	VAL
1	D	35	LEU
1	D	44	VAL
1	D	73	LEU
1	D	391	VAL
1	D	415	ALA
1	D	515	ASP
2	E	33	ILE
2	E	43	PHE
2	E	44	ASP
2	E	46	VAL
2	E	55	TRP
2	E	57	GLU
2	E	72	HIS
2	E	73	ASN
2	E	146	LYS
2	E	161	PHE
2	E	165	ASP
2	E	166	PRO
2	E	167	ARG
2	E	229	LEU
2	E	367	ASN
2	E	368	SER
2	E	390	MSE
2	E	413	MSE
3	F	94	VAL
3	F	254	ARG
3	F	265	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	23	GLU
1	A	86	VAL
1	A	89	LEU
1	A	238	GLU
1	A	254	ASP
1	A	274	VAL
1	A	318	ARG
1	A	349	ILE
1	A	373	LEU
1	A	415	ALA
1	A	465	ASN
1	A	474	GLY
1	A	490	SER
1	A	500	THR
1	A	513	GLY
1	A	515	ASP
1	A	553	ASN
2	B	72	HIS
2	B	76	VAL
2	B	125	GLN
2	B	135	LEU
2	B	223	ASN
2	B	287	HIS
2	B	314	MSE
2	B	374	LYS
2	B	389	GLU
3	C	41	LYS
3	C	135	ARG
3	C	161	GLY
3	C	207	GLY
3	C	240	ALA
3	C	253	ASP
3	C	270	GLY
1	D	76	PHE
1	D	86	VAL
1	D	147	ALA
1	D	254	ASP
1	D	263	VAL
1	D	274	VAL
1	D	297	GLU
1	D	317	CYS
1	D	349	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	412	ALA
1	D	513	GLY
1	D	529	ALA
1	D	560	VAL
1	D	576	LYS
2	E	51	SER
2	E	76	VAL
2	E	81	ILE
2	E	104	THR
2	E	125	GLN
2	E	160	LEU
2	E	223	ASN
2	E	251	SER
2	E	313	ILE
2	E	351	ASP
2	E	374	LYS
2	E	389	GLU
2	E	414	LYS
3	F	108	ARG
3	F	129	PHE
3	F	161	GLY
3	F	207	GLY
3	F	240	ALA
3	F	269	CYS
1	A	37	THR
1	A	152	SER
1	A	484	PRO
1	A	529	ALA
2	B	51	SER
2	B	90	ALA
2	B	163	SER
2	B	170	ASP
2	B	204	GLU
2	B	251	SER
2	B	284	PRO
2	B	362	PRO
3	C	108	ARG
3	C	231	ALA
1	D	23	GLU
1	D	318	ARG
1	D	344	ALA
1	D	399	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	416	LYS
1	D	428	PRO
1	D	490	SER
1	D	553	ASN
2	E	36	LEU
2	E	62	ALA
2	E	90	ALA
2	E	135	LEU
2	E	287	HIS
2	E	361	PHE
2	E	400	GLN
3	F	41	LYS
3	F	60	GLY
3	F	107	TYR
3	F	173	SER
3	F	186	LEU
3	F	253	ASP
1	A	99	VAL
1	A	117	HIS
1	A	297	GLU
1	A	334	VAL
2	B	62	ALA
2	B	66	MSE
2	B	133	ARG
2	B	196	ASN
2	B	313	ILE
2	B	361	PHE
2	B	400	GLN
2	B	414	LYS
3	C	36	LYS
3	C	129	PHE
3	C	186	LEU
3	C	282	LEU
1	D	12	PRO
1	D	100	GLU
1	D	103	VAL
1	D	298	VAL
1	D	533	VAL
1	D	577	TYR
2	E	66	MSE
2	E	84	GLU
2	E	103	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	170	ASP
2	E	268	ASP
2	E	271	LEU
2	E	362	PRO
1	A	12	PRO
1	A	87	HIS
1	A	237	GLN
1	A	271	GLN
1	A	416	LYS
1	A	428	PRO
1	A	506	ASN
2	B	141	GLN
2	B	330	PHE
3	C	107	TYR
1	D	28	ARG
1	D	45	GLU
1	D	87	HIS
1	D	117	HIS
1	D	516	ILE
1	D	547	ILE
1	D	581	GLU
2	E	86	VAL
2	E	133	ARG
2	E	163	SER
2	E	196	ASN
2	E	330	PHE
3	F	43	SER
3	F	282	LEU
1	A	516	ILE
1	A	523	PRO
1	A	576	LYS
2	B	79	GLU
2	B	303	ASP
2	B	328	PRO
3	C	88	ASP
1	D	396	GLY
1	D	492	ASP
1	D	532	PRO
2	E	343	GLU
2	B	228	PRO
1	D	91	PRO
2	E	141	GLN

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Mol	Chain	Res	Type
2	E	305	ILE
3	F	28	VAL
1	A	13	ILE
1	A	158	VAL
1	A	492	ASP
2	B	91	VAL
1	D	484	PRO
2	E	284	PRO
2	B	115	PRO
2	B	288	SER
1	D	13	ILE
1	D	99	VAL
2	E	79	GLU
2	E	228	PRO
2	E	262	VAL
3	C	90	GLY
1	D	523	PRO

### 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	509/496 (103%)	438 (86%)	71 (14%)	3	18
1	D	509/496 (103%)	440 (86%)	69 (14%)	3	18
2	B	331/351 (94%)	297 (90%)	34 (10%)	7	27
2	E	331/351 (94%)	290 (88%)	41 (12%)	4	21
3	C	259/259 (100%)	243 (94%)	16 (6%)	16	42
3	F	259/259 (100%)	244 (94%)	15 (6%)	18	44
4	G	2/2 (100%)	2 (100%)	0	100	100
4	H	2/2 (100%)	2 (100%)	0	100	100
All	All	2202/2216 (99%)	1956 (89%)	246 (11%)	6	24

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	15	VAL
1	A	18	ASP
1	A	32	ILE
1	A	44	VAL
1	A	48	ARG
1	A	62	GLU
1	A	65	VAL
1	A	77	THR
1	A	86	VAL
1	A	89	LEU
1	A	91	PRO
1	A	95	SER
1	A	101	GLU
1	A	104	VAL
1	A	107	LYS
1	A	122	SER
1	A	129	VAL
1	A	130	PRO
1	A	139	ASP
1	A	145	THR
1	A	153	VAL
1	A	177	ASP
1	A	180	MSE
1	A	197	GLU
1	A	198	LEU
1	A	204	GLU
1	A	211	ASN
1	A	214	SER
1	A	222	LEU
1	A	225	VAL
1	A	230	ASN
1	A	237	GLN
1	A	268	THR
1	A	278	ILE
1	A	294	CYS
1	A	295	GLU
1	A	297	GLU
1	A	306	VAL
1	A	313	LEU
1	A	345	LEU
1	A	348	VAL
1	A	373	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	379	GLU
1	A	382	LEU
1	A	383	ASN
1	A	384	ILE
1	A	385	ILE
1	A	391	VAL
1	A	395	ILE
1	A	398	ARG
1	A	399	GLN
1	A	404	LEU
1	A	414	ASP
1	A	419	VAL
1	A	427	MSE
1	A	437	GLU
1	A	438	PHE
1	A	443	LEU
1	A	446	LEU
1	A	447	CYS
1	A	451	LEU
1	A	475	LYS
1	A	476	GLU
1	A	489	MSE
1	A	508	LEU
1	A	515	ASP
1	A	524	THR
1	A	540	VAL
1	A	556	LEU
1	A	575	VAL
2	B	95	ARG
2	B	96	THR
2	B	101	SER
2	B	107	GLU
2	B	123	HIS
2	B	129	GLU
2	B	134	PHE
2	B	135	LEU
2	B	139	ASP
2	B	162	ASP
2	B	164	GLU
2	B	166	PRO
2	B	167	ARG
2	B	170	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	183	PHE
2	B	186	LEU
2	B	209	ASN
2	B	225	PHE
2	B	231	GLU
2	B	235	ILE
2	B	246	LYS
2	B	253	TYR
2	B	256	GLN
2	B	263	GLN
2	B	264	PHE
2	B	289	PRO
2	B	305	ILE
2	B	338	TYR
2	B	357	LEU
2	B	361	PHE
2	B	375	THR
2	B	380	ILE
2	B	386	LEU
2	B	387	PHE
3	C	71	ILE
3	C	75	SER
3	C	78	THR
3	C	81	LEU
3	C	99	LEU
3	C	110	ARG
3	C	119	GLU
3	C	159	VAL
3	C	160	ASP
3	C	173	SER
3	C	187	GLN
3	C	235	THR
3	C	239	ARG
3	C	242	GLN
3	C	284	TYR
3	C	294	ARG
1	D	8	ASP
1	D	15	VAL
1	D	18	ASP
1	D	42	LEU
1	D	44	VAL
1	D	53	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	62	GLU
1	D	65	VAL
1	D	71	GLU
1	D	77	THR
1	D	79	LEU
1	D	83	PRO
1	D	86	VAL
1	D	89	LEU
1	D	91	PRO
1	D	95	SER
1	D	101	GLU
1	D	104	VAL
1	D	107	LYS
1	D	115	ILE
1	D	116	SER
1	D	129	VAL
1	D	131	LEU
1	D	139	ASP
1	D	145	THR
1	D	179	PRO
1	D	180	MSE
1	D	195	VAL
1	D	197	GLU
1	D	198	LEU
1	D	204	GLU
1	D	214	SER
1	D	217	GLN
1	D	220	VAL
1	D	222	LEU
1	D	230	ASN
1	D	237	GLN
1	D	278	ILE
1	D	294	CYS
1	D	295	GLU
1	D	306	VAL
1	D	321	VAL
1	D	345	LEU
1	D	348	VAL
1	D	350	MSE
1	D	373	LEU
1	D	378	PRO
1	D	379	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	382	LEU
1	D	384	ILE
1	D	389	ASP
1	D	391	VAL
1	D	398	ARG
1	D	399	GLN
1	D	411	LEU
1	D	414	ASP
1	D	419	VAL
1	D	427	MSE
1	D	437	GLU
1	D	438	PHE
1	D	446	LEU
1	D	475	LYS
1	D	476	GLU
1	D	489	MSE
1	D	500	THR
1	D	515	ASP
1	D	524	THR
1	D	540	VAL
1	D	556	LEU
2	E	83	PRO
2	E	92	ASN
2	E	95	ARG
2	E	96	THR
2	E	98	PRO
2	E	101	SER
2	E	107	GLU
2	E	118	GLU
2	E	129	GLU
2	E	134	PHE
2	E	135	LEU
2	E	139	ASP
2	E	149	ILE
2	E	162	ASP
2	E	164	GLU
2	E	166	PRO
2	E	167	ARG
2	E	170	ASP
2	E	183	PHE
2	E	186	LEU
2	E	197	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	E	209	ASN
2	E	215	LEU
2	E	225	PHE
2	E	235	ILE
2	E	253	TYR
2	E	256	GLN
2	E	263	GLN
2	E	264	PHE
2	E	289	PRO
2	E	298	LEU
2	E	303	ASP
2	E	305	ILE
2	E	357	LEU
2	E	361	PHE
2	E	370	THR
2	E	375	THR
2	E	379	LEU
2	E	380	ILE
2	E	386	LEU
2	E	387	PHE
3	F	65	LEU
3	F	68	LEU
3	F	71	ILE
3	F	81	LEU
3	F	110	ARG
3	F	119	GLU
3	F	159	VAL
3	F	160	ASP
3	F	166	LEU
3	F	235	THR
3	F	239	ARG
3	F	242	GLN
3	F	256	VAL
3	F	284	TYR
3	F	294	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	22	ASN
1	A	119	HIS
1	A	168	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	172	ASN
1	A	200	ASN
1	A	211	ASN
1	A	230	ASN
1	A	237	GLN
1	A	271	GLN
1	A	338	ASN
1	A	339	GLN
1	A	383	ASN
1	A	399	GLN
1	A	444	ASN
1	A	465	ASN
1	A	506	ASN
1	A	580	GLN
2	B	72	HIS
2	B	87	HIS
2	B	92	ASN
2	B	177	HIS
2	B	208	HIS
2	B	209	ASN
2	B	233	HIS
2	B	254	HIS
2	B	320	GLN
2	B	329	HIS
2	B	373	ASN
2	B	392	GLN
3	C	12	GLN
3	C	27	GLN
3	C	63	HIS
3	C	141	ASN
3	C	179	HIS
3	C	187	GLN
3	C	191	HIS
3	C	288	GLN
1	D	22	ASN
1	D	119	HIS
1	D	127	HIS
1	D	200	ASN
1	D	211	ASN
1	D	230	ASN
1	D	271	GLN
1	D	338	ASN

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Mol	Chain	Res	Type
1	D	372	GLN
1	D	392	ASN
1	D	399	GLN
1	D	465	ASN
1	D	506	ASN
1	D	539	ASN
1	D	580	GLN
2	E	72	HIS
2	E	87	HIS
2	E	92	ASN
2	E	125	GLN
2	E	143	ASN
2	E	177	HIS
2	E	208	HIS
2	E	209	ASN
2	E	223	ASN
2	E	254	HIS
2	E	329	HIS
2	E	373	ASN
2	E	392	GLN
3	F	12	GLN
3	F	16	GLN
3	F	18	ASN
3	F	27	GLN
3	F	44	ASN
3	F	63	HIS
3	F	141	ASN
3	F	179	HIS
3	F	187	GLN
3	F	272	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	DAM	H	7	4,3	4,5,6	1.90	1 (25%)	3,5,7	4.37	3 (100%)
4	DAM	G	7	4,3	4,5,6	1.86	1 (25%)	3,5,7	4.04	3 (100%)
4	ACB	H	3	-	7,8,9	1.30	0	8,10,12	0.91	0
4	ACB	G	3	-	7,8,9	1.17	0	8,10,12	0.79	0
4	1ZN	G	5	4	21,23,24	1.24	2 (9%)	25,29,31	0.92	1 (4%)
4	FGA	H	6	4	6,8,9	2.70	2 (33%)	6,9,11	0.57	0
4	1ZN	H	5	4	21,23,24	1.05	0	25,29,31	0.81	0
4	FGA	G	6	4	6,8,9	2.57	2 (33%)	6,9,11	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DAM	H	7	4,3	-	0/0/4/6	-
4	DAM	G	7	4,3	-	0/0/4/6	-
4	ACB	H	3	-	-	2/10/10/12	-
4	ACB	G	3	-	-	2/10/10/12	-
4	1ZN	G	5	4	-	3/23/25/27	0/1/1/1
4	FGA	H	6	4	-	2/8/8/9	-
4	1ZN	H	5	4	-	3/23/25/27	0/1/1/1
4	FGA	G	6	4	-	3/8/8/9	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	6	FGA	O-C	5.45	1.38	1.22
4	G	6	FGA	O-C	5.32	1.37	1.22
4	G	7	DAM	C-CA	3.31	1.50	1.45
4	H	7	DAM	C-CA	3.30	1.50	1.45
4	H	6	FGA	OXT-C	-2.93	1.21	1.30
4	G	6	FGA	OXT-C	-2.42	1.22	1.30
4	G	5	1ZN	C5-C4	2.06	1.43	1.38
4	G	5	1ZN	C8-C9	2.03	1.42	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	7	DAM	CM-N-CA	-5.25	116.01	123.98
4	G	7	DAM	CM-N-CA	-5.19	116.11	123.98
4	H	7	DAM	O-C-CA	-4.98	118.85	125.33
4	G	7	DAM	O-C-CA	-4.22	119.85	125.33
4	H	7	DAM	CB-CA-N	-2.23	120.35	125.84
4	G	7	DAM	CB-CA-N	-2.07	120.75	125.84
4	G	5	1ZN	CA-C16-C15	-2.06	120.26	123.62

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3	ACB	CA-CB-CG-OD1
4	G	3	ACB	C4-CB-CG-OD1
4	H	3	ACB	C4-CB-CG-OD1
4	G	5	1ZN	C12-C13-C15-C16
4	G	5	1ZN	C14-C13-C15-C16
4	H	5	1ZN	C12-C13-C15-C16
4	H	5	1ZN	C14-C13-C15-C16
4	G	6	FGA	O-C-CA-N
4	G	6	FGA	OXT-C-CA-N
4	H	6	FGA	OXT-C-CA-N
4	G	6	FGA	CA-CB-CG-CD
4	H	3	ACB	CA-CB-CG-OD1
4	G	5	1ZN	C10-C2-C3-C4
4	H	5	1ZN	C10-C2-C3-C4
4	H	6	FGA	O-C-CA-N

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	7	DAM	2	0
4	G	7	DAM	1	0
4	G	6	FGA	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.