



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:35 AM UTC

PDB ID : 1GYL / pdb_00001gyl
Title : INVOLVEMENT OF TYR24 AND TRP108 IN SUBSTRATE BINDING AND
SUBSTRATE SPECIFICITY OF GLYCOLATE OXIDASE
Authors : Lindqvist, Y.; Stenberg, K.
Deposited on : 1995-01-30
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

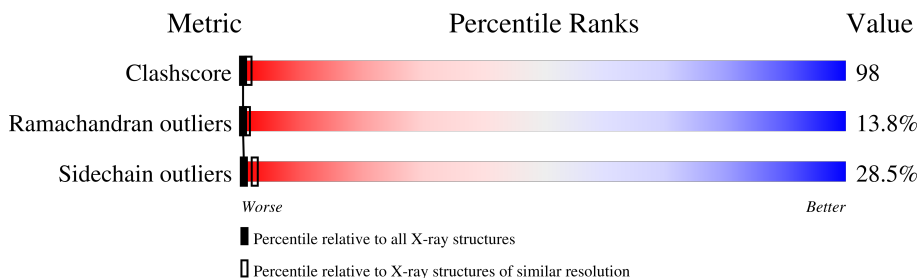
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

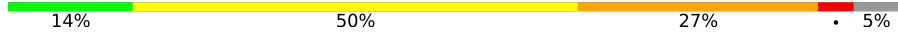
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	369	
1	B	369	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5436 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 GLYCOLATE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2708	1726	474	495	13			
1	B	350	Total	C	N	O	S	0	0	0
			2695	1718	471	493	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	PHE	TYR	conflict	UNP P05414
B	24	PHE	TYR	conflict	UNP P05414

- Molecule 2 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	1	Total	O	0	0
			1	1		

V242	A303	SER
Q243	G304	ARG
H244	V305	ALA
G245	F306	VAL
A246	I307	ALA
A247	G308	ARG
G248	R309	LEU
I249	P310	
I250	V311	
V251	F312	
S252	F313	
N253	S314	
H254	L315	
G255	A316	
A256	A317	
R257	E318	
Q258	G319	
L259	E320	
D260	A321	
Y261	G322	
V262	V323	
P263	K324	
A264	K325	
T265	V326	
I266	I327	
N267	Q328	
A268	M329	
L269	M330	
E270	R331	
E271	D332	
V272	F333	
V273	F334	
K274	E335	
A275	L336	
A276	T337	
Q277	M338	
G278	A339	
R279	L340	
I280	S341	
P281	G342	
V282	C343	
F283	R344	
L284	S345	
D285	L346	
	K347	
	E348	
V288	I349	
R289	S350	
R290	R351	
G291	S352	
T292	H353	
D293	I354	
V294	A355	
F295	A356	
K296	D357	
A297	W358	
L298	D359	
A299	GLY	
L300	PRO	
G301	SER	
A302		

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	145.50Å 145.50Å 100.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.254 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5436	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.95	1/2756 (0.0%)	1.67	63/3729 (1.7%)
1	B	1.01	5/2743 (0.2%)	1.70	85/3713 (2.3%)
All	All	0.98	6/5499 (0.1%)	1.68	148/7442 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	20	MET	SD-CE	6.43	1.95	1.79
1	B	20	MET	SD-CE	6.41	1.95	1.79
1	B	200	SER	CA-C	5.93	1.57	1.52
1	B	262	VAL	CA-CB	5.62	1.61	1.53
1	B	251	VAL	CA-CB	5.55	1.60	1.54
1	B	223	THR	CA-CB	5.00	1.61	1.53

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ALA	N-CA-C	-14.55	93.57	112.93
1	B	60	MET	N-CA-C	-13.02	95.61	112.93
1	A	120	GLY	CA-C-N	12.55	135.53	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	GLY	C-N-CA	12.55	135.53	119.84
1	A	183	PHE	N-CA-C	-12.49	96.56	113.18
1	A	202	TYR	N-CA-C	-12.31	94.31	112.04
1	A	8	GLU	N-CA-C	-12.00	97.74	112.38
1	A	76	ALA	CA-C-N	10.99	133.58	119.84
1	A	76	ALA	C-N-CA	10.99	133.58	119.84
1	A	204	ALA	N-CA-C	-10.94	100.21	112.57
1	B	158	THR	CA-C-N	10.64	133.14	119.84
1	B	158	THR	C-N-CA	10.64	133.14	119.84
1	B	262	VAL	N-CA-C	-10.42	99.33	109.02
1	A	51	ILE	N-CA-C	10.41	121.24	108.53
1	A	170	ASN	N-CA-C	-10.38	95.07	109.71
1	B	141	VAL	N-CA-C	-10.22	100.61	110.42
1	A	352	SER	N-CA-C	-10.14	98.36	112.45
1	B	315	LEU	N-CA-C	-10.00	98.55	112.45
1	A	336	LEU	N-CA-C	-9.66	98.90	112.13
1	B	213	TRP	N-CA-C	-9.65	101.50	113.28
1	B	172	PHE	N-CA-C	9.63	124.08	110.50
1	A	160	ARG	N-CA-C	-9.61	93.51	109.46
1	B	69	ILE	N-CA-C	9.61	122.34	109.37
1	B	280	ILE	CA-C-N	9.36	131.54	119.84
1	B	280	ILE	C-N-CA	9.36	131.54	119.84
1	A	215	ASP	N-CA-C	-9.36	100.18	111.69
1	A	280	ILE	CA-C-N	9.36	130.06	120.14
1	A	280	ILE	C-N-CA	9.36	130.06	120.14
1	A	174	LEU	CA-C-N	9.29	129.94	120.38
1	A	174	LEU	C-N-CA	9.29	129.94	120.38
1	A	269	LEU	N-CA-C	9.22	121.02	110.97
1	B	135	ASN	N-CA-C	-9.15	101.55	112.89
1	A	325	LYS	N-CA-C	-9.14	102.03	113.55
1	B	313	PHE	N-CA-C	-9.12	99.48	111.24
1	B	245	GLY	N-CA-C	9.00	123.07	110.74
1	A	115	GLU	N-CA-C	8.88	120.57	111.07
1	B	246	ALA	N-CA-C	8.84	123.96	112.12
1	A	69	ILE	N-CA-C	-8.78	95.54	108.54
1	A	175	PRO	CA-C-N	8.77	130.80	119.84
1	A	175	PRO	C-N-CA	8.77	130.80	119.84
1	B	239	ARG	N-CA-C	-8.77	101.63	111.71
1	B	115	GLU	N-CA-C	8.75	120.44	111.07
1	B	354	ILE	N-CA-C	-8.63	96.15	108.58
1	B	158	THR	N-CA-C	8.62	122.12	109.62
1	B	187	ASP	N-CA-C	-8.27	102.75	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	SER	N-CA-C	-8.05	103.35	113.01
1	A	82	LYS	N-CA-C	-7.79	103.80	113.38
1	B	58	ILE	N-CA-C	7.78	119.69	108.48
1	B	306	PHE	N-CA-C	7.73	121.44	110.23
1	B	336	LEU	N-CA-C	-7.67	101.66	111.02
1	B	57	ASN	N-CA-C	7.57	120.75	108.41
1	B	140	LEU	N-CA-C	-7.52	102.75	112.23
1	A	83	MET	N-CA-C	-7.49	102.48	111.69
1	B	348	GLU	N-CA-C	-7.43	103.67	112.89
1	B	108	TRP	N-CA-C	-7.34	103.30	111.82
1	A	188	LEU	N-CA-C	-7.33	95.18	110.80
1	B	163	ARG	N-CA-C	7.32	121.72	108.17
1	A	50	ARG	N-CA-C	-7.27	96.70	109.06
1	B	332	ASP	N-CA-C	-7.21	101.94	111.24
1	B	217	ALA	N-CA-C	-7.10	103.88	112.54
1	B	150	LYS	N-CA-C	7.08	125.89	110.80
1	A	28	GLY	N-CA-C	-7.03	100.43	110.91
1	B	42	PHE	N-CA-C	-7.02	104.18	112.89
1	A	3	ILE	N-CA-C	7.00	117.95	107.80
1	A	59	ASP	N-CA-C	6.93	119.41	107.28
1	B	62	THR	N-CA-C	6.92	119.59	109.07
1	B	145	GLU	N-CA-C	6.83	120.50	110.59
1	B	99	ALA	N-CA-C	-6.79	96.33	110.80
1	A	158	THR	N-CA-C	6.72	119.31	109.30
1	B	132	LYS	N-CA-C	6.71	125.09	110.80
1	B	88	GLY	N-CA-C	6.68	121.32	111.76
1	B	50	ARG	N-CA-C	-6.66	99.68	110.20
1	A	168	ILE	N-CA-C	6.53	122.93	109.34
1	B	90	TYR	N-CA-C	-6.46	105.38	113.20
1	A	292	THR	N-CA-C	-6.36	103.97	111.03
1	A	89	GLU	N-CA-C	-6.35	97.28	110.80
1	B	39	ARG	N-CA-C	-6.34	104.17	112.41
1	B	203	VAL	N-CA-C	6.33	118.96	111.05
1	B	51	ILE	N-CA-C	6.33	116.95	110.05
1	A	133	ASP	N-CA-C	-6.30	98.92	109.07
1	A	329	MET	N-CA-C	-6.26	104.53	111.36
1	B	166	ALA	N-CA-C	-6.26	97.47	110.80
1	B	161	LEU	N-CA-C	6.25	119.60	109.40
1	A	155	THR	N-CA-C	6.24	119.42	108.56
1	A	4	THR	N-CA-C	6.24	118.57	108.41
1	B	8	GLU	N-CA-C	-6.21	104.40	112.23
1	B	61	THR	N-CA-C	-6.16	100.72	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	ILE	N-CA-C	6.14	117.62	108.23
1	B	281	PRO	N-CA-C	6.13	125.10	112.47
1	B	120	GLY	N-CA-C	6.11	124.80	112.34
1	B	292	THR	N-CA-C	-6.11	104.81	112.93
1	B	233	ILE	N-CA-C	6.08	121.98	109.34
1	A	288	VAL	N-CA-C	6.06	121.95	109.34
1	B	357	ASP	N-CA-C	-6.05	104.32	111.03
1	A	262	VAL	N-CA-C	-6.04	100.92	108.05
1	A	114	GLU	N-CA-C	-6.00	104.37	111.03
1	A	224	SER	N-CA-C	-5.96	98.12	110.80
1	B	109	ALA	N-CA-C	-5.93	98.18	110.80
1	B	264	ALA	N-CA-C	-5.87	102.37	110.35
1	A	273	VAL	N-CA-C	-5.86	105.41	110.74
1	A	303	ALA	N-CA-C	5.86	123.28	110.80
1	B	21	VAL	N-CA-C	5.85	115.97	110.30
1	A	2	GLU	N-CA-C	-5.84	101.83	110.48
1	B	335	GLU	N-CA-C	-5.84	105.00	111.36
1	A	321	ALA	N-CA-C	-5.79	106.06	113.23
1	B	182	ASN	N-CA-C	-5.78	98.50	110.80
1	B	262	VAL	CA-C-N	-5.77	114.32	120.03
1	B	262	VAL	C-N-CA	-5.77	114.32	120.03
1	B	241	ALA	N-CA-C	-5.74	106.32	113.15
1	B	307	ILE	N-CA-C	5.74	121.28	109.34
1	B	103	MET	N-CA-C	-5.72	99.92	109.24
1	A	134	ARG	N-CA-C	5.69	119.00	112.97
1	A	161	LEU	N-CA-C	5.60	118.75	109.46
1	B	317	ALA	N-CA-C	5.57	121.31	113.02
1	B	343	CYS	N-CA-C	5.55	122.63	110.80
1	A	252	SER	N-CA-C	5.52	116.65	108.60
1	A	163	ARG	N-CA-C	5.51	117.88	109.62
1	A	315	LEU	N-CA-C	-5.51	105.18	111.07
1	B	224	SER	N-CA-C	-5.50	106.62	113.38
1	B	80	MET	N-CA-C	5.42	122.34	110.80
1	A	277	GLN	N-CA-C	5.39	117.53	108.96
1	B	171	ARG	N-CA-C	5.39	118.86	112.72
1	B	294	VAL	CB-CA-C	-5.38	103.54	112.26
1	B	350	SER	N-CA-C	5.36	116.14	108.74
1	A	72	PRO	N-CA-C	5.36	123.51	112.47
1	B	342	GLY	N-CA-C	5.34	125.83	113.18
1	B	10	GLU	N-CA-C	5.33	117.84	111.71
1	A	98	ALA	N-CA-C	-5.32	105.65	111.82
1	A	214	LYS	N-CA-C	-5.30	106.94	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	PHE	N-CA-C	5.29	122.07	110.80
1	B	344	ARG	N-CA-C	5.24	119.89	111.81
1	A	179	THR	N-CA-C	5.23	117.63	109.52
1	B	151	ALA	N-CA-C	5.23	118.59	110.17
1	B	126	PHE	N-CA-C	5.22	118.20	110.48
1	B	40	ASN	N-CA-C	5.21	121.32	114.75
1	B	100	GLY	N-CA-C	5.21	117.46	111.36
1	B	125	PHE	N-CA-C	5.19	117.10	108.02
1	B	83	MET	N-CA-C	-5.16	107.15	112.93
1	B	90	TYR	CA-C-N	5.16	127.45	120.44
1	B	90	TYR	C-N-CA	5.16	127.45	120.44
1	B	277	GLN	N-CA-C	5.15	121.76	110.80
1	A	38	ASN	N-CA-C	-5.13	107.06	113.38
1	A	239	ARG	N-CA-C	-5.13	105.81	111.71
1	B	124	ARG	N-CA-C	5.13	116.86	108.55
1	A	114	GLU	CA-C-N	5.12	127.09	120.44
1	A	114	GLU	C-N-CA	5.12	127.09	120.44
1	A	200	SER	N-CA-C	5.12	121.69	110.80
1	B	230	LYS	N-CA-C	5.10	117.11	110.53

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	TYR	Sidechain
1	B	90	TYR	Sidechain

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	2708	0	2771	422	0
1	B	2695	0	2755	712	0
2	A	31	0	19	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	5436	0	5545	1072	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 98.

All (1072) 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:B:235:ALA:HA	1:B:238:ALA:HB3	1.18	1.14
1:A:80:MET:HG2	1:A:110:THR:HG23	1.27	1.14
1:B:82:LYS:HB2	1:B:178:LEU:HD11	1.22	1.13
1:B:227:ILE:HB	1:B:246:ALA:HB1	1.17	1.09
1:B:165:GLU:HA	1:B:168:ILE:HB	1.16	1.09
1:B:144:ALA:HA	1:B:149:PHE:HB3	1.35	1.08
1:B:132:LYS:HG3	1:B:208:ASP:HB2	1.37	1.06
1:A:146:ARG:HB2	1:B:114:GLU:HA	1.31	1.04
1:B:47:PHE:HA	1:B:355:ALA:H	1.24	1.02
1:A:142:ARG:NH1	1:B:184:GLU:HG3	1.74	1.01
1:A:181:LYS:HA	1:A:184:GLU:HB2	1.45	0.98
1:A:143:ARG:NE	1:B:142:ARG:HA	1.79	0.97
1:B:25:TYR:HE2	1:B:81:GLN:HB3	1.28	0.97
1:A:112:SER:HB2	1:A:181:LYS:O	1.66	0.96
1:B:229:VAL:HG22	1:B:246:ALA:HB3	1.47	0.95
1:B:67:PHE:HA	1:B:68:LYS:HZ1	1.31	0.95
1:B:131:TYR:HB3	1:B:136:VAL:HB	1.46	0.95
1:B:307:ILE:HB	1:B:310:PRO:HG3	1.47	0.94
1:A:5:ASN:HB3	1:A:8:GLU:HB2	1.48	0.94
1:B:228:LEU:HA	1:B:247:ALA:O	1.68	0.94
1:B:74:MET:HB2	1:B:102:ILE:HB	1.49	0.94
1:B:82:LYS:HD3	1:B:178:LEU:HD21	1.49	0.93
1:A:60:MET:O	1:A:72:PRO:HD3	1.68	0.93
1:B:248:GLY:HA2	1:B:281:PRO:HB2	1.47	0.93
1:B:41:ALA:O	1:B:44:ARG:HB3	1.67	0.93
1:B:45:ILE:HG13	1:B:357:ASP:H	1.32	0.93
1:B:98:ALA:HB1	1:B:324:LYS:HE2	1.50	0.93
1:B:74:MET:CB	1:B:102:ILE:HB	1.99	0.93
1:B:24:PHE:HA	1:B:164:ARG:HH21	1.33	0.92
1:B:300:LEU:HD21	1:B:354:ILE:HG21	1.52	0.92
1:B:232:VAL:H	1:B:251:VAL:HA	1.33	0.91
1:A:28:GLY:HA3	1:A:35:LEU:HD11	1.52	0.91
1:B:298:LEU:HA	1:B:302:ALA:HB3	1.48	0.91
1:B:247:ALA:HA	1:B:280:ILE:HB	1.53	0.90
1:B:291:GLY:HA2	1:B:330:MET:SD	2.11	0.90
1:B:132:LYS:HB2	1:B:206:GLN:HA	1.55	0.89
1:A:82:LYS:HB3	1:A:110:THR:HG21	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ARG:HB2	1:A:354:ILE:HA	1.53	0.89
1:A:114:GLU:HG3	1:A:115:GLU:HG3	1.56	0.88
1:B:229:VAL:HG23	1:B:249:ILE:HG12	1.53	0.88
1:A:136:VAL:HA	1:B:139:GLN:HG3	1.54	0.88
1:A:152:ILE:HD12	1:A:227:ILE:HD11	1.56	0.88
1:B:30:GLU:HG3	1:B:259:LEU:HA	1.56	0.87
1:B:61:THR:HG23	1:B:70:SER:HA	1.56	0.87
1:B:31:ASP:O	1:B:260:ASP:HB3	1.74	0.87
1:B:268:ALA:O	1:B:272:VAL:HG22	1.75	0.87
1:A:12:ILE:O	1:A:15:GLN:HG3	1.74	0.87
1:B:37:GLU:HG3	1:B:264:ALA:HB2	1.54	0.87
1:A:45:ILE:HD11	1:A:266:ILE:HD11	1.57	0.87
1:A:87:GLU:O	1:A:90:TYR:HB2	1.75	0.87
1:B:346:LEU:HA	1:B:349:ILE:HG12	1.57	0.86
1:B:73:ILE:HA	1:B:305:VAL:HB	1.57	0.86
1:A:151:ALA:HA	1:A:225:LEU:O	1.76	0.86
1:B:152:ILE:HD11	1:B:225:LEU:HD12	1.56	0.86
1:B:283:PHE:HE1	1:B:303:ALA:HB3	1.39	0.86
1:B:283:PHE:CE1	1:B:303:ALA:HB3	2.11	0.85
1:A:186:ILE:HG12	1:B:142:ARG:NH1	1.90	0.85
1:B:273:VAL:HA	1:B:282:VAL:HG21	1.56	0.85
1:B:152:ILE:HB	1:B:226:PRO:O	1.76	0.85
1:B:235:ALA:CA	1:B:238:ALA:HB3	2.05	0.85
1:B:29:ALA:HA	1:B:164:ARG:HB3	1.55	0.85
1:A:74:MET:O	1:A:307:ILE:HG12	1.75	0.85
1:B:22:TYR:HA	1:B:25:TYR:CD1	2.12	0.85
1:B:264:ALA:O	1:B:267:MET:SD	2.35	0.85
1:A:284:LEU:HD11	1:A:297:ALA:HB1	1.59	0.84
1:A:60:MET:SD	1:A:331:ARG:HG3	2.18	0.84
1:A:143:ARG:CZ	1:B:142:ARG:HA	2.06	0.84
1:B:233:ILE:HA	1:B:251:VAL:HG13	1.60	0.84
1:A:64:ILE:HG13	1:A:283:PHE:CE1	2.12	0.84
1:A:146:ARG:HB2	1:B:114:GLU:CA	2.09	0.83
1:A:274:LYS:HE2	1:A:274:LYS:HA	1.58	0.83
1:A:354:ILE:HG12	1:A:355:ALA:H	1.42	0.83
1:B:230:LYS:HG2	1:B:250:ILE:CG2	2.09	0.83
1:A:63:THR:HA	1:A:67:PHE:O	1.79	0.83
1:A:88:GLY:O	1:A:89:GLU:HB2	1.79	0.83
1:B:270:GLU:HA	1:B:273:VAL:HG12	1.59	0.82
1:B:186:ILE:HG13	1:B:188:LEU:HB3	1.61	0.82
1:B:23:ASP:HB2	1:B:167:ASP:HB3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HD3	1:A:289:ARG:HH21	1.45	0.81
1:A:116:VAL:O	1:A:119:THR:HG23	1.80	0.81
1:B:131:TYR:CD1	1:B:206:GLN:HG2	2.16	0.81
1:A:113:VAL:CG2	1:A:143:ARG:HD3	2.10	0.80
1:B:96:ALA:C	1:B:100:GLY:HA2	2.06	0.80
1:A:188:LEU:HD12	1:B:135:ASN:ND2	1.96	0.80
1:B:141:VAL:HG22	1:B:223:THR:HB	1.64	0.80
1:B:53:ILE:HG13	1:B:342:GLY:HA3	1.63	0.80
1:B:269:LEU:HD21	1:B:300:LEU:HB3	1.64	0.80
1:B:237:ASP:HA	1:B:240:LEU:HD12	1.64	0.79
1:B:20:MET:HG2	1:B:172:PHE:HB2	1.65	0.79
1:B:184:GLU:O	1:B:186:ILE:HG12	1.82	0.79
1:B:295:PHE:HA	1:B:298:LEU:HG	1.64	0.79
1:B:71:MET:HG2	1:B:73:ILE:HG13	1.64	0.79
1:B:24:PHE:HA	1:B:164:ARG:NH2	1.97	0.79
1:A:106:SER:HA	1:A:127:GLN:HB3	1.62	0.79
1:B:266:ILE:HG23	1:B:267:MET:SD	2.23	0.79
1:A:164:ARG:NH1	1:A:257:ARG:HB3	1.98	0.79
1:A:222:ILE:HG22	1:B:185:GLY:HA3	1.63	0.78
1:B:25:TYR:CE2	1:B:81:GLN:HB3	2.16	0.78
1:B:125:PHE:CZ	1:B:151:ALA:HB3	2.18	0.78
1:A:48:ARG:CB	1:A:354:ILE:HA	2.14	0.78
1:A:300:LEU:HA	1:A:351:ARG:HD3	1.66	0.78
1:B:333:GLU:O	1:B:336:LEU:HB2	1.83	0.78
1:B:91:ALA:CA	1:B:320:GLU:HA	2.14	0.78
1:B:307:ILE:HB	1:B:310:PRO:CG	2.12	0.78
1:A:131:TYR:HD1	1:A:207:ILE:HA	1.48	0.78
1:B:188:LEU:HD13	1:B:198:GLY:HA2	1.66	0.78
1:A:103:MET:SD	1:A:103:MET:C	2.67	0.77
1:A:291:GLY:HA2	1:A:294:VAL:HB	1.66	0.77
1:B:35:LEU:HD13	1:B:256:ALA:HB3	1.66	0.77
1:B:26:ALA:HA	1:B:309:ARG:CZ	2.15	0.77
1:A:273:VAL:HG22	1:A:282:VAL:HG21	1.65	0.77
1:B:75:ILE:HA	1:B:307:ILE:HG13	1.67	0.77
1:B:267:MET:SD	1:B:267:MET:N	2.57	0.77
1:B:298:LEU:HA	1:B:302:ALA:CB	2.15	0.77
1:B:24:PHE:CD2	1:B:80:MET:HB2	2.20	0.77
1:B:209:ARG:H	1:B:209:ARG:HE	1.31	0.77
1:B:110:THR:HB	1:B:181:LYS:HB2	1.67	0.76
1:B:143:ARG:O	1:B:145:GLU:HG2	1.85	0.76
1:B:251:VAL:HG12	1:B:265:THR:HG22	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:SER:HA	1:A:204:ALA:HB3	1.65	0.76
1:A:131:TYR:HA	1:A:207:ILE:HA	1.65	0.76
1:A:267:MET:SD	1:A:358:TRP:CZ3	2.79	0.76
1:B:308:GLY:C	1:B:310:PRO:HD2	2.11	0.76
1:B:269:LEU:HD23	1:B:270:GLU:HG3	1.67	0.76
1:A:39:ARG:NH2	1:A:289:ARG:HB2	2.01	0.76
1:B:75:ILE:HG22	1:B:308:GLY:N	2.01	0.76
1:B:126:PHE:HD1	1:B:127:GLN:N	1.82	0.76
1:A:142:ARG:HH12	1:B:184:GLU:HG3	1.50	0.75
1:A:64:ILE:HG13	1:A:283:PHE:HE1	1.49	0.75
1:A:128:LEU:HD21	1:A:130:VAL:HG23	1.68	0.75
1:A:284:LEU:O	1:A:305:VAL:HG23	1.85	0.75
1:B:164:ARG:HD2	1:B:164:ARG:O	1.86	0.75
1:A:146:ARG:HH11	1:B:117:ALA:HB1	1.50	0.75
1:B:235:ALA:HB2	1:B:271:GLU:O	1.87	0.75
1:A:73:ILE:O	1:A:101:THR:HG21	1.87	0.75
1:B:75:ILE:HG22	1:B:308:GLY:CA	2.16	0.75
1:B:26:ALA:HB2	1:B:309:ARG:HD3	1.69	0.75
1:B:106:SER:HA	1:B:127:GLN:HB3	1.69	0.74
1:B:250:ILE:HB	1:B:283:PHE:HB2	1.67	0.74
1:B:300:LEU:H	1:B:300:LEU:HD22	1.51	0.74
1:A:80:MET:CG	1:A:110:THR:HG23	2.13	0.74
1:A:143:ARG:HA	1:B:143:ARG:HG2	1.69	0.74
1:B:47:PHE:HA	1:B:355:ALA:N	2.00	0.74
1:B:199:LEU:H	1:B:199:LEU:HD12	1.52	0.74
1:A:285:ASP:HB3	1:A:306:PHE:HB2	1.69	0.74
1:B:18:PRO:HG2	1:B:21:VAL:HB	1.68	0.74
1:A:132:LYS:NZ	1:A:132:LYS:HB3	2.02	0.74
1:B:136:VAL:HG11	1:B:206:GLN:NE2	2.03	0.74
1:B:134:ARG:HD2	1:B:218:TRP:HH2	1.53	0.74
1:B:242:VAL:HG21	1:B:276:ALA:HB2	1.70	0.73
1:B:331:ARG:HA	1:B:334:PHE:CE1	2.23	0.73
1:A:143:ARG:HA	1:B:143:ARG:HA	1.70	0.73
1:B:27:SER:O	1:B:257:ARG:HD2	1.87	0.73
1:B:91:ALA:CB	1:B:320:GLU:HA	2.19	0.73
1:B:22:TYR:HA	1:B:25:TYR:CE1	2.24	0.73
1:B:75:ILE:HG22	1:B:308:GLY:HA2	1.69	0.73
1:B:131:TYR:HB2	1:B:137:VAL:HG22	1.70	0.73
1:B:309:ARG:O	1:B:312:VAL:HB	1.89	0.73
1:B:346:LEU:HD12	1:B:349:ILE:HG13	1.69	0.73
1:B:108:TRP:CH2	1:B:129:TYR:HE2	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ARG:HH21	1:B:225:LEU:HA	1.55	0.72
1:B:254:HIS:HB2	1:B:258:GLN:HB2	1.70	0.72
1:A:59:ASP:HB3	1:A:345:SER:HB3	1.71	0.72
1:B:153:ALA:HB1	1:B:228:LEU:O	1.88	0.72
1:B:184:GLU:HA	1:B:199:LEU:HD23	1.71	0.72
1:A:113:VAL:HG21	1:A:143:ARG:HD3	1.70	0.72
1:B:2:GLU:HG2	1:B:3:ILE:N	2.05	0.72
1:B:139:GLN:HA	1:B:142:ARG:HD2	1.72	0.72
1:B:209:ARG:H	1:B:209:ARG:NE	1.87	0.72
1:A:269:LEU:HD23	1:A:300:LEU:HB2	1.71	0.71
1:B:91:ALA:HB1	1:B:320:GLU:HA	1.72	0.71
1:B:294:VAL:HG21	1:B:330:MET:HG3	1.71	0.71
1:A:135:ASN:O	1:A:139:GLN:HG3	1.89	0.71
1:A:184:GLU:O	1:A:199:LEU:HB3	1.89	0.71
1:B:248:GLY:HA2	1:B:281:PRO:CB	2.20	0.71
1:A:58:ILE:HG22	1:A:59:ASP:H	1.54	0.71
1:B:229:VAL:CG2	1:B:246:ALA:HB3	2.20	0.71
1:B:20:MET:SD	1:B:172:PHE:HD1	2.13	0.71
1:A:189:GLY:HA3	1:B:133:ASP:HA	1.72	0.70
1:A:142:ARG:HB2	1:B:143:ARG:NE	2.06	0.70
1:B:183:PHE:O	1:B:186:ILE:HG23	1.92	0.70
1:A:143:ARG:HB2	1:B:142:ARG:O	1.91	0.70
1:B:236:GLU:HA	1:B:239:ARG:NH1	2.06	0.70
1:A:144:ALA:HB1	1:A:149:PHE:HB2	1.73	0.70
1:B:91:ALA:HA	1:B:320:GLU:HA	1.71	0.70
1:A:159:PRO:HG2	1:A:160:ARG:H	1.54	0.70
1:B:215:ASP:HA	1:B:218:TRP:CD2	2.27	0.70
1:B:239:ARG:HG3	1:B:240:LEU:HG	1.74	0.69
1:A:101:THR:HG22	1:A:102:ILE:H	1.57	0.69
1:B:329:MET:O	1:B:333:GLU:HB2	1.93	0.69
1:A:152:ILE:HD12	1:A:227:ILE:CD1	2.22	0.69
1:B:61:THR:HG22	1:B:68:LYS:O	1.92	0.69
1:B:63:THR:HA	1:B:67:PHE:O	1.93	0.69
1:B:266:ILE:HA	1:B:284:LEU:CD1	2.21	0.69
1:B:64:ILE:CD1	1:B:69:ILE:HG12	2.22	0.69
1:B:188:LEU:HB2	1:B:198:GLY:C	2.18	0.69
1:B:249:ILE:HD11	1:B:280:ILE:HD12	1.75	0.69
1:B:233:ILE:CA	1:B:251:VAL:HG13	2.22	0.69
1:B:30:GLU:HB2	1:B:260:ASP:HB2	1.75	0.69
1:A:82:LYS:HD2	1:A:110:THR:HB	1.75	0.68
1:A:110:THR:O	1:A:181:LYS:HE2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:HG2	1:B:289:ARG:HD2	1.74	0.68
1:B:61:THR:HG23	1:B:70:SER:CA	2.22	0.68
1:B:260:ASP:O	1:B:261:TYR:HB2	1.92	0.68
1:B:144:ALA:HA	1:B:149:PHE:CB	2.20	0.68
1:B:73:ILE:HA	1:B:305:VAL:CB	2.22	0.68
1:A:222:ILE:HG13	1:A:222:ILE:O	1.93	0.68
1:B:6:VAL:HG13	1:B:329:MET:HE3	1.75	0.68
1:B:74:MET:HB3	1:B:102:ILE:HB	1.74	0.68
1:B:130:VAL:O	1:B:130:VAL:HG13	1.94	0.68
1:B:50:ARG:H	1:B:341:SER:HB3	1.59	0.68
1:B:144:ALA:O	1:B:225:LEU:HD13	1.94	0.68
1:A:44:ARG:HD3	1:A:357:ASP:CG	2.19	0.68
1:B:132:LYS:HB2	1:B:206:GLN:CA	2.24	0.68
1:A:59:ASP:CB	1:A:345:SER:HB3	2.23	0.67
1:A:186:ILE:HB	1:A:202:TYR:CE2	2.29	0.67
1:A:222:ILE:CG2	1:B:185:GLY:HA3	2.23	0.67
1:B:163:ARG:HG3	1:B:163:ARG:HH11	1.59	0.67
1:A:31:ASP:HB2	1:A:261:TYR:OH	1.95	0.67
1:B:345:SER:O	1:B:349:ILE:HG12	1.95	0.67
1:A:126:PHE:HB2	1:A:149:PHE:CD2	2.30	0.67
1:A:273:VAL:HG22	1:A:282:VAL:CG2	2.24	0.67
1:B:6:VAL:HG22	1:B:329:MET:SD	2.34	0.67
1:B:49:PRO:HB3	1:B:341:SER:OG	1.94	0.67
1:B:35:LEU:HD13	1:B:256:ALA:CB	2.24	0.67
1:A:136:VAL:HG11	1:A:186:ILE:HG21	1.77	0.67
1:B:232:VAL:N	1:B:251:VAL:HA	2.09	0.67
1:B:238:ALA:O	1:B:242:VAL:HG23	1.95	0.67
1:A:162:GLY:O	1:A:164:ARG:HD3	1.95	0.66
1:B:219:LEU:O	1:B:222:ILE:HB	1.96	0.66
1:A:288:VAL:HG11	1:A:305:VAL:HG21	1.75	0.66
1:B:124:ARG:HB3	1:B:149:PHE:CD1	2.30	0.66
1:B:232:VAL:O	1:B:251:VAL:HG22	1.95	0.66
1:B:242:VAL:HG21	1:B:275:ALA:O	1.95	0.66
1:B:307:ILE:CB	1:B:310:PRO:HG3	2.24	0.66
1:B:60:MET:HB3	1:B:338:MET:HE1	1.78	0.66
1:A:171:ARG:HG2	1:A:171:ARG:HH11	1.60	0.66
1:A:180:LEU:HD11	1:A:200:SER:HA	1.77	0.66
1:A:267:MET:SD	1:A:358:TRP:HZ3	2.19	0.66
1:B:289:ARG:HB3	1:B:289:ARG:NH1	2.09	0.66
1:A:312:VAL:O	1:A:315:LEU:HD23	1.95	0.66
1:B:212:SER:HB2	1:B:214:LYS:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:GLU:HB2	1:B:322:GLY:CA	2.26	0.66
1:A:114:GLU:HA	1:B:145:GLU:HB3	1.78	0.66
1:B:22:TYR:HA	1:B:25:TYR:HD1	1.60	0.66
1:A:128:LEU:HD13	1:A:154:LEU:HD13	1.77	0.66
1:B:134:ARG:HD2	1:B:218:TRP:CH2	2.31	0.66
1:B:152:ILE:HG22	1:B:153:ALA:N	2.11	0.66
1:B:131:TYR:HD1	1:B:206:GLN:HG2	1.61	0.65
1:B:58:ILE:HA	1:B:344:ARG:HB3	1.78	0.65
1:B:209:ARG:NE	1:B:209:ARG:N	2.45	0.65
1:B:29:ALA:O	1:B:260:ASP:HB2	1.96	0.65
1:B:288:VAL:HG12	1:B:293:ASP:CB	2.26	0.65
1:A:113:VAL:HG23	1:A:143:ARG:HD3	1.79	0.65
1:A:114:GLU:HB2	1:B:225:LEU:HD21	1.78	0.65
1:B:138:ALA:O	1:B:141:VAL:HB	1.97	0.65
1:B:232:VAL:O	1:B:232:VAL:HG13	1.97	0.65
1:B:311:VAL:O	1:B:315:LEU:N	2.30	0.65
1:A:227:ILE:HG22	1:A:227:ILE:O	1.97	0.65
1:B:5:ASN:HA	1:B:290:ARG:NH1	2.12	0.65
1:A:39:ARG:HD3	1:A:289:ARG:NH2	2.11	0.65
1:A:69:ILE:HB	1:A:101:THR:HG23	1.79	0.65
1:A:98:ALA:HB3	1:A:324:LYS:NZ	2.12	0.65
1:B:45:ILE:HG13	1:B:357:ASP:N	2.09	0.65
1:B:126:PHE:HD2	1:B:144:ALA:HB2	1.62	0.65
1:B:252:SER:HA	1:B:265:THR:HG21	1.78	0.65
1:A:146:ARG:NH1	1:B:117:ALA:HB1	2.11	0.65
1:B:74:MET:SD	1:B:305:VAL:N	2.70	0.65
1:B:77:PRO:HD2	1:B:230:LYS:HZ2	1.62	0.65
1:B:108:TRP:O	1:B:110:THR:HG23	1.97	0.65
1:B:266:ILE:HA	1:B:284:LEU:HD11	1.78	0.65
1:A:293:ASP:HA	1:A:296:LYS:HD2	1.78	0.64
1:B:288:VAL:HB	1:B:294:VAL:HG13	1.79	0.64
1:B:45:ILE:HG23	1:B:356:ALA:HA	1.79	0.64
1:B:105:LEU:O	1:B:127:GLN:HB2	1.97	0.64
1:A:274:LYS:HE2	1:A:274:LYS:CA	2.26	0.64
1:A:64:ILE:O	1:A:67:PHE:HB2	1.97	0.64
1:A:232:VAL:O	1:A:251:VAL:HG12	1.97	0.64
1:B:48:ARG:O	1:B:353:HIS:HD2	1.81	0.64
1:B:106:SER:HA	1:B:127:GLN:CB	2.27	0.64
1:B:291:GLY:HA3	1:B:333:GLU:HB3	1.79	0.64
1:A:202:TYR:CD1	1:A:202:TYR:C	2.76	0.64
1:B:108:TRP:CH2	1:B:129:TYR:CE2	2.86	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:THR:HG22	1:B:125:PHE:CB	2.28	0.63
1:A:249:ILE:CG2	1:A:251:VAL:HG22	2.28	0.63
1:A:325:LYS:HB3	1:A:329:MET:HE2	1.78	0.63
1:B:178:LEU:HD23	1:B:181:LYS:HE3	1.80	0.63
1:B:208:ASP:HA	1:B:209:ARG:CZ	2.28	0.63
1:A:80:MET:HG2	1:A:110:THR:CG2	2.17	0.63
1:A:273:VAL:CG2	1:A:282:VAL:HG21	2.28	0.63
1:B:227:ILE:HB	1:B:246:ALA:CB	2.12	0.63
1:A:107:SER:HB3	1:A:183:PHE:HE1	1.63	0.63
1:A:277:GLN:O	1:A:279:ARG:HD2	1.98	0.63
1:B:75:ILE:HG13	1:B:103:MET:HE2	1.79	0.63
1:A:62:THR:HG22	1:A:63:THR:H	1.64	0.63
1:A:32:GLN:HB3	1:A:35:LEU:HD13	1.80	0.62
1:A:300:LEU:HD23	1:A:351:ARG:HD2	1.81	0.62
1:A:242:VAL:HG11	1:A:279:ARG:HG2	1.81	0.62
1:B:47:PHE:CA	1:B:355:ALA:H	2.06	0.62
1:B:321:ALA:HB1	1:B:325:LYS:HE3	1.80	0.62
1:A:33:TRP:CE3	1:A:261:TYR:HA	2.33	0.62
1:B:321:ALA:HA	1:B:324:LYS:HG2	1.81	0.62
1:A:139:GLN:HB2	1:B:139:GLN:HB3	1.82	0.62
1:A:20:MET:SD	1:A:172:PHE:CD1	2.92	0.62
1:A:20:MET:SD	1:A:173:VAL:O	2.58	0.62
1:A:179:THR:OG1	1:A:181:LYS:HG3	1.99	0.62
1:A:84:ALA:HB1	1:A:316:ALA:HB2	1.82	0.62
1:A:276:ALA:HA	1:A:279:ARG:NE	2.14	0.62
1:B:6:VAL:HG23	1:B:290:ARG:HD3	1.80	0.62
1:A:186:ILE:HD11	1:B:139:GLN:HE21	1.64	0.62
1:A:265:THR:CG2	1:A:284:LEU:HB2	2.30	0.62
1:B:9:TYR:HA	1:B:12:ILE:HD12	1.82	0.62
1:B:233:ILE:HG22	1:B:251:VAL:CG1	2.29	0.62
1:B:311:VAL:HB	1:B:323:VAL:HG12	1.82	0.62
1:A:248:GLY:N	1:A:280:ILE:HD13	2.15	0.61
1:B:156:VAL:HG22	1:B:230:LYS:O	1.99	0.61
1:B:334:PHE:CD1	1:B:335:GLU:N	2.68	0.61
1:A:199:LEU:O	1:A:201:SER:N	2.33	0.61
1:A:218:TRP:NE1	1:A:222:ILE:HG21	2.14	0.61
1:B:254:HIS:HB3	1:B:257:ARG:HG2	1.80	0.61
1:B:263:PRO:HB2	1:B:267:MET:HE2	1.83	0.61
1:B:237:ASP:O	1:B:240:LEU:HB2	2.00	0.61
1:B:336:LEU:O	1:B:340:LEU:HB2	2.00	0.61
1:A:285:ASP:CB	1:A:306:PHE:HB2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:TYR:HE2	1:B:140:LEU:HD21	1.66	0.61
1:A:60:MET:HB3	1:A:72:PRO:HD2	1.81	0.61
1:B:273:VAL:HG23	1:B:282:VAL:CB	2.30	0.61
1:A:172:PHE:CD1	1:A:172:PHE:C	2.78	0.61
1:B:251:VAL:HG12	1:B:265:THR:CG2	2.30	0.61
1:B:270:GLU:HA	1:B:273:VAL:CG1	2.28	0.61
1:B:74:MET:HE1	1:B:304:GLY:HA3	1.83	0.61
1:B:123:ILE:HB	1:B:150:LYS:HB2	1.83	0.61
1:B:25:TYR:OH	1:B:83:MET:SD	2.59	0.61
1:B:35:LEU:HD22	1:B:256:ALA:O	2.00	0.61
1:B:102:ILE:HG22	1:B:104:THR:HG23	1.82	0.61
1:A:115:GLU:OE2	1:A:181:LYS:HB3	2.00	0.60
1:A:132:LYS:HA	1:A:208:ASP:OD1	2.01	0.60
1:A:102:ILE:HG23	1:A:124:ARG:HA	1.82	0.60
1:A:142:ARG:HB2	1:B:143:ARG:HE	1.64	0.60
1:B:318:GLU:HB2	1:B:322:GLY:HA3	1.82	0.60
1:B:269:LEU:HD21	1:B:300:LEU:CB	2.30	0.60
1:A:151:ALA:HB1	1:A:228:LEU:HD21	1.82	0.60
1:B:253:ASN:HB2	1:B:262:VAL:HG21	1.82	0.60
1:B:324:LYS:HG3	1:B:325:LYS:HG3	1.83	0.60
1:B:240:LEU:HA	1:B:243:GLN:HB3	1.82	0.60
1:A:45:ILE:CD1	1:A:266:ILE:HD11	2.30	0.60
1:B:27:SER:HB3	1:B:164:ARG:HD3	1.84	0.60
1:B:233:ILE:HG22	1:B:251:VAL:HG12	1.83	0.60
1:B:324:LYS:HG3	1:B:325:LYS:N	2.17	0.60
1:B:110:THR:HG22	1:B:180:LEU:HA	1.83	0.60
1:B:234:THR:HA	1:B:271:GLU:OE1	2.02	0.60
1:A:226:PRO:O	1:A:228:LEU:HD22	2.02	0.60
1:A:228:LEU:HD22	1:A:228:LEU:H	1.66	0.60
1:A:275:ALA:O	1:A:277:GLN:HG3	2.01	0.60
1:A:328:GLN:O	1:A:332:ASP:HB2	2.01	0.60
1:B:248:GLY:CA	1:B:281:PRO:HB2	2.28	0.60
1:A:172:PHE:C	1:A:172:PHE:HD1	2.09	0.59
1:A:188:LEU:HD12	1:B:135:ASN:CG	2.27	0.59
1:B:62:THR:O	1:B:68:LYS:HA	2.01	0.59
1:A:76:ALA:HB1	2:A:370:FMN:H3'	1.84	0.59
1:B:74:MET:HE2	1:B:306:PHE:CE1	2.37	0.59
1:A:114:GLU:HB3	1:B:145:GLU:OE2	2.01	0.59
1:B:20:MET:SD	1:B:172:PHE:CD1	2.94	0.59
1:B:331:ARG:O	1:B:335:GLU:HB2	2.03	0.59
1:A:161:LEU:HA	1:A:258:GLN:HE22	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:HG23	1:B:282:VAL:HB	1.83	0.59
1:A:110:THR:O	1:A:181:LYS:HB2	2.02	0.59
1:B:21:VAL:HG22	1:B:172:PHE:CZ	2.36	0.59
1:B:250:ILE:HG12	1:B:251:VAL:O	2.02	0.59
1:B:146:ARG:NH2	1:B:224:SER:O	2.35	0.59
1:B:20:MET:CE	1:B:171:ARG:HB3	2.33	0.59
1:B:228:LEU:O	1:B:228:LEU:HD12	2.03	0.59
1:A:128:LEU:CD2	1:A:130:VAL:HG23	2.33	0.59
1:B:20:MET:HE2	1:B:171:ARG:HB3	1.85	0.59
1:B:230:LYS:HG2	1:B:250:ILE:HG21	1.84	0.59
1:A:111:SER:HB2	1:A:116:VAL:HG22	1.85	0.58
1:A:274:LYS:HA	1:A:274:LYS:CE	2.32	0.58
1:A:347:LYS:HD3	1:A:348:GLU:HG3	1.85	0.58
1:B:64:ILE:HD11	1:B:69:ILE:HG12	1.84	0.58
1:B:213:TRP:CH2	1:B:240:LEU:HB3	2.38	0.58
1:B:216:VAL:CG1	1:B:217:ALA:N	2.65	0.58
1:B:242:VAL:HG11	1:B:276:ALA:HA	1.84	0.58
1:B:321:ALA:O	1:B:324:LYS:N	2.35	0.58
1:A:312:VAL:HA	1:A:315:LEU:CD2	2.34	0.58
1:B:90:TYR:CD1	1:B:116:VAL:HA	2.36	0.58
1:A:186:ILE:HG12	1:B:142:ARG:HH11	1.63	0.58
1:B:139:GLN:HA	1:B:142:ARG:CD	2.32	0.58
1:B:253:ASN:ND2	1:B:263:PRO:O	2.36	0.58
1:A:254:HIS:O	1:A:257:ARG:HB2	2.03	0.58
1:B:19:LYS:O	1:B:20:MET:C	2.47	0.58
1:B:82:LYS:CB	1:B:178:LEU:HD11	2.15	0.58
1:B:186:ILE:HG13	1:B:188:LEU:CB	2.32	0.58
1:A:18:PRO:HD2	1:A:21:VAL:HG21	1.84	0.58
1:A:90:TYR:HA	1:A:116:VAL:HG13	1.86	0.58
1:A:98:ALA:HB3	1:A:324:LYS:HZ3	1.69	0.58
1:B:188:LEU:HB2	1:B:198:GLY:CA	2.34	0.58
1:B:61:THR:HA	1:B:70:SER:HA	1.85	0.58
1:B:126:PHE:HB2	1:B:144:ALA:HB2	1.86	0.58
1:B:154:LEU:H	1:B:227:ILE:HG22	1.68	0.58
1:B:279:ARG:HG2	1:B:280:ILE:HG12	1.85	0.58
1:A:39:ARG:HH21	1:A:289:ARG:HB2	1.69	0.58
1:A:267:MET:SD	1:A:358:TRP:CE3	2.97	0.58
1:B:9:TYR:HB3	1:B:313:PHE:HB3	1.85	0.58
1:B:142:ARG:NH2	1:B:222:ILE:HG23	2.19	0.58
1:A:158:THR:HG23	1:A:258:GLN:CD	2.28	0.58
1:A:187:ASP:O	1:B:134:ARG:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ALA:HB3	1:B:300:LEU:HD22	1.85	0.58
1:B:67:PHE:CA	1:B:68:LYS:HZ1	2.12	0.57
1:A:17:LEU:HD21	1:A:316:ALA:HB1	1.86	0.57
1:B:64:ILE:HD13	1:B:67:PHE:O	2.04	0.57
1:B:295:PHE:O	1:B:298:LEU:HG	2.03	0.57
1:B:17:LEU:HB2	1:B:18:PRO:HD2	1.85	0.57
1:B:83:MET:HB3	1:B:175:PRO:HG3	1.86	0.57
1:B:266:ILE:HG13	1:B:267:MET:N	2.19	0.57
1:B:6:VAL:HG13	1:B:329:MET:CE	2.34	0.57
1:B:46:LEU:HB2	1:B:355:ALA:HB3	1.86	0.57
1:B:219:LEU:O	1:B:219:LEU:HD23	2.04	0.57
1:B:251:VAL:HG11	1:B:268:ALA:HB3	1.87	0.57
1:A:131:TYR:HB3	1:A:206:GLN:CD	2.29	0.57
1:A:213:TRP:HA	1:A:216:VAL:HB	1.85	0.57
1:B:75:ILE:HG13	1:B:103:MET:CE	2.34	0.57
1:B:104:THR:HG22	1:B:125:PHE:HB3	1.86	0.57
1:A:246:ALA:O	1:A:280:ILE:HG21	2.05	0.57
1:A:131:TYR:O	1:A:134:ARG:HD3	2.04	0.56
1:B:259:LEU:O	1:B:262:VAL:HG22	2.04	0.56
1:A:64:ILE:HG23	1:A:65:LEU:HD13	1.86	0.56
1:A:131:TYR:HA	1:A:207:ILE:CA	2.34	0.56
1:A:162:GLY:HA3	1:A:258:GLN:HA	1.88	0.56
1:A:247:ALA:HA	1:A:280:ILE:HG21	1.85	0.56
1:B:34:THR:HA	1:B:37:GLU:OE2	2.06	0.56
1:B:110:THR:HG22	1:B:181:LYS:H	1.70	0.56
1:B:156:VAL:HG13	1:B:229:VAL:HG12	1.86	0.56
1:B:240:LEU:O	1:B:244:HIS:HD2	1.87	0.56
1:B:288:VAL:HG12	1:B:293:ASP:HB3	1.86	0.56
1:A:107:SER:HB3	1:A:183:PHE:CE1	2.41	0.56
1:B:125:PHE:CE2	1:B:151:ALA:HB3	2.40	0.56
1:B:232:VAL:HG12	1:B:251:VAL:N	2.19	0.56
1:A:164:ARG:CD	1:A:164:ARG:H	2.19	0.56
1:B:126:PHE:CD2	1:B:144:ALA:HB2	2.40	0.56
1:B:294:VAL:HG21	1:B:330:MET:CG	2.36	0.56
1:B:320:GLU:O	1:B:323:VAL:HG22	2.05	0.56
1:A:103:MET:CE	1:A:105:LEU:HD22	2.36	0.56
1:A:326:VAL:O	1:A:330:MET:HE2	2.05	0.56
1:B:132:LYS:CG	1:B:208:ASP:HB2	2.24	0.56
1:A:265:THR:HG21	1:A:284:LEU:HB2	1.88	0.56
1:A:323:VAL:HA	1:A:326:VAL:HB	1.88	0.56
1:B:103:MET:HE2	1:B:104:THR:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HG	1:B:175:PRO:CD	2.35	0.56
1:B:309:ARG:N	1:B:310:PRO:HD2	2.20	0.56
1:A:39:ARG:C	1:A:41:ALA:H	2.14	0.56
1:B:75:ILE:HG22	1:B:308:GLY:H	1.70	0.56
1:B:227:ILE:CB	1:B:246:ALA:HB1	2.11	0.56
1:A:46:LEU:O	1:A:354:ILE:HG12	2.05	0.56
1:A:228:LEU:HD22	1:A:228:LEU:N	2.21	0.56
1:A:164:ARG:HD3	1:A:164:ARG:H	1.69	0.56
1:B:6:VAL:HG21	1:B:289:ARG:O	2.06	0.56
1:B:34:THR:O	1:B:38:ASN:OD1	2.24	0.56
1:B:69:ILE:HD12	1:B:72:PRO:HA	1.88	0.56
1:B:72:PRO:O	1:B:74:MET:N	2.39	0.56
1:B:126:PHE:CD1	1:B:127:GLN:N	2.71	0.56
1:A:45:ILE:HA	1:A:356:ALA:HA	1.88	0.55
1:A:263:PRO:HB2	1:A:268:ALA:HB2	1.87	0.55
1:B:141:VAL:HG21	1:B:222:ILE:HG22	1.87	0.55
1:B:288:VAL:H	1:B:289:ARG:HH21	1.52	0.55
1:A:18:PRO:O	1:A:21:VAL:N	2.38	0.55
1:A:218:TRP:HE1	1:B:185:GLY:C	2.13	0.55
1:B:99:ALA:CB	1:B:324:LYS:HA	2.36	0.55
1:B:131:TYR:CB	1:B:136:VAL:HB	2.29	0.55
1:B:300:LEU:HD22	1:B:300:LEU:N	2.21	0.55
1:A:61:THR:O	1:A:346:LEU:HD21	2.06	0.55
1:A:113:VAL:HG12	1:A:149:PHE:CZ	2.42	0.55
1:A:139:GLN:HB2	1:B:139:GLN:OE1	2.06	0.55
1:B:32:GLN:OE1	1:B:35:LEU:HB2	2.07	0.55
1:B:159:PRO:CG	1:B:211:LEU:HD21	2.37	0.55
1:B:246:ALA:O	1:B:247:ALA:HB2	2.06	0.55
1:A:3:ILE:HD12	1:A:8:GLU:OE1	2.07	0.55
1:B:53:ILE:HG21	1:B:342:GLY:CA	2.37	0.55
1:A:38:ASN:O	1:A:42:PHE:HE1	1.89	0.55
1:A:69:ILE:O	1:A:69:ILE:HG13	2.07	0.55
1:A:146:ARG:CB	1:B:114:GLU:HA	2.21	0.55
1:B:73:ILE:HG23	1:B:305:VAL:HB	1.88	0.55
1:B:77:PRO:HD2	1:B:230:LYS:NZ	2.21	0.55
1:B:174:LEU:HG	1:B:175:PRO:N	2.22	0.55
1:B:64:ILE:HD12	1:B:69:ILE:HG12	1.87	0.55
1:B:73:ILE:HD13	1:B:330:MET:HB3	1.89	0.55
1:A:171:ARG:HG2	1:A:171:ARG:NH1	2.22	0.54
1:B:104:THR:HG22	1:B:125:PHE:HB2	1.89	0.54
1:B:279:ARG:CG	1:B:280:ILE:HG12	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ILE:HG13	1:B:356:ALA:HA	1.90	0.54
1:B:216:VAL:HG12	1:B:217:ALA:H	1.73	0.54
1:B:318:GLU:HB2	1:B:322:GLY:HA2	1.88	0.54
1:A:139:GLN:HE22	1:B:140:LEU:HD12	1.72	0.54
1:B:145:GLU:HA	1:B:225:LEU:HD22	1.89	0.54
1:A:103:MET:HE1	1:A:105:LEU:HD22	1.89	0.54
1:A:358:TRP:CD1	1:A:359:ASP:N	2.75	0.54
1:A:158:THR:HG23	1:A:258:GLN:NE2	2.23	0.54
1:B:95:ALA:C	1:B:97:SER:H	2.14	0.54
1:B:101:THR:HG23	1:B:102:ILE:N	2.21	0.54
1:B:239:ARG:HG3	1:B:240:LEU:N	2.22	0.54
1:B:242:VAL:CG2	1:B:276:ALA:HB2	2.36	0.54
1:A:56:THR:C	1:A:57:ASN:HD22	2.15	0.54
1:A:312:VAL:C	1:A:314:SER:H	2.15	0.54
1:B:216:VAL:CG1	1:B:217:ALA:H	2.21	0.54
1:B:289:ARG:HB3	1:B:289:ARG:HH11	1.71	0.54
1:A:55:VAL:HG12	1:A:55:VAL:O	2.06	0.54
1:A:219:LEU:O	1:A:223:THR:HG22	2.08	0.54
1:B:240:LEU:C	1:B:242:VAL:H	2.15	0.54
1:B:61:THR:CG2	1:B:70:SER:HA	2.34	0.53
1:B:72:PRO:C	1:B:305:VAL:HG23	2.33	0.53
1:B:107:SER:HA	1:B:182:ASN:CG	2.33	0.53
1:B:152:ILE:HG22	1:B:227:ILE:HG23	1.90	0.53
1:B:188:LEU:HB2	1:B:198:GLY:HA2	1.89	0.53
1:B:239:ARG:O	1:B:243:GLN:N	2.39	0.53
1:B:288:VAL:CG2	1:B:294:VAL:HG12	2.38	0.53
1:A:84:ALA:O	1:A:85:HIS:HB3	2.08	0.53
1:A:105:LEU:HG	1:A:126:PHE:HD1	1.72	0.53
1:A:145:GLU:C	1:A:147:ALA:H	2.16	0.53
1:B:238:ALA:C	1:B:241:ALA:H	2.16	0.53
1:A:99:ALA:CB	1:A:327:LEU:HD13	2.38	0.53
1:A:139:GLN:CB	1:B:139:GLN:HB3	2.39	0.53
1:B:346:LEU:CD1	1:B:349:ILE:HG13	2.37	0.53
1:B:21:VAL:HG11	1:B:83:MET:HG2	1.90	0.53
1:B:326:VAL:O	1:B:329:MET:N	2.41	0.53
1:A:126:PHE:CZ	1:A:182:ASN:ND2	2.76	0.53
1:A:213:TRP:O	1:A:216:VAL:HG12	2.09	0.53
1:B:295:PHE:CA	1:B:298:LEU:HG	2.36	0.53
1:B:218:TRP:CE3	1:B:219:LEU:HB2	2.44	0.53
1:B:291:GLY:HA3	1:B:333:GLU:CB	2.38	0.53
1:B:24:PHE:CE2	1:B:80:MET:HB2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:THR:HG21	1:B:262:VAL:HG23	1.90	0.53
1:B:78:THR:O	1:B:79:ALA:HB2	2.09	0.53
1:A:59:ASP:HB3	1:A:345:SER:CB	2.38	0.53
1:B:23:ASP:O	1:B:164:ARG:NE	2.42	0.53
1:B:106:SER:O	1:B:109:ALA:HB3	2.09	0.53
1:B:6:VAL:HA	1:B:329:MET:SD	2.49	0.53
1:B:20:MET:O	1:B:23:ASP:HB2	2.09	0.53
1:B:251:VAL:CG1	1:B:265:THR:HG22	2.38	0.53
1:B:324:LYS:HG3	1:B:325:LYS:H	1.72	0.53
1:A:143:ARG:CA	1:B:143:ARG:HG2	2.39	0.52
1:A:247:ALA:HA	1:A:280:ILE:CG2	2.39	0.52
1:A:270:GLU:O	1:A:274:LYS:HB2	2.09	0.52
1:A:329:MET:O	1:A:333:GLU:HG3	2.09	0.52
1:B:24:PHE:HE2	1:B:79:ALA:C	2.17	0.52
1:B:71:MET:HB3	1:B:331:ARG:HG3	1.90	0.52
1:A:69:ILE:CD1	1:A:74:MET:HE2	2.39	0.52
1:B:128:LEU:HG	1:B:140:LEU:HD23	1.91	0.52
1:B:220:GLN:NE2	1:B:246:ALA:HA	2.24	0.52
1:A:249:ILE:HG21	1:A:251:VAL:HG22	1.91	0.52
1:B:5:ASN:HA	1:B:290:ARG:HH12	1.74	0.52
1:A:82:LYS:CB	1:A:110:THR:HG21	2.36	0.52
1:A:142:ARG:HB2	1:B:143:ARG:CZ	2.39	0.52
1:A:143:ARG:HG3	1:B:143:ARG:HA	1.91	0.52
1:B:247:ALA:HA	1:B:280:ILE:CB	2.35	0.52
1:A:146:ARG:HD3	1:B:117:ALA:HB3	1.91	0.52
1:B:165:GLU:O	1:B:169:LYS:HB3	2.09	0.52
1:A:42:PHE:HB3	1:A:296:LYS:HZ2	1.74	0.52
1:B:111:SER:HB3	1:B:116:VAL:HG23	1.91	0.52
1:B:111:SER:HB3	1:B:116:VAL:CG2	2.39	0.52
1:B:266:ILE:HA	1:B:284:LEU:HD12	1.91	0.52
1:A:314:SER:OG	1:A:326:VAL:HG21	2.09	0.52
1:B:110:THR:HG22	1:B:181:LYS:N	2.23	0.52
1:B:152:ILE:CG2	1:B:153:ALA:N	2.73	0.52
1:B:307:ILE:CG2	1:B:310:PRO:HG3	2.40	0.52
1:A:71:MET:HG2	1:A:73:ILE:HD12	1.91	0.52
1:B:23:ASP:HB2	1:B:167:ASP:CB	2.36	0.52
1:B:265:THR:OG1	1:B:285:ASP:O	2.27	0.52
1:B:330:MET:O	1:B:334:PHE:CD1	2.63	0.52
1:A:296:LYS:O	1:A:299:ALA:N	2.42	0.51
1:B:45:ILE:HA	1:B:357:ASP:OD1	2.10	0.51
1:B:95:ALA:O	1:B:97:SER:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ASN:HD22	1:B:262:VAL:HG23	1.75	0.51
1:A:117:ALA:CB	1:B:147:ALA:HB3	2.41	0.51
1:B:76:ALA:N	1:B:104:THR:OG1	2.43	0.51
1:A:18:PRO:O	1:A:19:LYS:C	2.52	0.51
1:B:291:GLY:CA	1:B:330:MET:SD	2.92	0.51
1:B:60:MET:HG2	1:B:61:THR:H	1.75	0.51
1:B:63:THR:HG23	1:B:66:GLY:O	2.11	0.51
1:B:126:PHE:HD1	1:B:127:GLN:H	1.55	0.51
1:B:89:GLU:C	1:B:91:ALA:H	2.17	0.51
1:B:152:ILE:HG22	1:B:153:ALA:H	1.75	0.51
1:A:34:THR:HG21	1:A:262:VAL:O	2.10	0.51
1:A:136:VAL:O	1:B:139:GLN:OE1	2.29	0.51
1:A:290:ARG:O	1:A:294:VAL:HG23	2.11	0.51
1:B:40:ASN:HA	1:B:43:SER:OG	2.11	0.51
1:B:30:GLU:HB2	1:B:260:ASP:CB	2.40	0.51
1:B:68:LYS:N	1:B:68:LYS:NZ	2.58	0.51
1:B:73:ILE:HA	1:B:305:VAL:O	2.11	0.51
1:B:171:ARG:HG3	1:B:171:ARG:O	2.10	0.51
1:A:67:PHE:CZ	1:A:150:LYS:HG3	2.45	0.51
1:B:71:MET:SD	1:B:100:GLY:O	2.69	0.51
1:B:209:ARG:N	1:B:209:ARG:CD	2.74	0.51
1:A:132:LYS:HB3	1:A:132:LYS:HZ3	1.76	0.50
1:B:38:ASN:O	1:B:42:PHE:HE1	1.94	0.50
1:B:62:THR:C	1:B:68:LYS:HA	2.36	0.50
1:B:89:GLU:OE2	1:B:105:LEU:HD23	2.11	0.50
1:B:112:SER:O	1:B:115:GLU:N	2.44	0.50
1:B:232:VAL:HG13	1:B:251:VAL:HG22	1.93	0.50
1:B:240:LEU:O	1:B:244:HIS:CD2	2.63	0.50
1:B:108:TRP:HA	1:B:180:LEU:HG	1.92	0.50
1:A:159:PRO:CG	1:A:160:ARG:H	2.23	0.50
1:A:295:PHE:HB2	1:A:337:THR:HG21	1.93	0.50
1:B:71:MET:SD	1:B:71:MET:O	2.69	0.50
1:B:266:ILE:O	1:B:269:LEU:HB2	2.12	0.50
1:A:28:GLY:HA3	1:A:35:LEU:CD1	2.36	0.50
1:A:64:ILE:HG23	1:A:65:LEU:CD1	2.41	0.50
1:A:235:ALA:HB1	1:A:275:ALA:HB2	1.92	0.50
1:A:184:GLU:OE2	1:B:222:ILE:HA	2.11	0.50
1:A:143:ARG:C	1:A:145:GLU:H	2.20	0.50
1:A:186:ILE:HG22	1:A:187:ASP:N	2.26	0.50
1:B:8:GLU:O	1:B:12:ILE:HD12	2.12	0.50
1:B:250:ILE:CB	1:B:283:PHE:HB2	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:VAL:O	1:B:315:LEU:HB2	2.12	0.50
1:B:294:VAL:HG23	1:B:295:PHE:N	2.26	0.50
1:A:202:TYR:CD1	1:A:203:VAL:N	2.80	0.50
1:A:283:PHE:HB2	1:A:306:PHE:HE1	1.77	0.50
1:A:131:TYR:HB3	1:A:206:GLN:NE2	2.27	0.49
1:B:20:MET:O	1:B:167:ASP:HB3	2.12	0.49
1:B:74:MET:SD	1:B:304:GLY:HA3	2.52	0.49
1:B:144:ALA:C	1:B:149:PHE:O	2.55	0.49
1:B:145:GLU:O	1:B:150:LYS:N	2.46	0.49
1:B:264:ALA:HB3	1:B:266:ILE:HG22	1.93	0.49
1:B:288:VAL:HG21	1:B:294:VAL:HG12	1.94	0.49
1:A:6:VAL:O	1:A:7:ASN:HB2	2.11	0.49
1:A:280:ILE:HB	1:A:281:PRO:HD2	1.93	0.49
1:B:20:MET:CG	1:B:172:PHE:HB2	2.39	0.49
1:B:33:TRP:CD2	1:B:261:TYR:HA	2.47	0.49
1:B:41:ALA:C	1:B:44:ARG:HB3	2.33	0.49
1:B:239:ARG:O	1:B:242:VAL:HB	2.12	0.49
1:A:183:PHE:C	1:A:185:GLY:H	2.20	0.49
1:B:67:PHE:HA	1:B:68:LYS:NZ	2.17	0.49
1:B:82:LYS:HG3	1:B:110:THR:OG1	2.12	0.49
1:A:44:ARG:HB3	1:A:357:ASP:HB3	1.94	0.49
1:B:74:MET:CE	1:B:304:GLY:HA3	2.42	0.49
1:B:269:LEU:O	1:B:273:VAL:HB	2.12	0.49
1:A:32:GLN:O	1:A:35:LEU:HB2	2.13	0.49
1:A:42:PHE:HB3	1:A:296:LYS:NZ	2.28	0.49
1:A:186:ILE:CD1	1:B:139:GLN:HE21	2.25	0.49
1:B:214:LYS:N	1:B:214:LYS:HD2	2.27	0.49
1:B:60:MET:HG2	1:B:61:THR:N	2.28	0.49
1:B:129:TYR:O	1:B:137:VAL:HG13	2.13	0.49
1:B:175:PRO:HG2	1:B:178:LEU:HD12	1.94	0.49
1:B:300:LEU:H	1:B:300:LEU:CD2	2.23	0.49
1:B:176:PRO:HG2	1:B:177:PHE:H	1.78	0.49
1:A:173:VAL:O	1:A:175:PRO:HD3	2.13	0.49
1:B:53:ILE:CG1	1:B:342:GLY:HA3	2.39	0.49
1:B:60:MET:HB3	1:B:335:GLU:HG2	1.95	0.49
1:B:73:ILE:CD1	1:B:330:MET:HB3	2.42	0.49
1:B:131:TYR:N	1:B:137:VAL:HG22	2.28	0.49
1:A:131:TYR:HD1	1:A:207:ILE:CA	2.24	0.49
1:B:132:LYS:HB2	1:B:206:GLN:C	2.37	0.49
1:B:141:VAL:CG2	1:B:219:LEU:HD21	2.43	0.49
1:B:159:PRO:HG3	1:B:211:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLN:HB3	1:A:35:LEU:HD22	1.95	0.49
1:A:53:ILE:HG22	1:A:54:ASP:H	1.78	0.49
1:B:159:PRO:HG3	1:B:211:LEU:HD11	1.94	0.49
1:A:7:ASN:C	1:A:9:TYR:N	2.68	0.48
1:B:152:ILE:O	1:B:227:ILE:HA	2.13	0.48
1:A:62:THR:OG1	1:A:69:ILE:HG13	2.13	0.48
1:A:160:ARG:HG3	1:A:209:ARG:NE	2.28	0.48
1:B:253:ASN:C	1:B:255:GLY:H	2.21	0.48
1:A:61:THR:HA	1:A:70:SER:O	2.13	0.48
1:B:207:ILE:HG13	1:B:207:ILE:O	2.13	0.48
1:A:91:ALA:HB1	1:A:320:GLU:HG2	1.95	0.48
1:A:140:LEU:HD11	1:A:182:ASN:OD1	2.13	0.48
1:B:80:MET:HG3	1:B:108:TRP:HB3	1.95	0.48
1:B:94:ARG:HD3	1:B:119:THR:OG1	2.13	0.48
1:B:123:ILE:HB	1:B:150:LYS:CB	2.41	0.48
1:B:128:LEU:HD11	1:B:152:ILE:HG23	1.94	0.48
1:B:295:PHE:HE2	1:B:338:MET:HG3	1.79	0.48
1:B:334:PHE:O	1:B:337:THR:HB	2.14	0.48
1:A:39:ARG:NH1	1:A:287:GLY:O	2.47	0.48
1:B:295:PHE:HA	1:B:298:LEU:CG	2.40	0.48
1:A:117:ALA:HB1	1:B:147:ALA:HB3	1.95	0.48
1:A:186:ILE:O	1:A:187:ASP:HB2	2.12	0.48
1:A:277:GLN:H	1:A:279:ARG:CZ	2.26	0.48
1:A:342:GLY:O	1:A:353:HIS:HE1	1.96	0.48
1:B:83:MET:SD	1:B:83:MET:N	2.82	0.48
1:B:184:GLU:O	1:B:186:ILE:N	2.46	0.48
1:B:236:GLU:HA	1:B:239:ARG:HH12	1.75	0.48
1:B:290:ARG:C	1:B:292:THR:H	2.21	0.48
1:B:333:GLU:HA	1:B:336:LEU:HD12	1.95	0.48
1:A:25:TYR:HE2	1:A:84:ALA:HB2	1.79	0.48
1:A:250:ILE:HA	1:A:283:PHE:O	2.13	0.48
1:B:112:SER:HB3	1:B:115:GLU:HB2	1.94	0.48
1:A:81:GLN:O	1:A:315:LEU:HD11	2.14	0.48
1:A:103:MET:O	1:A:124:ARG:HB2	2.13	0.48
1:B:35:LEU:CD1	1:B:256:ALA:HB3	2.40	0.48
1:B:131:TYR:CB	1:B:137:VAL:HG22	2.40	0.48
1:B:145:GLU:O	1:B:150:LYS:HA	2.13	0.48
1:B:215:ASP:HA	1:B:218:TRP:CG	2.48	0.48
1:B:90:TYR:CE2	1:B:115:GLU:O	2.67	0.48
1:B:270:GLU:O	1:B:274:LYS:HG3	2.14	0.48
1:A:165:GLU:HB3	1:A:166:ALA:H	1.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLU:O	1:A:322:GLY:N	2.45	0.48
1:B:134:ARG:O	1:B:138:ALA:HB3	2.14	0.48
1:B:152:ILE:CG2	1:B:153:ALA:H	2.26	0.48
1:B:204:ALA:O	1:B:206:GLN:N	2.43	0.48
1:B:253:ASN:O	1:B:255:GLY:N	2.47	0.48
1:A:111:SER:HB2	1:A:116:VAL:CG2	2.43	0.47
1:A:289:ARG:HH12	2:A:370:FMN:P	2.37	0.47
1:B:22:TYR:CA	1:B:25:TYR:HD1	2.26	0.47
1:A:62:THR:HB	1:A:69:ILE:HG12	1.96	0.47
1:A:300:LEU:HD23	1:A:351:ARG:CD	2.42	0.47
1:A:354:ILE:HG23	1:A:355:ALA:N	2.29	0.47
1:B:10:GLU:HG2	1:B:313:PHE:HE2	1.79	0.47
1:B:34:THR:HG21	1:B:253:ASN:ND2	2.28	0.47
1:A:9:TYR:O	1:A:10:GLU:C	2.57	0.47
1:A:81:GLN:O	1:A:88:GLY:HA3	2.15	0.47
1:A:103:MET:SD	1:A:103:MET:O	2.72	0.47
1:A:125:PHE:CE1	1:A:150:LYS:HB2	2.49	0.47
1:A:350:SER:C	1:A:352:SER:H	2.21	0.47
1:B:2:GLU:HG2	1:B:3:ILE:H	1.80	0.47
1:B:106:SER:HB2	1:B:127:GLN:OE1	2.14	0.47
1:B:144:ALA:CA	1:B:149:PHE:HB3	2.26	0.47
1:B:294:VAL:O	1:B:298:LEU:HB3	2.14	0.47
1:A:25:TYR:CE2	1:A:84:ALA:HB2	2.50	0.47
1:A:188:LEU:O	1:B:134:ARG:HB2	2.15	0.47
1:A:207:ILE:HG23	1:A:208:ASP:N	2.29	0.47
1:B:218:TRP:HE3	1:B:219:LEU:HB2	1.78	0.47
1:B:254:HIS:HB2	1:B:257:ARG:O	2.13	0.47
1:B:58:ILE:N	1:B:58:ILE:HD13	2.29	0.47
1:B:137:VAL:O	1:B:139:GLN:N	2.43	0.47
1:B:250:ILE:HG23	1:B:250:ILE:O	2.15	0.47
1:A:146:ARG:CZ	1:B:117:ALA:O	2.62	0.47
1:A:222:ILE:O	1:A:223:THR:HB	2.13	0.47
1:B:16:LYS:HB3	1:B:17:LEU:HD23	1.96	0.47
1:A:9:TYR:HA	1:A:12:ILE:CG1	2.45	0.47
1:A:58:ILE:HG21	1:A:338:MET:HE3	1.97	0.47
1:A:101:THR:HG22	1:A:102:ILE:N	2.25	0.47
1:A:265:THR:HG22	1:A:284:LEU:HB2	1.95	0.47
1:B:16:LYS:C	1:B:17:LEU:HD23	2.40	0.47
1:B:151:ALA:HA	1:B:226:PRO:HD2	1.96	0.47
1:B:250:ILE:HD12	1:B:306:PHE:CE2	2.49	0.47
1:A:172:PHE:HE1	1:A:174:LEU:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:ASN:O	1:B:8:GLU:HB2	2.15	0.47
1:B:80:MET:SD	1:B:108:TRP:HD1	2.38	0.47
1:A:60:MET:HB3	1:A:72:PRO:CD	2.45	0.47
1:A:131:TYR:CD1	1:A:207:ILE:HA	2.39	0.47
1:A:188:LEU:O	1:B:134:ARG:N	2.48	0.47
1:B:110:THR:HG21	1:B:179:THR:O	2.15	0.47
1:A:155:THR:HA	1:A:230:LYS:HB3	1.97	0.47
1:A:188:LEU:O	1:B:134:ARG:CB	2.64	0.47
1:A:308:GLY:O	1:A:309:ARG:C	2.57	0.47
1:A:107:SER:C	1:A:109:ALA:H	2.23	0.46
1:B:213:TRP:CH2	1:B:240:LEU:CB	2.98	0.46
1:B:230:LYS:HG2	1:B:250:ILE:HG23	1.94	0.46
1:B:298:LEU:HD12	1:B:299:ALA:N	2.30	0.46
1:B:31:ASP:O	1:B:33:TRP:N	2.48	0.46
1:B:70:SER:HB2	1:B:71:MET:HE3	1.97	0.46
1:B:154:LEU:O	1:B:229:VAL:HG12	2.15	0.46
1:B:252:SER:HA	1:B:265:THR:CG2	2.44	0.46
1:B:289:ARG:N	1:B:289:ARG:NE	2.63	0.46
1:A:130:VAL:HG22	1:A:137:VAL:HG11	1.96	0.46
1:A:284:LEU:HD12	1:A:302:ALA:CB	2.46	0.46
1:B:7:ASN:O	1:B:10:GLU:HB2	2.16	0.46
1:B:48:ARG:O	1:B:353:HIS:CD2	2.65	0.46
1:B:234:THR:O	1:B:238:ALA:HB2	2.15	0.46
1:B:295:PHE:CE2	1:B:338:MET:HG3	2.51	0.46
1:A:21:VAL:HG12	1:A:25:TYR:CE2	2.49	0.46
1:A:27:SER:HB2	1:A:164:ARG:HB2	1.97	0.46
1:A:146:ARG:NH1	1:B:117:ALA:O	2.49	0.46
1:B:6:VAL:HG21	1:B:290:ARG:HA	1.97	0.46
1:B:30:GLU:HB2	1:B:260:ASP:N	2.31	0.46
1:B:74:MET:HE2	1:B:306:PHE:HE1	1.81	0.46
1:B:105:LEU:HD12	1:B:105:LEU:N	2.30	0.46
1:B:117:ALA:C	1:B:119:THR:H	2.23	0.46
1:B:129:TYR:HB2	1:B:131:TYR:CZ	2.50	0.46
1:B:244:HIS:CD2	1:B:244:HIS:N	2.83	0.46
1:B:42:PHE:CE2	1:B:288:VAL:CG1	2.98	0.46
1:A:34:THR:HA	1:A:37:GLU:HB3	1.98	0.46
1:A:107:SER:HB2	1:A:129:TYR:HD2	1.80	0.46
1:A:265:THR:HB	1:A:284:LEU:HD23	1.97	0.46
1:B:78:THR:O	1:B:79:ALA:CB	2.63	0.46
1:B:238:ALA:HA	1:B:241:ALA:CB	2.46	0.46
1:B:308:GLY:O	1:B:311:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG11	1:A:339:ALA:CB	2.45	0.46
1:A:80:MET:HB3	1:A:83:MET:HG3	1.97	0.46
1:A:108:TRP:HA	1:A:108:TRP:CE3	2.51	0.46
1:B:273:VAL:O	1:B:277:GLN:HB3	2.16	0.46
1:A:9:TYR:O	1:A:12:ILE:N	2.48	0.46
1:A:254:HIS:CE1	2:A:370:FMN:C2	2.98	0.46
1:B:216:VAL:HG13	1:B:217:ALA:N	2.31	0.46
1:B:235:ALA:CB	1:B:271:GLU:O	2.61	0.46
1:B:292:THR:O	1:B:295:PHE:N	2.49	0.46
1:B:345:SER:OG	1:B:348:GLU:HG2	2.15	0.46
1:A:82:LYS:HB2	1:A:110:THR:OG1	2.16	0.46
1:A:214:LYS:HG3	1:A:215:ASP:N	2.30	0.46
1:B:90:TYR:HA	1:B:116:VAL:HG13	1.98	0.46
1:B:326:VAL:O	1:B:329:MET:HB3	2.16	0.46
1:A:55:VAL:HG11	1:A:339:ALA:HB1	1.98	0.45
1:A:289:ARG:HG2	1:A:310:PRO:HG3	1.98	0.45
1:B:186:ILE:CG1	1:B:188:LEU:HB3	2.37	0.45
1:B:269:LEU:CD2	1:B:270:GLU:HG3	2.42	0.45
1:A:24:PHE:CD1	1:A:172:PHE:HE2	2.34	0.45
1:B:131:TYR:O	1:B:137:VAL:CG2	2.65	0.45
1:B:235:ALA:HB1	1:B:275:ALA:CB	2.46	0.45
1:B:344:ARG:HD3	1:B:344:ARG:N	2.31	0.45
1:A:71:MET:HE3	1:A:331:ARG:NH1	2.32	0.45
1:A:142:ARG:CB	1:B:143:ARG:NE	2.77	0.45
1:A:165:GLU:O	1:A:166:ALA:C	2.58	0.45
1:A:254:HIS:CG	1:A:258:GLN:HG2	2.51	0.45
1:B:18:PRO:HG2	1:B:21:VAL:CB	2.43	0.45
1:B:125:PHE:CE2	1:B:228:LEU:HD23	2.51	0.45
1:A:133:ASP:HB3	1:B:187:ASP:OD2	2.17	0.45
1:A:158:THR:HA	1:A:258:GLN:NE2	2.32	0.45
1:A:235:ALA:CB	1:A:275:ALA:HB2	2.46	0.45
1:B:131:TYR:HB3	1:B:206:GLN:HG3	1.99	0.45
1:B:150:LYS:HD2	1:B:151:ALA:HB2	1.99	0.45
1:B:172:PHE:CZ	1:B:174:LEU:HA	2.51	0.45
1:B:233:ILE:CD1	1:B:263:PRO:HD2	2.46	0.45
1:B:298:LEU:CA	1:B:302:ALA:HB3	2.32	0.45
1:A:59:ASP:HB2	1:A:345:SER:HB3	1.96	0.45
1:A:103:MET:SD	1:A:105:LEU:HD22	2.57	0.45
1:A:331:ARG:C	1:A:333:GLU:H	2.25	0.45
1:B:10:GLU:CG	1:B:313:PHE:HE2	2.30	0.45
1:B:76:ALA:O	1:B:77:PRO:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ALA:HB1	1:A:228:LEU:CD2	2.47	0.45
1:A:202:TYR:HD1	1:A:203:VAL:N	2.14	0.45
1:B:25:TYR:HB3	1:B:312:VAL:HG11	1.99	0.45
1:B:208:ASP:HA	1:B:209:ARG:NH2	2.31	0.45
1:A:146:ARG:HH11	1:B:117:ALA:CB	2.23	0.45
1:B:186:ILE:HB	1:B:187:ASP:H	1.55	0.45
1:B:213:TRP:CE3	1:B:244:HIS:HB2	2.52	0.45
1:B:213:TRP:HA	1:B:216:VAL:HB	1.98	0.45
1:B:238:ALA:O	1:B:241:ALA:N	2.49	0.45
1:A:150:LYS:O	1:A:225:LEU:HA	2.17	0.45
1:B:23:ASP:O	1:B:164:ARG:NH2	2.50	0.45
1:B:158:THR:HA	1:B:159:PRO:HD3	1.37	0.45
1:A:30:GLU:CD	1:A:163:ARG:HH11	2.24	0.45
1:A:236:GLU:OE1	1:A:236:GLU:N	2.50	0.45
1:B:89:GLU:OE1	1:B:116:VAL:HG21	2.16	0.45
1:B:90:TYR:HD1	1:B:90:TYR:N	2.14	0.45
1:B:94:ARG:CA	1:B:119:THR:HG21	2.47	0.45
1:B:290:ARG:O	1:B:292:THR:N	2.44	0.45
1:A:77:PRO:HB2	1:A:106:SER:HB2	1.99	0.44
1:A:132:LYS:HB2	1:A:206:GLN:OE1	2.17	0.44
1:A:143:ARG:HG3	1:B:143:ARG:N	2.32	0.44
1:A:277:GLN:N	1:A:279:ARG:CD	2.80	0.44
1:B:131:TYR:O	1:B:133:ASP:N	2.46	0.44
1:B:270:GLU:CA	1:B:273:VAL:HG12	2.39	0.44
1:B:273:VAL:HG23	1:B:282:VAL:HG11	1.99	0.44
1:A:98:ALA:CB	1:A:324:LYS:HZ1	2.30	0.44
1:A:108:TRP:HZ3	1:A:131:TYR:OH	2.00	0.44
1:B:42:PHE:HB3	1:B:296:LYS:HG2	1.97	0.44
1:B:131:TYR:CE2	1:B:140:LEU:HD11	2.51	0.44
1:B:154:LEU:C	1:B:154:LEU:HD13	2.43	0.44
1:B:295:PHE:O	1:B:296:LYS:C	2.59	0.44
1:B:334:PHE:CD1	1:B:334:PHE:C	2.95	0.44
1:A:62:THR:HG21	1:A:69:ILE:HD11	2.00	0.44
1:A:96:ALA:O	1:A:100:GLY:N	2.51	0.44
1:A:296:LYS:O	1:A:299:ALA:HB3	2.17	0.44
1:B:90:TYR:CD1	1:B:90:TYR:N	2.85	0.44
1:B:99:ALA:HB2	1:B:324:LYS:HA	1.99	0.44
1:B:131:TYR:CA	1:B:137:VAL:HG22	2.48	0.44
1:B:266:ILE:C	1:B:266:ILE:HD12	2.42	0.44
1:A:315:LEU:HG	1:A:316:ALA:N	2.33	0.44
1:B:47:PHE:HD2	1:B:296:LYS:NZ	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PHE:CD1	1:B:127:GLN:O	2.70	0.44
1:B:127:GLN:NE2	1:B:131:TYR:OH	2.50	0.44
1:B:238:ALA:HA	1:B:241:ALA:HB3	1.97	0.44
1:B:334:PHE:HD1	1:B:335:GLU:H	1.65	0.44
1:A:105:LEU:HD21	1:A:149:PHE:HE2	1.82	0.44
1:A:114:GLU:OE1	1:B:225:LEU:HG	2.18	0.44
1:A:277:GLN:H	1:A:279:ARG:NH1	2.14	0.44
1:A:326:VAL:O	1:A:330:MET:HB2	2.18	0.44
1:B:40:ASN:HA	1:B:43:SER:CB	2.48	0.44
1:B:61:THR:HA	1:B:70:SER:CA	2.45	0.44
1:B:76:ALA:HB3	1:B:307:ILE:O	2.18	0.44
1:B:298:LEU:HD12	1:B:298:LEU:C	2.42	0.44
1:B:90:TYR:CG	1:B:116:VAL:HA	2.53	0.44
1:B:259:LEU:HB3	1:B:262:VAL:HG13	2.00	0.44
1:B:294:VAL:CG2	1:B:330:MET:HG3	2.44	0.44
1:A:53:ILE:HG22	1:A:54:ASP:N	2.32	0.44
1:B:46:LEU:HG	1:B:355:ALA:O	2.18	0.44
1:B:152:ILE:C	1:B:227:ILE:HA	2.42	0.44
1:B:229:VAL:O	1:B:249:ILE:HG23	2.17	0.44
1:B:248:GLY:HA2	1:B:281:PRO:CA	2.47	0.44
1:B:253:ASN:HD22	1:B:262:VAL:CG2	2.31	0.44
1:A:18:PRO:HD2	1:A:21:VAL:CG2	2.47	0.44
1:A:250:ILE:HG22	1:A:285:ASP:OD1	2.18	0.44
1:A:269:LEU:HD23	1:A:300:LEU:CB	2.44	0.44
1:A:277:GLN:C	1:A:279:ARG:HD2	2.43	0.44
1:B:94:ARG:HG3	1:B:94:ARG:O	2.18	0.44
1:B:130:VAL:O	1:B:130:VAL:CG1	2.63	0.44
1:B:288:VAL:HG12	1:B:293:ASP:HB2	1.97	0.44
1:A:274:LYS:NZ	1:A:277:GLN:HG2	2.32	0.44
1:A:358:TRP:NE1	1:A:359:ASP:OD2	2.51	0.44
1:B:20:MET:SD	1:B:172:PHE:HA	2.58	0.44
1:B:29:ALA:C	1:B:30:GLU:HG2	2.41	0.44
1:B:98:ALA:CB	1:B:324:LYS:HE2	2.36	0.44
1:B:323:VAL:O	1:B:326:VAL:HB	2.18	0.44
1:B:353:HIS:CD2	1:B:353:HIS:O	2.71	0.44
1:A:142:ARG:HD3	1:A:222:ILE:O	2.18	0.43
1:B:33:TRP:CD1	1:B:261:TYR:CE1	3.06	0.43
1:B:42:PHE:H	1:B:42:PHE:HD1	1.61	0.43
1:B:295:PHE:HD2	1:B:334:PHE:HB2	1.83	0.43
1:B:334:PHE:HD1	1:B:335:GLU:N	2.16	0.43
1:B:312:VAL:O	1:B:312:VAL:CG1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PHE:C	1:B:68:LYS:HZ1	2.25	0.43
1:B:80:MET:HB3	1:B:83:MET:HE1	2.00	0.43
1:B:328:GLN:C	1:B:330:MET:N	2.76	0.43
1:A:214:LYS:O	1:A:217:ALA:HB3	2.19	0.43
1:A:248:GLY:HA2	1:A:281:PRO:O	2.18	0.43
1:B:112:SER:O	1:B:114:GLU:N	2.51	0.43
1:B:175:PRO:CG	1:B:178:LEU:HD12	2.48	0.43
1:B:325:LYS:O	1:B:329:MET:N	2.52	0.43
1:A:200:SER:O	1:A:203:VAL:HG23	2.18	0.43
1:A:252:SER:OG	1:A:253:ASN:N	2.51	0.43
1:A:274:LYS:HE2	1:A:274:LYS:O	2.19	0.43
1:A:36:ALA:HB1	1:A:40:ASN:ND2	2.34	0.43
1:B:71:MET:C	1:B:73:ILE:H	2.26	0.43
1:B:90:TYR:OH	1:B:115:GLU:HB3	2.19	0.43
1:B:273:VAL:HG23	1:B:282:VAL:CG1	2.48	0.43
1:B:344:ARG:HD3	1:B:344:ARG:H	1.84	0.43
1:A:22:TYR:O	1:A:26:ALA:N	2.48	0.43
1:A:39:ARG:HH11	1:A:39:ARG:HA	1.83	0.43
1:A:105:LEU:O	1:A:126:PHE:HA	2.18	0.43
1:A:188:LEU:CD1	1:B:135:ASN:ND2	2.75	0.43
1:A:189:GLY:CA	1:B:133:ASP:HA	2.46	0.43
1:B:50:ARG:HD2	1:B:53:ILE:HD11	2.00	0.43
1:B:71:MET:CG	1:B:73:ILE:HG13	2.43	0.43
1:A:42:PHE:CD2	1:A:293:ASP:HB2	2.54	0.43
1:A:67:PHE:CE1	1:A:150:LYS:HG3	2.53	0.43
1:B:64:ILE:HD12	1:B:69:ILE:CG1	2.49	0.43
1:B:131:TYR:HB3	1:B:206:GLN:CG	2.48	0.43
1:B:215:ASP:O	1:B:218:TRP:CE3	2.72	0.43
1:B:233:ILE:HA	1:B:251:VAL:CG1	2.40	0.43
1:A:325:LYS:O	1:A:329:MET:HG3	2.19	0.43
1:B:86:PRO:HB2	1:B:87:GLU:H	1.65	0.43
1:B:186:ILE:C	1:B:188:LEU:H	2.25	0.43
1:B:215:ASP:C	1:B:218:TRP:CE3	2.97	0.43
1:B:232:VAL:H	1:B:251:VAL:CA	2.16	0.43
1:B:295:PHE:HE2	1:B:338:MET:CG	2.32	0.43
2:A:370:FMN:H9	2:A:370:FMN:H1'2	1.61	0.43
1:B:98:ALA:HB1	1:B:324:LYS:CE	2.35	0.43
1:B:150:LYS:HD2	1:B:151:ALA:N	2.33	0.43
1:B:288:VAL:HB	1:B:294:VAL:CG1	2.47	0.43
1:A:188:LEU:C	1:B:134:ARG:H	2.27	0.42
1:A:296:LYS:O	1:A:297:ALA:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:ALA:HA	1:B:320:GLU:CA	2.44	0.42
1:B:128:LEU:O	1:B:129:TYR:CG	2.72	0.42
1:B:129:TYR:HB2	1:B:131:TYR:CE1	2.53	0.42
1:B:78:THR:H	1:B:105:LEU:HA	1.84	0.42
1:B:131:TYR:CE2	1:B:140:LEU:HD21	2.50	0.42
1:A:13:ALA:O	1:A:17:LEU:HG	2.19	0.42
1:A:84:ALA:O	1:A:85:HIS:CB	2.67	0.42
1:A:145:GLU:CD	1:B:113:VAL:HB	2.45	0.42
1:A:236:GLU:O	1:A:240:LEU:HD23	2.19	0.42
1:A:249:ILE:HG23	1:A:251:VAL:HG22	2.01	0.42
1:B:229:VAL:CG2	1:B:249:ILE:HG12	2.36	0.42
1:A:58:ILE:HG22	1:A:59:ASP:N	2.27	0.42
1:A:266:ILE:HG23	1:A:267:MET:H	1.83	0.42
1:A:292:THR:O	1:A:295:PHE:HB3	2.19	0.42
1:A:42:PHE:HA	1:A:266:ILE:HD12	2.02	0.42
1:A:57:ASN:HD22	1:A:57:ASN:N	2.18	0.42
1:A:96:ALA:O	1:A:99:ALA:N	2.52	0.42
1:A:127:GLN:HA	1:A:153:ALA:O	2.20	0.42
1:A:155:THR:O	1:A:155:THR:HG22	2.19	0.42
1:A:289:ARG:HH11	1:A:310:PRO:HD3	1.84	0.42
1:B:59:ASP:OD1	1:B:62:THR:HB	2.19	0.42
1:B:247:ALA:O	1:B:248:GLY:C	2.63	0.42
1:B:309:ARG:O	1:B:312:VAL:N	2.43	0.42
1:A:131:TYR:H	1:A:137:VAL:HG21	1.85	0.42
1:A:142:ARG:HH11	1:B:184:GLU:HG3	1.71	0.42
1:A:188:LEU:HB3	1:A:189:GLY:H	1.69	0.42
1:B:132:LYS:O	1:B:133:ASP:CG	2.62	0.42
1:A:143:ARG:NE	1:B:145:GLU:OE2	2.53	0.42
1:A:270:GLU:OE2	1:A:351:ARG:NE	2.53	0.42
1:B:75:ILE:HD13	1:B:75:ILE:N	2.34	0.42
1:B:100:GLY:O	1:B:101:THR:HB	2.19	0.42
1:B:213:TRP:CD1	1:B:213:TRP:H	2.38	0.42
1:A:39:ARG:C	1:A:41:ALA:N	2.77	0.42
1:A:235:ALA:HB1	1:A:275:ALA:CB	2.50	0.42
1:B:142:ARG:HD2	1:B:142:ARG:H	1.85	0.42
1:B:214:LYS:HD2	1:B:214:LYS:H	1.83	0.42
1:A:14:LYS:HA	1:A:22:TYR:CD1	2.55	0.42
1:A:35:LEU:O	1:A:38:ASN:HB2	2.20	0.42
1:A:36:ALA:C	1:A:38:ASN:H	2.27	0.42
1:A:112:SER:OG	1:A:113:VAL:N	2.53	0.42
1:A:114:GLU:HB3	1:B:145:GLU:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ALA:HA	1:A:280:ILE:CB	2.50	0.42
1:A:143:ARG:HG3	1:B:143:ARG:CA	2.50	0.41
1:B:145:GLU:O	1:B:149:PHE:C	2.63	0.41
1:B:253:ASN:C	1:B:255:GLY:N	2.78	0.41
1:A:151:ALA:HB1	1:A:226:PRO:O	2.20	0.41
1:B:59:ASP:HB3	1:B:345:SER:HA	2.03	0.41
1:B:71:MET:HB3	1:B:331:ARG:CG	2.50	0.41
1:B:75:ILE:HB	1:B:104:THR:OG1	2.20	0.41
1:B:220:GLN:HE21	1:B:246:ALA:HA	1.85	0.41
1:B:346:LEU:HD12	1:B:349:ILE:CG1	2.44	0.41
1:A:27:SER:OG	1:A:257:ARG:NH1	2.53	0.41
1:A:44:ARG:O	1:A:357:ASP:N	2.54	0.41
1:A:161:LEU:HD12	1:A:161:LEU:H	1.85	0.41
1:A:354:ILE:HG12	1:A:355:ALA:N	2.22	0.41
1:B:85:HIS:HE2	1:B:315:LEU:HD23	1.84	0.41
1:B:159:PRO:HG2	1:B:211:LEU:HD21	2.01	0.41
1:B:172:PHE:CG	1:B:173:VAL:N	2.89	0.41
1:B:213:TRP:HH2	1:B:240:LEU:CB	2.33	0.41
1:A:228:LEU:H	1:A:228:LEU:CD2	2.31	0.41
1:A:299:ALA:O	1:A:351:ARG:N	2.54	0.41
1:B:126:PHE:HB2	1:B:144:ALA:CB	2.50	0.41
1:B:163:ARG:NH1	1:B:163:ARG:CG	2.82	0.41
1:B:309:ARG:N	1:B:310:PRO:CD	2.84	0.41
1:A:80:MET:HE3	1:A:80:MET:HB2	1.79	0.41
1:B:64:ILE:HD13	1:B:64:ILE:N	2.35	0.41
1:B:73:ILE:N	1:B:305:VAL:HG23	2.35	0.41
1:B:233:ILE:HG22	1:B:251:VAL:HG13	2.00	0.41
1:B:234:THR:O	1:B:238:ALA:CB	2.68	0.41
1:B:19:LYS:O	1:B:23:ASP:CG	2.63	0.41
1:B:20:MET:HE1	1:B:171:ARG:HB3	2.03	0.41
1:B:91:ALA:HA	1:B:320:GLU:HG2	2.01	0.41
1:B:133:ASP:HB2	1:B:136:VAL:HG22	2.02	0.41
1:B:298:LEU:C	1:B:298:LEU:CD1	2.93	0.41
1:B:343:CYS:HB3	1:B:349:ILE:HD13	2.03	0.41
1:A:37:GLU:O	1:A:264:ALA:HB2	2.20	0.41
1:A:130:VAL:HG13	1:A:134:ARG:HE	1.86	0.41
1:A:238:ALA:O	1:A:241:ALA:N	2.52	0.41
1:B:38:ASN:O	1:B:42:PHE:CE1	2.72	0.41
1:B:81:GLN:HE21	1:B:81:GLN:HB2	1.60	0.41
1:B:103:MET:HE2	1:B:104:THR:N	2.36	0.41
1:B:271:GLU:O	1:B:271:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:PHE:O	1:B:307:ILE:HG23	2.20	0.41
1:B:358:TRP:CD1	1:B:358:TRP:C	2.99	0.41
1:A:24:PHE:HE2	1:A:79:ALA:HB3	1.85	0.41
1:A:175:PRO:HA	1:A:176:PRO:HD2	1.50	0.41
1:A:323:VAL:O	1:A:327:LEU:HG	2.20	0.41
1:A:330:MET:HE2	1:A:330:MET:HB2	1.85	0.41
1:B:14:LYS:HA	1:B:14:LYS:HD3	1.77	0.41
1:B:59:ASP:HB3	1:B:344:ARG:O	2.21	0.41
1:B:89:GLU:C	1:B:91:ALA:N	2.79	0.41
1:B:310:PRO:C	1:B:312:VAL:N	2.78	0.41
1:A:24:PHE:CD1	1:A:172:PHE:CE2	3.09	0.41
1:A:69:ILE:O	1:A:70:SER:C	2.62	0.41
1:A:142:ARG:HE	1:B:143:ARG:NH2	2.19	0.41
1:A:143:ARG:C	1:A:145:GLU:N	2.79	0.41
1:A:183:PHE:O	1:A:185:GLY:N	2.47	0.41
1:A:184:GLU:CD	1:B:222:ILE:HA	2.45	0.41
1:B:92:THR:HA	1:B:323:VAL:HG21	2.03	0.41
1:B:128:LEU:HD13	1:B:153:ALA:O	2.21	0.41
1:B:328:GLN:NE2	1:B:331:ARG:HB3	2.35	0.41
1:A:39:ARG:CZ	1:A:287:GLY:O	2.69	0.41
1:A:127:GLN:NE2	2:A:370:FMN:HN3	2.19	0.41
1:A:162:GLY:O	1:A:164:ARG:CD	2.66	0.41
1:A:162:GLY:HA3	1:A:257:ARG:O	2.20	0.41
1:B:37:GLU:CG	1:B:264:ALA:HB2	2.39	0.41
1:B:82:LYS:C	1:B:84:ALA:H	2.27	0.41
1:B:134:ARG:NH1	1:B:218:TRP:CH2	2.88	0.41
1:B:146:ARG:NH2	1:B:225:LEU:HA	2.31	0.41
1:B:204:ALA:C	1:B:206:GLN:H	2.26	0.41
1:B:238:ALA:C	1:B:240:LEU:N	2.76	0.40
1:B:266:ILE:O	1:B:269:LEU:N	2.47	0.40
1:A:24:PHE:CE2	1:A:79:ALA:HB3	2.57	0.40
1:A:117:ALA:O	1:B:147:ALA:CB	2.69	0.40
1:B:128:LEU:HG	1:B:140:LEU:CD2	2.50	0.40
1:B:131:TYR:HE2	1:B:140:LEU:HD11	1.87	0.40
1:B:311:VAL:HG11	1:B:323:VAL:HB	2.02	0.40
1:A:165:GLU:O	1:A:167:ASP:N	2.54	0.40
1:B:45:ILE:CG2	1:B:356:ALA:HA	2.47	0.40
1:A:93:ALA:HA	1:A:103:MET:HG3	2.02	0.40
1:A:269:LEU:HA	1:A:269:LEU:HD12	1.92	0.40
1:B:72:PRO:HB2	1:B:304:GLY:HA2	2.03	0.40
1:B:107:SER:O	1:B:182:ASN:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:VAL:HB	1:B:323:VAL:CG1	2.50	0.40
1:A:141:VAL:HG11	1:A:222:ILE:HD11	2.04	0.40
1:A:186:ILE:HD11	1:B:139:GLN:NE2	2.33	0.40
1:B:64:ILE:HG12	1:B:67:PHE:CD1	2.56	0.40
1:B:73:ILE:CA	1:B:305:VAL:HB	2.39	0.40
1:B:75:ILE:C	1:B:104:THR:OG1	2.64	0.40
1:B:77:PRO:HB3	1:B:127:GLN:HB2	2.03	0.40
1:B:163:ARG:HG3	1:B:163:ARG:NH1	2.31	0.40
1:B:243:GLN:HB3	1:B:244:HIS:CD2	2.56	0.40
1:B:307:ILE:HG13	1:B:308:GLY:H	1.86	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	279/369 (76%)	190 (68%)	55 (20%)	34 (12%)	0	1
1	B	346/369 (94%)	203 (59%)	91 (26%)	52 (15%)	0	0
All	All	625/738 (85%)	393 (63%)	146 (23%)	86 (14%)	0	1

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	19	LYS
1	A	89	GLU
1	A	200	SER
1	A	207	ILE
1	A	226	PRO
1	A	303	ALA
1	A	357	ASP

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Mol	Chain	Res	Type
1	B	25	TYR
1	B	30	GLU
1	B	67	PHE
1	B	86	PRO
1	B	113	VAL
1	B	132	LYS
1	B	133	ASP
1	B	144	ALA
1	B	150	LYS
1	B	159	PRO
1	B	184	GLU
1	B	237	ASP
1	B	254	HIS
1	B	261	TYR
1	B	277	GLN
1	B	281	PRO
1	B	291	GLY
1	B	307	ILE
1	A	63	THR
1	A	85	HIS
1	A	87	GLU
1	A	181	LYS
1	A	254	HIS
1	A	275	ALA
1	A	288	VAL
1	A	350	SER
1	A	354	ILE
1	B	79	ALA
1	B	80	MET
1	B	96	ALA
1	B	101	THR
1	B	118	SER
1	B	143	ARG
1	B	181	LYS
1	B	182	ASN
1	B	185	GLY
1	B	249	ILE
1	B	258	GLN
1	B	322	GLY
1	B	347	LYS
1	A	30	GLU
1	A	77	PRO

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Mol	Chain	Res	Type
1	A	79	ALA
1	A	80	MET
1	A	145	GLU
1	A	263	PRO
1	B	64	ILE
1	B	129	TYR
1	B	227	ILE
1	B	267	MET
1	B	301	GLY
1	B	333	GLU
1	B	353	HIS
1	A	108	TRP
1	A	188	LEU
1	A	233	ILE
1	A	276	ALA
1	B	73	ILE
1	B	110	THR
1	B	131	TYR
1	B	266	ILE
1	B	276	ALA
1	B	296	LYS
1	B	343	CYS
1	A	86	PRO
1	A	88	GLY
1	A	332	ASP
1	A	342	GLY
1	A	349	ILE
1	B	207	ILE
1	B	248	GLY
1	A	10	GLU
1	B	75	ILE
1	B	174	LEU
1	B	137	VAL
1	A	319	GLY
1	B	173	VAL
1	B	130	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	281/294 (96%)	213 (76%)	68 (24%)	1	4
1	B	280/294 (95%)	188 (67%)	92 (33%)	0	1
All	All	561/588 (95%)	401 (72%)	160 (28%)	0	2

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	12	ILE
1	A	15	GLN
1	A	17	LEU
1	A	34	THR
1	A	38	ASN
1	A	48	ARG
1	A	49	PRO
1	A	51	ILE
1	A	53	ILE
1	A	57	ASN
1	A	59	ASP
1	A	62	THR
1	A	64	ILE
1	A	68	LYS
1	A	71	MET
1	A	85	HIS
1	A	87	GLU
1	A	89	GLU
1	A	90	TYR
1	A	103	MET
1	A	108	TRP
1	A	110	THR
1	A	113	VAL
1	A	123	ILE
1	A	129	TYR
1	A	130	VAL
1	A	135	ASN
1	A	152	ILE
1	A	161	LEU
1	A	164	ARG
1	A	165	GLU
1	A	168	ILE

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Mol	Chain	Res	Type
1	A	174	LEU
1	A	177	PHE
1	A	180	LEU
1	A	188	LEU
1	A	190	LYS
1	A	199	LEU
1	A	202	TYR
1	A	206	GLN
1	A	207	ILE
1	A	211	LEU
1	A	212	SER
1	A	216	VAL
1	A	222	ILE
1	A	226	PRO
1	A	228	LEU
1	A	240	LEU
1	A	251	VAL
1	A	253	ASN
1	A	260	ASP
1	A	265	THR
1	A	266	ILE
1	A	267	MET
1	A	271	GLU
1	A	274	LYS
1	A	284	LEU
1	A	292	THR
1	A	298	LEU
1	A	305	VAL
1	A	311	VAL
1	A	318	GLU
1	A	325	LYS
1	A	326	VAL
1	A	328	GLN
1	A	346	LEU
1	A	347	LYS
1	B	2	GLU
1	B	3	ILE
1	B	16	LYS
1	B	17	LEU
1	B	32	GLN
1	B	35	LEU
1	B	42	PHE

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Mol	Chain	Res	Type
1	B	43	SER
1	B	46	LEU
1	B	55	VAL
1	B	57	ASN
1	B	58	ILE
1	B	60	MET
1	B	61	THR
1	B	64	ILE
1	B	65	LEU
1	B	67	PHE
1	B	68	LYS
1	B	70	SER
1	B	74	MET
1	B	75	ILE
1	B	77	PRO
1	B	81	GLN
1	B	83	MET
1	B	85	HIS
1	B	87	GLU
1	B	90	TYR
1	B	94	ARG
1	B	103	MET
1	B	105	LEU
1	B	121	PRO
1	B	124	ARG
1	B	127	GLN
1	B	129	TYR
1	B	130	VAL
1	B	132	LYS
1	B	136	VAL
1	B	137	VAL
1	B	142	ARG
1	B	145	GLU
1	B	150	LYS
1	B	158	THR
1	B	160	ARG
1	B	163	ARG
1	B	165	GLU
1	B	174	LEU
1	B	177	PHE
1	B	180	LEU
1	B	181	LYS

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Mol	Chain	Res	Type
1	B	199	LEU
1	B	200	SER
1	B	208	ASP
1	B	209	ARG
1	B	211	LEU
1	B	213	TRP
1	B	216	VAL
1	B	218	TRP
1	B	221	THR
1	B	228	LEU
1	B	229	VAL
1	B	233	ILE
1	B	234	THR
1	B	244	HIS
1	B	250	ILE
1	B	254	HIS
1	B	260	ASP
1	B	261	TYR
1	B	262	VAL
1	B	265	THR
1	B	266	ILE
1	B	267	MET
1	B	273	VAL
1	B	277	GLN
1	B	280	ILE
1	B	281	PRO
1	B	284	LEU
1	B	288	VAL
1	B	289	ARG
1	B	298	LEU
1	B	305	VAL
1	B	312	VAL
1	B	314	SER
1	B	324	LYS
1	B	328	GLN
1	B	333	GLU
1	B	334	PHE
1	B	335	GLU
1	B	344	ARG
1	B	346	LEU
1	B	347	LYS
1	B	351	ARG

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Mol	Chain	Res	Type
1	B	358	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	40	ASN
1	A	57	ASN
1	A	139	GLN
1	A	253	ASN
1	A	254	HIS
1	A	353	HIS
1	B	40	ASN
1	B	81	GLN
1	B	135	ASN
1	B	244	HIS
1	B	277	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
2	FMN	A	370	-	33,33,33	3.12	14 (42%)	48,50,50	2.14	20 (41%)

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
2	FMN	A	370	-	-	7/18/18/18	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	370	FMN	C5'-C4'	12.27	1.68	1.51
2	A	370	FMN	C4'-C3'	5.78	1.63	1.53
2	A	370	FMN	C10-N1	4.66	1.42	1.33
2	A	370	FMN	C4A-N5	4.33	1.40	1.30
2	A	370	FMN	C1'-N10	-3.70	1.38	1.47
2	A	370	FMN	P-O5'	3.45	1.71	1.60
2	A	370	FMN	C10-N10	3.19	1.44	1.37
2	A	370	FMN	C2-N1	3.11	1.43	1.36
2	A	370	FMN	C1'-C2'	-2.97	1.48	1.52
2	A	370	FMN	C6-C7	2.83	1.43	1.39
2	A	370	FMN	O4'-C4'	2.55	1.48	1.43
2	A	370	FMN	C9-C8	-2.19	1.36	1.39
2	A	370	FMN	C6-C5A	-2.11	1.36	1.40
2	A	370	FMN	C4-N3	2.01	1.42	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	370	FMN	C4A-C10-N10	4.46	122.86	116.48
2	A	370	FMN	C9-C9A-N10	-4.19	116.22	121.85
2	A	370	FMN	C4A-C10-N1	-4.11	114.50	124.59
2	A	370	FMN	C10-N1-C2	3.99	125.48	116.85
2	A	370	FMN	O2'-C2'-C3'	3.40	117.20	109.25
2	A	370	FMN	C10-C4A-N5	-3.38	117.91	124.81
2	A	370	FMN	C4-C4A-C10	3.30	122.59	116.93
2	A	370	FMN	O2'-C2'-C1'	3.01	122.58	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	370	FMN	C9A-N10-C10	-2.90	116.33	120.75
2	A	370	FMN	O2P-P-O5'	-2.79	99.39	106.67
2	A	370	FMN	O4'-C4'-C5'	2.65	115.83	109.99
2	A	370	FMN	O5'-C5'-C4'	-2.55	102.54	109.36
2	A	370	FMN	N3-C2-N1	-2.52	114.16	119.50
2	A	370	FMN	O4'-C4'-C3'	2.41	114.89	109.25
2	A	370	FMN	C7M-C7-C8	-2.33	115.99	120.76
2	A	370	FMN	C5A-N5-C4A	2.28	121.77	118.09
2	A	370	FMN	C5A-C9A-N10	2.19	119.95	117.97
2	A	370	FMN	C9A-C5A-N5	-2.16	120.17	122.45
2	A	370	FMN	O3P-P-O2P	2.02	115.38	107.80
2	A	370	FMN	O3'-C3'-C4'	-2.00	104.38	108.93

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	370	FMN	C2'-C3'-C4'-O4'
2	A	370	FMN	O3'-C3'-C4'-O4'
2	A	370	FMN	O2'-C2'-C3'-O3'
2	A	370	FMN	O2'-C2'-C3'-C4'
2	A	370	FMN	C5'-O5'-P-O3P
2	A	370	FMN	N10-C1'-C2'-O2'
2	A	370	FMN	C4'-C5'-O5'-P

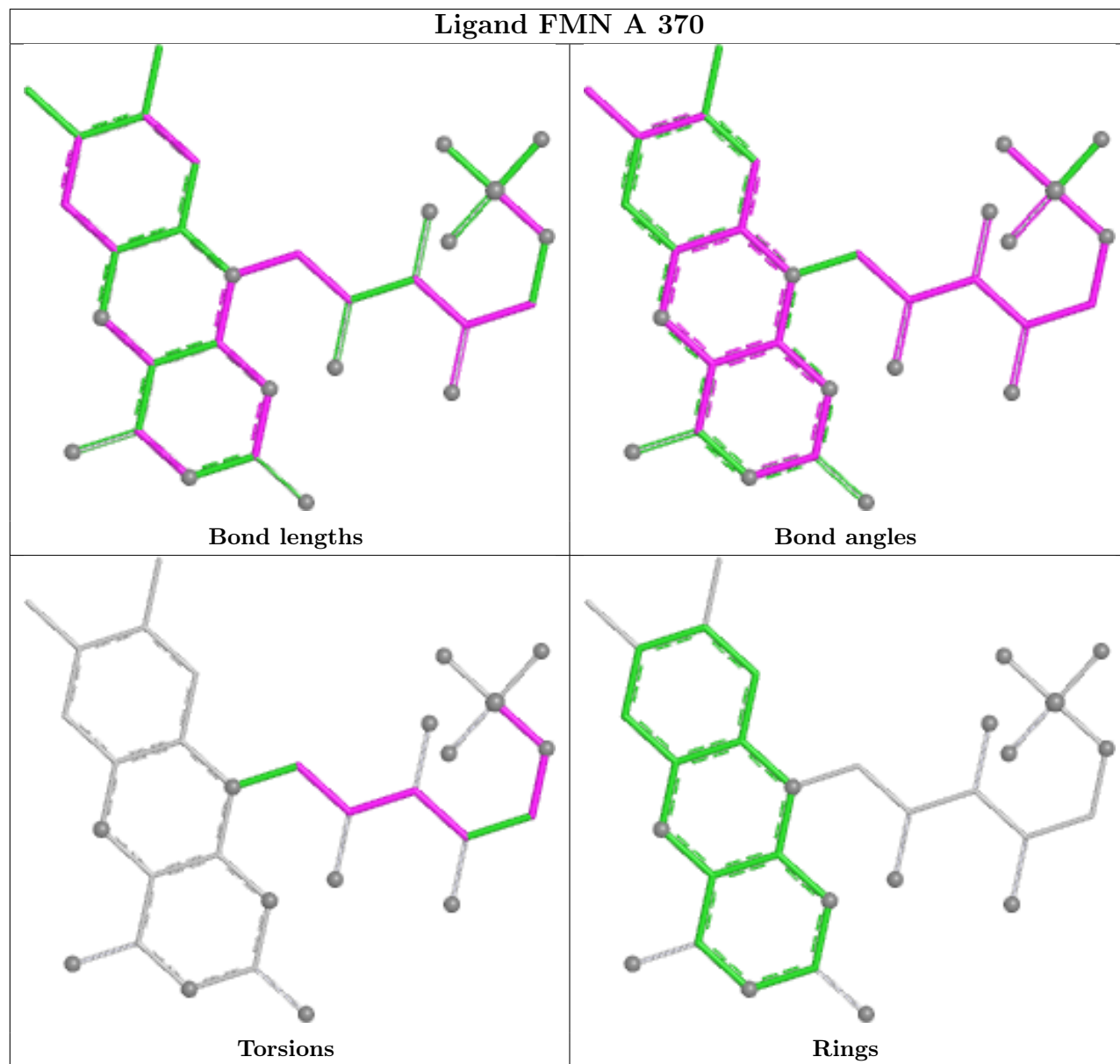
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	370	FMN	5	0

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

equivalents in the CSD to analyse the geometry.



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.