



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:37 AM UTC

PDB ID : 1DXL / pdb_00001dxl
Title : Dihydrolipoamide dehydrogenase of glycine decarboxylase from Pisum Sativum
Authors : Faure, M.; Cohen-Addad, C.; Bourguignon, J.; Macherel, D.; Neuburger, M.; Douce, R.
Deposited on : 2000-01-10
Resolution : 3.15 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

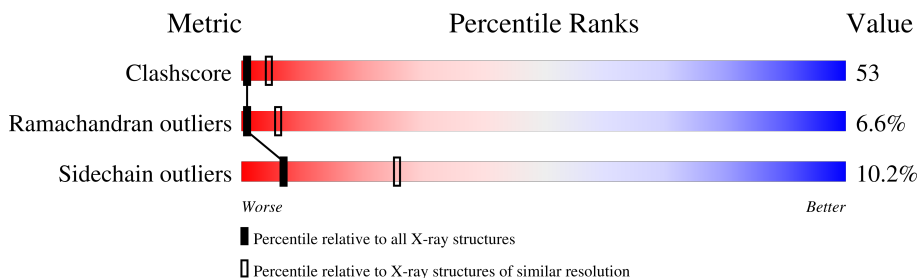
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)

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	470	
1	B	470	
1	C	470	
1	D	470	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14240 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 DIHYDROLIPOAMIDE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	48	1	0
			3487	2203	591	677	16			
1	B	467	Total	C	N	O	S	50	1	0
			3487	2203	591	677	16			
1	C	467	Total	C	N	O	S	77	0	0
			3475	2194	590	675	16			
1	D	467	Total	C	N	O	S	38	0	0
			3475	2194	590	675	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	HIS	ASN	conflict	UNP P31023
B	449	HIS	ASN	conflict	UNP P31023
C	449	HIS	ASN	conflict	UNP P31023
D	449	HIS	ASN	conflict	UNP P31023

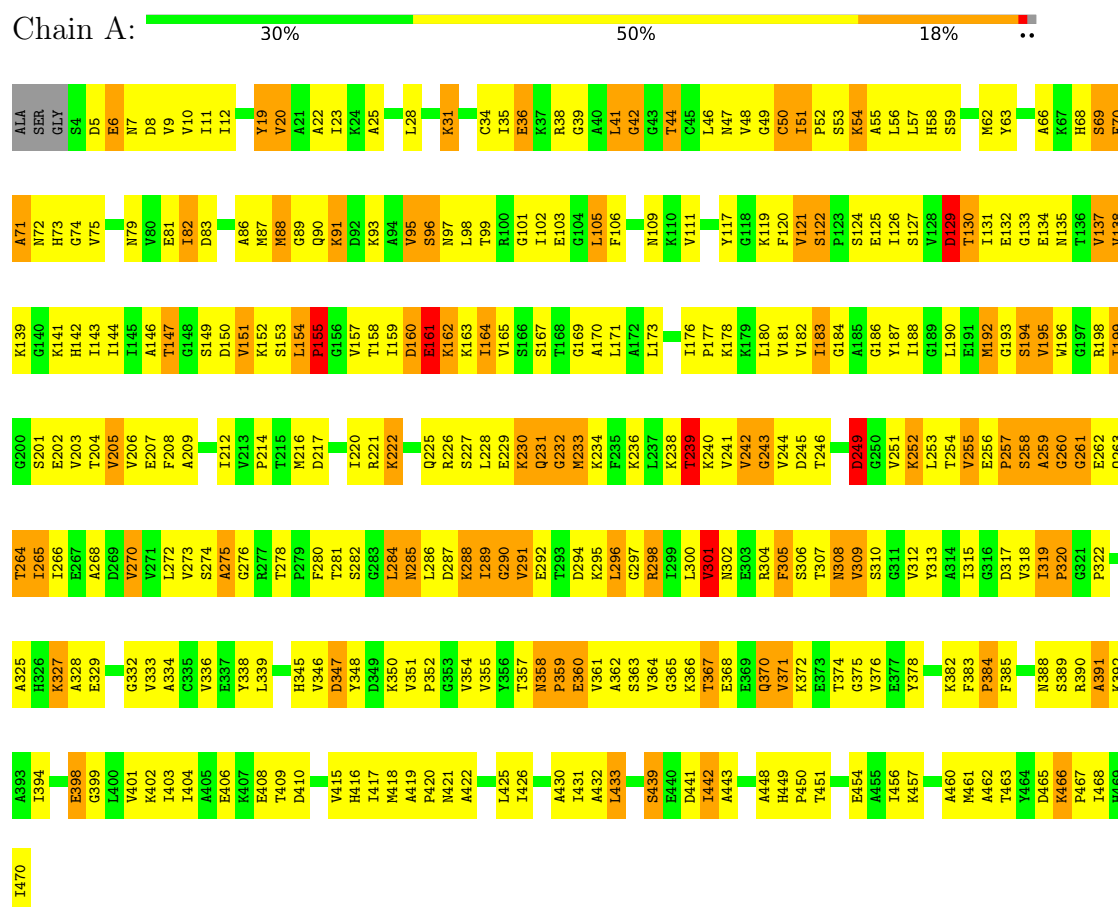
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

3 Residue-property plots

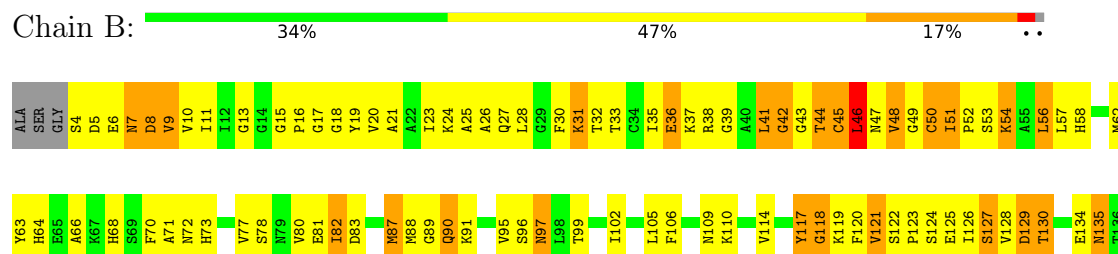
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

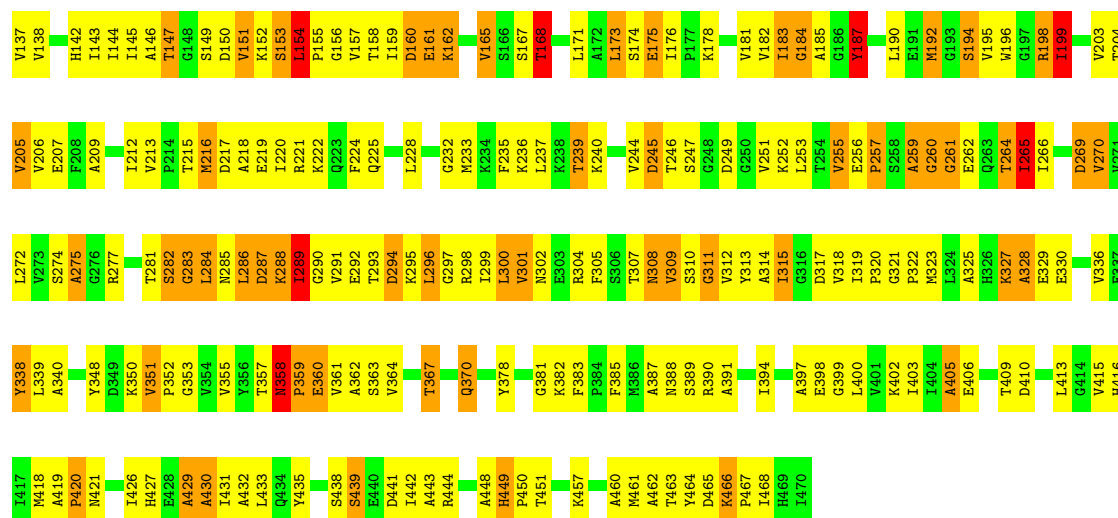
Note EDS was not executed.

• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE



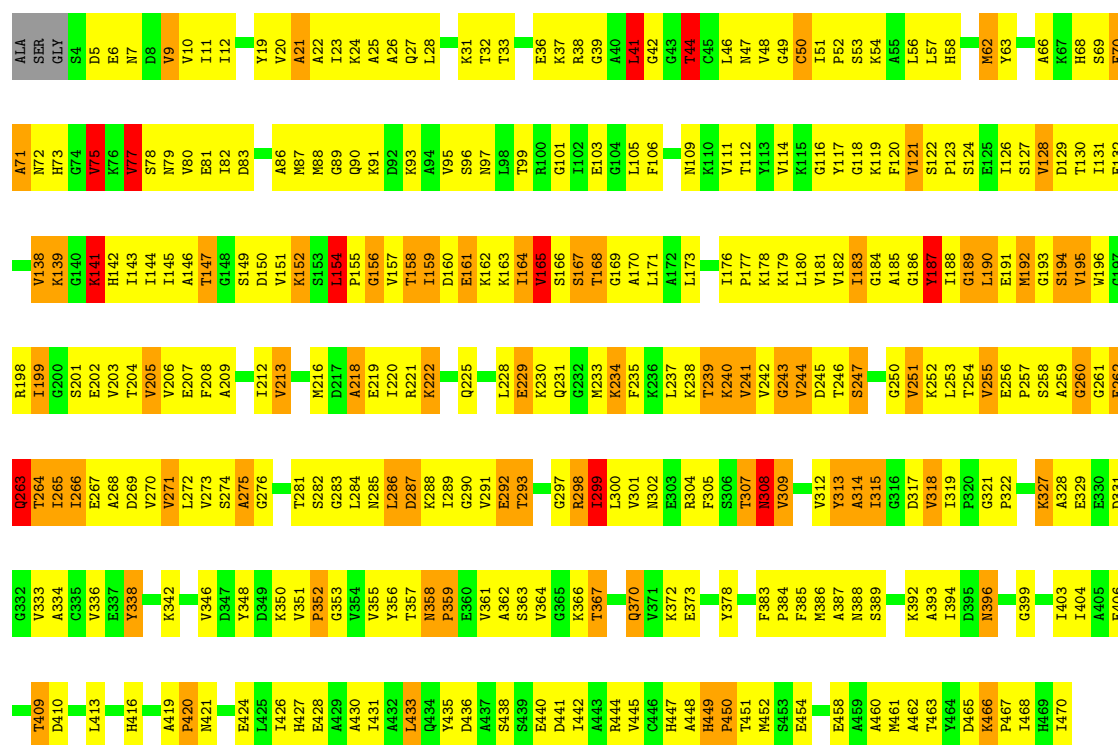
• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE





• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain C: 30% 52% 15% ..



• Molecule 1: DIHYDROLIPOAMIDE DEHYDROGENASE

Chain D: 34% 50% 13% ..



A422	P352	G283	V205	V138	N72
G423	G353	L284	V206	H142	H73
E424	V354	N285	E207	I143	G74
L425	V355	L286	F208	I144	V75
I426	Y356	D287	A209	I145	K76
H427	T357	K288	I212	A146	V77
E428	H358	I289	V213	T147	S78
A429	F359	G290	V213	G148	N79
A430	V361	V291	M216	S149	V80
I431	E292	E292	D217	D150	E81
A432	A362	T293	A218	D150	I82
L433	S363	D294	E219	V151	D83
S438	V364	K295	I220	K152	L84
S439	G365	R298	R221	S153	A85
E440	K366		K222	L154	A86
D441	T367			P155	M87
E442	E368			G156	M88
	Q370	N302	Q225	V157	G89
	V371	F303	R226	T158	O90
	V376	R304	L228	I159	K91
A448	E377	F305	E229	D160	
H449			K230	E161	A94
P450	V380	N308	Q231	K162	V95
T451		V309	Q231	K163	S96
H452	F383	S310	G232	I164	N97
A455	E454	G311	M233	V165	L98
A456	V312	V312	K234	S166	
K457	F385	A314	L237	S167	G101
E458	M386	I315	K238	L171	I102
A459			T239	A172	E103
A460	S389	V318	K240	L173	G104
M461	R390	I319	V241	I176	F106
A462	A391	P320	V242	P177	
T463	K392	G321	G243		N109
Y464	A393	P322	V244	L180	K110
D465	I394	M323		V181	V111
K466		L324	D249	V182	T112
P467	E398	A325	L253	I183	Y113
I468	G399	H326	T254	G184	G116
H469	L400	K327	V255	A185	Y117
H469	V401	A328	E262	G186	G118
I470	K402	E329	Q263	Y187	K119
	I403	F330	T264		F120
	I404	D331	I265	L190	V121
	A405	G332		E191	S122
	E406	V333	V270	M192	P123
		A334		G193	S124
	T409	G335		S194	E125
	D410	V336		V195	I126
				W196	S127
	L413	L339		G197	V128
	G414			R198	D129
	V415	H345		I199	T130
	H416	V346		G200	I131
	I417	D347		S201	E132
	M418	Y348		E202	
	A419	D349		V203	T136
	P420	K350		T204	
	N421	V351			

4 Data and refinement statistics

Xtriage (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, α , β , γ	100.56Å 108.33Å 202.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.15	Depositor
% Data completeness (in resolution range)	86.1 (15.00-3.15)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.226 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14240	wwPDB-VP
Average B, all atoms (Å ²)	74.0	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: FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.11	14/3541 (0.4%)	1.49	55/4783 (1.1%)
1	B	1.00	4/3541 (0.1%)	1.46	61/4783 (1.3%)
1	C	1.05	9/3527 (0.3%)	1.46	53/4762 (1.1%)
1	D	1.04	8/3528 (0.2%)	1.43	47/4765 (1.0%)
All	All	1.05	35/14137 (0.2%)	1.46	216/19093 (1.1%)

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
1	C	0	1
All	All	0	3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	GLN	C-N	-9.67	1.20	1.33
1	D	301	VAL	CA-CB	-7.79	1.47	1.55
1	A	301	VAL	CA-CB	-6.95	1.45	1.55
1	A	289	ILE	CA-CB	-6.62	1.47	1.54
1	C	315	ILE	CA-CB	-6.50	1.43	1.55
1	D	393	ALA	C-O	-6.50	1.15	1.24
1	A	147	THR	CA-CB	-6.46	1.43	1.53
1	A	9	VAL	CA-CB	6.36	1.62	1.55
1	A	151	VAL	CA-CB	-6.20	1.47	1.54
1	B	430	ALA	CA-CB	-6.17	1.43	1.53
1	C	146	ALA	CA-CB	-6.09	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	9	VAL	CA-CB	6.04	1.62	1.54
1	B	87	MET	SD-CE	-5.85	1.65	1.79
1	B	216	MET	SD-CE	-5.80	1.65	1.79
1	A	319	ILE	CA-CB	5.79	1.61	1.54
1	A	88	MET	SD-CE	5.76	1.94	1.79
1	D	404	ILE	CA-CB	-5.72	1.47	1.54
1	C	313	TYR	CA-C	5.72	1.59	1.52
1	A	95	VAL	CA-CB	-5.69	1.48	1.54
1	A	164	ILE	CA-CB	-5.67	1.46	1.54
1	A	255	VAL	CA-CB	5.62	1.60	1.54
1	A	430	ALA	CA-CB	-5.61	1.44	1.53
1	A	51	ILE	CA-C	5.57	1.58	1.52
1	A	371	VAL	CA-CB	5.51	1.60	1.54
1	C	66	ALA	CA-CB	-5.51	1.44	1.53
1	D	426	ILE	CA-CB	-5.45	1.45	1.54
1	C	299	ILE	CA-CB	-5.42	1.46	1.54
1	C	75	VAL	CA-CB	-5.30	1.47	1.54
1	D	418	MET	CA-C	-5.27	1.46	1.52
1	D	455	ALA	CA-CB	-5.22	1.45	1.53
1	B	439	SER	CA-C	-5.20	1.45	1.52
1	C	404	ILE	CA-CB	-5.18	1.48	1.54
1	D	380	VAL	CA-CB	-5.12	1.48	1.54
1	D	183	ILE	CA-C	-5.10	1.46	1.52
1	A	10	VAL	CA-C	-5.06	1.46	1.52

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	ASN	CA-C-N	-15.87	103.32	120.14
1	C	358	ASN	C-N-CA	-15.87	103.32	120.14
1	B	44	THR	N-CA-C	-15.03	95.40	114.04
1	B	162	LYS	N-CA-C	12.91	129.24	113.23
1	D	399	GLY	N-CA-C	12.28	124.57	112.04
1	D	466	LYS	CA-C-N	11.78	132.53	119.92
1	D	466	LYS	C-N-CA	11.78	132.53	119.92
1	A	131	ILE	N-CA-C	-11.58	102.18	113.53
1	A	44	THR	N-CA-C	-11.46	99.43	113.41
1	B	294	ASP	N-CA-C	11.35	126.70	113.19
1	A	383	PHE	CA-C-N	10.73	131.58	119.99
1	A	383	PHE	C-N-CA	10.73	131.58	119.99
1	A	284	LEU	N-CA-C	-10.46	95.75	110.50
1	B	260	GLY	N-CA-C	-10.44	98.44	115.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	THR	N-CA-C	-10.25	100.77	113.18
1	D	237	LEU	N-CA-C	10.06	126.08	112.90
1	A	154	LEU	CA-C-N	9.92	132.24	119.84
1	A	154	LEU	C-N-CA	9.92	132.24	119.84
1	B	358	ASN	CA-C-N	-9.91	108.93	120.13
1	B	358	ASN	C-N-CA	-9.91	108.93	120.13
1	D	165	VAL	N-CA-C	9.49	120.40	108.82
1	C	165	VAL	N-CA-C	9.49	123.68	108.97
1	C	240	LYS	N-CA-C	9.21	120.81	108.38
1	B	165	VAL	N-CA-C	9.15	122.09	109.46
1	B	147	THR	N-CA-C	-9.13	98.55	110.33
1	B	466	LYS	CA-C-N	9.12	129.06	120.03
1	B	466	LYS	C-N-CA	9.12	129.06	120.03
1	B	351	VAL	CA-C-N	9.12	129.19	119.89
1	B	351	VAL	C-N-CA	9.12	129.19	119.89
1	D	31	LYS	N-CA-C	-9.06	95.35	109.76
1	A	358	ASN	CA-C-N	-9.03	109.93	120.13
1	A	358	ASN	C-N-CA	-9.03	109.93	120.13
1	C	47	ASN	N-CA-C	8.92	124.59	112.90
1	C	327	LYS	N-CA-C	-8.92	101.64	111.36
1	C	255	VAL	N-CA-C	8.91	121.63	108.45
1	B	327	LYS	N-CA-C	-8.85	101.32	110.97
1	C	260	GLY	CA-C-N	8.84	129.32	120.31
1	C	260	GLY	C-N-CA	8.84	129.32	120.31
1	D	44	THR	N-CA-C	-8.66	101.32	112.23
1	D	327	LYS	N-CA-C	-8.60	101.86	111.14
1	C	286	LEU	N-CA-C	-8.59	103.31	112.93
1	A	130	THR	N-CA-C	8.57	123.24	108.76
1	B	137	VAL	N-CA-C	8.57	120.34	106.72
1	B	31	LYS	N-CA-C	-8.48	96.28	109.25
1	D	358	ASN	CA-C-N	-8.45	111.31	119.76
1	D	358	ASN	C-N-CA	-8.45	111.31	119.76
1	D	152	LYS	N-CA-C	-8.43	96.35	109.76
1	D	147	THR	N-CA-C	-8.40	98.92	110.35
1	B	167	SER	N-CA-C	-8.28	101.94	110.97
1	A	147	THR	N-CA-C	-8.16	99.81	110.33
1	C	359	PRO	N-CA-C	-8.08	98.19	111.68
1	C	308	ASN	N-CA-C	-8.05	102.93	114.12
1	A	68	HIS	N-CA-C	8.01	123.64	113.55
1	B	399	GLY	N-CA-C	8.00	120.20	112.04
1	B	45	CYS	N-CA-C	-7.97	102.37	113.20
1	A	121	VAL	N-CA-C	-7.89	105.50	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	327	LYS	N-CA-C	-7.89	102.62	111.07
1	C	466	LYS	CA-C-N	7.86	127.87	119.78
1	C	466	LYS	C-N-CA	7.86	127.87	119.78
1	C	399	GLY	N-CA-C	7.83	121.24	111.85
1	B	301	VAL	N-CA-C	7.80	119.39	108.23
1	B	168	THR	N-CA-C	7.78	120.44	111.11
1	A	309	VAL	N-CA-C	7.77	118.40	107.37
1	C	409	THR	N-CA-C	7.75	119.81	111.36
1	A	165	VAL	N-CA-C	7.51	119.96	109.29
1	A	20	VAL	N-CA-C	-7.40	104.57	111.45
1	C	147	THR	N-CA-C	-7.40	100.74	110.43
1	A	34	CYS	N-CA-C	-7.36	98.62	110.32
1	A	466	LYS	CA-C-N	7.25	127.24	119.78
1	A	466	LYS	C-N-CA	7.25	127.24	119.78
1	B	360	GLU	N-CA-C	-7.24	100.36	110.35
1	C	299	ILE	CB-CA-C	-7.23	102.17	110.41
1	D	238	LYS	N-CA-C	-7.20	104.12	113.12
1	B	36	GLU	N-CA-C	7.19	120.19	108.26
1	D	163	LYS	N-CA-C	-7.17	106.45	114.62
1	B	383	PHE	CA-C-N	7.15	127.72	120.14
1	B	383	PHE	C-N-CA	7.15	127.72	120.14
1	B	359	PRO	N-CA-C	-7.14	98.90	110.55
1	B	184	GLY	N-CA-C	-7.08	104.54	112.33
1	A	359	PRO	N-CA-C	-7.03	99.08	110.55
1	A	161	GLU	N-CA-C	-7.01	95.88	110.80
1	C	420	PRO	N-CA-C	-6.95	101.01	111.57
1	C	164	ILE	N-CA-C	-6.85	98.46	108.87
1	D	242	VAL	CB-CA-C	-6.82	103.32	111.65
1	D	185	ALA	N-CA-C	6.82	118.62	110.44
1	C	103	GLU	N-CA-C	-6.81	103.86	111.28
1	C	245	ASP	N-CA-C	6.79	119.53	108.26
1	D	103	GLU	N-CA-C	-6.76	103.94	111.71
1	D	6	GLU	N-CA-C	6.73	120.57	110.14
1	B	173	LEU	N-CA-C	-6.71	101.88	110.19
1	C	293	THR	N-CA-C	6.70	120.25	109.86
1	D	263	GLN	N-CA-C	6.69	119.43	109.59
1	D	359	PRO	N-CA-C	-6.64	100.77	111.19
1	A	285	ASN	N-CA-C	-6.60	96.87	108.23
1	C	315	ILE	N-CA-C	6.55	119.42	108.81
1	D	198	ARG	N-CA-C	-6.54	104.08	111.14
1	B	130	THR	N-CA-C	6.53	117.09	107.88
1	C	141	LYS	N-CA-C	-6.53	104.20	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	SER	N-CA-C	6.49	119.62	111.24
1	A	264	THR	N-CA-C	-6.47	99.81	108.74
1	C	260	GLY	O-C-N	6.47	130.75	123.12
1	C	68	HIS	N-CA-C	6.47	121.58	113.43
1	C	356	TYR	N-CA-C	6.44	119.79	112.97
1	B	308	ASN	N-CA-C	-6.28	99.41	109.39
1	D	383	PHE	CA-C-N	6.26	128.71	120.25
1	D	383	PHE	C-N-CA	6.26	128.71	120.25
1	B	41	LEU	N-CA-C	6.23	120.74	113.20
1	B	232	GLY	N-CA-C	6.22	123.25	114.85
1	A	165	VAL	CB-CA-C	-6.20	103.27	111.70
1	B	286	LEU	N-CA-C	-6.14	105.81	113.55
1	B	255	VAL	N-CA-C	6.14	117.25	107.98
1	C	111	VAL	N-CA-C	-6.10	100.92	109.21
1	C	121	VAL	N-CA-C	-6.08	107.20	113.10
1	A	103	GLU	N-CA-C	-6.07	104.67	111.28
1	C	31	LYS	N-CA-C	-6.04	100.01	109.25
1	A	202	GLU	N-CA-C	-6.02	97.48	108.02
1	D	275	ALA	N-CA-C	-6.02	102.72	110.19
1	D	121	VAL	N-CA-C	-6.00	106.89	113.43
1	D	362	ALA	N-CA-C	-5.99	99.23	109.24
1	A	42	GLY	N-CA-C	-5.98	103.37	112.51
1	B	420	PRO	N-CA-C	-5.96	101.72	111.68
1	B	397	ALA	N-CA-C	5.96	119.86	112.59
1	D	159	ILE	N-CA-C	5.93	116.84	108.36
1	A	378	TYR	N-CA-C	5.92	118.87	109.81
1	B	432	ALA	N-CA-C	-5.90	104.76	111.14
1	D	295	LYS	N-CA-C	-5.89	104.20	111.33
1	B	42	GLY	N-CA-C	-5.87	103.54	112.51
1	B	68	HIS	N-CA-C	5.85	120.80	113.43
1	B	429	ALA	N-CA-C	-5.85	104.27	111.40
1	D	345	HIS	N-CA-C	5.82	117.89	108.34
1	C	77	VAL	N-CA-C	-5.80	99.40	108.86
1	B	198	ARG	N-CA-C	-5.78	104.62	111.03
1	A	91	LYS	N-CA-C	-5.76	104.69	110.97
1	C	41	LEU	N-CA-C	5.76	120.17	113.20
1	C	396	ASN	N-CA-C	-5.75	98.55	110.80
1	C	321	GLY	CA-C-N	5.71	125.73	119.90
1	C	321	GLY	C-N-CA	5.71	125.73	119.90
1	B	351	VAL	CA-C-O	5.71	122.32	119.12
1	B	213	VAL	CA-C-N	5.68	125.36	119.05
1	B	213	VAL	C-N-CA	5.68	125.36	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	GLU	N-CA-C	-5.68	99.15	108.41
1	D	460	ALA	N-CA-C	-5.68	104.73	111.03
1	D	7	ASN	N-CA-C	5.67	122.88	110.80
1	A	83	ASP	N-CA-C	-5.65	101.14	109.62
1	A	96	SER	CA-CB-OG	-5.65	99.81	111.10
1	B	275	ALA	N-CA-C	-5.62	98.82	110.80
1	B	160	ASP	N-CA-C	5.61	118.00	108.02
1	C	314	ALA	N-CA-C	5.60	118.60	108.69
1	C	297	GLY	N-CA-C	5.59	123.16	115.27
1	C	428	GLU	N-CA-C	-5.58	105.20	111.28
1	D	321	GLY	CA-C-N	5.58	125.85	119.83
1	D	321	GLY	C-N-CA	5.58	125.85	119.83
1	D	301	VAL	N-CA-C	5.56	115.56	107.88
1	A	151	VAL	N-CA-C	5.55	117.62	109.63
1	A	129	ASP	N-CA-C	5.54	122.61	110.80
1	B	330	GLU	N-CA-C	5.54	117.32	111.28
1	B	117	TYR	N-CA-C	5.54	117.70	107.73
1	B	83	ASP	N-CA-C	-5.53	101.33	109.62
1	C	62	MET	N-CA-C	-5.53	105.17	111.14
1	A	8	ASP	N-CA-C	5.52	120.08	113.23
1	A	291	VAL	N-CA-C	-5.52	100.48	108.87
1	D	9	VAL	N-CA-C	5.52	116.93	108.71
1	B	37	LYS	N-CA-C	5.51	118.05	111.71
1	A	59	SER	N-CA-C	-5.51	105.35	111.36
1	A	305	PHE	N-CA-C	5.51	119.18	111.90
1	D	420	PRO	N-CA-C	-5.49	100.87	111.69
1	A	162	LYS	N-CA-C	5.49	122.50	110.80
1	A	239	THR	N-CA-C	5.48	117.33	108.34
1	C	292	GLU	N-CA-C	5.44	117.61	107.99
1	B	121	VAL	N-CA-C	-5.41	107.53	113.43
1	A	158	THR	N-CA-C	-5.41	102.48	110.48
1	B	287	ASP	N-CA-C	-5.39	105.33	112.34
1	C	154	LEU	N-CA-C	5.38	116.73	109.24
1	D	239	THR	N-CA-C	5.38	122.26	110.80
1	A	47	ASN	N-CA-C	5.38	119.97	113.41
1	C	162	LYS	N-CA-C	5.37	119.54	113.15
1	A	36	GLU	N-CA-C	5.36	118.18	108.69
1	D	111	VAL	N-CA-C	-5.36	101.93	109.21
1	B	127	SER	N-CA-C	5.32	117.90	107.57
1	B	239	THR	N-CA-C	5.31	117.49	109.41
1	D	48	VAL	N-CA-C	5.31	120.39	109.34
1	B	405	ALA	N-CA-C	5.28	117.70	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	428	GLU	N-CA-C	-5.27	105.53	111.28
1	C	69	SER	N-CA-C	5.25	119.61	112.04
1	A	233	MET	N-CA-C	-5.25	99.62	110.80
1	A	398	GLU	N-CA-C	-5.25	103.10	110.50
1	A	31	LYS	N-CA-C	-5.24	101.89	109.59
1	C	21	ALA	N-CA-C	-5.24	104.83	111.11
1	B	265	ILE	N-CA-C	5.23	116.26	108.46
1	B	165	VAL	CB-CA-C	-5.23	103.92	112.03
1	B	315	ILE	CB-CA-C	-5.23	104.03	111.40
1	A	9	VAL	N-CA-C	5.22	114.75	108.06
1	A	360	GLU	N-CA-C	-5.22	103.80	110.53
1	D	415	VAL	N-CA-C	-5.19	100.09	107.77
1	A	137	VAL	N-CA-C	5.18	115.04	107.37
1	D	244	VAL	N-CA-C	5.17	115.92	108.48
1	C	342	LYS	CA-C-N	-5.16	116.42	123.12
1	C	342	LYS	C-N-CA	-5.16	116.42	123.12
1	B	145	ILE	N-CA-C	-5.15	102.21	109.21
1	A	155	PRO	N-CA-C	5.14	123.06	112.47
1	A	354	VAL	N-CA-C	5.14	115.44	107.78
1	D	173	LEU	N-CA-C	-5.12	103.77	110.53
1	A	105	LEU	N-CA-C	-5.09	106.23	112.90
1	C	213	VAL	CA-C-N	5.06	124.37	118.85
1	C	213	VAL	C-N-CA	5.06	124.37	118.85
1	D	312	VAL	N-CA-C	5.06	115.20	108.11
1	C	352	PRO	N-CA-C	5.06	119.18	111.34
1	A	243	GLY	N-CA-C	5.06	119.99	111.04
1	C	309	VAL	CB-CA-C	-5.06	104.16	111.19
1	A	111	VAL	N-CA-C	-5.04	102.24	108.89
1	D	409	THR	N-CA-C	5.03	119.49	112.90
1	B	321	GLY	CA-C-N	5.02	124.78	119.76
1	B	321	GLY	C-N-CA	5.02	124.78	119.76
1	A	69	SER	N-CA-C	5.01	117.52	111.40
1	B	249	ASP	N-CA-C	5.00	117.43	108.17
1	D	249	ASP	N-CA-C	5.00	117.68	108.58

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	B	187[A]	TYR	Sidechain
1	C	263	GLN	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3487	0	3552	356	0
1	B	3487	0	3552	388	0
1	C	3475	0	3543	441	0
1	D	3475	0	3544	359	0
2	A	53	0	31	2	0
2	B	53	0	31	2	0
2	C	53	0	31	3	0
2	D	53	0	31	3	0
3	A	33	0	0	2	0
3	B	23	0	0	3	0
3	C	25	0	0	6	0
3	D	23	0	0	6	0
All	All	14240	0	14315	1495	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 (1495) 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:322:PRO:HG2	1:B:327:LYS:HG3	1.25	1.18
1:C:254:THR:HG23	1:C:265:ILE:HD11	1.25	1.18
1:D:243:GLY:HA3	1:D:254:THR:HB	1.25	1.13
1:A:12:ILE:HD11	1:A:126:ILE:CD1	1.81	1.11
1:B:147:THR:HG21	1:B:284:LEU:HD22	1.15	1.11
1:C:192:MET:HE3	1:C:192:MET:HA	1.24	1.09
1:C:212:ILE:HG21	1:C:235:PHE:CE2	1.89	1.07
1:C:180:LEU:HD12	1:C:270:VAL:O	1.56	1.05
1:B:239:THR:HA	1:B:257:PRO:HA	1.37	1.03
1:C:51:ILE:HB	1:C:52:PRO:HD3	1.39	1.02
1:B:120:PHE:HA	1:B:126:ILE:HG22	1.39	1.02
1:C:118:GLY:HA2	1:C:127:SER:O	1.58	1.01
1:C:262:GLU:O	1:C:263:GLN:HB2	1.59	1.01
1:B:82:ILE:HD12	1:B:82:ILE:N	1.74	1.01
1:D:364:VAL:HG23	1:D:426:ILE:HD11	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:TYR:O	1:C:128:VAL:HA	1.63	0.97
1:C:258:SER:C	1:C:259:ALA:N	2.22	0.97
1:D:192:MET:HE3	1:D:192:MET:HA	1.46	0.97
1:A:117:TYR:HB3	1:A:129:ASP:HB2	1.45	0.97
1:B:308:ASN:O	1:B:309:VAL:HG23	1.63	0.97
1:C:462:ALA:HA	1:C:467:PRO:HD3	1.48	0.96
1:A:358:ASN:HB3	1:A:359:PRO:HD3	1.45	0.95
1:C:182:VAL:HB	1:C:205:VAL:HG13	1.44	0.95
1:C:250:GLY:O	1:C:251:VAL:HG23	1.65	0.95
1:C:257:PRO:HG2	1:C:260:GLY:O	1.67	0.95
1:A:157:VAL:HG13	1:A:244:VAL:HG21	1.46	0.94
1:C:123:PRO:HG3	1:C:289:ILE:HG22	1.46	0.94
1:D:448:ALA:O	1:D:451:THR:HG23	1.67	0.94
1:A:192:MET:HA	1:A:192:MET:CE	1.97	0.94
1:A:355:VAL:HG12	1:A:357:THR:HG23	1.48	0.94
1:B:192:MET:HE3	1:B:192:MET:HA	1.46	0.94
1:C:242:VAL:HG21	1:C:256:GLU:H	1.31	0.94
1:A:12:ILE:HD11	1:A:126:ILE:HD11	1.47	0.93
1:B:367:THR:HG23	1:B:370:GLN:NE2	1.84	0.93
1:A:160:ASP:O	1:A:161:GLU:HG3	1.68	0.93
1:D:81:GLU:C	1:D:82:ILE:HD12	1.93	0.93
1:D:242:VAL:HG23	1:D:254:THR:HG22	1.50	0.93
1:C:152:LYS:HB2	1:C:276:GLY:O	1.69	0.93
1:A:296:LEU:N	1:A:296:LEU:HD23	1.83	0.92
1:C:164:ILE:HD11	1:C:251:VAL:HG11	1.52	0.92
1:C:88:MET:HB3	3:C:2007:HOH:O	1.69	0.92
1:C:242:VAL:HB	1:C:255:VAL:HA	1.52	0.91
1:A:241:VAL:O	1:A:241:VAL:HG23	1.70	0.91
1:C:180:LEU:O	1:C:203:VAL:HA	1.69	0.91
1:C:63:TYR:CZ	1:C:82:ILE:HD11	2.05	0.91
1:D:284:LEU:HD12	1:D:285:ASN:H	1.36	0.91
1:D:161:GLU:HA	1:D:165:VAL:HG12	1.53	0.90
1:A:6:GLU:OE2	1:A:141:LYS:HE2	1.71	0.90
1:C:367:THR:H	1:C:370:GLN:HE21	1.20	0.89
1:A:12:ILE:HD11	1:A:126:ILE:HD13	1.49	0.89
1:B:300:LEU:H	1:B:300:LEU:HD22	1.37	0.88
1:B:35:ILE:HD11	1:B:138:VAL:HG21	1.55	0.87
1:B:117:TYR:CE2	1:B:283:GLY:HA3	2.09	0.87
1:C:212:ILE:HD13	1:C:235:PHE:HE2	1.38	0.87
1:D:117:TYR:CE2	1:D:283:GLY:HA3	2.10	0.86
1:C:165:VAL:HG23	1:C:272:LEU:HA	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:THR:H	1:B:370:GLN:HE21	1.21	0.85
1:C:427:HIS:O	1:C:431:ILE:HG22	1.76	0.85
1:D:38:ARG:HD3	1:D:47:ASN:ND2	1.92	0.85
1:C:286:LEU:HD22	1:C:291:VAL:HB	1.59	0.85
1:C:212:ILE:HG21	1:C:235:PHE:HE2	1.39	0.84
1:A:284:LEU:HD23	1:A:285:ASN:H	1.41	0.84
1:C:119:LYS:HB3	1:C:127:SER:HB3	1.58	0.84
1:B:9:VAL:HG23	1:B:30:PHE:HB3	1.60	0.84
1:C:364:VAL:HG23	1:C:426:ILE:HD11	1.59	0.84
1:D:129:ASP:O	1:D:130:THR:HG23	1.78	0.84
1:B:153:SER:O	1:B:154:LEU:HB2	1.78	0.84
1:D:54:LYS:HA	1:D:57:LEU:HD12	1.59	0.84
1:B:4:SER:HB2	3:B:2001:HOH:O	1.78	0.83
1:C:78:SER:HB2	1:D:78:SER:HB2	1.59	0.83
1:A:227:SER:HA	1:A:230:LYS:HD3	1.58	0.83
1:A:322:PRO:HG2	1:A:327:LYS:HG3	1.58	0.83
1:B:147:THR:HG21	1:B:284:LEU:CD2	2.06	0.83
1:B:154:LEU:HG	1:B:155:PRO:HD2	1.60	0.83
1:D:43:GLY:O	3:D:2001:HOH:O	1.95	0.83
1:B:117:TYR:HE2	1:B:283:GLY:HA3	1.42	0.83
1:A:119:LYS:HG2	1:A:285:ASN:CG	2.03	0.83
1:D:120:PHE:HD1	1:D:284:LEU:HD11	1.41	0.82
1:D:364:VAL:HG23	1:D:426:ILE:CD1	2.08	0.82
1:C:63:TYR:CE1	1:C:82:ILE:HD11	2.14	0.82
1:A:448:ALA:O	1:A:451:THR:HG23	1.80	0.82
1:C:152:LYS:HB2	1:C:276:GLY:C	2.05	0.82
1:D:117:TYR:CZ	1:D:283:GLY:HA3	2.15	0.82
1:A:41:LEU:HD11	1:A:106:PHE:CE1	2.16	0.81
1:C:50:CYS:O	1:C:54:LYS:HE2	1.80	0.81
1:C:212:ILE:HD13	1:C:235:PHE:CE2	2.15	0.81
1:D:82:ILE:HD12	1:D:82:ILE:N	1.93	0.81
1:C:192:MET:HE3	1:C:192:MET:CA	2.08	0.81
1:A:284:LEU:HD23	1:A:285:ASN:N	1.96	0.80
1:A:367:THR:HG23	1:A:370:GLN:NE2	1.97	0.80
1:B:253:LEU:HB2	1:B:266:ILE:HB	1.61	0.80
1:A:251:VAL:N	1:A:268:ALA:O	2.13	0.80
1:C:192:MET:HA	1:C:192:MET:CE	2.08	0.80
1:C:242:VAL:CG2	1:C:256:GLU:H	1.94	0.80
1:B:10:VAL:HB	1:B:143:ILE:HG12	1.63	0.80
1:A:364:VAL:HG23	1:A:426:ILE:CD1	2.11	0.80
1:A:367:THR:H	1:A:370:GLN:HE21	1.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:VAL:HA	1:A:288:LYS:NZ	1.96	0.80
1:A:355:VAL:CG1	1:A:357:THR:HG23	2.11	0.80
1:D:383:PHE:CD1	1:D:458:GLU:HB3	2.16	0.80
1:B:28:LEU:HD12	1:B:336:VAL:HG12	1.64	0.79
1:B:358:ASN:HB3	1:B:359:PRO:HD3	1.64	0.79
1:C:139:LYS:H	1:C:139:LYS:HD2	1.47	0.79
1:D:41:LEU:HD11	1:D:106:PHE:CE1	2.17	0.79
1:A:49:GLY:O	1:A:53:SER:CB	2.31	0.79
1:B:129:ASP:HB3	1:B:135:ASN:OD1	1.83	0.79
1:C:204:THR:HA	1:C:233:MET:O	1.83	0.79
1:C:253:LEU:HB2	1:C:266:ILE:HB	1.65	0.79
1:A:408:GLU:OE2	1:D:386:MET:HE2	1.83	0.79
1:D:42:GLY:HA3	1:D:46:LEU:HB3	1.64	0.79
1:D:88:MET:HE1	1:D:171:LEU:O	1.82	0.79
1:B:184:GLY:HA3	1:B:274:SER:O	1.83	0.79
1:B:295:LYS:C	1:B:297:GLY:H	1.90	0.79
1:C:154:LEU:HD12	1:C:156:GLY:H	1.48	0.79
1:B:300:LEU:H	1:B:300:LEU:CD2	1.95	0.78
1:D:439:SER:O	1:D:442:ILE:HG22	1.82	0.78
1:B:239:THR:HG22	1:B:257:PRO:HB3	1.64	0.78
1:C:176:ILE:HD13	1:C:199:ILE:HG23	1.64	0.78
1:C:204:THR:HG22	1:C:234:LYS:HB2	1.64	0.78
1:D:449:HIS:CE1	1:D:450:PRO:HB3	2.18	0.78
1:A:192:MET:HA	1:A:192:MET:HE3	1.63	0.78
1:D:117:TYR:HB3	1:D:129:ASP:OD1	1.84	0.78
1:A:28:LEU:HD12	1:A:336:VAL:HG12	1.66	0.78
1:C:254:THR:CG2	1:C:265:ILE:HD11	2.10	0.78
1:D:51:ILE:HB	1:D:52:PRO:HD3	1.66	0.78
1:B:48:VAL:CG1	1:B:168:THR:HG23	2.14	0.78
1:B:269:ASP:O	1:B:270:VAL:HG23	1.83	0.78
1:C:427:HIS:HA	1:C:430:ALA:HB3	1.64	0.78
1:B:48:VAL:HG11	1:B:168:THR:HG23	1.64	0.78
1:D:50:CYS:O	1:D:54:LYS:HE2	1.84	0.78
1:A:95:VAL:O	1:A:99:THR:HG23	1.84	0.78
1:C:165:VAL:N	1:C:271:VAL:O	2.17	0.78
1:D:309:VAL:O	1:D:312:VAL:HG23	1.84	0.78
1:C:261:GLY:O	1:C:262:GLU:CB	2.30	0.77
1:B:129:ASP:HA	1:B:135:ASN:HA	1.64	0.77
1:A:120:PHE:HB2	1:A:285:ASN:O	1.83	0.77
1:A:239:THR:HG22	1:A:255:VAL:HG22	1.66	0.77
1:C:154:LEU:HD11	1:C:241:VAL:HG11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TYR:CZ	1:A:82:ILE:HD11	2.20	0.77
1:B:82:ILE:N	1:B:82:ILE:CD1	2.46	0.77
1:C:126:ILE:CD1	1:C:143:ILE:HD13	2.15	0.77
1:A:298:ARG:HB2	1:A:320:PRO:HD3	1.67	0.76
1:B:123:PRO:HG3	1:B:289:ILE:HG21	1.67	0.76
1:B:16:PRO:O	1:B:20:VAL:HG23	1.85	0.76
1:C:187:TYR:HD1	1:C:188:ILE:H	1.30	0.76
1:A:119:LYS:HG2	1:A:285:ASN:ND2	2.00	0.76
1:A:371:VAL:HG21	1:A:404:ILE:HG21	1.65	0.76
1:C:240:LYS:H	1:C:255:VAL:HG11	1.50	0.76
1:D:10:VAL:CG2	1:D:143:ILE:HG12	2.15	0.75
1:C:150:ASP:CG	1:C:151:VAL:H	1.94	0.75
1:B:228:LEU:HB3	1:B:233:MET:HE3	1.68	0.75
1:D:49:GLY:O	1:D:53:SER:HB3	1.86	0.75
1:A:259:ALA:O	1:A:261:GLY:N	2.19	0.75
1:A:245:ASP:HB2	1:A:252:LYS:HB3	1.69	0.75
1:B:15:GLY:HA2	1:B:43:GLY:CA	2.17	0.75
1:C:242:VAL:HG21	1:C:256:GLU:N	2.01	0.75
1:B:82:ILE:HD12	1:B:82:ILE:H	1.50	0.75
1:C:126:ILE:HD11	1:C:143:ILE:HG21	1.68	0.74
1:D:161:GLU:O	1:D:162:LYS:HG3	1.87	0.74
1:C:243:GLY:O	1:C:254:THR:HB	1.88	0.74
1:D:86:ALA:O	1:D:89:GLY:N	2.20	0.74
1:B:51:ILE:HB	1:B:52:PRO:HD3	1.67	0.74
1:D:239:THR:HB	1:D:255:VAL:CG1	2.17	0.74
1:B:292:GLU:C	1:B:300:LEU:HD23	2.12	0.74
1:C:394:ILE:HD12	1:D:58:HIS:CG	2.23	0.74
1:B:54:LYS:HA	1:B:57:LEU:HD12	1.69	0.74
1:D:358:ASN:HB3	1:D:359:PRO:HD3	1.68	0.73
1:C:117:TYR:N	1:C:128:VAL:HG13	2.03	0.73
1:A:6:GLU:CD	1:A:141:LYS:HE2	2.13	0.73
1:D:217:ASP:HB2	1:D:416:HIS:CD2	2.23	0.73
1:B:119:LYS:O	1:B:127:SER:N	2.20	0.73
1:A:239:THR:CG2	1:A:255:VAL:HG22	2.18	0.73
1:B:176:ILE:HD13	1:B:199:ILE:HG23	1.70	0.73
1:C:242:VAL:HG21	1:C:256:GLU:HB3	1.70	0.73
1:C:42:GLY:HA3	1:C:46:LEU:HB3	1.70	0.73
1:D:44:THR:HA	3:D:2001:HOH:O	1.88	0.73
1:A:12:ILE:CD1	1:A:126:ILE:HD13	2.19	0.72
1:A:121:VAL:HG21	1:A:127:SER:HB2	1.72	0.72
1:B:88:MET:HE1	1:B:171:LEU:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:THR:HG23	1:C:370:GLN:NE2	2.04	0.72
1:A:42:GLY:HA3	1:A:46:LEU:HB3	1.69	0.72
1:C:282:SER:C	1:C:284:LEU:H	1.96	0.72
1:C:355:VAL:HG12	1:C:357:THR:HG23	1.72	0.72
1:B:8:ASP:HB2	1:B:31:LYS:O	1.90	0.72
1:B:23:ILE:HG23	1:B:109:ASN:ND2	2.04	0.72
1:B:183:ILE:O	1:B:206:VAL:O	2.06	0.72
1:C:164:ILE:HG13	1:C:271:VAL:HB	1.71	0.72
1:A:119:LYS:HG2	1:A:285:ASN:CB	2.19	0.72
1:B:244:VAL:HG12	1:B:245:ASP:H	1.53	0.72
1:C:154:LEU:CD1	1:C:156:GLY:H	2.03	0.72
1:C:184:GLY:HA3	1:C:274:SER:O	1.88	0.72
1:C:187:TYR:HD1	1:C:188:ILE:N	1.88	0.72
1:C:198:ARG:O	3:C:2010:HOH:O	2.07	0.72
1:C:264:THR:HG22	1:C:265:ILE:H	1.55	0.72
1:D:12:ILE:HD11	1:D:126:ILE:HD11	1.72	0.72
1:B:294:ASP:H	1:B:300:LEU:HD21	1.54	0.72
1:C:251:VAL:O	1:C:268:ALA:O	2.08	0.71
1:A:291:VAL:HA	1:A:308:ASN:HD21	1.55	0.71
1:A:5:ASP:CB	1:A:31:LYS:HE2	2.20	0.71
1:D:96:SER:O	1:D:97:ASN:C	2.33	0.71
1:D:118:GLY:HA2	1:D:127:SER:O	1.90	0.71
1:B:367:THR:N	1:B:370:GLN:HE21	1.89	0.71
1:C:165:VAL:O	1:C:272:LEU:HD12	1.90	0.71
1:A:367:THR:HG23	1:A:370:GLN:HE21	1.55	0.71
1:B:322:PRO:CG	1:B:327:LYS:HG3	2.15	0.71
1:C:54:LYS:HA	1:C:57:LEU:HD12	1.72	0.71
1:A:86:ALA:O	1:A:89:GLY:N	2.23	0.71
1:D:243:GLY:CA	1:D:254:THR:HB	2.14	0.71
1:A:403:ILE:HG23	1:A:415:VAL:HG22	1.72	0.70
1:C:286:LEU:HD22	1:C:291:VAL:CB	2.20	0.70
1:A:346:VAL:O	1:A:347:ASP:HB2	1.89	0.70
1:A:5:ASP:CA	1:A:31:LYS:HE2	2.22	0.70
1:B:151:VAL:HG12	1:B:152:LYS:N	2.06	0.70
1:B:284:LEU:CD1	1:B:286:LEU:HD11	2.22	0.70
1:B:50:CYS:O	1:B:53:SER:HB3	1.92	0.70
1:A:241:VAL:O	1:A:241:VAL:CG2	2.40	0.70
1:C:42:GLY:HA3	1:C:46:LEU:HD23	1.72	0.70
1:A:49:GLY:O	1:A:53:SER:HB3	1.91	0.69
1:B:438:SER:O	1:B:441:ASP:HB2	1.92	0.69
1:C:42:GLY:CA	1:C:46:LEU:HD23	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:HG2	1:A:285:ASN:HB2	1.73	0.69
1:B:427:HIS:O	1:B:431:ILE:HG22	1.92	0.69
1:C:362:ALA:HB1	1:C:426:ILE:HD12	1.74	0.69
1:A:5:ASP:HB3	1:A:31:LYS:HE2	1.75	0.69
1:A:183:ILE:HG22	1:A:184:GLY:N	2.05	0.69
1:B:15:GLY:HA2	1:B:43:GLY:HA2	1.75	0.69
1:C:183:ILE:O	1:C:206:VAL:O	2.09	0.69
1:B:304:ARG:HA	1:B:338:TYR:CE1	2.28	0.69
1:D:216:MET:HE2	1:D:221:ARG:N	2.08	0.69
1:B:294:ASP:N	1:B:300:LEU:HD21	2.07	0.69
1:A:121:VAL:HA	1:A:288:LYS:HZ2	1.58	0.69
1:A:164:ILE:HD11	1:A:244:VAL:HG11	1.74	0.69
1:B:97:ASN:C	1:B:97:ASN:HD22	1.99	0.69
1:B:362:ALA:HB1	1:B:426:ILE:HD12	1.75	0.69
1:C:300:LEU:HD23	1:C:301:VAL:N	2.07	0.69
1:A:51:ILE:HB	1:A:52:PRO:HD3	1.74	0.69
1:C:86:ALA:O	1:C:89:GLY:N	2.23	0.69
1:C:229:GLU:O	1:C:231:GLN:N	2.25	0.69
1:A:55:ALA:HB1	1:A:90:GLN:HE22	1.58	0.69
1:C:166:SER:O	1:C:167:SER:C	2.35	0.69
1:A:81:GLU:C	1:A:82:ILE:HD12	2.18	0.69
1:A:246:THR:HG22	1:A:251:VAL:HG22	1.75	0.69
1:C:117:TYR:N	1:C:128:VAL:CG1	2.55	0.69
1:C:358:ASN:HB3	1:C:359:PRO:HD3	1.75	0.69
1:A:82:ILE:HD12	1:A:82:ILE:N	2.08	0.68
1:C:261:GLY:O	1:C:262:GLU:HB2	1.93	0.68
1:D:345:HIS:O	1:D:345:HIS:ND1	2.26	0.68
1:D:183:ILE:HG22	1:D:184:GLY:N	2.08	0.68
1:C:393:ALA:HB2	1:D:51:ILE:HG23	1.74	0.68
1:A:192:MET:HA	1:A:192:MET:HE2	1.75	0.68
1:A:367:THR:N	1:A:370:GLN:HE21	1.92	0.68
1:C:141:LYS:HB3	1:C:142:HIS:CE1	2.28	0.68
1:A:35:ILE:HD11	1:A:138:VAL:HG11	1.75	0.68
1:A:130:THR:HG23	1:A:133:GLY:N	2.08	0.68
1:B:185:ALA:CB	1:B:207:GLU:HB2	2.24	0.68
1:B:328:ALA:O	1:B:329:GLU:C	2.36	0.68
1:D:63:TYR:CZ	1:D:82:ILE:HD11	2.28	0.68
1:A:48:VAL:HG12	1:A:48:VAL:O	1.93	0.68
1:C:229:GLU:C	1:C:231:GLN:H	2.01	0.68
1:C:262:GLU:O	1:C:263:GLN:CB	2.33	0.68
1:A:364:VAL:HG23	1:A:426:ILE:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:THR:HG23	1:D:370:GLN:HE21	1.57	0.68
1:B:462:ALA:HB2	1:B:467:PRO:HG3	1.73	0.67
1:C:12:ILE:HD11	1:C:126:ILE:HD13	1.75	0.67
1:C:364:VAL:HG23	1:C:426:ILE:CD1	2.23	0.67
1:A:88:MET:HE3	1:A:91:LYS:HD3	1.75	0.67
1:D:9:VAL:HB	1:D:32:THR:HG23	1.74	0.67
1:C:139:LYS:HD2	1:C:139:LYS:N	2.08	0.67
1:D:284:LEU:CD1	1:D:285:ASN:H	2.07	0.67
1:D:121:VAL:CG2	1:D:127:SER:HB2	2.25	0.67
1:A:48:VAL:O	1:A:48:VAL:CG1	2.43	0.67
1:A:120:PHE:N	1:A:285:ASN:HB2	2.10	0.67
1:B:151:VAL:HG12	1:B:152:LYS:H	1.59	0.67
1:C:51:ILE:HB	1:C:52:PRO:CD	2.18	0.67
1:C:203:VAL:CG2	1:C:233:MET:HG3	2.25	0.67
1:D:161:GLU:OE1	1:D:165:VAL:HB	1.95	0.67
1:B:44:THR:C	1:B:46:LEU:H	2.03	0.66
1:B:300:LEU:HD22	1:B:300:LEU:N	2.08	0.66
1:B:367:THR:HG23	1:B:370:GLN:HE21	1.61	0.66
1:C:289:ILE:HG13	1:C:290:GLY:H	1.59	0.66
1:D:120:PHE:HD1	1:D:284:LEU:CD1	2.07	0.66
1:B:158:THR:O	1:B:160:ASP:N	2.29	0.66
1:C:163:LYS:O	1:C:270:VAL:HG13	1.95	0.66
1:D:36:GLU:OE2	2:D:480:FAD:H4B	1.95	0.66
1:D:180:LEU:O	1:D:203:VAL:HA	1.95	0.66
1:A:58:HIS:CG	1:B:394:ILE:HD12	2.30	0.66
1:C:157:VAL:HG12	1:C:158:THR:H	1.60	0.66
1:D:286:LEU:HA	1:D:289:ILE:HG13	1.76	0.66
1:A:187[B]:TYR:CD2	1:A:355:VAL:HG22	2.31	0.66
1:A:367:THR:H	1:A:370:GLN:HG3	1.61	0.66
1:D:91:LYS:O	1:D:94:ALA:HB3	1.96	0.66
1:D:142:HIS:ND1	3:D:2004:HOH:O	2.21	0.66
1:A:125:GLU:HB2	1:A:139:LYS:HG2	1.78	0.66
1:C:367:THR:HG23	1:C:370:GLN:HE21	1.60	0.66
1:A:88:MET:HE1	1:A:171:LEU:O	1.96	0.65
1:A:366:LYS:HA	1:A:370:GLN:NE2	2.11	0.65
1:C:254:THR:HA	1:C:265:ILE:CD1	2.26	0.65
1:A:284:LEU:CD2	1:A:285:ASN:N	2.60	0.65
1:A:394:ILE:HD12	1:B:58:HIS:CG	2.31	0.65
1:C:239:THR:HG22	1:C:255:VAL:HG12	1.76	0.65
1:D:448:ALA:O	1:D:451:THR:CG2	2.44	0.65
1:A:130:THR:HG23	1:A:133:GLY:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:HD3	1:B:47:ASN:ND2	2.12	0.65
1:D:273:VAL:HG12	1:D:273:VAL:O	1.96	0.65
1:A:58:HIS:O	1:A:62:MET:HG3	1.96	0.65
1:C:145:ILE:N	1:C:313:TYR:O	2.23	0.65
1:C:240:LYS:H	1:C:255:VAL:CG1	2.10	0.65
1:D:360:GLU:N	1:D:419:ALA:O	2.24	0.65
1:C:62:MET:HE2	1:D:70:PHE:CD1	2.31	0.65
1:C:225:GLN:HG3	1:C:235:PHE:CE2	2.32	0.65
1:A:119:LYS:C	1:A:285:ASN:HB2	2.22	0.65
1:A:227:SER:O	1:A:230:LYS:HG2	1.96	0.65
1:A:291:VAL:HA	1:A:308:ASN:ND2	2.11	0.65
1:A:358:ASN:HB3	1:A:359:PRO:CD	2.21	0.65
1:D:117:TYR:OH	1:D:283:GLY:N	2.30	0.65
1:D:120:PHE:CD1	1:D:284:LEU:HD11	2.27	0.65
1:A:362:ALA:C	1:A:426:ILE:HD12	2.23	0.64
1:B:82:ILE:HG21	1:B:199:ILE:CD1	2.26	0.64
1:C:367:THR:N	1:C:370:GLN:HE21	1.93	0.64
1:A:96:SER:O	1:A:97:ASN:C	2.40	0.64
1:A:152:LYS:HB2	1:A:276:GLY:C	2.22	0.64
1:D:126:ILE:HD13	1:D:143:ILE:HD13	1.78	0.64
1:A:216:MET:HE3	1:A:361:VAL:HG11	1.77	0.64
1:B:128:VAL:HG12	1:B:129:ASP:H	1.63	0.64
1:C:462:ALA:CA	1:C:467:PRO:HD3	2.26	0.64
1:D:161:GLU:C	1:D:162:LYS:HG3	2.23	0.64
1:D:304:ARG:O	1:D:305:PHE:HB2	1.96	0.64
1:B:284:LEU:HD11	1:B:286:LEU:HD11	1.78	0.64
1:D:367:THR:HG23	1:D:370:GLN:NE2	2.12	0.64
1:B:160:ASP:O	1:B:160:ASP:OD2	2.16	0.64
1:D:38:ARG:CD	1:D:47:ASN:ND2	2.61	0.64
1:D:358:ASN:HB3	1:D:359:PRO:CD	2.27	0.64
1:C:448:ALA:O	1:C:451:THR:HG23	1.97	0.64
1:A:62:MET:HE2	1:B:70:PHE:CD1	2.33	0.64
1:D:121:VAL:HG23	1:D:127:SER:HB2	1.80	0.64
1:D:243:GLY:HA3	1:D:254:THR:CB	2.17	0.64
1:A:443:ALA:O	1:A:457:LYS:NZ	2.30	0.64
1:D:462:ALA:HB2	1:D:467:PRO:HG3	1.80	0.64
1:C:187:TYR:CD1	1:C:188:ILE:N	2.63	0.63
1:C:176:ILE:HD13	1:C:199:ILE:CG2	2.28	0.63
1:D:45:CYS:O	1:D:50:CYS:HB2	1.98	0.63
1:A:253:LEU:O	1:A:265:ILE:HD12	1.98	0.63
1:B:176:ILE:HD13	1:B:199:ILE:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LEU:HD12	1:C:336:VAL:HG12	1.79	0.63
1:C:285:ASN:C	1:C:287:ASP:H	2.03	0.63
1:D:126:ILE:CD1	1:D:143:ILE:HD13	2.28	0.63
1:A:149:SER:HB3	1:A:317:ASP:HB3	1.80	0.63
1:B:228:LEU:HD13	1:B:233:MET:CE	2.28	0.63
1:B:460:ALA:O	1:B:463:THR:HB	1.99	0.63
1:C:193:GLY:C	1:C:233:MET:HE2	2.23	0.63
1:C:242:VAL:O	1:C:254:THR:O	2.15	0.63
1:B:153:SER:C	1:B:157:VAL:HG21	2.23	0.63
1:B:367:THR:H	1:B:370:GLN:HG3	1.63	0.63
1:C:95:VAL:O	1:C:99:THR:HG23	1.99	0.63
1:C:333:VAL:O	1:C:334:ALA:C	2.42	0.63
1:C:445:VAL:HG21	1:D:431:ILE:HG13	1.81	0.63
1:A:229:GLU:O	1:A:231:GLN:N	2.31	0.63
1:C:262:GLU:HG2	1:C:263:GLN:N	2.12	0.63
1:A:462:ALA:HB2	1:A:467:PRO:HG3	1.79	0.63
1:C:150:ASP:CG	1:C:151:VAL:N	2.56	0.63
1:D:171:LEU:HD23	1:D:192:MET:HE1	1.80	0.63
1:D:367:THR:H	1:D:370:GLN:HE21	1.47	0.63
1:B:301:VAL:HG22	1:B:302:ASN:H	1.62	0.63
1:B:415:VAL:HG21	1:B:429:ALA:HB1	1.79	0.63
1:B:216:MET:HE3	1:B:361:VAL:HG11	1.81	0.63
1:D:152:LYS:HG3	1:D:278:THR:HG23	1.79	0.63
1:D:426:ILE:HG12	1:D:426:ILE:O	1.98	0.63
1:C:181:VAL:HG22	1:C:204:THR:OG1	1.99	0.62
1:A:12:ILE:CD1	1:A:126:ILE:CD1	2.70	0.62
1:A:117:TYR:HB3	1:A:129:ASP:CB	2.23	0.62
1:A:121:VAL:CG2	1:A:127:SER:HB2	2.29	0.62
1:C:183:ILE:HG22	1:C:184:GLY:N	2.13	0.62
1:C:286:LEU:HD22	1:C:291:VAL:CG2	2.30	0.62
1:D:12:ILE:HD11	1:D:126:ILE:CD1	2.28	0.62
1:D:28:LEU:HD12	1:D:336:VAL:HG12	1.82	0.62
1:C:154:LEU:HD12	1:C:155:PRO:N	2.14	0.62
1:C:460:ALA:O	1:C:463:THR:HB	1.98	0.62
1:B:304:ARG:HA	1:B:338:TYR:CD1	2.35	0.62
1:D:7:ASN:ND2	1:D:33:THR:OG1	2.32	0.62
1:A:120:PHE:N	1:A:285:ASN:CB	2.63	0.62
1:C:299:ILE:HG13	1:C:318:VAL:O	1.99	0.62
1:C:424:GLU:OE2	1:D:451:THR:HB	1.98	0.62
1:A:54:LYS:HA	1:A:57:LEU:HD12	1.81	0.62
1:C:164:ILE:HG13	1:C:271:VAL:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:THR:HB	1:D:255:VAL:HG11	1.81	0.62
1:B:161:GLU:HG2	1:B:162:LYS:HG2	1.82	0.61
1:D:242:VAL:HG23	1:D:254:THR:CG2	2.28	0.61
1:C:262:GLU:HG2	1:C:263:GLN:H	1.65	0.61
1:D:119:LYS:HB3	1:D:127:SER:HB3	1.82	0.61
1:A:212:ILE:HG13	1:A:212:ILE:O	1.98	0.61
1:A:245:ASP:HB2	1:A:252:LYS:CB	2.30	0.61
1:B:8:ASP:HB2	1:B:31:LYS:N	2.15	0.61
1:A:184:GLY:HA3	1:A:274:SER:O	2.01	0.61
1:C:156:GLY:HA3	1:C:241:VAL:HG11	1.82	0.61
1:B:295:LYS:C	1:B:297:GLY:N	2.59	0.61
1:B:364:VAL:HG12	1:B:433:LEU:HD22	1.83	0.61
1:B:183:ILE:HG22	1:B:184:GLY:N	2.15	0.61
1:C:300:LEU:HD23	1:C:300:LEU:C	2.26	0.61
1:D:49:GLY:O	1:D:53:SER:CB	2.48	0.61
1:A:350:LYS:HD3	1:A:433:LEU:HD23	1.82	0.61
1:B:295:LYS:O	1:B:297:GLY:N	2.32	0.61
1:C:216:MET:HE3	1:C:361:VAL:HG11	1.83	0.61
1:B:185:ALA:HB3	1:B:207:GLU:HB2	1.82	0.61
1:B:207:GLU:HG3	1:B:209:ALA:H	1.65	0.61
1:B:146:ALA:C	1:B:147:THR:O	2.42	0.60
1:B:171:LEU:HD23	1:B:192:MET:HE1	1.83	0.60
1:C:114:VAL:HG12	1:C:114:VAL:O	2.00	0.60
1:A:208:PHE:CE2	1:A:258:SER:HB3	2.36	0.60
1:B:281:THR:HA	1:B:284:LEU:HD21	1.83	0.60
1:B:389:SER:O	1:B:390:ARG:C	2.43	0.60
1:B:468:ILE:O	1:B:468:ILE:HG22	2.00	0.60
1:D:286:LEU:HD13	1:D:291:VAL:N	2.15	0.60
1:B:367:THR:HG23	1:B:370:GLN:CD	2.25	0.60
1:C:263:GLN:C	1:C:264:THR:O	2.38	0.60
1:A:208:PHE:O	1:A:238:LYS:HA	2.01	0.60
1:C:154:LEU:HD12	1:C:155:PRO:CD	2.32	0.60
1:B:41:LEU:HD11	1:B:106:PHE:CE1	2.37	0.60
1:B:212:ILE:HG21	1:B:235:PHE:CE2	2.36	0.60
1:D:46:LEU:HD11	1:D:98:LEU:HB2	1.83	0.60
1:A:164:ILE:CD1	1:A:244:VAL:HG11	2.32	0.60
1:C:51:ILE:HD13	1:C:51:ILE:N	2.16	0.60
1:B:49:GLY:O	1:B:50:CYS:C	2.44	0.60
1:A:374:THR:O	1:A:376:VAL:HG23	2.02	0.59
1:C:5:ASP:CG	1:C:6:GLU:H	2.10	0.59
1:C:121:VAL:HG12	1:C:121:VAL:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ILE:HD11	1:C:126:ILE:CD1	2.33	0.59
1:C:378:TYR:CD1	1:C:378:TYR:C	2.79	0.59
1:D:403:ILE:HG12	1:D:415:VAL:HG22	1.84	0.59
1:B:367:THR:H	1:B:370:GLN:NE2	1.95	0.59
1:A:260:GLY:O	1:A:262:GLU:N	2.35	0.59
1:C:86:ALA:O	1:C:87:MET:C	2.44	0.59
1:C:127:SER:C	1:C:128:VAL:HG23	2.27	0.59
1:D:284:LEU:HD12	1:D:285:ASN:N	2.13	0.59
1:C:394:ILE:HD12	1:D:58:HIS:CD2	2.36	0.59
1:D:462:ALA:HA	1:D:467:PRO:HD3	1.83	0.59
1:A:418:MET:O	1:A:419:ALA:HB2	2.01	0.59
1:A:448:ALA:O	1:A:451:THR:CG2	2.51	0.59
1:C:242:VAL:CB	1:C:255:VAL:HA	2.31	0.59
1:D:183:ILE:O	1:D:206:VAL:O	2.20	0.59
1:A:225:GLN:O	1:A:229:GLU:HG3	2.02	0.59
1:B:265:ILE:N	1:B:265:ILE:HD12	2.18	0.59
1:B:293:THR:HG22	1:B:293:THR:O	2.01	0.59
1:C:117:TYR:C	1:C:128:VAL:HA	2.28	0.59
1:D:130:THR:O	1:D:131:ILE:HD13	2.03	0.59
1:C:366:LYS:O	1:C:416:HIS:HE1	1.85	0.59
1:D:182:VAL:HB	1:D:205:VAL:HG13	1.84	0.59
1:D:128:VAL:O	1:D:129:ASP:O	2.20	0.59
1:B:8:ASP:HB2	1:B:31:LYS:H	1.67	0.58
1:C:184:GLY:HA3	1:C:274:SER:C	2.28	0.58
1:C:246:THR:O	1:C:247:SER:HB2	2.02	0.58
1:D:185:ALA:CB	1:D:207:GLU:HB2	2.33	0.58
1:C:122:SER:C	1:C:124:SER:H	2.09	0.58
1:C:270:VAL:CG1	1:C:271:VAL:N	2.67	0.58
1:D:227:SER:OG	1:D:231:GLN:NE2	2.37	0.58
1:D:325:ALA:O	1:D:328:ALA:HB3	2.03	0.58
1:A:364:VAL:HG23	1:A:426:ILE:HD13	1.85	0.58
1:C:160:ASP:O	1:C:161:GLU:C	2.47	0.58
1:C:357:THR:OG1	1:C:359:PRO:O	2.21	0.58
1:D:126:ILE:HG23	1:D:127:SER:O	2.03	0.58
1:A:176:ILE:HD13	1:A:199:ILE:HG23	1.85	0.58
1:B:212:ILE:HG21	1:B:235:PHE:CD2	2.38	0.58
1:C:357:THR:O	1:C:358:ASN:C	2.44	0.58
1:A:49:GLY:O	1:A:53:SER:HB2	2.02	0.58
1:B:8:ASP:CB	1:B:31:LYS:H	2.17	0.58
1:B:216:MET:HE2	1:B:221:ARG:HA	1.85	0.58
1:B:123:PRO:HG3	1:B:289:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:PHE:CZ	1:D:70:PHE:CZ	2.92	0.58
1:C:242:VAL:HG21	1:C:256:GLU:CB	2.34	0.58
1:D:401:VAL:HG11	1:D:456:ILE:HA	1.86	0.58
1:B:296:LEU:HD12	1:B:296:LEU:H	1.68	0.58
1:B:419:ALA:HB1	1:B:420:PRO:HD2	1.85	0.58
1:A:150:ASP:CG	1:A:151:VAL:H	2.11	0.58
1:A:221:ARG:HG2	1:A:221:ARG:HH11	1.69	0.58
1:C:62:MET:SD	1:D:73:HIS:CG	2.97	0.57
1:D:120:PHE:H	1:D:284:LEU:HD13	1.70	0.57
1:B:36:GLU:OE2	2:B:480:FAD:H4B	2.04	0.57
1:B:265:ILE:HD12	1:B:265:ILE:H	1.68	0.57
1:C:185:ALA:CB	1:C:207:GLU:HB2	2.34	0.57
1:C:253:LEU:N	1:C:266:ILE:O	2.36	0.57
1:C:38:ARG:O	3:C:2004:HOH:O	2.17	0.57
1:B:286:LEU:C	1:B:288:LYS:N	2.59	0.57
1:C:216:MET:HE2	1:C:221:ARG:HA	1.86	0.57
1:A:58:HIS:CD2	1:B:394:ILE:HD12	2.39	0.57
1:A:468:ILE:HG22	1:A:468:ILE:O	2.04	0.57
1:B:81:GLU:C	1:B:82:ILE:HD12	2.27	0.57
1:B:190:LEU:HD13	1:B:228:LEU:HD11	1.86	0.57
1:D:329:GLU:OE2	3:D:2011:HOH:O	2.17	0.57
1:A:66:ALA:HB2	1:B:70:PHE:CE2	2.39	0.57
1:B:358:ASN:HB3	1:B:359:PRO:CD	2.35	0.57
1:B:443:ALA:O	1:B:457:LYS:NZ	2.37	0.57
1:C:203:VAL:HG21	1:C:233:MET:HG3	1.87	0.57
1:D:53:SER:O	1:D:57:LEU:HG	2.04	0.57
1:D:166:SER:O	1:D:167:SER:C	2.47	0.57
1:D:425:LEU:HB3	1:D:456:ILE:HD11	1.85	0.57
1:A:154:LEU:HD12	1:A:155:PRO:HD2	1.87	0.57
1:A:160:ASP:O	1:A:161:GLU:CG	2.50	0.57
1:A:163:LYS:O	1:A:270:VAL:HA	2.04	0.57
1:A:206:VAL:HG22	1:A:236:LYS:HB2	1.85	0.57
1:C:468:ILE:HG22	1:C:468:ILE:O	2.03	0.57
1:A:401:VAL:HG11	1:A:456:ILE:HA	1.85	0.57
1:D:192:MET:HE3	1:D:192:MET:CA	2.25	0.57
1:D:427:HIS:O	1:D:431:ILE:HG22	2.05	0.57
1:A:96:SER:O	1:A:99:THR:N	2.37	0.57
1:A:465:ASP:CG	1:A:466:LYS:H	2.12	0.57
1:D:120:PHE:H	1:D:284:LEU:CD1	2.18	0.57
1:D:243:GLY:O	1:D:253:LEU:HA	2.04	0.57
1:D:284:LEU:CG	1:D:285:ASN:N	2.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:PRO:HG2	1:D:327:LYS:HG3	1.87	0.57
1:B:49:GLY:O	1:B:50:CYS:O	2.23	0.56
1:B:142:HIS:HB3	1:B:313:TYR:HE1	1.69	0.56
1:C:48:VAL:HG12	1:C:48:VAL:O	2.05	0.56
1:C:195:VAL:HG12	1:C:196:TRP:N	2.19	0.56
1:C:293:THR:HG22	1:C:298:ARG:O	2.04	0.56
1:D:358:ASN:CB	1:D:359:PRO:HD3	2.34	0.56
1:A:38:ARG:NH1	3:A:2007:HOH:O	2.24	0.56
1:C:181:VAL:HA	1:C:204:THR:O	2.06	0.56
1:C:393:ALA:CB	1:D:51:ILE:HG23	2.35	0.56
1:C:409:THR:O	1:C:410:ASP:HB3	2.05	0.56
1:D:28:LEU:HD12	1:D:336:VAL:CG1	2.35	0.56
1:B:82:ILE:HG21	1:B:199:ILE:HD11	1.86	0.56
1:B:119:LYS:O	1:B:126:ILE:HA	2.05	0.56
1:B:244:VAL:HG12	1:B:251:VAL:HG13	1.87	0.56
1:B:362:ALA:CB	1:B:426:ILE:HD12	2.34	0.56
1:C:406:GLU:HB2	1:C:409:THR:OG1	2.05	0.56
1:D:207:GLU:HG3	1:D:209:ALA:H	1.70	0.56
1:A:441:ASP:O	1:B:435:TYR:OH	2.22	0.56
1:C:81:GLU:C	1:C:82:ILE:HD12	2.30	0.56
1:C:185:ALA:HB3	1:C:207:GLU:HB2	1.87	0.56
1:D:150:ASP:CG	1:D:151:VAL:H	2.13	0.56
1:D:309:VAL:O	1:D:309:VAL:HG12	2.04	0.56
1:A:157:VAL:CG1	1:A:244:VAL:HG21	2.28	0.56
1:B:292:GLU:HB3	1:B:300:LEU:HB2	1.86	0.56
1:C:36:GLU:OE2	2:C:480:FAD:H4B	2.05	0.56
1:C:139:LYS:N	1:C:139:LYS:CD	2.69	0.56
1:D:75:VAL:HG12	1:D:75:VAL:O	2.05	0.56
1:B:400:LEU:N	1:B:400:LEU:HD23	2.20	0.56
1:C:11:ILE:HG12	1:C:144:ILE:HB	1.87	0.56
1:C:118:GLY:HA2	1:C:128:VAL:HG22	1.87	0.56
1:C:154:LEU:HD12	1:C:156:GLY:N	2.20	0.56
1:A:227:SER:OG	1:A:230:LYS:NZ	2.38	0.56
1:C:73:HIS:O	1:D:87:MET:HG3	2.05	0.56
1:A:138:VAL:HG12	1:A:138:VAL:O	2.06	0.56
1:A:152:LYS:HB2	1:A:276:GLY:O	2.05	0.56
1:B:259:ALA:C	1:B:261:GLY:H	2.12	0.56
1:B:406:GLU:HB2	1:B:409:THR:OG1	2.06	0.56
1:C:123:PRO:CG	1:C:289:ILE:HG22	2.28	0.56
1:D:284:LEU:HG	1:D:285:ASN:N	2.20	0.56
1:A:367:THR:H	1:A:370:GLN:NE2	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HD13	1:B:233:MET:HE1	1.88	0.56
1:B:299:ILE:HG22	1:B:299:ILE:O	2.06	0.56
1:C:122:SER:C	1:C:124:SER:N	2.64	0.56
1:C:322:PRO:HG2	1:C:327:LYS:HG3	1.87	0.56
1:D:438:SER:O	1:D:441:ASP:HB2	2.06	0.56
1:A:281:THR:O	1:A:284:LEU:HB2	2.06	0.56
1:B:15:GLY:HA2	1:B:43:GLY:HA3	1.87	0.56
1:C:62:MET:HE2	1:D:70:PHE:CE1	2.41	0.56
1:C:88:MET:HE3	3:C:2007:HOH:O	2.05	0.56
1:C:118:GLY:CA	1:C:127:SER:O	2.43	0.56
1:C:461:MET:C	1:C:463:THR:H	2.14	0.56
1:D:184:GLY:HA3	1:D:274:SER:O	2.06	0.56
1:A:120:PHE:O	1:A:285:ASN:ND2	2.39	0.55
1:A:229:GLU:C	1:A:231:GLN:N	2.61	0.55
1:A:419:ALA:HB1	1:A:420:PRO:HD2	1.87	0.55
1:C:190:LEU:HD13	1:C:228:LEU:HD11	1.87	0.55
1:C:348:TYR:HA	1:C:351:VAL:HG23	1.88	0.55
1:C:438:SER:O	1:C:441:ASP:HB2	2.06	0.55
1:A:208:PHE:CZ	1:A:258:SER:HB3	2.41	0.55
1:B:128:VAL:HG12	1:B:129:ASP:N	2.20	0.55
1:B:315:ILE:O	1:B:315:ILE:HG13	2.05	0.55
1:C:42:GLY:HA3	1:C:46:LEU:CB	2.36	0.55
1:D:11:ILE:HG12	1:D:144:ILE:HB	1.87	0.55
1:D:154:LEU:HD23	1:D:157:VAL:HB	1.89	0.55
1:C:156:GLY:HA3	1:C:241:VAL:CG1	2.37	0.55
1:A:249:ASP:OD1	1:A:249:ASP:N	2.39	0.55
1:A:82:ILE:HG21	1:A:199:ILE:CD1	2.37	0.55
1:A:350:LYS:O	1:A:352:PRO:HD3	2.06	0.55
1:C:70:PHE:HB3	1:C:75:VAL:O	2.06	0.55
1:C:265:ILE:HG22	1:C:265:ILE:O	2.05	0.55
1:A:63:TYR:CE1	1:A:82:ILE:HD11	2.41	0.55
1:A:96:SER:OG	1:A:97:ASN:N	2.35	0.55
1:B:253:LEU:O	1:B:265:ILE:HG22	2.06	0.55
1:B:260:GLY:O	1:B:261:GLY:O	2.23	0.55
1:C:165:VAL:HG11	1:C:173:LEU:HD21	1.87	0.55
1:A:207:GLU:HG3	1:A:209:ALA:H	1.72	0.55
1:A:240:LYS:HG2	1:A:241:VAL:N	2.21	0.55
1:B:35:ILE:CD1	1:B:138:VAL:HG21	2.33	0.55
1:C:164:ILE:HG13	1:C:271:VAL:CB	2.35	0.55
1:C:355:VAL:CG1	1:C:357:THR:HG23	2.37	0.55
1:D:419:ALA:HB1	1:D:420:PRO:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:SER:C	1:B:124:SER:H	2.15	0.55
1:C:126:ILE:N	1:C:138:VAL:O	2.35	0.55
1:C:352:PRO:HB3	1:C:364:VAL:CG2	2.36	0.55
1:A:253:LEU:O	1:A:265:ILE:HA	2.07	0.55
1:B:216:MET:HE2	1:B:221:ARG:N	2.22	0.55
1:B:239:THR:CA	1:B:257:PRO:HA	2.24	0.55
1:C:179:LYS:O	1:C:269:ASP:HB2	2.06	0.55
1:C:193:GLY:HA3	1:C:233:MET:HE2	1.89	0.55
1:C:216:MET:HE3	1:C:220:ILE:HG22	1.88	0.55
1:A:119:LYS:CA	1:A:285:ASN:HB2	2.37	0.54
1:A:216:MET:HE2	1:A:221:ARG:N	2.22	0.54
1:B:216:MET:HE2	1:B:221:ARG:CA	2.37	0.54
1:C:127:SER:C	1:C:128:VAL:CG2	2.80	0.54
1:C:244:VAL:HG11	1:C:253:LEU:CD2	2.38	0.54
1:D:348:TYR:N	1:D:348:TYR:CD2	2.69	0.54
1:A:292:GLU:N	1:A:308:ASN:HD21	2.04	0.54
1:B:448:ALA:O	1:B:451:THR:HG23	2.07	0.54
1:C:149:SER:HB3	1:C:317:ASP:HB3	1.88	0.54
1:A:253:LEU:HB2	1:A:266:ILE:HB	1.90	0.54
1:B:310:SER:C	1:B:312:VAL:H	2.15	0.54
1:C:282:SER:O	1:C:284:LEU:N	2.41	0.54
1:D:313:TYR:CE1	1:D:339:LEU:HD21	2.43	0.54
1:D:357:THR:O	1:D:358:ASN:C	2.49	0.54
1:B:310:SER:O	1:B:312:VAL:N	2.41	0.54
1:B:415:VAL:C	1:B:416:HIS:ND1	2.66	0.54
1:C:19:TYR:O	1:C:23:ILE:HG13	2.08	0.54
1:D:42:GLY:HA3	1:D:46:LEU:CB	2.37	0.54
1:A:192:MET:CE	1:A:192:MET:CA	2.77	0.54
1:B:44:THR:C	1:B:46:LEU:N	2.66	0.54
1:B:173:LEU:HD12	1:B:196:TRP:CZ2	2.43	0.54
1:B:450:PRO:O	1:B:450:PRO:HG2	2.07	0.54
1:C:181:VAL:HG23	1:C:268:ALA:HB2	1.90	0.54
1:C:203:VAL:HG23	1:C:233:MET:HG3	1.89	0.54
1:A:287:ASP:O	1:A:288:LYS:C	2.50	0.54
1:A:363:SER:C	1:A:426:ILE:HD11	2.32	0.54
1:B:17:GLY:O	1:B:21:ALA:HB2	2.07	0.54
1:C:305:PHE:CE2	1:C:331:ASP:HB3	2.43	0.54
1:B:409:THR:O	1:B:410:ASP:HB3	2.08	0.54
1:D:44:THR:N	2:D:480:FAD:O1A	2.41	0.54
1:B:310:SER:O	1:B:312:VAL:HG23	2.08	0.53
1:C:207:GLU:HG3	1:C:209:ALA:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ILE:HG23	1:C:237:LEU:HD21	1.91	0.53
1:D:51:ILE:O	1:D:54:LYS:N	2.41	0.53
1:A:229:GLU:O	1:A:230:LYS:C	2.50	0.53
1:B:228:LEU:HD22	1:B:233:MET:CE	2.38	0.53
1:C:70:PHE:HB3	1:C:75:VAL:HB	1.91	0.53
1:D:204:THR:HA	1:D:234:LYS:O	2.09	0.53
1:D:243:GLY:O	1:D:254:THR:N	2.40	0.53
1:A:221:ARG:O	1:A:222:LYS:C	2.52	0.53
1:B:11:ILE:HG12	1:B:144:ILE:HB	1.91	0.53
1:C:216:MET:CE	1:C:220:ILE:HG22	2.39	0.53
1:B:283:GLY:O	1:B:284:LEU:O	2.25	0.53
1:B:292:GLU:O	1:B:300:LEU:HD23	2.07	0.53
1:C:265:ILE:O	1:C:265:ILE:CG2	2.56	0.53
1:D:82:ILE:N	1:D:82:ILE:CD1	2.64	0.53
1:D:149:SER:HA	1:D:280:PHE:N	2.23	0.53
1:B:308:ASN:O	1:B:308:ASN:CG	2.49	0.53
1:C:126:ILE:HD11	1:C:143:ILE:CG2	2.35	0.53
1:C:264:THR:HG22	1:C:265:ILE:N	2.23	0.53
1:B:53:SER:O	1:B:57:LEU:HG	2.08	0.53
1:B:71:ALA:O	1:B:73:HIS:N	2.41	0.53
1:C:9:VAL:HB	1:C:32:THR:HG23	1.89	0.53
1:C:58:HIS:CG	1:D:394:ILE:HD12	2.44	0.53
1:C:157:VAL:HG11	1:C:164:ILE:HG21	1.90	0.53
1:C:353:GLY:O	1:C:362:ALA:HA	2.09	0.53
1:D:216:MET:HE2	1:D:221:ARG:CA	2.38	0.53
1:D:460:ALA:O	1:D:463:THR:HB	2.08	0.53
1:A:121:VAL:HA	1:A:288:LYS:HZ3	1.71	0.53
1:B:46:LEU:O	1:B:46:LEU:HD12	2.07	0.53
1:C:123:PRO:HG3	1:C:289:ILE:CG2	2.31	0.53
1:C:367:THR:H	1:C:370:GLN:NE2	1.97	0.53
1:C:449:HIS:C	1:C:449:HIS:ND1	2.66	0.53
1:D:22:ALA:O	1:D:25:ALA:HB3	2.09	0.53
1:A:195:VAL:HG12	1:A:196:TRP:N	2.24	0.53
1:A:358:ASN:CB	1:A:359:PRO:HD3	2.31	0.53
1:B:182:VAL:HB	1:B:205:VAL:HG13	1.90	0.53
1:B:313:TYR:CZ	1:B:339:LEU:HD21	2.44	0.53
1:D:204:THR:HG22	1:D:234:LYS:HB2	1.91	0.53
1:A:152:LYS:HD2	1:A:278:THR:HG23	1.90	0.53
1:A:291:VAL:CA	1:A:308:ASN:HD21	2.20	0.53
1:C:163:LYS:O	1:C:270:VAL:HG22	2.08	0.53
1:D:142:HIS:HB2	3:D:2004:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:CE2	1:B:66:ALA:HB2	2.43	0.53
1:B:88:MET:CE	1:B:91:LYS:NZ	2.72	0.53
1:C:41:LEU:HD11	1:C:106:PHE:CE1	2.44	0.53
1:A:416:HIS:ND1	1:A:416:HIS:N	2.57	0.52
1:B:364:VAL:CG1	1:B:433:LEU:HD22	2.38	0.52
1:B:367:THR:N	1:B:370:GLN:HG3	2.23	0.52
1:B:462:ALA:CB	1:B:467:PRO:HG3	2.39	0.52
1:C:70:PHE:HZ	1:D:70:PHE:CZ	2.27	0.52
1:C:164:ILE:HD11	1:C:251:VAL:CG1	2.34	0.52
1:C:221:ARG:O	1:C:222:LYS:C	2.51	0.52
1:C:127:SER:O	1:C:128:VAL:CG2	2.57	0.52
1:C:282:SER:C	1:C:284:LEU:N	2.63	0.52
1:B:216:MET:HE1	1:B:224:PHE:CB	2.39	0.52
1:B:362:ALA:C	1:B:426:ILE:HD12	2.34	0.52
1:C:62:MET:SD	1:D:73:HIS:CD2	3.03	0.52
1:A:465:ASP:CG	1:A:466:LYS:N	2.67	0.52
1:B:42:GLY:HA3	1:B:46:LEU:HB3	1.91	0.52
1:C:63:TYR:CE1	1:C:82:ILE:CD1	2.89	0.52
1:D:185:ALA:HB3	1:D:207:GLU:HB2	1.89	0.52
1:A:184:GLY:HA3	1:A:274:SER:C	2.35	0.52
1:B:400:LEU:HD23	1:B:400:LEU:H	1.74	0.52
1:C:130:THR:C	1:C:132:GLU:H	2.16	0.52
1:A:227:SER:OG	1:A:230:LYS:CE	2.58	0.52
1:A:295:LYS:C	1:A:296:LEU:HD23	2.33	0.52
1:B:160:ASP:O	1:B:161:GLU:C	2.53	0.52
1:B:194:SER:O	1:B:198:ARG:HG3	2.09	0.52
1:B:302:ASN:OD1	1:B:302:ASN:C	2.53	0.52
1:C:131:ILE:HG12	1:C:131:ILE:O	2.09	0.52
1:C:212:ILE:O	1:C:212:ILE:HG13	2.10	0.52
1:D:284:LEU:CD1	1:D:285:ASN:N	2.72	0.52
1:D:294:ASP:HB2	1:D:298:ARG:HB2	1.90	0.52
1:D:332:GLY:O	1:D:335:CYS:HB3	2.09	0.52
1:A:46:LEU:HD11	1:A:98:LEU:CB	2.40	0.52
1:C:289:ILE:HB	1:C:309:VAL:HG21	1.92	0.52
1:C:304:ARG:HA	1:C:338:TYR:CD1	2.45	0.52
1:D:298:ARG:HD2	1:D:320:PRO:CA	2.39	0.52
1:A:274:SER:C	1:A:275:ALA:O	2.48	0.52
1:A:315:ILE:HA	1:A:319:ILE:HD13	1.91	0.52
1:B:357:THR:O	1:B:358:ASN:C	2.51	0.52
1:C:254:THR:HA	1:C:265:ILE:HD12	1.89	0.52
1:C:273:VAL:HG12	1:C:273:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:VAL:HG11	1:B:168:THR:CG2	2.37	0.52
1:B:192:MET:HE3	1:B:192:MET:CA	2.31	0.52
1:C:157:VAL:HG12	1:C:158:THR:N	2.24	0.52
1:C:180:LEU:HD12	1:C:270:VAL:C	2.32	0.52
1:D:51:ILE:HB	1:D:52:PRO:CD	2.38	0.52
1:D:298:ARG:HD2	1:D:320:PRO:N	2.25	0.52
1:A:192:MET:HG3	1:A:272:LEU:CD2	2.40	0.52
1:B:228:LEU:HD13	1:B:233:MET:HE3	1.92	0.52
1:B:301:VAL:HG22	1:B:302:ASN:N	2.24	0.52
1:B:427:HIS:HA	1:B:430:ALA:HB3	1.91	0.52
1:C:12:ILE:CD1	1:C:126:ILE:HD13	2.40	0.52
1:C:44:THR:N	2:C:480:FAD:O1A	2.43	0.52
1:C:93:LYS:O	1:C:96:SER:OG	2.26	0.52
1:C:193:GLY:CA	1:C:233:MET:HE2	2.40	0.52
1:A:119:LYS:HA	1:A:285:ASN:H	1.75	0.51
1:B:23:ILE:O	1:B:27:GLN:HG3	2.10	0.51
1:C:56:LEU:HD22	1:C:87:MET:HE3	1.91	0.51
1:C:71:ALA:O	1:C:73:HIS:N	2.43	0.51
1:C:302:ASN:C	1:C:302:ASN:OD1	2.52	0.51
1:D:298:ARG:NE	1:D:320:PRO:HA	2.25	0.51
1:B:82:ILE:HG21	1:B:199:ILE:HD12	1.91	0.51
1:A:409:THR:O	1:A:410:ASP:HB3	2.11	0.51
1:D:81:GLU:CA	1:D:82:ILE:HD12	2.41	0.51
1:D:149:SER:C	1:D:280:PHE:HB2	2.35	0.51
1:D:209:ALA:O	1:D:237:LEU:O	2.28	0.51
1:A:360:GLU:HB2	1:A:422:ALA:HB3	1.92	0.51
1:B:56:LEU:HD13	1:B:195:VAL:HG11	1.91	0.51
1:C:36:GLU:O	3:C:2004:HOH:O	2.19	0.51
1:C:78:SER:HB2	1:D:78:SER:CB	2.36	0.51
1:D:264:THR:O	1:D:265:ILE:HD13	2.11	0.51
1:D:359:PRO:HG2	1:D:398:GLU:OE2	2.11	0.51
1:B:38:ARG:CD	1:B:47:ASN:ND2	2.73	0.51
1:B:358:ASN:CB	1:B:359:PRO:HD3	2.38	0.51
1:C:88:MET:HE3	1:C:91:LYS:HD3	1.92	0.51
1:B:48:VAL:HG12	1:B:168:THR:HG23	1.91	0.51
1:B:119:LYS:O	1:B:126:ILE:CA	2.58	0.51
1:B:353:GLY:O	1:B:362:ALA:HA	2.10	0.51
1:C:77:VAL:HG12	1:D:79:ASN:O	2.11	0.51
1:C:117:TYR:C	1:C:128:VAL:HG13	2.36	0.51
1:C:203:VAL:HG23	1:C:233:MET:HA	1.93	0.51
1:C:383:PHE:CD1	1:C:458:GLU:HB3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ASP:OD2	1:D:298:ARG:NH1	2.43	0.51
1:D:298:ARG:HD2	1:D:320:PRO:HA	1.92	0.51
1:D:353:GLY:O	1:D:362:ALA:HA	2.10	0.51
1:D:420:PRO:O	1:D:421:ASN:HB2	2.09	0.51
1:B:82:ILE:CD1	1:B:82:ILE:H	2.19	0.51
1:C:244:VAL:HG12	1:C:254:THR:H	1.75	0.51
1:C:461:MET:C	1:C:463:THR:N	2.68	0.51
1:D:277:ARG:O	1:D:323:MET:HE1	2.11	0.51
1:D:389:SER:O	1:D:390:ARG:C	2.51	0.51
1:B:240:LYS:N	1:B:256:GLU:O	2.34	0.51
1:B:308:ASN:O	1:B:309:VAL:CG2	2.49	0.51
1:C:46:LEU:CD2	1:C:99:THR:HG22	2.40	0.51
1:C:258:SER:CA	1:C:259:ALA:N	2.74	0.51
1:C:406:GLU:HG2	1:C:413:LEU:HD21	1.92	0.51
1:D:358:ASN:CB	1:D:359:PRO:CD	2.89	0.51
1:B:51:ILE:O	1:B:52:PRO:C	2.53	0.51
1:B:292:GLU:CB	1:B:300:LEU:HB2	2.41	0.51
1:C:450:PRO:HG2	1:C:450:PRO:O	2.10	0.51
1:D:367:THR:H	1:D:370:GLN:HG3	1.76	0.51
1:A:50:CYS:O	1:A:54:LYS:N	2.35	0.51
1:A:245:ASP:N	1:A:252:LYS:O	2.38	0.51
1:A:333:VAL:O	1:A:334:ALA:C	2.53	0.51
1:A:406:GLU:HB2	1:A:409:THR:OG1	2.11	0.51
1:C:12:ILE:CG1	1:C:126:ILE:HD13	2.41	0.51
1:A:315:ILE:CD1	1:A:332:GLY:HA2	2.41	0.50
1:B:9:VAL:CG2	1:B:30:PHE:HB3	2.36	0.50
1:C:241:VAL:HG12	1:C:241:VAL:O	2.12	0.50
1:C:261:GLY:O	1:C:262:GLU:HB3	2.11	0.50
1:D:327:LYS:HE2	1:D:348:TYR:CE1	2.46	0.50
1:D:352:PRO:HB3	1:D:364:VAL:CG2	2.41	0.50
1:A:62:MET:HE2	1:B:70:PHE:CE1	2.46	0.50
1:A:256:GLU:OE2	1:A:261:GLY:HA2	2.11	0.50
1:B:96:SER:O	1:B:97:ASN:C	2.53	0.50
1:B:363:SER:C	1:B:426:ILE:HD11	2.36	0.50
1:C:88:MET:CE	3:C:2007:HOH:O	2.58	0.50
1:C:182:VAL:O	1:C:205:VAL:HA	2.11	0.50
1:C:244:VAL:HG11	1:C:253:LEU:HD23	1.92	0.50
1:C:385:PHE:CE1	1:C:419:ALA:HB2	2.47	0.50
1:D:33:THR:HG23	1:D:112:THR:O	2.11	0.50
1:D:129:ASP:O	1:D:130:THR:CG2	2.56	0.50
1:D:212:ILE:HD13	1:D:225:GLN:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:LYS:HE3	1:D:242:VAL:HG13	1.92	0.50
1:A:11:ILE:HG12	1:A:144:ILE:HB	1.92	0.50
1:A:169:GLY:O	1:A:173:LEU:HD23	2.11	0.50
1:A:292:GLU:H	1:A:308:ASN:HD21	1.58	0.50
1:B:158:THR:HG22	1:B:160:ASP:CG	2.36	0.50
1:B:171:LEU:HD23	1:B:192:MET:CE	2.41	0.50
1:C:7:ASN:ND2	1:C:33:THR:OG1	2.44	0.50
1:C:154:LEU:HD12	1:C:154:LEU:C	2.36	0.50
1:A:119:LYS:CG	1:A:285:ASN:HB2	2.39	0.50
1:B:244:VAL:O	1:B:245:ASP:HB2	2.11	0.50
1:B:245:ASP:OD2	1:B:247:SER:HB3	2.12	0.50
1:B:286:LEU:O	1:B:288:LYS:N	2.45	0.50
1:B:294:ASP:H	1:B:300:LEU:CD2	2.24	0.50
1:B:309:VAL:HG12	1:B:310:SER:O	2.11	0.50
1:C:165:VAL:HG22	1:C:270:VAL:CG1	2.41	0.50
1:D:20:VAL:O	1:D:21:ALA:C	2.55	0.50
1:D:348:TYR:N	1:D:348:TYR:HD2	2.09	0.50
1:B:38:ARG:HD3	1:B:47:ASN:HD22	1.76	0.50
1:B:117:TYR:CE2	1:B:283:GLY:CA	2.88	0.50
1:B:192:MET:HA	1:B:192:MET:CE	2.31	0.50
1:C:126:ILE:HD12	1:C:143:ILE:HD13	1.92	0.50
1:D:51:ILE:O	1:D:52:PRO:C	2.53	0.50
1:A:41:LEU:HD11	1:A:106:PHE:CD1	2.46	0.50
1:A:82:ILE:HG21	1:A:199:ILE:HD12	1.94	0.50
1:A:313:TYR:CZ	1:A:339:LEU:HD21	2.47	0.50
1:A:325:ALA:O	1:A:328:ALA:HB3	2.12	0.50
1:B:45:CYS:O	1:B:46:LEU:HB2	2.11	0.50
1:B:274:SER:C	1:B:275:ALA:O	2.49	0.50
1:D:449:HIS:ND1	1:D:450:PRO:HB3	2.27	0.50
1:B:449:HIS:CE1	1:B:450:PRO:HB3	2.45	0.50
1:C:97:ASN:C	1:C:97:ASN:HD22	2.19	0.50
1:C:409:THR:O	1:C:410:ASP:CB	2.59	0.50
1:D:350:LYS:O	1:D:352:PRO:HD3	2.11	0.50
1:A:208:PHE:CD1	1:A:208:PHE:C	2.89	0.50
1:B:88:MET:HE1	1:B:91:LYS:HZ2	1.76	0.50
1:B:95:VAL:O	1:B:99:THR:HG23	2.11	0.50
1:B:118:GLY:HA2	1:B:126:ILE:HD13	1.93	0.50
1:C:48:VAL:HG13	1:C:168:THR:HG23	1.94	0.50
1:C:246:THR:HA	1:C:251:VAL:HG22	1.94	0.50
1:C:254:THR:HG23	1:C:265:ILE:CD1	2.17	0.50
1:D:403:ILE:HD12	1:D:460:ALA:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:O	1:A:433:LEU:HG	2.12	0.50
1:C:290:GLY:O	1:C:291:VAL:C	2.55	0.50
1:C:388:ASN:O	1:C:389:SER:C	2.54	0.50
1:D:195:VAL:HG12	1:D:196:TRP:N	2.25	0.50
1:D:220:ILE:O	1:D:221:ARG:C	2.52	0.50
1:D:346:VAL:O	1:D:347:ASP:HB2	2.12	0.49
1:C:33:THR:HG23	1:C:112:THR:O	2.12	0.49
1:D:345:HIS:ND1	1:D:345:HIS:C	2.70	0.49
1:A:240:LYS:HG2	1:A:241:VAL:H	1.76	0.49
1:A:287:ASP:O	1:A:289:ILE:N	2.46	0.49
1:A:328:ALA:O	1:A:329:GLU:C	2.55	0.49
1:B:28:LEU:HD12	1:B:336:VAL:CG1	2.36	0.49
1:C:49:GLY:O	1:C:52:PRO:HD2	2.13	0.49
1:D:451:THR:OG1	1:D:453:SER:HB2	2.13	0.49
1:A:120:PHE:HD1	1:A:284:LEU:CD2	2.24	0.49
1:D:366:LYS:O	1:D:416:HIS:HE1	1.94	0.49
1:D:409:THR:O	1:D:410:ASP:HB3	2.12	0.49
1:B:117:TYR:CZ	1:B:283:GLY:HA3	2.45	0.49
1:C:73:HIS:CD2	1:D:62:MET:SD	3.05	0.49
1:C:203:VAL:CG2	1:C:233:MET:HA	2.42	0.49
1:C:307:THR:HB	1:C:308:ASN:OD1	2.12	0.49
1:B:348:TYR:N	1:B:348:TYR:CD2	2.80	0.49
1:C:86:ALA:HB3	1:D:74:GLY:HA2	1.94	0.49
1:C:182:VAL:HB	1:C:205:VAL:CG1	2.32	0.49
1:C:308:ASN:OD1	1:C:308:ASN:N	2.45	0.49
1:B:82:ILE:HG12	1:B:199:ILE:HD12	1.93	0.49
1:C:242:VAL:HG21	1:C:256:GLU:CA	2.43	0.49
1:D:315:ILE:HA	1:D:319:ILE:HD13	1.93	0.49
1:A:262:GLU:HG3	1:A:262:GLU:O	2.13	0.49
1:A:367:THR:HG23	1:A:370:GLN:CG	2.42	0.49
1:B:282:SER:O	1:B:283:GLY:C	2.56	0.49
1:C:79:ASN:HB2	1:D:78:SER:OG	2.13	0.49
1:C:350:LYS:HD3	1:C:433:LEU:HD23	1.94	0.49
1:A:307:THR:OG1	1:A:312:VAL:HB	2.13	0.49
1:B:122:SER:C	1:B:124:SER:N	2.69	0.49
1:B:185:ALA:HB2	1:B:207:GLU:HB2	1.95	0.49
1:B:283:GLY:C	1:B:284:LEU:O	2.56	0.49
1:C:49:GLY:O	1:C:53:SER:N	2.39	0.49
1:A:51:ILE:HG21	1:A:98:LEU:HD12	1.94	0.48
1:A:164:ILE:O	1:A:164:ILE:HG22	2.13	0.48
1:A:186:GLY:O	1:A:190:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HE2	1:B:285:ASN:ND2	2.28	0.48
1:B:119:LYS:HE2	1:B:285:ASN:HD22	1.78	0.48
1:A:70:PHE:HE2	1:B:66:ALA:HB2	1.78	0.48
1:C:101:GLY:O	1:C:105:LEU:HG	2.13	0.48
1:C:159:ILE:HD12	1:C:159:ILE:H	1.77	0.48
1:C:212:ILE:CG2	1:C:237:LEU:HD21	2.43	0.48
1:B:245:ASP:HB3	1:B:252:LYS:HB2	1.93	0.48
1:C:122:SER:O	1:C:124:SER:N	2.47	0.48
1:D:184:GLY:HA3	1:D:274:SER:C	2.39	0.48
1:A:462:ALA:CB	1:A:467:PRO:HG3	2.43	0.48
1:C:88:MET:HE1	1:C:171:LEU:O	2.13	0.48
1:C:189:GLY:O	1:C:191:GLU:N	2.46	0.48
1:C:204:THR:HG22	1:C:234:LYS:CB	2.38	0.48
1:D:10:VAL:HG21	1:D:143:ILE:HG12	1.95	0.48
1:B:122:SER:O	1:B:124:SER:N	2.47	0.48
1:B:286:LEU:O	1:B:287:ASP:C	2.55	0.48
1:C:127:SER:O	1:C:128:VAL:HG22	2.13	0.48
1:C:181:VAL:HG11	1:C:253:LEU:HD11	1.94	0.48
1:D:163:LYS:O	1:D:270:VAL:HA	2.13	0.48
1:D:468:ILE:O	1:D:468:ILE:HG22	2.14	0.48
1:B:403:ILE:HD12	1:B:460:ALA:HA	1.95	0.48
1:B:461:MET:C	1:B:463:THR:H	2.21	0.48
1:C:120:PHE:HB2	1:C:285:ASN:O	2.13	0.48
1:D:158:THR:O	1:D:164:ILE:HG21	2.13	0.48
1:B:149:SER:HB3	1:B:317:ASP:HB3	1.96	0.48
1:D:176:ILE:HD13	1:D:199:ILE:HG23	1.96	0.48
1:D:364:VAL:HG12	1:D:433:LEU:HD13	1.96	0.48
1:A:56:LEU:HD22	1:A:87:MET:HE3	1.96	0.48
1:A:367:THR:HG23	1:A:370:GLN:CD	2.39	0.48
1:A:370:GLN:O	1:A:371:VAL:C	2.57	0.48
1:B:217:ASP:HB2	1:B:416:HIS:CD2	2.48	0.48
1:D:216:MET:HE2	1:D:221:ARG:HA	1.95	0.48
1:D:383:PHE:CD1	1:D:458:GLU:CB	2.94	0.48
1:B:216:MET:CE	1:B:220:ILE:HG22	2.44	0.48
1:C:406:GLU:CG	1:C:413:LEU:HD21	2.44	0.48
1:B:114:VAL:HG12	1:B:114:VAL:O	2.14	0.48
1:B:150:ASP:CG	1:B:151:VAL:N	2.72	0.48
1:B:438:SER:O	1:B:441:ASP:N	2.47	0.48
1:C:119:LYS:N	1:C:127:SER:O	2.47	0.48
1:D:192:MET:HA	1:D:192:MET:CE	2.33	0.48
1:D:333:VAL:O	1:D:334:ALA:C	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:TYR:O	1:A:23:ILE:HG13	2.14	0.47
1:A:182:VAL:HB	1:A:205:VAL:HG13	1.96	0.47
1:A:227:SER:HA	1:A:230:LYS:CD	2.37	0.47
1:B:9:VAL:HG23	1:B:30:PHE:CB	2.39	0.47
1:C:315:ILE:HA	1:C:319:ILE:HD13	1.94	0.47
1:A:188:ILE:O	1:A:192:MET:HG2	2.14	0.47
1:A:439:SER:O	1:A:442:ILE:HG22	2.14	0.47
1:C:46:LEU:HD21	1:C:99:THR:HG22	1.96	0.47
1:C:170:ALA:HB2	1:C:272:LEU:HD13	1.96	0.47
1:D:122:SER:O	1:D:124:SER:N	2.47	0.47
1:D:221:ARG:HG2	1:D:221:ARG:HH11	1.79	0.47
1:D:280:PHE:C	1:D:280:PHE:CD2	2.91	0.47
1:D:367:THR:O	1:D:371:VAL:HG23	2.14	0.47
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.77	0.47
1:A:305:PHE:O	1:A:313:TYR:HB3	2.14	0.47
1:A:425:LEU:HB3	1:A:456:ILE:HD11	1.95	0.47
1:A:460:ALA:O	1:A:463:THR:HB	2.13	0.47
1:B:109:ASN:O	1:B:110:LYS:HB2	2.14	0.47
1:C:42:GLY:HA3	1:C:46:LEU:CD2	2.42	0.47
1:C:189:GLY:O	1:C:190:LEU:C	2.56	0.47
1:B:147:THR:CG2	1:B:284:LEU:HD22	2.11	0.47
1:C:126:ILE:HD11	1:C:143:ILE:HD13	1.96	0.47
1:C:192:MET:O	1:C:193:GLY:C	2.57	0.47
1:C:314:ALA:O	1:C:319:ILE:HG21	2.15	0.47
1:D:10:VAL:HG23	1:D:142:HIS:O	2.14	0.47
1:D:298:ARG:CD	1:D:320:PRO:HA	2.44	0.47
1:D:352:PRO:HB3	1:D:364:VAL:HG22	1.95	0.47
1:B:8:ASP:CG	1:B:31:LYS:H	2.22	0.47
1:B:46:LEU:HD13	1:B:51:ILE:HG13	1.96	0.47
1:B:128:VAL:O	1:B:129:ASP:CB	2.63	0.47
1:C:286:LEU:HD22	1:C:291:VAL:HG21	1.97	0.47
1:D:157:VAL:CG2	1:D:241:VAL:HG11	2.45	0.47
1:D:218:ALA:HB2	1:D:369:GLU:OE2	2.13	0.47
1:D:286:LEU:CD2	1:D:291:VAL:HB	2.44	0.47
1:B:8:ASP:HB3	1:B:30:PHE:HB3	1.95	0.47
1:B:174:SER:O	1:B:175:GLU:HB2	2.15	0.47
1:B:400:LEU:N	1:B:400:LEU:CD2	2.78	0.47
1:C:119:LYS:O	1:C:127:SER:HB3	2.15	0.47
1:D:121:VAL:O	1:D:288:LYS:HD2	2.14	0.47
1:D:227:SER:C	1:D:229:GLU:N	2.72	0.47
1:A:371:VAL:O	1:A:372:LYS:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:HIS:ND1	1:A:449:HIS:C	2.72	0.47
1:B:142:HIS:HB3	1:B:313:TYR:CE1	2.48	0.47
1:B:444:ARG:HG3	1:B:444:ARG:HH11	1.78	0.47
1:D:10:VAL:HG23	1:D:143:ILE:HG12	1.94	0.47
1:D:161:GLU:O	1:D:162:LYS:CG	2.62	0.47
1:D:286:LEU:CA	1:D:289:ILE:HG13	2.44	0.47
1:D:294:ASP:O	1:D:295:LYS:C	2.57	0.47
1:D:302:ASN:OD1	1:D:302:ASN:C	2.57	0.47
1:A:79:ASN:O	1:B:77:VAL:HA	2.14	0.47
1:A:357:THR:O	1:A:358:ASN:C	2.55	0.47
1:A:461:MET:C	1:A:463:THR:H	2.22	0.47
1:B:117:TYR:C	1:B:117:TYR:CD2	2.93	0.47
1:B:255:VAL:HG23	1:B:264:THR:OG1	2.15	0.47
1:C:20:VAL:O	1:C:21:ALA:C	2.58	0.47
1:C:403:ILE:HD12	1:C:460:ALA:HA	1.96	0.47
1:A:90:GLN:HA	1:A:93:LYS:HB3	1.97	0.47
1:A:264:THR:HG22	1:A:265:ILE:N	2.30	0.47
1:A:352:PRO:HB3	1:A:364:VAL:HG22	1.97	0.47
1:B:296:LEU:HD12	1:B:296:LEU:N	2.30	0.47
1:B:406:GLU:CG	1:B:413:LEU:HD21	2.45	0.47
1:C:82:ILE:HD12	1:C:82:ILE:N	2.29	0.47
1:D:63:TYR:CE1	1:D:82:ILE:HD11	2.49	0.47
1:A:181:VAL:HG22	1:A:204:THR:OG1	2.15	0.47
1:B:216:MET:CE	1:B:221:ARG:HA	2.45	0.47
1:C:363:SER:C	1:C:426:ILE:HD11	2.39	0.47
1:D:212:ILE:O	1:D:212:ILE:HG13	2.14	0.47
1:A:66:ALA:HB2	1:B:70:PHE:HE2	1.78	0.46
1:A:184:GLY:H	1:A:274:SER:H	1.64	0.46
1:A:304:ARG:HA	1:A:338:TYR:CE1	2.50	0.46
1:B:281:THR:HG22	1:B:299:ILE:HD11	1.96	0.46
1:C:117:TYR:N	1:C:128:VAL:HG12	2.31	0.46
1:D:404:ILE:HG22	1:D:413:LEU:HB2	1.98	0.46
1:A:22:ALA:O	1:A:25:ALA:HB3	2.16	0.46
1:A:180:LEU:HD12	1:A:270:VAL:O	2.16	0.46
1:A:315:ILE:HD12	1:A:332:GLY:HA2	1.97	0.46
1:B:119:LYS:HA	1:B:284:LEU:HA	1.97	0.46
1:C:87:MET:O	1:C:88:MET:C	2.57	0.46
1:C:218:ALA:O	1:C:219:GLU:C	2.56	0.46
1:A:50:CYS:HB2	1:A:51:ILE:H	1.40	0.46
1:B:63:TYR:O	1:B:64:HIS:C	2.57	0.46
1:C:165:VAL:HG23	1:C:272:LEU:CA	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:PHE:HZ	1:C:346:VAL:HG11	1.79	0.46
1:A:86:ALA:O	1:A:89:GLY:CA	2.64	0.46
1:A:225:GLN:O	1:A:226:ARG:C	2.58	0.46
1:C:130:THR:C	1:C:132:GLU:N	2.73	0.46
1:C:315:ILE:HG13	1:C:315:ILE:O	2.16	0.46
1:D:199:ILE:HD13	1:D:199:ILE:HA	1.62	0.46
1:D:293:THR:CG2	1:D:294:ASP:N	2.77	0.46
1:A:120:PHE:HD1	1:A:284:LEU:HD21	1.80	0.46
1:A:363:SER:N	1:A:426:ILE:HD12	2.30	0.46
1:A:468:ILE:HG21	1:B:20:VAL:HG13	1.98	0.46
1:B:118:GLY:CA	1:B:126:ILE:HD13	2.45	0.46
1:B:291:VAL:HG12	1:B:292:GLU:N	2.29	0.46
1:C:182:VAL:N	1:C:204:THR:O	2.45	0.46
1:C:396:ASN:HD21	1:C:420:PRO:HG3	1.80	0.46
1:D:439:SER:O	1:D:442:ILE:CG2	2.59	0.46
1:A:177:PRO:HB3	1:A:270:VAL:CG2	2.46	0.46
1:B:461:MET:C	1:B:463:THR:N	2.74	0.46
1:C:73:HIS:CG	1:D:62:MET:SD	3.09	0.46
1:D:227:SER:O	1:D:229:GLU:N	2.49	0.46
1:D:237:LEU:HD12	1:D:237:LEU:H	1.80	0.46
1:A:95:VAL:O	1:A:98:LEU:HB2	2.14	0.46
1:B:216:MET:HE3	1:B:220:ILE:HG22	1.97	0.46
1:B:221:ARG:HG2	1:B:221:ARG:HH11	1.80	0.46
1:B:381:GLY:O	1:B:402:LYS:HA	2.16	0.46
1:C:150:ASP:OD1	1:C:151:VAL:N	2.43	0.46
1:C:246:THR:HG22	1:C:251:VAL:CG2	2.46	0.46
1:D:357:THR:O	1:D:358:ASN:O	2.33	0.46
1:D:361:VAL:HA	1:D:417:ILE:O	2.16	0.46
1:D:386:MET:HE1	1:D:392:LYS:HZ3	1.80	0.46
1:A:199:ILE:HD13	1:A:199:ILE:HA	1.59	0.46
1:A:296:LEU:N	1:A:296:LEU:CD2	2.56	0.46
1:A:302:ASN:OD1	1:A:302:ASN:C	2.57	0.46
1:A:374:THR:O	1:A:376:VAL:N	2.49	0.46
1:B:51:ILE:HB	1:B:52:PRO:CD	2.43	0.46
1:B:388:ASN:OD1	1:B:391:ALA:N	2.39	0.46
1:C:166:SER:O	1:C:169:GLY:N	2.48	0.46
1:C:177:PRO:HG2	1:C:201:SER:OG	2.14	0.46
1:C:420:PRO:O	1:C:421:ASN:HB2	2.15	0.46
1:A:450:PRO:HA	1:A:454:GLU:OE1	2.16	0.46
1:B:88:MET:CE	1:B:91:LYS:HZ3	2.29	0.46
1:D:97:ASN:C	1:D:97:ASN:HD22	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASN:HB2	1:B:78:SER:OG	2.16	0.46
1:A:88:MET:HE3	1:A:88:MET:HA	1.97	0.46
1:A:192:MET:HG3	1:A:272:LEU:HD21	1.98	0.46
1:B:151:VAL:CG1	1:B:152:LYS:N	2.75	0.46
1:C:37:LYS:HD3	1:C:117:TYR:CE1	2.50	0.46
1:C:116:GLY:C	1:C:128:VAL:CG1	2.89	0.46
1:D:95:VAL:O	1:D:96:SER:C	2.59	0.46
1:A:5:ASP:HA	1:A:31:LYS:HE2	1.94	0.45
1:A:178:LYS:HA	1:A:178:LYS:HD3	1.72	0.45
1:A:292:GLU:H	1:A:308:ASN:ND2	2.13	0.45
1:A:304:ARG:HA	1:A:338:TYR:CD1	2.51	0.45
1:B:265:ILE:C	1:B:266:ILE:HD13	2.41	0.45
1:B:277:ARG:O	1:B:323:MET:HE1	2.16	0.45
1:B:388:ASN:HB3	1:B:391:ALA:HB3	1.96	0.45
1:B:439:SER:OG	1:B:463:THR:HG21	2.16	0.45
1:D:70:PHE:HB3	1:D:75:VAL:O	2.15	0.45
1:D:87:MET:C	1:D:89:GLY:N	2.74	0.45
1:D:207:GLU:HG3	1:D:209:ALA:N	2.31	0.45
1:D:440:GLU:OE2	1:D:464:TYR:CE2	2.69	0.45
1:B:25:ALA:O	1:B:28:LEU:N	2.48	0.45
1:D:400:LEU:N	1:D:400:LEU:HD23	2.32	0.45
1:A:120:PHE:CD1	1:A:284:LEU:HD21	2.51	0.45
1:A:449:HIS:CE1	1:A:450:PRO:HB3	2.52	0.45
1:B:32:THR:HG22	1:B:33:THR:N	2.31	0.45
1:B:150:ASP:CG	1:B:151:VAL:H	2.24	0.45
1:C:449:HIS:ND1	1:C:450:PRO:N	2.64	0.45
1:D:10:VAL:HB	1:D:143:ILE:HG12	1.98	0.45
1:D:254:THR:HG22	1:D:254:THR:O	2.15	0.45
1:D:285:ASN:OD1	1:D:286:LEU:N	2.49	0.45
1:A:230:LYS:HE3	1:A:398:GLU:OE1	2.16	0.45
1:A:390:ARG:O	1:A:391:ALA:C	2.59	0.45
1:B:291:VAL:CG1	1:B:292:GLU:N	2.78	0.45
1:B:409:THR:O	1:B:410:ASP:CB	2.64	0.45
1:C:121:VAL:O	1:C:121:VAL:CG1	2.63	0.45
1:C:147:THR:O	1:C:318:VAL:HG22	2.17	0.45
1:C:383:PHE:CZ	1:C:387:ALA:HB3	2.52	0.45
1:D:82:ILE:HG21	1:D:199:ILE:HD12	1.98	0.45
1:B:80:VAL:C	1:B:81:GLU:CG	2.90	0.45
1:B:87:MET:C	1:B:89:GLY:N	2.72	0.45
1:B:165:VAL:HG23	1:B:272:LEU:CD1	2.47	0.45
1:C:82:ILE:HG21	1:C:199:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:THR:OG1	1:D:370:GLN:HG3	2.17	0.45
1:A:46:LEU:HD11	1:A:98:LEU:HB2	1.98	0.45
1:B:16:PRO:HD2	2:B:480:FAD:O5'	2.16	0.45
1:C:78:SER:OG	1:D:79:ASN:HB2	2.16	0.45
1:C:435:TYR:O	1:C:436:ASP:C	2.59	0.45
1:A:51:ILE:O	1:A:52:PRO:C	2.59	0.45
1:A:142:HIS:HB3	1:A:313:TYR:HE1	1.81	0.45
1:A:146:ALA:C	1:A:147:THR:O	2.51	0.45
1:A:217:ASP:OD1	1:A:402:LYS:NZ	2.49	0.45
1:A:305:PHE:HE2	1:A:319:ILE:HD11	1.82	0.45
1:B:184:GLY:HA3	1:B:274:SER:C	2.41	0.45
1:C:178:LYS:HA	1:C:178:LYS:HD3	1.76	0.45
1:C:468:ILE:O	1:C:468:ILE:CG2	2.64	0.45
1:D:177:PRO:HG2	1:D:201:SER:OG	2.16	0.45
1:A:82:ILE:N	1:A:82:ILE:CD1	2.79	0.45
1:A:154:LEU:CD2	1:A:183:ILE:HG21	2.46	0.45
1:C:180:LEU:HG	1:C:181:VAL:N	2.30	0.45
1:C:194:SER:O	1:C:195:VAL:C	2.59	0.45
1:D:150:ASP:CG	1:D:151:VAL:N	2.75	0.45
1:D:376:VAL:HG12	1:D:377:GLU:N	2.31	0.45
1:B:9:VAL:HB	1:B:32:THR:HG23	1.98	0.45
1:B:295:LYS:HB3	1:B:296:LEU:H	1.69	0.45
1:B:351:VAL:HA	1:B:352:PRO:HD2	1.64	0.45
1:B:466:LYS:HA	1:B:467:PRO:HD3	1.75	0.45
1:C:48:VAL:HG11	1:C:168:THR:OG1	2.17	0.45
1:C:208:PHE:HA	1:C:239:THR:O	2.16	0.45
1:C:213:VAL:HG12	1:C:216:MET:HB2	1.98	0.45
1:D:145:ILE:N	1:D:313:TYR:O	2.41	0.45
1:D:345:HIS:O	1:D:345:HIS:CG	2.70	0.45
1:A:421:ASN:ND2	1:B:421:ASN:ND2	2.65	0.45
1:B:97:ASN:C	1:B:97:ASN:ND2	2.72	0.45
1:B:117:TYR:C	1:B:117:TYR:HD2	2.25	0.45
1:B:253:LEU:O	1:B:265:ILE:CG2	2.64	0.45
1:C:5:ASP:CG	1:C:6:GLU:N	2.74	0.45
1:C:435:TYR:OH	1:D:441:ASP:O	2.31	0.45
1:C:468:ILE:HG21	1:D:20:VAL:HG13	1.99	0.45
1:A:134:GLU:HB3	1:A:135:ASN:H	1.58	0.44
1:C:20:VAL:HG13	1:D:468:ILE:HG21	1.98	0.44
1:C:181:VAL:HG23	1:C:268:ALA:CB	2.46	0.44
1:C:389:SER:HB3	1:D:51:ILE:HD11	1.99	0.44
1:A:301:VAL:CG2	1:A:305:PHE:C	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:VAL:N	1:B:125:GLU:O	2.25	0.44
1:C:444:ARG:HG3	1:C:444:ARG:HH11	1.82	0.44
1:D:192:MET:CA	1:D:192:MET:CE	2.95	0.44
1:D:192:MET:O	1:D:193:GLY:C	2.57	0.44
1:D:351:VAL:O	1:D:351:VAL:HG12	2.16	0.44
1:A:160:ASP:HB2	1:A:162:LYS:H	1.82	0.44
1:B:123:PRO:CG	1:B:289:ILE:HD13	2.46	0.44
1:B:292:GLU:HB3	1:B:300:LEU:HD23	1.99	0.44
1:D:156:GLY:C	1:D:157:VAL:HG23	2.42	0.44
1:D:180:LEU:HB3	1:D:203:VAL:HG12	1.98	0.44
1:D:466:LYS:HA	1:D:467:PRO:HD3	1.72	0.44
1:A:87:MET:C	1:A:89:GLY:N	2.72	0.44
1:A:101:GLY:O	1:A:105:LEU:HG	2.17	0.44
1:A:280:PHE:CE1	1:A:282:SER:HB3	2.52	0.44
1:A:327:LYS:HE2	1:A:348:TYR:CE1	2.52	0.44
1:B:352:PRO:HB3	1:B:364:VAL:CG2	2.47	0.44
1:B:468:ILE:O	1:B:468:ILE:CG2	2.66	0.44
1:C:51:ILE:O	1:C:52:PRO:C	2.60	0.44
1:C:82:ILE:HG12	1:C:199:ILE:CD1	2.48	0.44
1:C:396:ASN:ND2	1:C:420:PRO:HG3	2.33	0.44
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.69	0.44
1:A:362:ALA:HB1	1:A:426:ILE:HD12	2.00	0.44
1:C:181:VAL:HG13	1:C:204:THR:O	2.17	0.44
1:C:305:PHE:CZ	1:C:346:VAL:HG11	2.52	0.44
1:C:448:ALA:O	1:C:451:THR:CG2	2.64	0.44
1:D:42:GLY:CA	1:D:46:LEU:HB3	2.43	0.44
1:D:217:ASP:CB	1:D:416:HIS:CD2	2.99	0.44
1:D:386:MET:HE1	1:D:392:LYS:NZ	2.32	0.44
1:A:122:SER:C	1:A:124:SER:N	2.76	0.44
1:B:38:ARG:CD	1:B:47:ASN:HD22	2.30	0.44
1:B:216:MET:HE1	1:B:224:PHE:HB2	1.99	0.44
1:C:246:THR:HG22	1:C:251:VAL:HG21	1.98	0.44
1:C:262:GLU:CG	1:C:263:GLN:N	2.79	0.44
1:C:358:ASN:CB	1:C:359:PRO:HD3	2.45	0.44
1:D:155:PRO:O	1:D:157:VAL:N	2.51	0.44
1:D:160:ASP:O	1:D:161:GLU:HB2	2.17	0.44
1:A:7:ASN:OD1	1:A:7:ASN:C	2.61	0.44
1:B:102:ILE:O	1:B:105:LEU:HB2	2.18	0.44
1:B:465:ASP:CG	1:B:466:LYS:N	2.76	0.44
1:C:38:ARG:HG2	1:C:39:GLY:N	2.32	0.44
1:C:50:CYS:HB3	1:C:51:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:ALA:HB1	1:D:109:ASN:O	2.17	0.44
1:D:41:LEU:HD11	1:D:106:PHE:CD1	2.51	0.44
1:D:64:HIS:O	1:D:65:GLU:C	2.61	0.44
1:A:120:PHE:N	1:A:285:ASN:HB3	2.31	0.44
1:A:159:ILE:HG23	1:A:164:ILE:HG22	2.00	0.44
1:B:385:PHE:C	1:B:387:ALA:N	2.73	0.44
1:C:63:TYR:CE1	1:C:80:VAL:HG12	2.53	0.44
1:C:451:THR:O	1:C:452:MET:C	2.61	0.44
1:D:142:HIS:CB	3:D:2004:HOH:O	2.64	0.44
1:D:171:LEU:HD23	1:D:192:MET:CE	2.45	0.44
1:D:400:LEU:HD23	1:D:400:LEU:H	1.83	0.44
1:D:449:HIS:ND1	1:D:450:PRO:CA	2.81	0.44
1:A:236:LYS:HD3	1:A:266:ILE:HD11	1.98	0.44
1:B:304:ARG:O	1:B:305:PHE:HB2	2.18	0.44
1:B:352:PRO:HA	1:B:364:VAL:HG22	1.99	0.44
1:C:154:LEU:CD1	1:C:156:GLY:N	2.77	0.44
1:C:154:LEU:HD21	1:C:241:VAL:CG1	2.48	0.44
1:C:262:GLU:CG	1:C:263:GLN:H	2.28	0.44
1:C:358:ASN:HB3	1:C:359:PRO:CD	2.46	0.44
1:D:116:GLY:HA3	1:D:128:VAL:HG12	2.00	0.44
1:A:163:LYS:HA	1:A:270:VAL:HG13	2.00	0.43
1:B:6:GLU:HB3	1:B:33:THR:OG1	2.18	0.43
1:B:88:MET:O	1:B:91:LYS:HB3	2.17	0.43
1:C:352:PRO:HB3	1:C:364:VAL:HG22	2.00	0.43
1:D:84:LEU:O	1:D:84:LEU:HG	2.18	0.43
1:D:86:ALA:O	1:D:87:MET:C	2.60	0.43
1:D:136:THR:HG22	1:D:136:THR:O	2.16	0.43
1:A:294:ASP:OD1	1:A:294:ASP:C	2.60	0.43
1:A:348:TYR:N	1:A:348:TYR:CD2	2.86	0.43
1:B:87:MET:O	1:B:88:MET:C	2.61	0.43
1:B:286:LEU:C	1:B:288:LYS:H	2.26	0.43
1:C:216:MET:HE2	1:C:221:ARG:CA	2.47	0.43
1:D:46:LEU:HD11	1:D:98:LEU:CB	2.46	0.43
1:A:150:ASP:CG	1:A:151:VAL:N	2.72	0.43
1:A:194:SER:O	1:A:198:ARG:HG3	2.18	0.43
1:A:264:THR:HG22	1:A:265:ILE:H	1.82	0.43
1:A:442:ILE:HD13	1:A:442:ILE:HG21	1.61	0.43
1:B:50:CYS:HB2	1:B:51:ILE:H	1.52	0.43
1:B:176:ILE:CD1	1:B:199:ILE:CG2	2.96	0.43
1:B:385:PHE:CB	3:B:2021:HOH:O	2.66	0.43
1:C:41:LEU:HA	1:C:41:LEU:HD23	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:PHE:O	1:C:71:ALA:C	2.61	0.43
1:C:447:HIS:CD2	1:D:427:HIS:CD2	3.06	0.43
1:D:52:PRO:HB3	1:D:91:LYS:HE3	2.00	0.43
1:D:54:LYS:HD3	1:D:57:LEU:CD1	2.47	0.43
1:D:187:TYR:CG	1:D:355:VAL:HG22	2.53	0.43
1:D:263:GLN:H	1:D:263:GLN:HG2	1.59	0.43
1:A:6:GLU:CD	1:A:141:LYS:CE	2.86	0.43
1:A:292:GLU:HB2	1:A:308:ASN:OD1	2.18	0.43
1:C:54:LYS:HD3	1:C:57:LEU:HD12	1.99	0.43
1:D:49:GLY:H	1:D:52:PRO:HG2	1.83	0.43
1:A:300:LEU:HD23	1:A:300:LEU:HA	1.87	0.43
1:B:13:GLY:O	1:B:18:GLY:HA3	2.18	0.43
1:C:41:LEU:C	1:C:42:GLY:O	2.59	0.43
1:C:86:ALA:HB3	1:D:74:GLY:CA	2.47	0.43
1:C:240:LYS:C	1:C:242:VAL:H	2.27	0.43
1:D:53:SER:O	1:D:57:LEU:CG	2.65	0.43
1:D:286:LEU:O	1:D:288:LYS:N	2.51	0.43
1:A:70:PHE:HB3	1:A:75:VAL:O	2.18	0.43
1:A:152:LYS:CB	1:A:276:GLY:O	2.66	0.43
1:A:461:MET:C	1:A:463:THR:N	2.74	0.43
1:B:128:VAL:C	1:B:129:ASP:OD1	2.62	0.43
1:C:6:GLU:HG2	1:C:139:LYS:HD3	1.99	0.43
1:C:181:VAL:HG11	1:C:253:LEU:CD1	2.49	0.43
1:D:364:VAL:HG12	1:D:365:GLY:N	2.33	0.43
1:A:74:GLY:O	1:B:82:ILE:HA	2.19	0.43
1:A:367:THR:N	1:A:370:GLN:HG3	2.30	0.43
1:A:470:ILE:HD12	1:A:470:ILE:HA	1.85	0.43
1:B:449:HIS:ND1	1:B:449:HIS:C	2.76	0.43
1:C:173:LEU:HD12	1:C:196:TRP:CE2	2.54	0.43
1:C:173:LEU:HD12	1:C:196:TRP:CZ2	2.54	0.43
1:D:117:TYR:OH	1:D:283:GLY:CA	2.67	0.43
1:D:439:SER:OG	1:D:463:THR:HG21	2.19	0.43
1:B:88:MET:HE3	1:B:91:LYS:HD3	2.01	0.43
1:B:153:SER:OG	1:B:154:LEU:N	2.41	0.43
1:B:382:LYS:HG2	1:B:402:LYS:HB2	2.01	0.43
1:C:23:ILE:HG23	1:C:109:ASN:ND2	2.34	0.43
1:C:270:VAL:HG13	1:C:271:VAL:H	1.83	0.43
1:D:282:SER:O	1:D:283:GLY:C	2.61	0.43
1:D:292:GLU:HG3	1:D:308:ASN:ND2	2.33	0.43
1:A:121:VAL:C	1:A:288:LYS:HD2	2.44	0.43
1:A:217:ASP:HB2	1:A:416:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:VAL:HG22	1:A:302:ASN:H	1.83	0.43
1:B:171:LEU:CD2	1:B:192:MET:HE1	2.47	0.43
1:B:176:ILE:CD1	1:B:199:ILE:HG23	2.45	0.43
1:C:26:ALA:HB1	1:C:109:ASN:O	2.18	0.43
1:C:290:GLY:O	1:C:308:ASN:ND2	2.51	0.43
1:C:301:VAL:HG22	1:C:302:ASN:H	1.83	0.43
1:D:229:GLU:C	1:D:231:GLN:N	2.76	0.43
1:D:367:THR:N	1:D:370:GLN:HE21	2.12	0.43
1:A:366:LYS:O	1:A:416:HIS:HE1	2.01	0.43
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.88	0.43
1:D:96:SER:O	1:D:97:ASN:O	2.36	0.43
1:D:155:PRO:C	1:D:157:VAL:N	2.77	0.43
1:D:286:LEU:HD22	1:D:291:VAL:HB	2.00	0.43
1:B:181:VAL:HA	1:B:204:THR:O	2.19	0.42
1:C:207:GLU:HG3	1:C:209:ALA:N	2.34	0.42
1:D:28:LEU:CD1	1:D:336:VAL:HG12	2.47	0.42
1:D:51:ILE:CB	1:D:52:PRO:HD3	2.44	0.42
1:A:69:SER:O	1:A:71:ALA:N	2.52	0.42
1:A:190:LEU:HD13	1:A:228:LEU:HD11	2.00	0.42
1:A:358:ASN:CB	1:A:359:PRO:CD	2.93	0.42
1:B:54:LYS:N	1:B:54:LYS:HE2	2.34	0.42
1:B:150:ASP:O	1:B:151:VAL:O	2.36	0.42
1:B:151:VAL:CG1	1:B:152:LYS:H	2.28	0.42
1:B:314:ALA:C	1:B:315:ILE:HG23	2.44	0.42
1:B:355:VAL:O	1:B:360:GLU:HA	2.19	0.42
1:B:416:HIS:ND1	1:B:416:HIS:N	2.66	0.42
1:C:10:VAL:C	1:C:11:ILE:HG13	2.44	0.42
1:C:242:VAL:HB	1:C:255:VAL:CA	2.36	0.42
1:D:159:ILE:HG23	1:D:165:VAL:HA	2.00	0.42
1:D:219:GLU:O	1:D:222:LYS:HB2	2.19	0.42
1:D:264:THR:C	1:D:265:ILE:HD13	2.43	0.42
1:D:282:SER:C	1:D:284:LEU:N	2.76	0.42
1:D:313:TYR:CZ	1:D:339:LEU:HD21	2.53	0.42
1:A:364:VAL:HG12	1:A:365:GLY:N	2.34	0.42
1:A:382:LYS:HB2	1:A:382:LYS:HE3	1.79	0.42
1:B:38:ARG:HG2	1:B:39:GLY:N	2.34	0.42
1:B:265:ILE:O	1:B:266:ILE:HD13	2.20	0.42
1:C:167:SER:O	1:C:170:ALA:HB3	2.19	0.42
1:C:179:LYS:O	1:C:269:ASP:N	2.51	0.42
1:C:465:ASP:CG	1:C:466:LYS:H	2.26	0.42
1:D:121:VAL:O	1:D:121:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:PHE:O	1:D:313:TYR:HA	2.19	0.42
1:A:164:ILE:HD11	1:A:244:VAL:CG1	2.47	0.42
1:B:253:LEU:O	1:B:265:ILE:HA	2.19	0.42
1:B:265:ILE:N	1:B:265:ILE:CD1	2.82	0.42
1:B:298:ARG:HH11	1:B:320:PRO:HA	1.84	0.42
1:C:70:PHE:O	1:C:71:ALA:O	2.37	0.42
1:C:212:ILE:HD13	1:C:225:GLN:HG3	1.99	0.42
1:D:315:ILE:O	1:D:318:VAL:HG23	2.19	0.42
1:D:400:LEU:N	1:D:400:LEU:CD2	2.83	0.42
1:A:71:ALA:O	1:A:73:HIS:N	2.52	0.42
1:A:98:LEU:HA	1:A:98:LEU:HD23	1.81	0.42
1:A:351:VAL:HA	1:A:352:PRO:HD2	1.89	0.42
1:B:6:GLU:O	1:B:7:ASN:CG	2.62	0.42
1:B:310:SER:OG	1:B:311:GLY:N	2.52	0.42
1:C:24:LYS:O	1:C:27:GLN:HB2	2.19	0.42
1:C:82:ILE:HG12	1:C:199:ILE:HD12	2.01	0.42
1:D:144:ILE:HA	1:D:313:TYR:O	2.19	0.42
1:D:149:SER:N	1:D:280:PHE:HB3	2.34	0.42
1:B:88:MET:HE1	1:B:91:LYS:NZ	2.34	0.42
1:B:120:PHE:HA	1:B:126:ILE:CG2	2.30	0.42
1:C:126:ILE:HG13	1:C:143:ILE:HD13	2.02	0.42
1:C:164:ILE:CG2	1:C:273:VAL:HG23	2.49	0.42
1:C:176:ILE:CG2	1:C:199:ILE:HG22	2.49	0.42
1:C:372:LYS:O	1:C:373:GLU:C	2.63	0.42
1:D:113:TYR:C	1:D:113:TYR:CD2	2.98	0.42
1:D:240:LYS:HE3	1:D:242:VAL:CG1	2.49	0.42
1:A:51:ILE:HG21	1:A:98:LEU:CD1	2.49	0.42
1:A:239:THR:HG21	1:A:255:VAL:HG22	1.98	0.42
1:B:283:GLY:O	1:B:284:LEU:C	2.62	0.42
1:B:350:LYS:NZ	3:B:2017:HOH:O	2.32	0.42
1:B:350:LYS:O	1:B:352:PRO:HD3	2.20	0.42
1:C:394:ILE:HD13	1:C:394:ILE:HA	1.80	0.42
1:C:450:PRO:HA	1:C:454:GLU:OE1	2.19	0.42
2:C:480:FAD:H9	2:C:480:FAD:H1'1	1.77	0.42
1:D:81:GLU:C	1:D:82:ILE:CD1	2.81	0.42
1:D:117:TYR:O	1:D:128:VAL:HA	2.19	0.42
1:D:186:GLY:O	1:D:190:LEU:HG	2.20	0.42
1:D:285:ASN:C	1:D:287:ASP:H	2.26	0.42
1:A:20:VAL:HG13	1:B:468:ILE:HG21	2.02	0.42
1:A:137:VAL:O	1:A:137:VAL:HG12	2.19	0.42
1:B:199:ILE:HG23	1:B:199:ILE:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:GLU:O	1:B:222:LYS:HB2	2.20	0.42
1:C:348:TYR:N	1:C:348:TYR:CD2	2.85	0.42
1:C:451:THR:HB	1:D:424:GLU:OE2	2.19	0.42
1:D:406:GLU:HB2	1:D:409:THR:OG1	2.19	0.42
1:D:449:HIS:ND1	1:D:450:PRO:N	2.68	0.42
1:A:367:THR:O	1:A:368:GLU:C	2.63	0.42
1:B:9:VAL:CG2	1:B:30:PHE:CB	2.98	0.42
1:C:56:LEU:HD13	1:C:195:VAL:HG11	2.02	0.42
1:C:242:VAL:CB	1:C:256:GLU:H	2.31	0.42
1:D:9:VAL:CB	1:D:32:THR:HG23	2.47	0.42
1:B:165:VAL:HG23	1:B:272:LEU:HD13	2.02	0.42
1:B:183:ILE:O	1:B:184:GLY:C	2.60	0.42
1:B:251:VAL:HG12	1:B:252:LYS:N	2.35	0.42
1:B:378:TYR:HB2	1:B:405:ALA:O	2.20	0.42
1:C:274:SER:C	1:C:275:ALA:O	2.59	0.42
1:D:54:LYS:HD3	1:D:57:LEU:HD12	2.02	0.42
1:D:148:GLY:HA3	2:D:480:FAD:O5B	2.20	0.42
1:D:161:GLU:CA	1:D:165:VAL:HG12	2.36	0.42
1:B:24:LYS:O	1:B:27:GLN:HB2	2.20	0.41
1:B:181:VAL:HG21	1:B:266:ILE:CG2	2.50	0.41
1:C:79:ASN:H	1:D:78:SER:HB2	1.85	0.41
1:C:366:LYS:O	1:C:416:HIS:CE1	2.70	0.41
1:D:10:VAL:CB	1:D:143:ILE:HG12	2.50	0.41
1:D:131:ILE:C	1:D:132:GLU:HG3	2.45	0.41
1:A:167:SER:HB3	2:A:480:FAD:HM71	2.00	0.41
1:A:439:SER:O	1:A:442:ILE:CG2	2.68	0.41
1:B:71:ALA:C	1:B:73:HIS:N	2.77	0.41
1:B:199:ILE:CG2	1:B:199:ILE:O	2.64	0.41
1:B:245:ASP:OD2	1:B:245:ASP:O	2.37	0.41
1:C:116:GLY:HA3	1:C:128:VAL:CG1	2.50	0.41
1:C:208:PHE:CD1	1:C:208:PHE:C	2.99	0.41
1:C:465:ASP:CG	1:C:466:LYS:N	2.76	0.41
1:D:101:GLY:O	1:D:105:LEU:HG	2.20	0.41
1:D:286:LEU:C	1:D:288:LYS:H	2.28	0.41
1:D:347:ASP:C	1:D:349:ASP:N	2.77	0.41
1:D:461:MET:C	1:D:463:THR:H	2.28	0.41
1:A:46:LEU:CD2	1:A:99:THR:HG22	2.50	0.41
1:A:170:ALA:HB2	1:A:272:LEU:HD13	2.02	0.41
1:A:192:MET:O	1:A:193:GLY:C	2.63	0.41
1:A:384:PRO:O	1:A:384:PRO:HG2	2.20	0.41
1:B:26:ALA:HB1	1:B:109:ASN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLU:HB3	1:B:300:LEU:CG	2.51	0.41
1:C:189:GLY:C	1:C:191:GLU:N	2.78	0.41
1:C:258:SER:N	1:C:259:ALA:N	2.68	0.41
1:C:289:ILE:HG13	1:C:290:GLY:N	2.32	0.41
1:C:328:ALA:O	1:C:329:GLU:C	2.63	0.41
1:D:171:LEU:CD2	1:D:192:MET:HE1	2.48	0.41
1:A:36:GLU:OE2	2:A:480:FAD:H4B	2.20	0.41
1:A:232:GLY:O	1:A:233:MET:HB2	2.19	0.41
1:A:345:HIS:CD2	3:A:2022:HOH:O	2.73	0.41
1:A:392:LYS:HA	1:A:392:LYS:HD2	1.81	0.41
1:B:5:ASP:O	1:B:31:LYS:HB3	2.20	0.41
1:B:461:MET:HA	1:B:464:TYR:CE1	2.55	0.41
1:C:180:LEU:HB3	1:C:203:VAL:HG12	2.03	0.41
1:D:350:LYS:HD3	1:D:433:LEU:HD23	2.01	0.41
1:A:181:VAL:HA	1:A:204:THR:O	2.21	0.41
1:A:241:VAL:O	1:A:242:VAL:C	2.63	0.41
1:A:241:VAL:O	1:A:242:VAL:O	2.38	0.41
1:A:243:GLY:O	1:A:254:THR:HG23	2.20	0.41
1:A:274:SER:O	1:A:274:SER:OG	2.31	0.41
1:A:364:VAL:HG12	1:A:433:LEU:HD22	2.02	0.41
1:D:38:ARG:HG2	1:D:39:GLY:N	2.35	0.41
1:D:305:PHE:CE2	1:D:331:ASP:HB3	2.55	0.41
1:A:233:MET:C	1:A:234:LYS:HG3	2.45	0.41
1:B:281:THR:CA	1:B:284:LEU:HD21	2.49	0.41
1:B:325:ALA:O	1:B:328:ALA:HB3	2.21	0.41
1:B:418:MET:O	1:B:419:ALA:HB2	2.20	0.41
1:C:83:ASP:O	1:C:86:ALA:N	2.51	0.41
1:C:176:ILE:CD1	1:C:199:ILE:HG23	2.44	0.41
1:D:23:ILE:O	1:D:24:LYS:C	2.59	0.41
1:D:51:ILE:N	1:D:52:PRO:CD	2.83	0.41
1:A:23:ILE:HG23	1:A:109:ASN:ND2	2.36	0.41
1:A:38:ARG:HG2	1:A:39:GLY:N	2.36	0.41
1:A:160:ASP:C	1:A:161:GLU:CG	2.93	0.41
1:B:199:ILE:HA	1:B:199:ILE:HD13	1.60	0.41
1:C:264:THR:O	1:C:265:ILE:HD12	2.21	0.41
1:C:266:ILE:H	1:C:266:ILE:HG13	1.76	0.41
1:C:386:MET:HE1	1:C:392:LYS:NZ	2.36	0.41
1:C:440:GLU:O	1:C:444:ARG:N	2.53	0.41
1:D:49:GLY:C	1:D:52:PRO:HD2	2.45	0.41
1:D:301:VAL:CG2	1:D:305:PHE:C	2.94	0.41
1:D:376:VAL:CG1	1:D:377:GLU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLY:CA	1:A:46:LEU:HD23	2.51	0.41
1:A:361:VAL:HA	1:A:417:ILE:O	2.20	0.41
1:B:295:LYS:HA	1:B:295:LYS:HD3	1.73	0.41
1:C:22:ALA:O	1:C:25:ALA:HB3	2.20	0.41
1:C:265:ILE:HD12	1:C:265:ILE:HA	1.84	0.41
1:D:87:MET:O	1:D:88:MET:C	2.60	0.41
1:A:75:VAL:HG22	1:B:63:TYR:HB2	2.02	0.41
1:A:102:ILE:O	1:A:105:LEU:HB2	2.20	0.41
1:A:154:LEU:HA	1:A:155:PRO:HD3	1.82	0.41
1:A:163:LYS:HE2	1:A:163:LYS:HB3	1.76	0.41
1:A:287:ASP:O	1:A:290:GLY:N	2.54	0.41
1:A:385:PHE:HD1	1:A:399:GLY:C	2.28	0.41
1:A:388:ASN:O	1:A:389:SER:C	2.63	0.41
1:B:50:CYS:O	1:B:54:LYS:HE2	2.21	0.41
1:B:119:LYS:C	1:B:126:ILE:HB	2.46	0.41
1:B:143:ILE:O	1:B:313:TYR:N	2.52	0.41
1:B:173:LEU:HD12	1:B:196:TRP:CE2	2.55	0.41
1:B:217:ASP:CB	1:B:416:HIS:CD2	3.04	0.41
1:B:358:ASN:CB	1:B:359:PRO:CD	2.99	0.41
1:B:448:ALA:O	1:B:451:THR:CG2	2.69	0.41
1:B:450:PRO:O	1:B:450:PRO:CG	2.68	0.41
1:C:70:PHE:CZ	1:D:70:PHE:HZ	2.38	0.41
1:C:442:ILE:H	1:C:442:ILE:HG22	1.52	0.41
1:C:444:ARG:HG3	1:C:444:ARG:NH1	2.36	0.41
1:C:445:VAL:HG21	1:D:431:ILE:CG1	2.51	0.41
1:D:109:ASN:O	1:D:110:LYS:HB2	2.21	0.41
1:D:148:GLY:C	1:D:280:PHE:HB3	2.46	0.41
1:D:364:VAL:CG1	1:D:365:GLY:N	2.83	0.41
1:D:422:ALA:HA	1:D:425:LEU:HD12	2.02	0.41
1:A:253:LEU:C	1:A:265:ILE:HD12	2.47	0.41
1:A:272:LEU:HD12	1:A:273:VAL:N	2.35	0.41
1:B:89:GLY:O	1:B:90:GLN:C	2.62	0.41
1:B:178:LYS:HD3	1:B:178:LYS:HA	1.87	0.41
1:B:292:GLU:N	1:B:308:ASN:OD1	2.46	0.41
1:D:53:SER:O	1:D:57:LEU:CD1	2.69	0.41
1:D:53:SER:O	1:D:57:LEU:HD12	2.21	0.41
1:D:203:VAL:HG21	1:D:233:MET:HE2	2.02	0.41
1:D:227:SER:O	1:D:228:LEU:C	2.63	0.41
1:A:216:MET:HE2	1:A:221:ARG:HA	2.03	0.40
1:A:309:VAL:O	1:A:310:SER:C	2.62	0.40
1:A:327:LYS:HE2	1:A:348:TYR:CZ	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:THR:O	1:A:410:ASP:CB	2.69	0.40
1:B:58:HIS:O	1:B:62:MET:HG3	2.21	0.40
1:B:348:TYR:N	1:B:348:TYR:HD2	2.19	0.40
1:C:50:CYS:O	1:C:54:LYS:HB2	2.21	0.40
1:C:121:VAL:O	1:C:122:SER:HB3	2.21	0.40
1:C:126:ILE:CG1	1:C:143:ILE:HD13	2.50	0.40
1:C:362:ALA:CB	1:C:426:ILE:HD12	2.49	0.40
1:D:177:PRO:HB3	1:D:270:VAL:HG23	2.02	0.40
1:A:420:PRO:O	1:A:421:ASN:C	2.64	0.40
1:A:466:LYS:HA	1:A:467:PRO:HD3	1.75	0.40
1:C:124:SER:O	1:C:139:LYS:CB	2.69	0.40
1:C:270:VAL:HG12	1:C:271:VAL:N	2.36	0.40
1:C:350:LYS:O	1:C:352:PRO:HD3	2.21	0.40
1:D:274:SER:O	1:D:274:SER:OG	2.37	0.40
1:A:208:PHE:O	1:A:208:PHE:CD1	2.75	0.40
1:B:28:LEU:HD13	1:B:340:ALA:HB2	2.02	0.40
1:B:449:HIS:ND1	1:B:450:PRO:N	2.69	0.40
1:D:415:VAL:HG21	1:D:429:ALA:HB1	2.02	0.40
1:D:461:MET:C	1:D:463:THR:N	2.78	0.40
1:A:284:LEU:CD2	1:A:284:LEU:C	2.95	0.40
1:A:301:VAL:HG22	1:A:302:ASN:N	2.36	0.40
1:A:394:ILE:HD13	1:A:394:ILE:HA	1.78	0.40
1:B:42:GLY:HA2	1:B:46:LEU:HD23	2.04	0.40
1:B:117:TYR:OH	1:B:283:GLY:CA	2.69	0.40
1:B:212:ILE:HD11	1:B:225:GLN:HB2	2.02	0.40
1:B:301:VAL:CG2	1:B:305:PHE:C	2.95	0.40
1:B:359:PRO:HG2	1:B:398:GLU:OE2	2.22	0.40
1:B:362:ALA:HB1	1:B:426:ILE:CD1	2.48	0.40
1:B:388:ASN:OD1	1:B:390:ARG:HB3	2.21	0.40
1:B:465:ASP:CG	1:B:466:LYS:H	2.28	0.40
1:C:54:LYS:HA	1:C:54:LYS:HD3	1.91	0.40
1:C:186:GLY:O	1:C:190:LEU:HG	2.22	0.40
1:C:292:GLU:N	1:C:308:ASN:HD21	2.19	0.40
1:A:220:ILE:HD12	1:A:220:ILE:HG23	1.78	0.40
1:A:391:ALA:O	1:A:392:LYS:C	2.64	0.40
1:A:431:ILE:HG23	1:A:432:ALA:N	2.36	0.40
1:C:46:LEU:HD21	1:C:99:THR:HA	2.03	0.40
1:C:49:GLY:O	1:C:50:CYS:C	2.64	0.40
1:C:187:TYR:CD1	1:C:187:TYR:N	2.90	0.40
1:C:252:LYS:HE2	1:C:267:GLU:OE2	2.22	0.40
1:D:38:ARG:HD3	1:D:47:ASN:CG	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:SER:C	1:D:128:VAL:CG2	2.95	0.40
1:D:213:VAL:HG12	1:D:216:MET:HB2	2.04	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	466/470 (99%)	368 (79%)	71 (15%)	27 (6%)	1	8
1	B	466/470 (99%)	357 (77%)	71 (15%)	38 (8%)	0	3
1	C	463/470 (98%)	367 (79%)	62 (13%)	34 (7%)	1	5
1	D	465/470 (99%)	350 (75%)	90 (19%)	25 (5%)	1	9
All	All	1860/1880 (99%)	1442 (78%)	294 (16%)	124 (7%)	1	6

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	129	ASP
1	A	161	GLU
1	A	201	SER
1	A	232	GLY
1	A	242	VAL
1	A	259	ALA
1	A	260	GLY
1	A	261	GLY
1	A	347	ASP
1	B	50	CYS
1	B	129	ASP
1	B	134	GLU

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Mol	Chain	Res	Type
1	B	151	VAL
1	B	153	SER
1	B	154	LEU
1	B	159	ILE
1	B	161	GLU
1	B	187[A]	TYR
1	B	187[B]	TYR
1	B	259	ALA
1	B	261	GLY
1	B	270	VAL
1	B	282	SER
1	B	284	LEU
1	B	290	GLY
1	C	72	ASN
1	C	187	TYR
1	C	230	LYS
1	C	247	SER
1	C	262	GLU
1	C	263	GLN
1	C	264	THR
1	C	287	ASP
1	D	7	ASN
1	D	129	ASP
1	D	130	THR
1	D	239	THR
1	D	347	ASP
1	A	70	PHE
1	A	72	ASN
1	A	195	VAL
1	A	230	LYS
1	A	275	ALA
1	A	288	LYS
1	A	290	GLY
1	B	72	ASN
1	B	118	GLY
1	B	283	GLY
1	B	289	ILE
1	B	296	LEU
1	B	311	GLY
1	C	50	CYS
1	C	71	ALA
1	C	128	VAL

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Mol	Chain	Res	Type
1	C	156	GLY
1	C	161	GLU
1	C	167	SER
1	C	190	LEU
1	C	195	VAL
1	C	229	GLU
1	C	234	LYS
1	C	288	LYS
1	D	50	CYS
1	D	80	VAL
1	D	276	GLY
1	D	287	ASP
1	D	310	SER
1	D	358	ASN
1	A	263	GLN
1	A	297	GLY
1	B	7	ASN
1	B	46	LEU
1	B	135	ASN
1	B	156	GLY
1	B	245	ASP
1	B	288	LYS
1	C	241	VAL
1	C	243	GLY
1	C	283	GLY
1	D	72	ASN
1	D	97	ASN
1	D	123	PRO
1	D	187	TYR
1	D	228	LEU
1	A	71	ALA
1	A	132	GLU
1	A	222	LYS
1	A	249	ASP
1	A	257	PRO
1	B	48	VAL
1	B	175	GLU
1	B	218	ALA
1	B	257	PRO
1	C	129	ASP
1	C	159	ILE
1	C	218	ALA

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Mol	Chain	Res	Type
1	C	222	LYS
1	C	275	ALA
1	C	298	ARG
1	C	307	THR
1	D	71	ALA
1	D	95	VAL
1	D	128	VAL
1	D	161	GLU
1	D	291	VAL
1	A	391	ALA
1	B	8	ASP
1	B	51	ILE
1	B	309	VAL
1	B	328	ALA
1	C	70	PHE
1	C	238	LYS
1	D	70	PHE
1	A	155	PRO
1	C	189	GLY
1	C	251	VAL
1	A	375	GLY
1	D	195	VAL
1	D	49	GLY
1	B	199	ILE
1	B	358	ASN
1	C	244	VAL
1	D	156	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/375 (100%)	333 (89%)	42 (11%)	6	22
1	B	375/375 (100%)	340 (91%)	35 (9%)	8	29
1	C	374/375 (100%)	338 (90%)	36 (10%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	374/375 (100%)	335 (90%)	39 (10%)	7	24
All	All	1498/1500 (100%)	1346 (90%)	152 (10%)	7	26

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	41	LEU
1	A	44	THR
1	A	54	LYS
1	A	82	ILE
1	A	122	SER
1	A	129	ASP
1	A	138	VAL
1	A	143	ILE
1	A	153	SER
1	A	155	PRO
1	A	160	ASP
1	A	161	GLU
1	A	183	ILE
1	A	192	MET
1	A	194	SER
1	A	199	ILE
1	A	203	VAL
1	A	205	VAL
1	A	214	PRO
1	A	231	GLN
1	A	239	THR
1	A	249	ASP
1	A	252	LYS
1	A	257	PRO
1	A	258	SER
1	A	265	ILE
1	A	270	VAL
1	A	286	LEU
1	A	296	LEU
1	A	298	ARG
1	A	301	VAL
1	A	306	SER
1	A	308	ASN
1	A	318	VAL
1	A	320	PRO

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Mol	Chain	Res	Type
1	A	367	THR
1	A	370	GLN
1	A	384	PRO
1	A	433	LEU
1	A	439	SER
1	A	442	ILE
1	B	9	VAL
1	B	19	TYR
1	B	46	LEU
1	B	54	LYS
1	B	56	LEU
1	B	82	ILE
1	B	90	GLN
1	B	97	ASN
1	B	130	THR
1	B	154	LEU
1	B	168	THR
1	B	183	ILE
1	B	192	MET
1	B	194	SER
1	B	199	ILE
1	B	203	VAL
1	B	205	VAL
1	B	215	THR
1	B	236	LYS
1	B	237	LEU
1	B	246	THR
1	B	262	GLU
1	B	264	THR
1	B	265	ILE
1	B	269	ASP
1	B	289	ILE
1	B	300	LEU
1	B	307	THR
1	B	318	VAL
1	B	319	ILE
1	B	338	TYR
1	B	367	THR
1	B	370	GLN
1	B	442	ILE
1	B	449	HIS
1	C	41	LEU

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Mol	Chain	Res	Type
1	C	44	THR
1	C	75	VAL
1	C	77	VAL
1	C	90	GLN
1	C	138	VAL
1	C	139	LYS
1	C	141	LYS
1	C	152	LYS
1	C	154	LEU
1	C	158	THR
1	C	165	VAL
1	C	168	THR
1	C	183	ILE
1	C	187	TYR
1	C	192	MET
1	C	194	SER
1	C	199	ILE
1	C	205	VAL
1	C	239	THR
1	C	265	ILE
1	C	266	ILE
1	C	271	VAL
1	C	281	THR
1	C	299	ILE
1	C	308	ASN
1	C	312	VAL
1	C	318	VAL
1	C	338	TYR
1	C	367	THR
1	C	370	GLN
1	C	384	PRO
1	C	433	LEU
1	C	449	HIS
1	C	450	PRO
1	C	470	ILE
1	D	10	VAL
1	D	19	TYR
1	D	34	CYS
1	D	41	LEU
1	D	46	LEU
1	D	54	LYS
1	D	76	LYS

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Mol	Chain	Res	Type
1	D	80	VAL
1	D	82	ILE
1	D	96	SER
1	D	126	ILE
1	D	138	VAL
1	D	158	THR
1	D	160	ASP
1	D	165	VAL
1	D	183	ILE
1	D	192	MET
1	D	194	SER
1	D	199	ILE
1	D	205	VAL
1	D	241	VAL
1	D	254	THR
1	D	262	GLU
1	D	264	THR
1	D	270	VAL
1	D	286	LEU
1	D	287	ASP
1	D	289	ILE
1	D	293	THR
1	D	294	ASP
1	D	298	ARG
1	D	301	VAL
1	D	312	VAL
1	D	318	VAL
1	D	327	LYS
1	D	345	HIS
1	D	346	VAL
1	D	384	PRO
1	D	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	58	HIS
1	A	64	HIS
1	A	90	GLN
1	A	97	ASN
1	A	109	ASN

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Mol	Chain	Res	Type
1	A	285	ASN
1	A	345	HIS
1	A	370	GLN
1	A	396	ASN
1	A	416	HIS
1	A	421	ASN
1	B	47	ASN
1	B	58	HIS
1	B	90	GLN
1	B	97	ASN
1	B	109	ASN
1	B	225	GLN
1	B	285	ASN
1	B	345	HIS
1	B	370	GLN
1	B	421	ASN
1	B	469	HIS
1	C	7	ASN
1	C	58	HIS
1	C	61	HIS
1	C	90	GLN
1	C	97	ASN
1	C	109	ASN
1	C	225	GLN
1	C	285	ASN
1	C	370	GLN
1	C	396	ASN
1	C	416	HIS
1	C	434	GLN
1	D	7	ASN
1	D	58	HIS
1	D	68	HIS
1	D	90	GLN
1	D	97	ASN
1	D	225	GLN
1	D	263	GLN
1	D	370	GLN
1	D	416	HIS
1	D	421	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands 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	$\# Z > 2$
2	FAD	A	480	-	58,58,58	2.58	17 (29%)	85,89,89	1.31	8 (9%)
2	FAD	B	480	-	58,58,58	2.34	16 (27%)	85,89,89	1.29	8 (9%)
2	FAD	D	480	-	58,58,58	2.31	16 (27%)	85,89,89	1.33	9 (10%)
2	FAD	C	480	-	58,58,58	2.30	19 (32%)	85,89,89	1.27	10 (11%)

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	FAD	A	480	-	-	4/34/50/50	0/6/6/6
2	FAD	B	480	-	-	4/34/50/50	0/6/6/6
2	FAD	D	480	-	-	4/34/50/50	0/6/6/6
2	FAD	C	480	-	-	4/34/50/50	0/6/6/6

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	480	FAD	P-O3P	-14.34	1.44	1.59
2	D	480	FAD	P-O3P	-11.96	1.46	1.59
2	B	480	FAD	P-O3P	-11.05	1.47	1.59
2	C	480	FAD	P-O3P	-10.52	1.48	1.59
2	C	480	FAD	PA-O2A	-5.26	1.31	1.55
2	D	480	FAD	PA-O2A	-5.07	1.31	1.55
2	A	480	FAD	PA-O2A	-4.93	1.32	1.55
2	B	480	FAD	C1'-C2'	4.40	1.58	1.52
2	A	480	FAD	P-O2P	-4.24	1.35	1.55
2	B	480	FAD	PA-O2A	-4.16	1.36	1.55
2	A	480	FAD	P-O5'	-4.05	1.43	1.59
2	B	480	FAD	O2-C2	-4.01	1.16	1.24
2	B	480	FAD	O5'-C5'	3.93	1.59	1.44
2	D	480	FAD	O5'-C5'	3.55	1.58	1.44
2	B	480	FAD	P-O2P	-3.46	1.39	1.55
2	B	480	FAD	C5A-C6A	3.40	1.50	1.41
2	A	480	FAD	C1'-C2'	3.39	1.57	1.52
2	B	480	FAD	C6-C7	-3.34	1.35	1.39
2	D	480	FAD	C5A-C6A	3.17	1.49	1.41
2	C	480	FAD	C8-C7	3.15	1.48	1.40
2	B	480	FAD	O4B-C1B	3.10	1.49	1.42
2	C	480	FAD	O2-C2	-3.06	1.18	1.24
2	B	480	FAD	C4A-N3A	3.01	1.40	1.34
2	C	480	FAD	C6-C7	-3.00	1.35	1.39
2	C	480	FAD	P-O2P	-2.98	1.41	1.55
2	A	480	FAD	O5'-C5'	2.97	1.55	1.44
2	C	480	FAD	P-O5'	-2.96	1.47	1.59
2	C	480	FAD	C5X-N5	-2.96	1.34	1.39
2	D	480	FAD	C9A-N10	2.85	1.46	1.41
2	D	480	FAD	P-O2P	-2.83	1.42	1.55
2	A	480	FAD	O2-C2	-2.78	1.18	1.24
2	C	480	FAD	C5'-C4'	-2.78	1.48	1.51
2	C	480	FAD	PA-O3P	-2.70	1.56	1.59
2	A	480	FAD	C5A-C6A	2.64	1.48	1.41
2	C	480	FAD	C2-N1	-2.62	1.30	1.36
2	D	480	FAD	C4A-N3A	2.60	1.39	1.34
2	A	480	FAD	C10-N1	2.51	1.38	1.33
2	A	480	FAD	C5X-N5	-2.49	1.34	1.39
2	C	480	FAD	C4A-N3A	2.46	1.39	1.34
2	C	480	FAD	C5A-C6A	2.45	1.47	1.41
2	A	480	FAD	C9-C9A	2.42	1.43	1.39
2	D	480	FAD	PA-O3P	-2.39	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	480	FAD	C1'-C2'	2.39	1.56	1.52
2	B	480	FAD	C5B-C4B	2.38	1.58	1.51
2	D	480	FAD	O2-C2	-2.38	1.19	1.24
2	D	480	FAD	P-O5'	-2.36	1.50	1.59
2	B	480	FAD	C4A-N9A	2.35	1.42	1.37
2	B	480	FAD	C5X-N5	-2.30	1.35	1.39
2	D	480	FAD	C10-N1	2.28	1.37	1.33
2	A	480	FAD	C6-C7	2.24	1.42	1.39
2	D	480	FAD	C2-N3	2.23	1.43	1.39
2	C	480	FAD	C2-N3	2.22	1.43	1.39
2	C	480	FAD	O5'-C5'	2.19	1.52	1.44
2	B	480	FAD	P-O5'	-2.19	1.50	1.59
2	B	480	FAD	C10-N1	2.18	1.37	1.33
2	A	480	FAD	C2-N3	2.16	1.43	1.39
2	D	480	FAD	C8-C7	2.15	1.46	1.40
2	A	480	FAD	C4A-N9A	2.14	1.42	1.37
2	A	480	FAD	O4B-C1B	2.14	1.46	1.42
2	D	480	FAD	O4B-C1B	2.13	1.46	1.42
2	D	480	FAD	C4A-N9A	2.10	1.42	1.37
2	B	480	FAD	C2-N1	-2.04	1.32	1.36
2	C	480	FAD	O4B-C1B	2.04	1.46	1.42
2	D	480	FAD	C9A-C5X	2.03	1.44	1.41
2	A	480	FAD	C8-C7	2.03	1.45	1.40
2	C	480	FAD	C6A-N6A	-2.02	1.29	1.34
2	C	480	FAD	C4A-N9A	2.00	1.41	1.37
2	A	480	FAD	C8A-N7A	2.00	1.35	1.31

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	480	FAD	O2A-PA-O3P	4.37	119.08	107.27
2	D	480	FAD	O4B-C1B-N9A	-4.25	99.92	108.09
2	B	480	FAD	O2A-PA-O3P	4.05	118.23	107.27
2	A	480	FAD	C4B-O4B-C1B	-3.99	100.65	109.47
2	D	480	FAD	C4B-O4B-C1B	-3.57	101.59	109.47
2	C	480	FAD	C4B-O4B-C1B	-3.55	101.63	109.47
2	B	480	FAD	C4B-O4B-C1B	-3.54	101.65	109.47
2	D	480	FAD	C2B-C1B-N9A	3.33	121.59	113.30
2	D	480	FAD	O2A-PA-O3P	3.22	115.98	107.27
2	C	480	FAD	O4B-C1B-N9A	-3.21	101.93	108.09
2	A	480	FAD	O4B-C1B-N9A	-3.19	101.95	108.09
2	A	480	FAD	C5'-C4'-C3'	-3.18	106.22	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	480	FAD	O2A-PA-O3P	2.97	115.31	107.27
2	D	480	FAD	O4B-C1B-C2B	-2.97	100.26	106.62
2	B	480	FAD	C5'-C4'-C3'	-2.82	106.90	112.22
2	D	480	FAD	C2A-N1A-C6A	2.82	123.36	118.73
2	C	480	FAD	O5'-C5'-C4'	-2.76	102.00	109.36
2	B	480	FAD	C2A-N1A-C6A	2.74	123.23	118.73
2	A	480	FAD	C2A-N1A-C6A	2.65	123.08	118.73
2	A	480	FAD	C2B-C1B-N9A	2.57	119.70	113.30
2	B	480	FAD	C4-N3-C2	-2.53	121.16	125.64
2	C	480	FAD	C2A-N1A-C6A	2.52	122.87	118.73
2	D	480	FAD	O5B-PA-O1A	-2.33	99.69	108.94
2	D	480	FAD	O3B-C3B-C2B	2.30	119.20	111.82
2	C	480	FAD	C5'-C4'-C3'	-2.24	107.99	112.22
2	C	480	FAD	C2B-C1B-N9A	2.24	118.86	113.30
2	A	480	FAD	O5'-P-O1P	-2.21	100.17	108.94
2	B	480	FAD	O4B-C1B-N9A	-2.20	103.86	108.09
2	A	480	FAD	C4-N3-C2	-2.12	121.89	125.64
2	B	480	FAD	O5B-PA-O1A	-2.09	100.66	108.94
2	B	480	FAD	O5'-P-O1P	-2.08	100.70	108.94
2	C	480	FAD	O4B-C1B-C2B	-2.05	102.24	106.62
2	D	480	FAD	C4-N3-C2	-2.04	122.02	125.64
2	C	480	FAD	C4-N3-C2	-2.03	122.04	125.64
2	C	480	FAD	O5B-PA-O1A	-2.01	100.96	108.94

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	480	FAD	O4B-C4B-C5B-O5B
2	C	480	FAD	O4B-C4B-C5B-O5B
2	C	480	FAD	P-O3P-PA-O1A
2	B	480	FAD	O4B-C4B-C5B-O5B
2	A	480	FAD	C3B-C4B-C5B-O5B
2	B	480	FAD	C3B-C4B-C5B-O5B
2	C	480	FAD	C3B-C4B-C5B-O5B
2	D	480	FAD	O4B-C4B-C5B-O5B
2	D	480	FAD	C3B-C4B-C5B-O5B
2	A	480	FAD	P-O3P-PA-O2A
2	B	480	FAD	P-O3P-PA-O2A
2	C	480	FAD	P-O3P-PA-O2A
2	D	480	FAD	P-O3P-PA-O1A
2	D	480	FAD	P-O3P-PA-O2A

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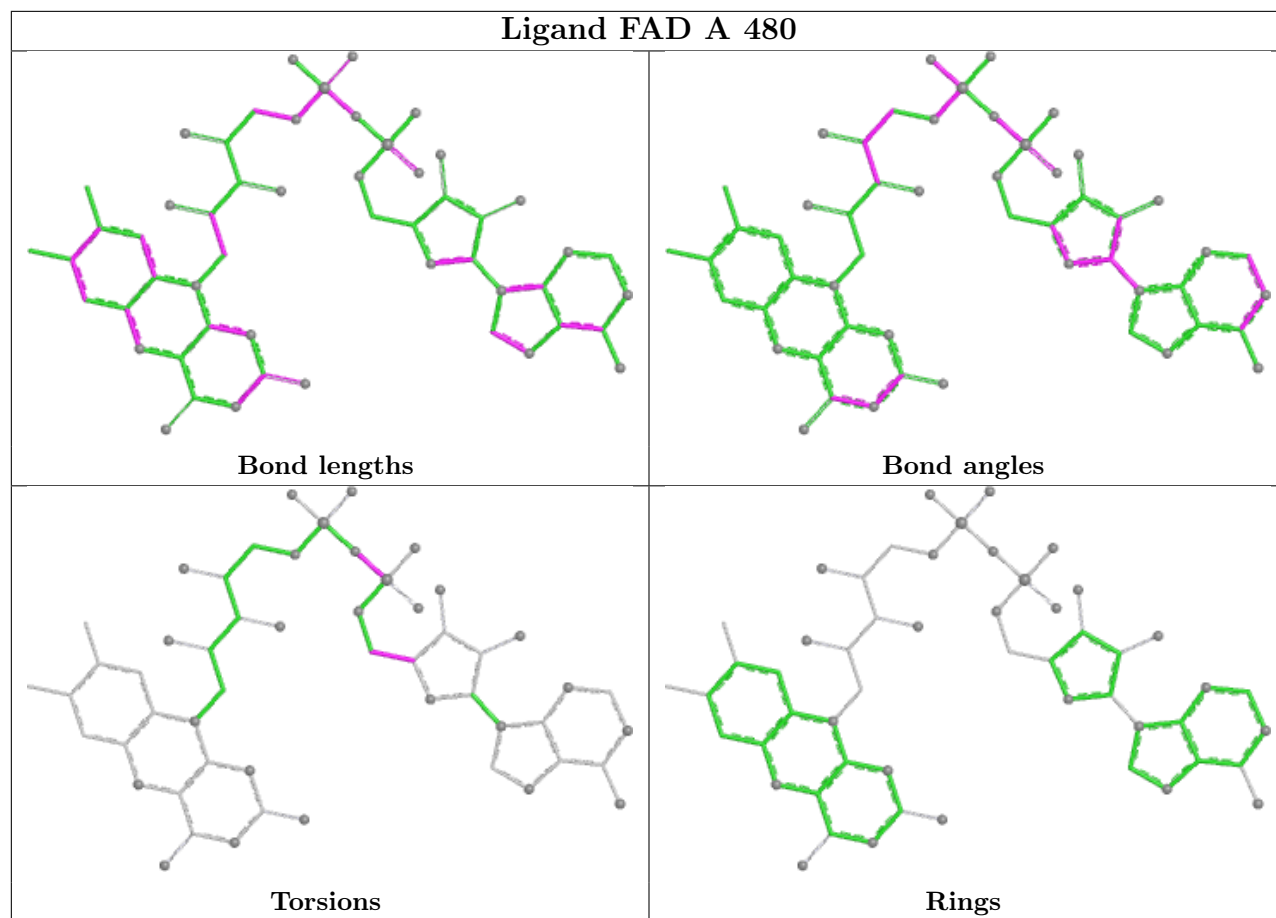
Mol	Chain	Res	Type	Atoms
2	B	480	FAD	P-O3P-PA-O1A
2	A	480	FAD	P-O3P-PA-O1A

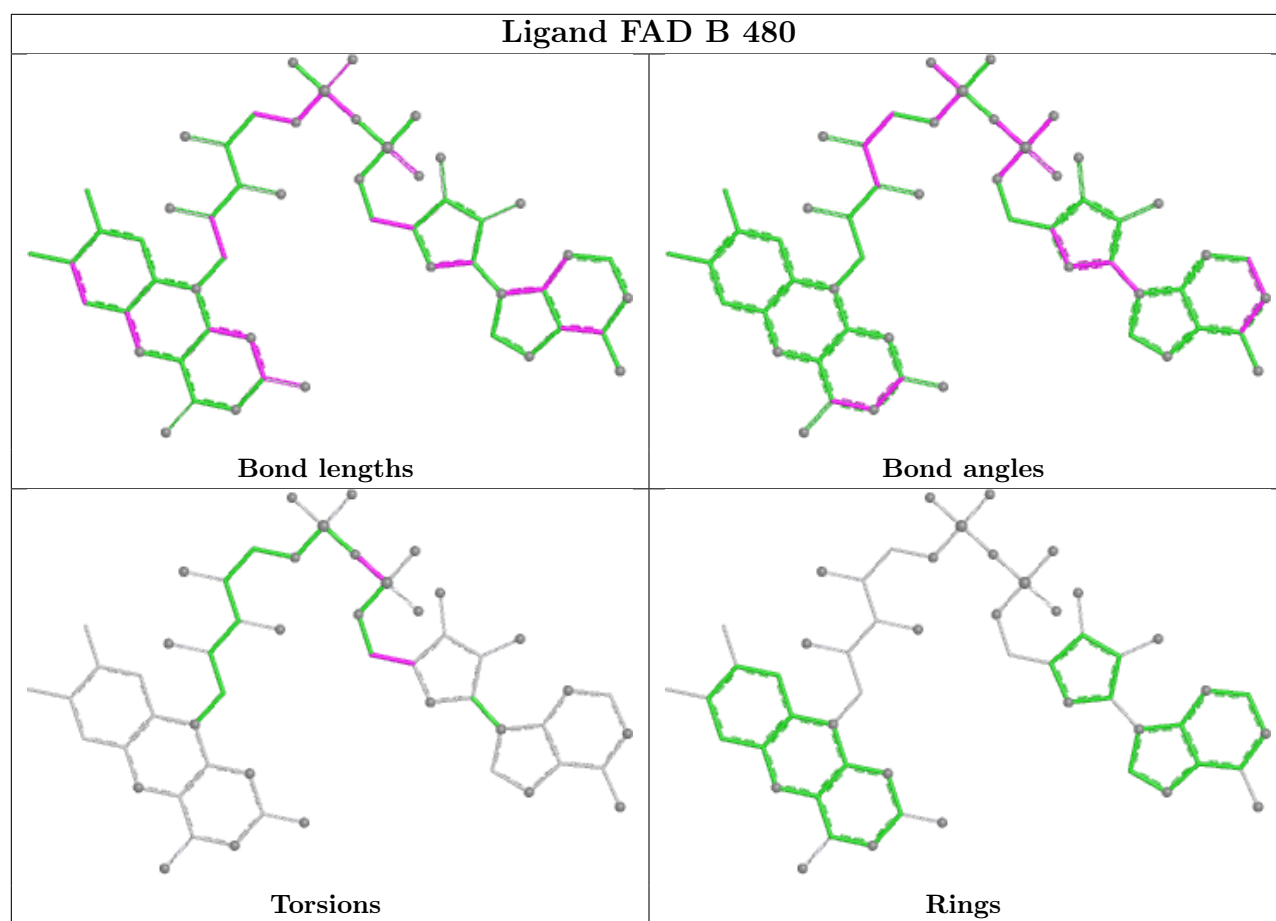
There are no ring outliers.

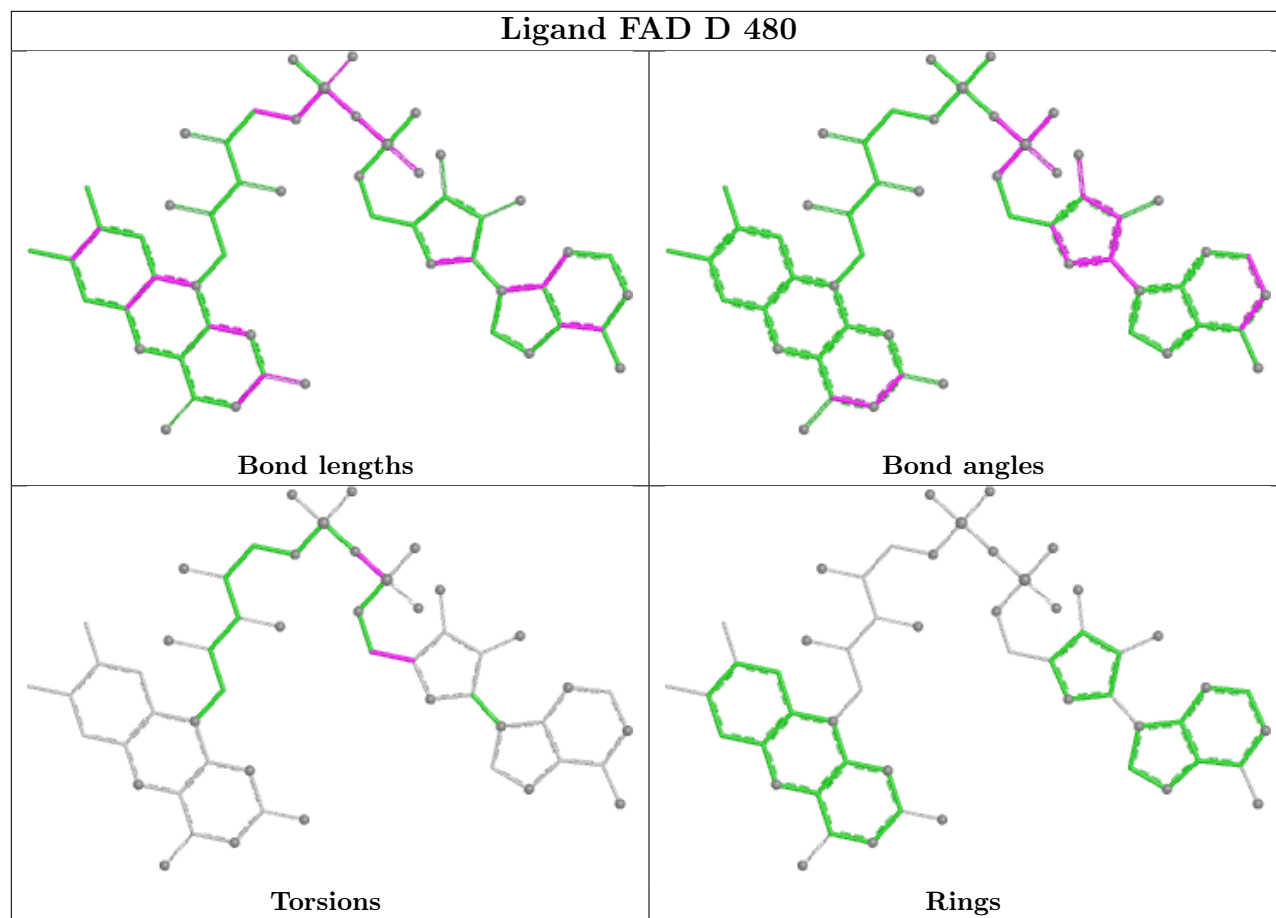
4 monomers are involved in 10 short contacts:

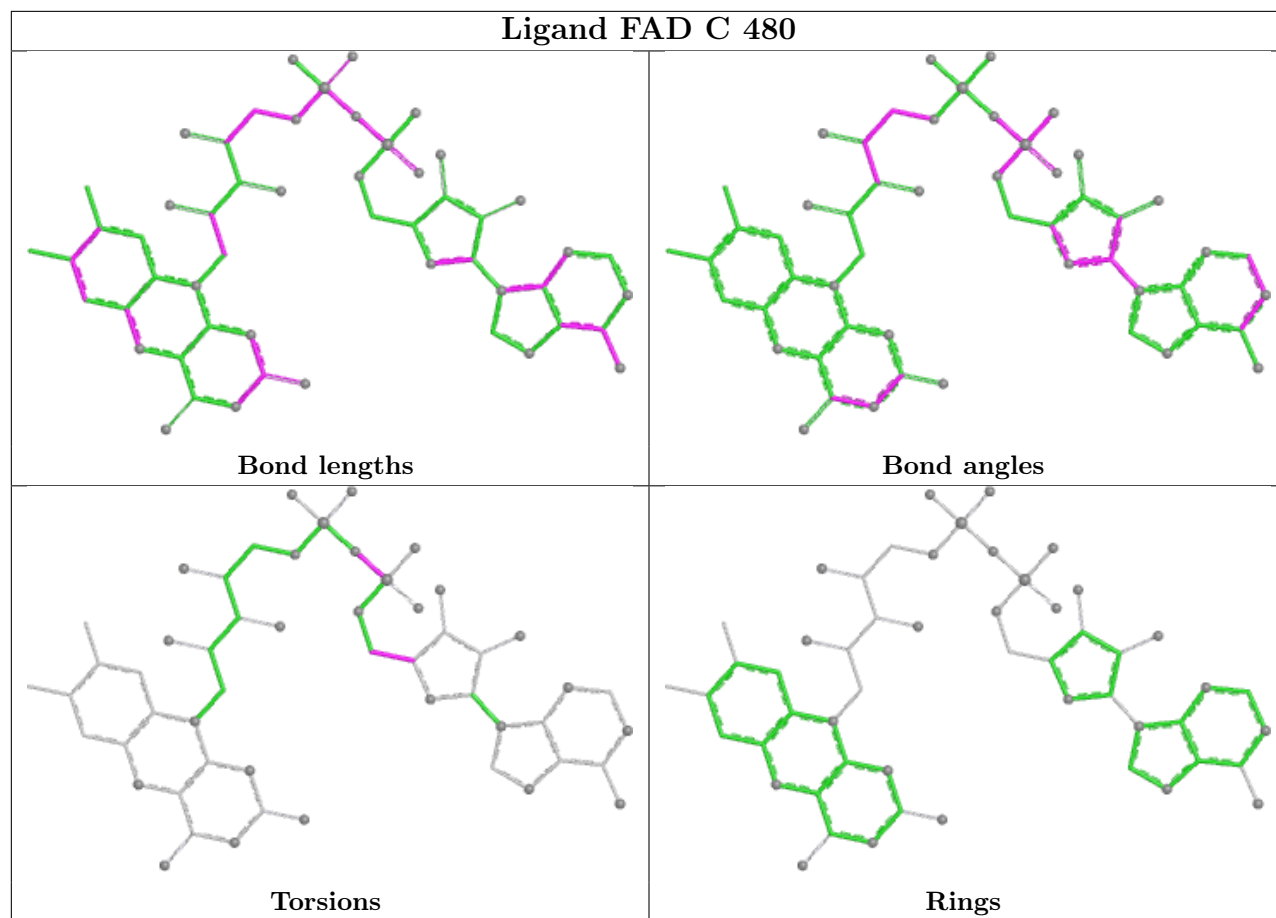
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	480	FAD	2	0
2	B	480	FAD	2	0
2	D	480	FAD	3	0
2	C	480	FAD	3	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	258:SER	C	259:ALA	N	2.22
1	C	263:GLN	C	264:THR	N	1.20

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.