



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:47 PM UTC

PDB ID : 2FIX / pdb\_00002fix  
Title : Structure of human liver FB Pase complexed with potent benzoxazole allosteric inhibitors  
Authors : Abad-Zapatero, C.  
Deposited on : 2005-12-30  
Resolution : 3.50 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
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

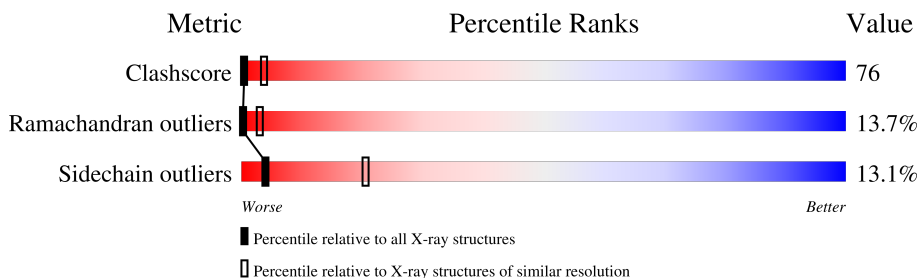
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	338	15% 56% 21% • 6%
1	D	338	13% 53% 26% • 6%
1	H	338	17% 55% 21% • 6%
1	L	338	17% 52% 22% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	870	H	901	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9848 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.

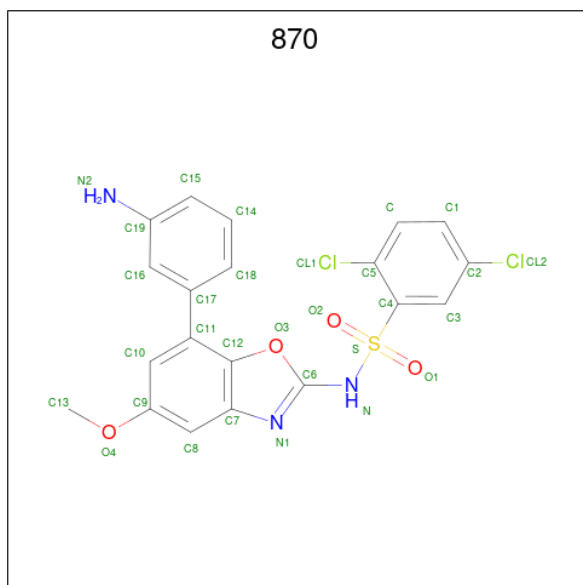
- Molecule 1 is a protein called Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2432	1548	408	459	17	0	0	1
1	D	319	2432	1548	408	459	17	0	0	1
1	H	319	2432	1548	408	459	17	0	0	1
1	L	319	2432	1548	408	459	17	0	0	1

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	ARG	variant	GB 15277851
D	217	LYS	ARG	variant	GB 15277851
H	217	LYS	ARG	variant	GB 15277851
L	217	LYS	ARG	variant	GB 15277851

- Molecule 2 is N-[7-(3-AMINOPHENYL)-5-METHOXY-1,3-BENZOXAZOL-2-YL]-2,5-DICHLOROBENZENESULFONAMIDE (CCD ID: 870) (formula: C<sub>20</sub>H<sub>15</sub>Cl<sub>2</sub>N<sub>3</sub>O<sub>4</sub>S).



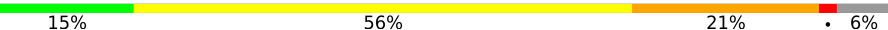
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	N	O			S
2	A	1	Total	C	Cl	N	O	S	0	0
			30	20	2	3	4	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			30	20	2	3	4	1		
2	H	1	Total	C	Cl	N	O	S	0	0
			30	20	2	3	4	1		
2	L	1	Total	C	Cl	N	O	S	0	0
			30	20	2	3	4	1		

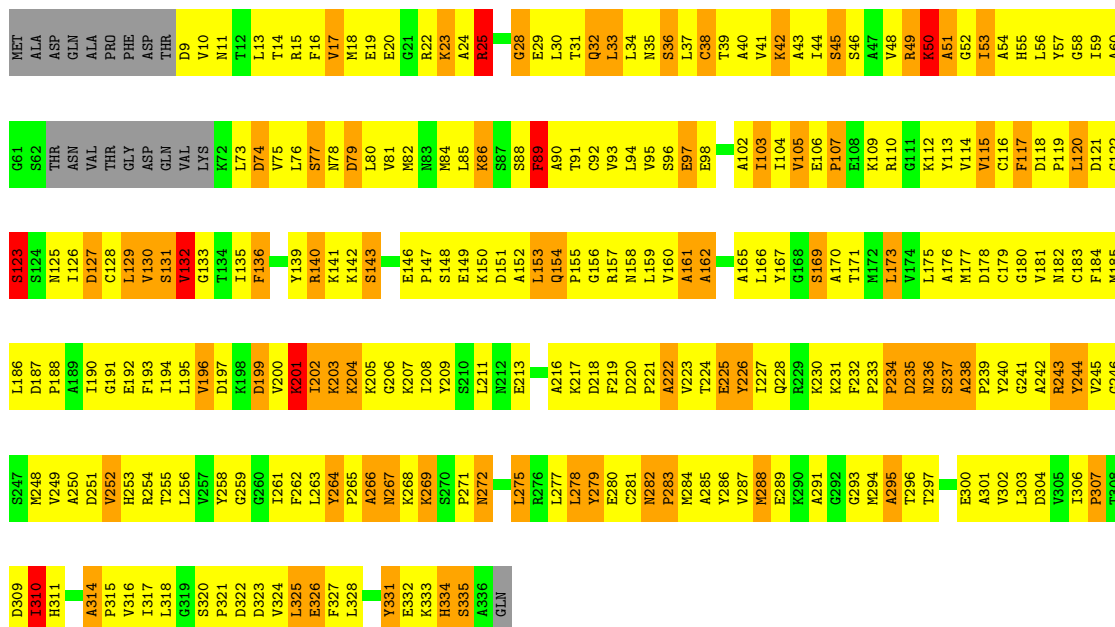
### 3 Residue-property plots

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.

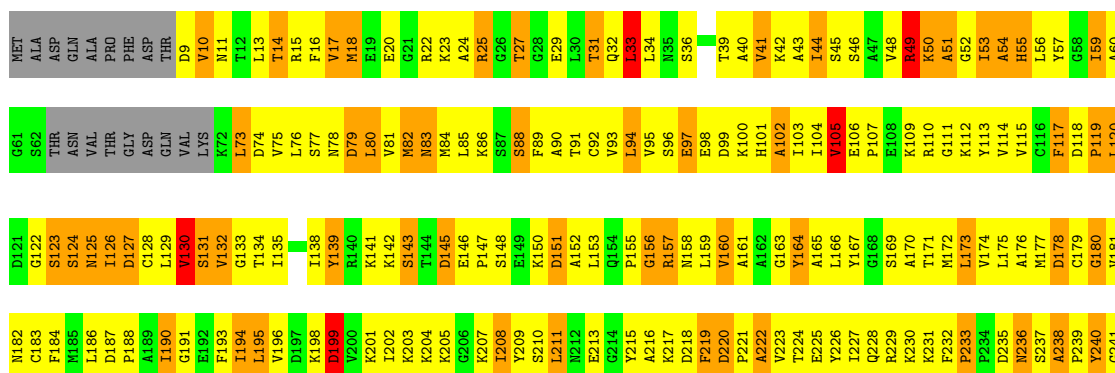
- Molecule 1: Fructose-1,6-bisphosphatase 1

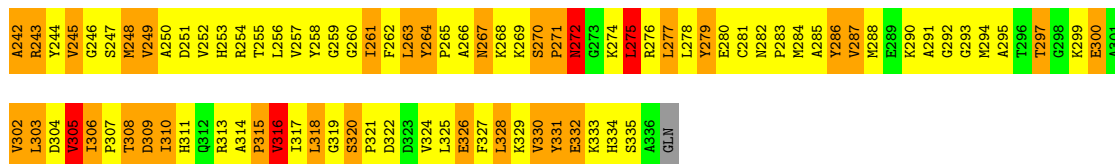
Chain A: 



- Molecule 1: Fructose-1,6-bisphosphatase 1

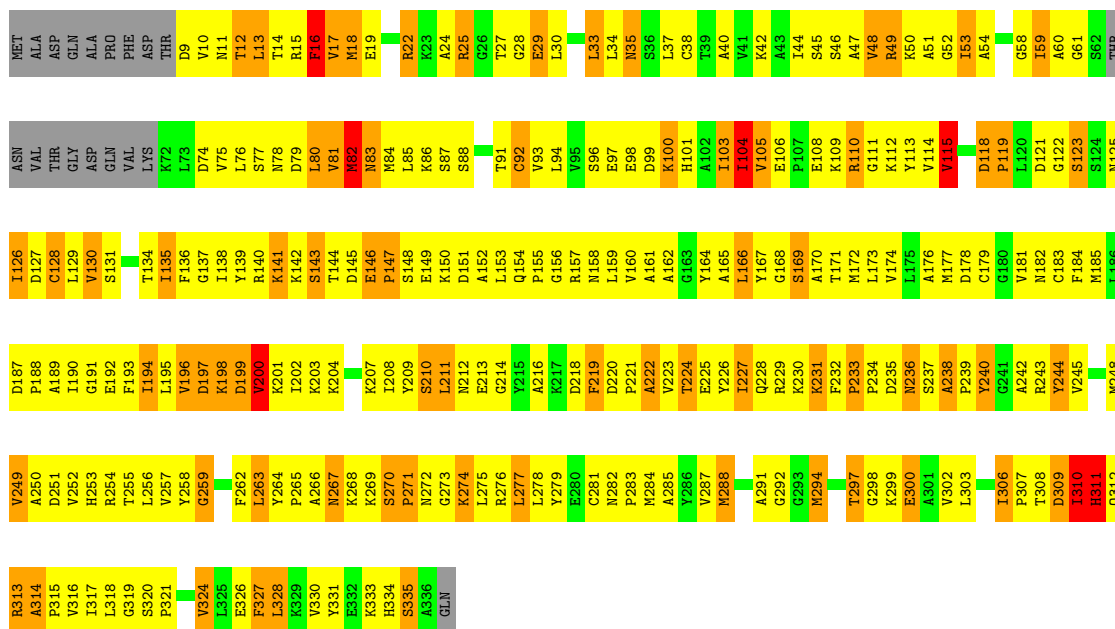
Chain D: 





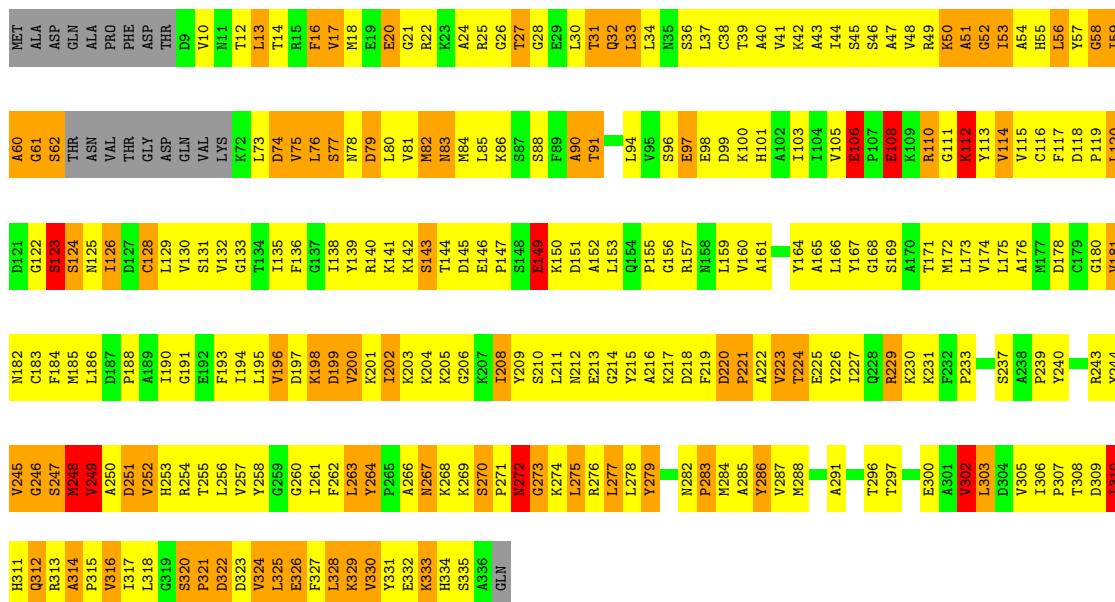
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain H: 17% 55% 21% 6%



• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain L: 17% 52% 22% 6%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.40Å 108.67Å 196.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.88 – 3.50	Depositor
% Data completeness (in resolution range)	61.6 (19.88-3.50)	Depositor
$R_{merge}$	0.24	Depositor
$R_{sym}$	0.24	Depositor
Refinement program	CNX 2002	Depositor
R, $R_{free}$	0.252 , 0.355	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 870

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.65	1/2475 (0.0%)	1.36	43/3343 (1.3%)
1	D	0.63	1/2475 (0.0%)	1.25	34/3343 (1.0%)
1	H	0.61	1/2475 (0.0%)	1.24	32/3343 (1.0%)
1	L	0.61	0/2475	1.27	31/3343 (0.9%)
All	All	0.63	3/9900 (0.0%)	1.28	140/13372 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	335	SER	C-N	-5.49	1.25	1.33
1	H	335	SER	C-N	-5.43	1.25	1.33
1	D	335	SER	C-N	-5.20	1.26	1.33

All (140) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	ILE	CA-C-N	13.51	133.67	119.76
1	A	306	ILE	C-N-CA	13.51	133.67	119.76
1	A	131	SER	CB-CA-C	-10.84	94.64	109.71
1	D	233	PRO	CA-C-N	10.62	130.23	119.82
1	D	233	PRO	C-N-CA	10.62	130.23	119.82
1	L	74	ASP	N-CA-C	-10.58	99.75	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	SER	N-CA-C	-10.37	99.67	110.97
1	A	131	SER	N-CA-C	10.11	125.18	110.42
1	A	326	GLU	N-CA-C	-10.10	100.35	111.36
1	A	132	VAL	N-CA-CB	-9.81	98.78	112.52
1	L	264	TYR	CA-C-N	9.79	132.08	119.84
1	L	264	TYR	C-N-CA	9.79	132.08	119.84
1	A	25	ARG	O-C-N	-9.55	110.70	122.55
1	D	272	ASN	N-CA-C	-9.45	100.33	112.23
1	A	28	GLY	N-CA-C	-9.44	103.48	113.58
1	A	238	ALA	CA-C-N	9.07	131.18	119.84
1	A	238	ALA	C-N-CA	9.07	131.18	119.84
1	H	270	SER	CA-C-N	9.06	131.17	119.84
1	H	270	SER	C-N-CA	9.06	131.17	119.84
1	D	264	TYR	CA-C-N	8.67	128.53	120.21
1	D	264	TYR	C-N-CA	8.67	128.53	120.21
1	L	53	ILE	N-CA-C	8.46	118.51	110.30
1	L	20	GLU	N-CA-C	-8.46	101.64	111.03
1	L	306	ILE	CA-C-N	8.40	128.90	119.83
1	L	306	ILE	C-N-CA	8.40	128.90	119.83
1	A	169	SER	N-CA-C	-8.35	101.87	110.97
1	H	144	THR	N-CA-C	-8.13	103.47	113.15
1	A	259	GLY	N-CA-C	-7.92	102.70	112.68
1	L	106	GLU	CA-C-N	7.88	129.68	119.84
1	L	106	GLU	C-N-CA	7.88	129.68	119.84
1	D	269	LYS	N-CA-C	-7.84	101.55	112.45
1	H	29	GLU	CB-CA-C	7.82	123.00	110.96
1	L	326	GLU	N-CA-C	-7.75	102.53	110.97
1	D	33	LEU	N-CA-C	-7.66	95.70	110.56
1	L	86	LYS	N-CA-C	-7.59	102.94	111.14
1	D	320	SER	CA-C-N	7.52	129.24	119.84
1	D	320	SER	C-N-CA	7.52	129.24	119.84
1	L	128	CYS	N-CA-C	-7.47	103.73	112.92
1	H	324	VAL	N-CA-C	-7.46	101.76	111.09
1	L	229	ARG	N-CA-C	-7.41	104.27	113.38
1	H	298	GLY	N-CA-C	-7.40	103.68	115.08
1	D	316	VAL	N-CA-C	7.28	118.96	108.48
1	H	146	GLU	CA-C-N	6.96	128.54	119.84
1	H	146	GLU	C-N-CA	6.96	128.54	119.84
1	L	220	ASP	CA-C-N	6.94	128.52	119.84
1	L	220	ASP	C-N-CA	6.94	128.52	119.84
1	A	136	PHE	N-CA-C	6.78	119.47	108.76
1	D	297	THR	N-CA-C	-6.78	105.01	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	TYR	N-CA-C	6.76	122.42	114.04
1	L	264	TYR	N-CA-C	-6.75	96.46	108.55
1	D	220	ASP	CA-C-N	6.72	128.24	119.84
1	D	220	ASP	C-N-CA	6.72	128.24	119.84
1	A	264	TYR	CA-C-N	6.65	128.15	119.84
1	A	264	TYR	C-N-CA	6.65	128.15	119.84
1	H	29	GLU	N-CA-C	-6.65	103.73	110.97
1	L	312	GLN	N-CA-C	-6.61	101.63	110.55
1	D	326	GLU	N-CA-C	-6.57	103.23	111.11
1	A	143	SER	N-CA-C	6.57	119.14	109.69
1	D	218	ASP	N-CA-C	-6.54	104.69	114.64
1	L	198	LYS	N-CA-C	6.53	118.45	110.41
1	H	297	THR	N-CA-C	-6.53	105.23	113.72
1	A	275	LEU	N-CA-C	6.53	119.49	110.35
1	H	316	VAL	N-CA-C	6.46	117.33	107.77
1	H	104	ILE	N-CA-C	6.45	116.69	106.88
1	A	325	LEU	N-CA-C	-6.40	104.51	112.90
1	D	279	TYR	N-CA-C	6.39	120.39	112.59
1	A	122	GLY	N-CA-C	-6.38	105.70	114.64
1	D	306	ILE	CA-C-N	6.36	127.79	119.84
1	D	306	ILE	C-N-CA	6.36	127.79	119.84
1	L	97	GLU	N-CA-C	-6.32	105.63	113.15
1	L	149	GLU	CB-CA-C	-6.31	97.86	110.42
1	L	118	ASP	N-CA-C	-6.31	98.61	109.15
1	L	17	VAL	CB-CA-C	-6.30	103.63	112.14
1	D	97	GLU	N-CA-C	-6.21	106.07	113.21
1	D	49	ARG	N-CA-C	-6.21	106.07	113.21
1	D	88	SER	N-CA-C	-6.20	103.83	112.45
1	H	110	ARG	N-CA-C	6.20	118.52	110.53
1	H	200	VAL	N-CA-C	6.18	118.63	108.99
1	D	215	TYR	N-CA-C	-6.17	106.43	112.97
1	D	41	VAL	N-CA-C	6.15	116.20	110.42
1	H	328	LEU	N-CA-C	6.13	117.63	111.07
1	H	231	LYS	N-CA-C	-6.11	103.92	111.75
1	A	86	LYS	N-CA-C	-6.05	103.84	111.11
1	A	288	MET	N-CA-C	-6.04	104.61	111.14
1	A	97	GLU	N-CA-C	-6.04	106.26	113.21
1	D	181	VAL	N-CA-C	6.04	116.56	108.11
1	H	115	VAL	N-CA-C	6.03	116.80	108.12
1	D	228	GLN	N-CA-C	-6.02	105.64	112.87
1	H	16	PHE	N-CA-C	-6.00	105.04	112.90
1	A	307	PRO	N-CA-C	5.99	120.48	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	208	ILE	N-CA-C	5.98	117.29	107.24
1	A	316	VAL	N-CA-C	5.92	116.16	108.35
1	H	204	LYS	N-CA-C	-5.90	103.55	112.04
1	A	306	ILE	N-CA-C	5.84	114.39	107.73
1	A	45	SER	N-CA-C	-5.81	104.85	111.07
1	A	202	ILE	N-CA-C	5.76	117.01	109.58
1	H	236	ASN	N-CA-C	5.74	123.03	110.80
1	A	127	ASP	N-CA-C	-5.72	104.41	111.33
1	A	115	VAL	N-CA-C	5.66	116.27	108.12
1	A	266	ALA	N-CA-C	5.66	117.83	110.53
1	A	154	GLN	CA-C-N	5.57	125.75	119.90
1	A	154	GLN	C-N-CA	5.57	125.75	119.90
1	A	314	ALA	CA-C-N	5.53	127.72	120.25
1	A	314	ALA	C-N-CA	5.53	127.72	120.25
1	D	302	VAL	N-CA-C	5.51	115.65	110.30
1	D	44	ILE	N-CA-C	-5.51	104.34	110.62
1	D	180	GLY	N-CA-C	5.48	117.58	110.45
1	L	112	LYS	N-CA-C	5.48	122.48	110.80
1	A	25	ARG	CA-C-N	5.45	129.73	122.75
1	A	25	ARG	C-N-CA	5.45	129.73	122.75
1	D	160	VAL	N-CA-C	-5.45	107.97	113.47
1	L	178	ASP	N-CA-C	-5.44	106.32	113.12
1	A	32	GLN	N-CA-C	-5.42	104.78	111.33
1	L	302	VAL	N-CA-C	5.41	120.58	109.34
1	A	42	LYS	N-CA-C	-5.39	105.57	111.82
1	A	226	TYR	N-CA-C	-5.37	106.56	113.01
1	H	196	VAL	N-CA-C	5.36	116.17	111.56
1	L	333	LYS	N-CA-C	-5.31	106.50	112.87
1	D	130	VAL	N-CA-C	-5.29	100.14	108.23
1	H	118	ASP	N-CA-C	-5.28	99.18	108.69
1	L	60	ALA	N-CA-C	-5.25	107.42	113.88
1	H	88	SER	N-CA-C	-5.24	105.75	113.61
1	H	143	SER	N-CA-C	5.23	118.34	109.76
1	D	102	ALA	N-CA-C	5.22	118.06	109.76
1	H	18	MET	N-CA-C	-5.17	106.23	112.54
1	H	128	CYS	N-CA-C	-5.17	107.04	113.19
1	L	16	PHE	N-CA-C	-5.17	105.33	111.69
1	D	157	ARG	N-CA-C	-5.15	106.15	112.90
1	H	233	PRO	N-CA-C	5.14	115.41	110.47
1	H	227	ILE	N-CA-C	-5.14	105.53	110.72
1	L	272	ASN	N-CA-C	5.12	115.76	107.32
1	L	114	VAL	N-CA-C	-5.11	103.00	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	VAL	N-CA-C	-5.11	105.40	112.50
1	D	139	TYR	CB-CA-C	-5.09	105.17	113.37
1	H	123	SER	N-CA-C	5.09	116.91	111.36
1	H	25	ARG	CD-NE-CZ	-5.06	117.32	124.40
1	D	127	ASP	N-CA-C	-5.04	105.30	111.75
1	H	210	SER	N-CA-C	5.04	117.61	108.69
1	A	250	ALA	N-CA-C	5.02	116.44	111.07
1	H	257	VAL	CB-CA-C	-5.02	105.78	111.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	ARG	Mainchain

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2432	0	2474	389	0
1	D	2432	0	2474	414	0
1	H	2432	0	2474	384	0
1	L	2432	0	2474	402	0
2	A	30	0	15	7	0
2	D	30	0	15	1	0
2	H	30	0	15	9	0
2	L	30	0	15	3	0
All	All	9848	0	9956	1499	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 76.

All (1499) 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:H:53:ILE:HD13	1:L:185:MET:HG2	1.25	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:THR:HB	1:D:94:LEU:HD21	1.38	1.05
1:H:194:ILE:HG12	1:L:54:ALA:HB2	1.31	1.05
1:D:27:THR:HA	2:H:901:870:HN22	1.18	1.03
1:A:191:GLY:HA3	1:L:191:GLY:HA3	1.37	1.02
1:D:27:THR:HA	2:H:901:870:N2	1.77	1.00
1:A:289:GLU:OE2	1:A:303:LEU:HD12	1.63	0.97
1:L:122:GLY:HA3	1:L:132:VAL:HG12	1.45	0.97
1:A:135:ILE:HD11	1:A:249:VAL:HG22	1.44	0.96
1:D:138:ILE:HB	1:D:161:ALA:HB3	1.48	0.96
1:A:11:ASN:HD21	1:A:16:PHE:HB2	1.30	0.96
1:A:85:LEU:HA	1:A:88:SER:HB3	1.47	0.95
1:L:91:THR:HG21	1:L:94:LEU:HD21	1.46	0.95
1:H:172:MET:HE2	1:H:183:CYS:HB3	1.47	0.95
1:D:252:VAL:HG21	1:D:284:MET:HE3	1.48	0.94
1:D:29:GLU:OE2	1:D:90:ALA:HA	1.68	0.94
1:L:156:GLY:HA3	1:L:303:LEU:HD22	1.50	0.92
1:L:99:ASP:HB3	1:L:103:ILE:HD11	1.50	0.91
1:D:293:GLY:HA2	1:D:321:PRO:HG3	1.51	0.91
1:H:272:ASN:O	1:H:314:ALA:HA	1.71	0.91
1:L:52:GLY:O	1:L:56:LEU:HD13	1.71	0.90
1:H:262:PHE:HB3	1:H:318:LEU:HG	1.52	0.90
1:A:82:MET:HG3	1:A:86:LYS:HE3	1.53	0.90
1:A:127:ASP:HB2	1:D:258:TYR:OH	1.72	0.90
1:H:44:ILE:HG12	1:H:80:LEU:HD12	1.52	0.89
1:A:10:VAL:HG22	1:A:11:ASN:H	1.39	0.88
1:H:190:ILE:HG13	1:H:191:GLY:N	1.87	0.88
1:A:220:ASP:HB2	1:A:221:PRO:HD2	1.54	0.88
1:H:44:ILE:HG12	1:H:80:LEU:CD1	2.04	0.88
1:A:261:ILE:HD12	1:A:323:ASP:O	1.74	0.87
1:A:17:VAL:HG13	1:A:34:LEU:HD12	1.55	0.87
1:D:242:ALA:O	1:D:243:ARG:HG2	1.75	0.87
1:L:273:GLY:H	1:L:315:PRO:HG3	1.40	0.86
1:A:282:ASN:HB2	1:A:283:PRO:HD3	1.56	0.86
1:A:245:VAL:O	1:D:243:ARG:HD2	1.74	0.85
1:D:93:VAL:O	1:D:114:VAL:HG13	1.77	0.85
1:H:150:LYS:HA	1:H:153:LEU:HD12	1.58	0.84
1:H:194:ILE:CG1	1:L:54:ALA:HB2	2.06	0.84
1:A:155:PRO:HG2	1:A:158:ASN:HD21	1.42	0.84
1:L:165:ALA:HA	1:L:173:LEU:HA	1.57	0.84
1:A:221:PRO:O	1:A:224:THR:HB	1.76	0.84
1:A:230:LYS:O	1:A:233:PRO:HD3	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:316:VAL:C	1:D:317:ILE:HD12	2.02	0.83
1:L:90:ALA:HA	1:L:111:GLY:HA3	1.58	0.83
1:A:155:PRO:HG2	1:A:158:ASN:ND2	1.94	0.83
1:L:288:MET:HG3	1:L:318:LEU:HD13	1.60	0.83
1:D:270:SER:C	1:D:272:ASN:H	1.84	0.83
1:H:276:ARG:HH21	1:H:313:ARG:HH12	1.24	0.83
1:D:202:ILE:HG12	1:D:203:LYS:H	1.43	0.83
1:L:209:TYR:HA	1:L:261:ILE:HG22	1.60	0.83
1:L:81:VAL:HG12	1:L:85:LEU:HD12	1.59	0.82
1:D:114:VAL:HG11	1:D:152:ALA:HB2	1.60	0.82
1:L:221:PRO:HB2	1:L:334:HIS:HD2	1.43	0.82
1:D:29:GLU:HG2	1:H:22:ARG:NH2	1.93	0.81
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.16	0.81
1:A:202:ILE:HB	1:A:256:LEU:HD12	1.61	0.81
1:A:186:LEU:O	1:A:188:PRO:HD3	1.81	0.80
1:D:202:ILE:HG12	1:D:203:LYS:N	1.95	0.80
1:D:13:LEU:HA	1:D:184:PHE:CE2	2.16	0.80
1:A:185:MET:HE3	1:D:50:LYS:HG2	1.64	0.80
1:H:15:ARG:O	1:H:19:GLU:HG2	1.81	0.80
1:H:214:GLY:C	1:H:216:ALA:H	1.90	0.80
1:A:272:ASN:N	1:A:272:ASN:HD22	1.80	0.79
1:D:27:THR:CA	2:H:901:870:HN22	1.95	0.79
1:A:139:TYR:CE1	1:A:159:LEU:HG	2.17	0.79
1:L:156:GLY:HA3	1:L:303:LEU:CD2	2.13	0.79
1:D:22:ARG:HH22	1:H:29:GLU:HG3	1.48	0.79
1:D:90:ALA:C	1:D:111:GLY:HA3	2.08	0.79
1:H:139:TYR:CE1	1:H:159:LEU:HG	2.17	0.79
1:L:153:LEU:HD21	1:L:308:THR:O	1.83	0.79
1:A:245:VAL:HG13	1:D:245:VAL:HG22	1.63	0.79
1:A:30:LEU:O	1:A:33:LEU:HB3	1.83	0.78
1:H:258:TYR:OH	1:L:125:ASN:HA	1.83	0.78
1:L:82:MET:O	1:L:85:LEU:N	2.14	0.78
1:A:88:SER:O	1:A:89:PHE:HB2	1.81	0.78
1:H:50:LYS:HG2	1:H:53:ILE:HD12	1.64	0.78
1:L:141:LYS:HG3	1:L:151:ASP:CG	2.09	0.78
1:H:245:VAL:HG22	1:L:245:VAL:HG22	1.66	0.78
1:A:285:ALA:HB3	1:A:303:LEU:HD21	1.64	0.78
1:H:82:MET:HG3	1:H:86:LYS:HE3	1.64	0.78
1:H:308:THR:HG22	1:H:312:GLN:OE1	1.83	0.77
1:A:17:VAL:CG1	1:A:34:LEU:HD12	2.14	0.77
1:H:187:ASP:OD2	1:L:53:ILE:HG22	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:252:VAL:HG21	1:L:284:MET:HE3	1.67	0.77
1:L:185:MET:O	1:L:193:PHE:HA	1.85	0.77
1:D:114:VAL:HG11	1:D:152:ALA:CB	2.16	0.76
1:H:53:ILE:HD13	1:L:185:MET:CG	2.12	0.76
1:A:204:LYS:O	1:A:320:SER:HB3	1.86	0.76
1:H:229:ARG:O	1:H:233:PRO:HA	1.85	0.76
1:L:50:LYS:HD2	1:L:50:LYS:N	2.00	0.76
1:H:181:VAL:O	1:H:199:ASP:HA	1.86	0.76
1:D:93:VAL:HG23	1:D:147:PRO:HB2	1.67	0.76
1:H:129:LEU:HD11	1:L:172:MET:HE3	1.66	0.76
1:L:91:THR:O	1:L:110:ARG:HA	1.85	0.76
1:L:50:LYS:HB3	1:L:53:ILE:HB	1.66	0.76
1:H:184:PHE:HB3	1:H:193:PHE:HB3	1.68	0.75
1:L:278:LEU:HA	1:L:282:ASN:OD1	1.86	0.75
1:L:58:GLY:HA2	1:L:62:SER:H	1.50	0.75
1:A:102:ALA:HB2	1:A:149:GLU:OE2	1.87	0.75
1:A:149:GLU:CG	1:A:310:ILE:HG21	2.17	0.75
1:D:194:ILE:N	1:D:194:ILE:HD12	2.01	0.75
1:H:190:ILE:HG13	1:H:191:GLY:H	1.50	0.74
1:A:44:ILE:O	1:A:48:VAL:HG23	1.87	0.74
1:A:129:LEU:HD22	1:D:170:ALA:HB3	1.68	0.74
1:A:234:PRO:HG2	1:A:235:ASP:H	1.52	0.74
1:L:318:LEU:C	1:L:318:LEU:HD12	2.12	0.74
1:D:27:THR:HG21	1:D:112:LYS:HZ2	1.52	0.74
1:D:263:LEU:HD12	1:D:263:LEU:N	2.03	0.74
1:H:195:LEU:HD21	1:H:198:LYS:HG2	1.68	0.74
1:D:157:ARG:HB2	1:D:303:LEU:O	1.88	0.74
1:H:91:THR:HB	1:H:94:LEU:HD21	1.69	0.74
1:D:11:ASN:O	1:D:194:ILE:HG23	1.88	0.74
1:H:94:LEU:O	1:H:103:ILE:HD12	1.87	0.74
1:A:149:GLU:OE2	1:A:310:ILE:HD13	1.87	0.73
1:L:201:LYS:HE2	1:L:201:LYS:HA	1.68	0.73
1:H:276:ARG:HG2	1:H:279:TYR:OH	1.88	0.73
1:A:185:MET:HG3	1:A:186:LEU:N	2.04	0.73
1:D:186:LEU:HD13	1:D:193:PHE:CE1	2.24	0.73
1:H:194:ILE:HD12	1:H:194:ILE:N	2.04	0.73
1:D:133:GLY:HA3	1:D:249:VAL:HG11	1.71	0.73
1:D:156:GLY:O	1:D:303:LEU:HD22	1.89	0.73
1:L:128:CYS:SG	1:L:130:VAL:HB	2.29	0.72
1:H:272:ASN:O	1:H:315:PRO:HD3	1.89	0.72
1:A:155:PRO:CG	1:A:158:ASN:HD21	2.01	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:194:ILE:HD12	1:H:194:ILE:H	1.54	0.72
1:D:119:PRO:O	1:D:134:THR:HA	1.90	0.72
1:A:95:VAL:HG13	1:A:310:ILE:HD12	1.69	0.72
1:A:104:ILE:HD11	1:A:148:SER:HA	1.71	0.72
1:A:278:LEU:HD12	1:A:310:ILE:O	1.89	0.72
1:D:29:GLU:HG2	1:H:22:ARG:HH22	1.51	0.72
1:L:272:ASN:HA	1:L:315:PRO:HD3	1.69	0.72
1:D:282:ASN:HB2	1:D:283:PRO:HD3	1.71	0.72
1:A:141:LYS:HZ1	1:A:147:PRO:HA	1.55	0.71
1:L:248:MET:HA	1:L:248:MET:CE	2.19	0.71
1:H:221:PRO:HB2	1:H:334:HIS:CE1	2.25	0.71
1:H:139:TYR:HE1	1:H:159:LEU:HG	1.55	0.71
1:D:82:MET:HE2	1:D:103:ILE:HG21	1.71	0.71
1:L:270:SER:C	1:L:272:ASN:H	1.98	0.71
1:L:53:ILE:HG23	1:L:54:ALA:N	2.04	0.71
1:A:49:ARG:NH2	1:A:171:THR:OG1	2.22	0.71
1:A:93:VAL:HG22	1:A:104:ILE:HD13	1.73	0.71
1:D:92:CYS:O	1:D:105:VAL:HB	1.90	0.71
1:L:112:LYS:HD2	1:L:140:ARG:NH1	2.06	0.71
1:L:156:GLY:CA	1:L:303:LEU:HD22	2.21	0.71
1:D:147:PRO:HA	1:D:151:ASP:OD2	1.90	0.71
1:L:183:CYS:HB2	1:L:196:VAL:HG22	1.72	0.71
1:L:276:ARG:HB2	1:L:279:TYR:CE1	2.26	0.71
1:D:186:LEU:O	1:D:188:PRO:HD3	1.91	0.70
1:H:269:LYS:NZ	1:H:274:LYS:HE2	2.06	0.70
1:L:237:SER:O	1:L:239:PRO:HD3	1.90	0.70
1:A:135:ILE:CD1	1:A:249:VAL:HG22	2.21	0.70
1:H:93:VAL:O	1:H:114:VAL:HG13	1.91	0.70
1:H:276:ARG:HD2	1:H:276:ARG:N	2.06	0.70
1:D:60:ALA:HB2	1:L:80:LEU:CD2	2.22	0.70
1:D:92:CYS:SG	1:D:93:VAL:N	2.63	0.70
1:D:107:PRO:HA	1:D:110:ARG:HE	1.56	0.70
1:D:204:LYS:HG2	1:D:322:ASP:OD1	1.92	0.70
1:D:225:GLU:O	1:D:229:ARG:HG2	1.91	0.70
1:D:270:SER:O	1:D:272:ASN:N	2.25	0.70
1:H:141:LYS:HE3	1:H:143:SER:O	1.90	0.70
1:A:11:ASN:HD21	1:A:16:PHE:CB	2.04	0.70
1:H:137:GLY:HA2	1:H:162:ALA:CB	2.22	0.70
1:A:10:VAL:HG22	1:A:11:ASN:N	2.03	0.70
1:A:235:ASP:OD2	1:A:237:SER:HB3	1.92	0.70
1:D:41:VAL:HG13	1:D:167:TYR:OH	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:313:ARG:O	1:L:314:ALA:HB2	1.91	0.70
1:H:50:LYS:HB3	1:H:53:ILE:HB	1.74	0.70
1:A:49:ARG:HH12	1:D:49:ARG:HH12	1.39	0.70
1:A:185:MET:HG3	1:A:186:LEU:H	1.56	0.70
1:H:137:GLY:HA2	1:H:162:ALA:HB2	1.73	0.70
1:D:86:LYS:O	1:D:109:LYS:HD3	1.92	0.70
1:A:226:TYR:O	1:A:230:LYS:CG	2.40	0.69
1:H:221:PRO:HB2	1:H:334:HIS:ND1	2.08	0.69
1:D:208:ILE:HD13	1:D:254:ARG:HD3	1.75	0.69
1:D:275:LEU:H	1:D:275:LEU:HD23	1.56	0.69
1:A:121:ASP:O	1:A:132:VAL:HG12	1.93	0.69
1:D:16:PHE:C	1:D:18:MET:H	1.99	0.69
1:D:82:MET:O	1:D:85:LEU:N	2.23	0.69
1:H:53:ILE:CD1	1:L:185:MET:HG2	2.15	0.69
1:L:302:VAL:HG12	1:L:303:LEU:N	2.06	0.69
1:H:150:LYS:HD3	1:H:150:LYS:C	2.18	0.69
1:L:288:MET:CG	1:L:318:LEU:HD13	2.22	0.69
1:A:95:VAL:HG12	1:A:96:SER:H	1.57	0.69
1:A:141:LYS:HZ1	1:A:147:PRO:CA	2.06	0.69
1:D:49:ARG:CD	1:D:49:ARG:N	2.56	0.69
1:L:13:LEU:O	1:L:17:VAL:HG23	1.93	0.69
1:L:106:GLU:O	1:L:110:ARG:HG3	1.92	0.69
1:L:276:ARG:HB2	1:L:279:TYR:HE1	1.57	0.69
1:A:227:ILE:HG22	1:A:231:LYS:CE	2.23	0.69
1:A:234:PRO:C	1:A:236:ASN:H	2.01	0.68
1:H:318:LEU:HD12	1:H:318:LEU:C	2.19	0.68
1:A:261:ILE:HD13	1:A:263:LEU:HD11	1.73	0.68
1:L:133:GLY:HA2	1:L:167:TYR:CD2	2.28	0.68
1:H:276:ARG:NH2	1:H:313:ARG:HH12	1.90	0.68
1:L:317:ILE:HG12	1:L:327:PHE:CE2	2.29	0.68
1:H:29:GLU:O	1:H:33:LEU:N	2.19	0.68
1:L:275:LEU:HD23	1:L:275:LEU:N	2.09	0.68
1:L:150:LYS:O	1:L:153:LEU:HB2	1.93	0.68
1:H:49:ARG:NH1	1:L:169:SER:O	2.27	0.68
1:A:226:TYR:O	1:A:230:LYS:HG2	1.92	0.68
1:L:184:PHE:HB3	1:L:193:PHE:HB3	1.76	0.68
1:D:274:LYS:O	1:D:313:ARG:HB3	1.94	0.67
1:L:183:CYS:O	1:L:195:LEU:HD12	1.93	0.67
1:A:94:LEU:CD2	1:A:115:VAL:HB	2.24	0.67
1:D:156:GLY:HA2	1:D:159:LEU:HG	1.75	0.67
1:L:133:GLY:HA2	1:L:167:TYR:HD2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:198:LYS:O	1:L:200:VAL:N	2.28	0.67
1:A:116:CYS:O	1:A:117:PHE:HB3	1.93	0.67
1:A:324:VAL:HA	1:A:327:PHE:HB3	1.76	0.67
1:A:248:MET:O	1:A:252:VAL:HG23	1.94	0.67
1:L:112:LYS:HD2	1:L:140:ARG:CZ	2.25	0.67
1:L:157:ARG:HG3	1:L:157:ARG:O	1.94	0.67
1:A:176:ALA:HB2	1:A:287:VAL:HG22	1.77	0.67
1:D:48:VAL:C	1:D:50:LYS:H	2.02	0.67
1:H:210:SER:O	1:H:211:LEU:HB3	1.94	0.67
1:L:112:LYS:HB2	1:L:140:ARG:NH1	2.09	0.67
1:A:216:ALA:HA	1:A:219:PHE:HD2	1.58	0.67
1:A:39:THR:HA	1:A:42:LYS:HE3	1.76	0.67
1:D:73:LEU:C	1:D:75:VAL:H	2.02	0.67
1:L:296:THR:HG21	1:L:328:LEU:HD21	1.76	0.67
1:A:227:ILE:HG22	1:A:231:LYS:HE2	1.77	0.67
1:D:54:ALA:O	1:D:57:TYR:N	2.26	0.66
1:D:153:LEU:HD22	1:D:307:PRO:O	1.96	0.66
1:L:181:VAL:HB	1:L:200:VAL:HB	1.77	0.66
1:L:305:VAL:O	1:L:307:PRO:HD3	1.94	0.66
1:D:120:LEU:HD23	1:D:123:SER:HB3	1.77	0.66
1:D:264:TYR:CE1	1:D:274:LYS:HB2	2.31	0.66
1:D:182:ASN:OD1	1:D:199:ASP:N	2.27	0.66
1:H:168:GLY:C	1:H:170:ALA:H	2.01	0.66
1:H:235:ASP:O	1:H:237:SER:N	2.29	0.66
1:A:234:PRO:O	1:A:236:ASN:N	2.27	0.66
1:H:9:ASP:CG	1:H:10:VAL:H	2.03	0.66
1:A:169:SER:O	1:D:49:ARG:NH1	2.29	0.66
1:H:58:GLY:O	1:H:60:ALA:N	2.28	0.66
1:H:13:LEU:HD12	1:H:13:LEU:O	1.95	0.66
1:L:185:MET:HB2	1:L:196:VAL:CG1	2.26	0.66
1:A:283:PRO:O	1:A:286:TYR:HB3	1.96	0.66
1:D:288:MET:SD	1:D:319:GLY:HA2	2.35	0.66
1:D:308:THR:HG22	1:D:309:ASP:N	2.11	0.66
1:H:299:LYS:O	1:H:300:GLU:HB3	1.95	0.66
1:D:309:ASP:O	1:D:311:HIS:N	2.28	0.66
1:H:82:MET:O	1:H:84:MET:N	2.29	0.66
1:A:19:GLU:HB3	1:A:23:LYS:NZ	2.11	0.66
1:A:165:ALA:HB2	1:A:173:LEU:HG	1.77	0.66
1:A:218:ASP:HB3	1:A:267:ASN:HB2	1.77	0.66
1:H:266:ALA:CB	1:H:271:PRO:HA	2.26	0.65
1:A:98:GLU:CG	1:A:119:PRO:HG3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:THR:CG2	1:D:112:LYS:HZ2	2.09	0.65
1:A:297:THR:HG22	1:A:302:VAL:HG22	1.78	0.65
1:D:60:ALA:HB2	1:L:80:LEU:HD23	1.77	0.65
1:D:278:LEU:HA	1:D:282:ASN:OD1	1.96	0.65
1:L:141:LYS:NZ	1:L:147:PRO:HA	2.11	0.65
1:L:313:ARG:HG2	1:L:313:ARG:HH11	1.60	0.65
1:D:92:CYS:SG	1:D:114:VAL:HG22	2.36	0.65
1:D:299:LYS:HG2	1:D:331:TYR:OH	1.97	0.65
1:H:218:ASP:O	1:H:267:ASN:HA	1.97	0.65
1:L:201:LYS:O	1:L:202:ILE:HB	1.97	0.65
1:D:104:ILE:HD12	1:D:148:SER:HA	1.79	0.65
1:H:168:GLY:C	1:H:170:ALA:N	2.50	0.65
1:D:73:LEU:O	1:D:75:VAL:N	2.30	0.64
1:L:111:GLY:O	1:L:113:TYR:N	2.30	0.64
1:A:196:VAL:HG12	1:D:57:TYR:CE2	2.33	0.64
1:D:46:SER:O	1:D:51:ALA:HB2	1.97	0.64
1:D:202:ILE:CG1	1:D:203:LYS:H	2.10	0.64
1:A:258:TYR:OH	1:D:125:ASN:HA	1.96	0.64
1:L:248:MET:HG3	1:L:249:VAL:N	2.12	0.64
1:A:39:THR:HG22	1:A:84:MET:HE2	1.78	0.64
1:D:207:LYS:HA	1:D:240:TYR:CE1	2.33	0.64
1:D:184:PHE:HB3	1:D:193:PHE:HB3	1.80	0.64
1:D:248:MET:O	1:D:251:ASP:N	2.31	0.64
1:H:230:LYS:HD2	1:H:230:LYS:N	2.13	0.64
1:H:317:ILE:HG12	1:H:327:PHE:CE2	2.33	0.64
1:L:97:GLU:HG3	1:L:276:ARG:CZ	2.28	0.64
1:L:211:LEU:HD22	1:L:263:LEU:HD13	1.78	0.64
1:D:221:PRO:C	1:D:223:VAL:N	2.55	0.64
1:H:169:SER:O	1:L:48:VAL:HG12	1.97	0.64
1:H:248:MET:SD	1:H:275:LEU:HD13	2.37	0.64
1:A:82:MET:HE2	1:A:103:ILE:HG21	1.80	0.63
1:H:112:LYS:HE2	1:H:113:TYR:CE2	2.33	0.63
1:H:128:CYS:HB3	1:L:258:TYR:HE2	1.62	0.63
1:L:46:SER:O	1:L:51:ALA:HB2	1.98	0.63
1:A:82:MET:CE	1:A:103:ILE:HG21	2.28	0.63
1:D:264:TYR:OH	1:D:274:LYS:HD2	1.98	0.63
1:H:294:MET:HB3	1:H:324:VAL:HG11	1.79	0.63
1:D:17:VAL:HG12	1:D:17:VAL:O	1.98	0.63
1:H:252:VAL:O	1:H:255:THR:HB	1.99	0.63
1:L:149:GLU:OE1	1:L:310:ILE:HD13	1.99	0.63
1:L:243:ARG:O	1:L:254:ARG:NH1	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:SER:O	1:A:84:MET:HE3	1.99	0.63
1:A:175:LEU:HD12	1:A:176:ALA:H	1.63	0.63
1:A:282:ASN:HB2	1:A:283:PRO:CD	2.28	0.63
1:A:77:SER:O	1:A:81:VAL:HG23	1.98	0.63
1:A:150:LYS:HA	1:A:153:LEU:HD12	1.79	0.63
1:A:169:SER:OG	1:D:129:LEU:HD22	1.99	0.63
1:D:91:THR:O	1:D:111:GLY:N	2.31	0.63
1:H:51:ALA:HA	1:L:188:PRO:CG	2.29	0.63
1:L:81:VAL:O	1:L:85:LEU:HB2	1.98	0.63
1:A:11:ASN:ND2	1:A:16:PHE:HB2	2.10	0.63
1:D:93:VAL:CG2	1:D:147:PRO:HB2	2.29	0.63
1:D:302:VAL:O	1:D:304:ASP:N	2.28	0.63
1:H:243:ARG:O	1:H:244:TYR:HB2	1.98	0.63
1:L:50:LYS:CG	1:L:53:ILE:HD12	2.29	0.63
1:A:49:ARG:NH1	1:D:49:ARG:HH12	1.96	0.63
1:D:73:LEU:C	1:D:75:VAL:N	2.53	0.63
1:D:229:ARG:C	1:D:230:LYS:HD2	2.24	0.63
1:H:49:ARG:HH11	1:H:49:ARG:HG3	1.63	0.63
1:H:155:PRO:HD2	1:H:158:ASN:ND2	2.14	0.63
1:A:40:ALA:HB2	1:A:84:MET:HG3	1.81	0.63
1:D:107:PRO:HA	1:D:110:ARG:NE	2.14	0.63
1:L:248:MET:HA	1:L:248:MET:HE3	1.81	0.63
1:D:138:ILE:CB	1:D:161:ALA:HB3	2.27	0.62
1:D:221:PRO:O	1:D:223:VAL:N	2.32	0.62
1:D:262:PHE:C	1:D:263:LEU:HD12	2.24	0.62
1:H:242:ALA:CB	1:L:213:GLU:HB2	2.29	0.62
1:A:141:LYS:NZ	1:A:147:PRO:HA	2.14	0.62
1:D:229:ARG:O	1:D:230:LYS:HD2	1.99	0.62
1:D:263:LEU:HA	1:D:317:ILE:HG13	1.80	0.62
1:L:203:LYS:HD2	1:L:258:TYR:O	1.99	0.62
1:A:205:LYS:HD2	1:A:240:TYR:OH	1.99	0.62
1:H:317:ILE:N	1:H:317:ILE:HD12	2.14	0.62
1:D:266:ALA:HB1	1:D:271:PRO:HA	1.82	0.62
1:H:269:LYS:HZ1	1:H:274:LYS:CE	2.12	0.62
1:L:302:VAL:O	1:L:305:VAL:HG23	1.98	0.62
1:D:91:THR:N	1:D:111:GLY:HA3	2.14	0.62
1:D:93:VAL:C	1:D:94:LEU:HD23	2.24	0.62
1:D:262:PHE:CE2	1:D:264:TYR:HB2	2.34	0.62
1:H:313:ARG:O	1:H:314:ALA:HB2	1.98	0.62
1:L:208:ILE:O	1:L:260:GLY:HA3	1.98	0.62
1:A:295:ALA:O	1:A:302:VAL:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:VAL:CG2	1:D:284:MET:HE3	2.26	0.62
1:A:25:ARG:HA	2:A:701:870:C18	2.30	0.62
1:A:46:SER:O	1:A:51:ALA:HB2	1.99	0.62
1:H:201:LYS:HG2	1:H:291:ALA:O	1.99	0.62
1:L:160:VAL:O	1:L:160:VAL:HG12	1.99	0.62
1:A:95:VAL:HG12	1:A:96:SER:N	2.15	0.61
1:A:252:VAL:HG11	1:A:284:MET:HE3	1.82	0.61
1:L:313:ARG:O	1:L:314:ALA:CB	2.48	0.61
1:A:193:PHE:C	1:A:194:ILE:HD12	2.26	0.61
1:H:172:MET:HE2	1:H:183:CYS:CB	2.25	0.61
1:L:274:LYS:O	1:L:274:LYS:HG2	2.01	0.61
1:A:317:ILE:HG12	1:A:327:PHE:CE2	2.35	0.61
1:A:318:LEU:HD12	1:A:318:LEU:C	2.24	0.61
1:H:157:ARG:N	1:H:303:LEU:HB3	2.16	0.61
1:D:252:VAL:O	1:D:255:THR:HB	2.01	0.61
1:L:221:PRO:HB2	1:L:334:HIS:CD2	2.31	0.61
1:A:175:LEU:HD12	1:A:176:ALA:N	2.15	0.61
1:D:117:PHE:HD1	1:D:117:PHE:H	1.47	0.61
1:H:172:MET:HB2	1:H:185:MET:SD	2.41	0.61
1:H:234:PRO:HG2	1:H:235:ASP:OD1	2.00	0.61
1:L:139:TYR:CE2	1:L:159:LEU:HD21	2.35	0.61
1:H:297:THR:HA	1:H:315:PRO:O	2.00	0.61
1:A:183:CYS:O	1:A:195:LEU:HD12	2.00	0.61
1:A:206:GLY:O	1:A:207:LYS:HG3	1.99	0.61
1:H:29:GLU:HB2	1:H:112:LYS:NZ	2.16	0.61
1:D:13:LEU:O	1:D:16:PHE:N	2.33	0.61
1:D:153:LEU:HD22	1:D:307:PRO:C	2.26	0.61
1:D:225:GLU:OE2	1:D:333:LYS:NZ	2.32	0.61
1:D:233:PRO:HG3	1:D:237:SER:O	2.00	0.61
1:D:278:LEU:HD23	1:D:282:ASN:OD1	2.01	0.61
1:H:252:VAL:HG22	1:H:318:LEU:HD21	1.83	0.61
1:L:153:LEU:HD22	1:L:307:PRO:O	2.01	0.61
1:L:308:THR:HG22	1:L:309:ASP:N	2.15	0.61
1:D:175:LEU:HD12	1:D:175:LEU:C	2.26	0.60
1:L:175:LEU:HD12	1:L:176:ALA:N	2.16	0.60
1:A:29:GLU:HB3	1:A:90:ALA:HB1	1.83	0.60
1:A:41:VAL:HG13	1:A:167:TYR:CE1	2.36	0.60
1:L:209:TYR:CA	1:L:261:ILE:HG22	2.29	0.60
1:D:207:LYS:HA	1:D:240:TYR:CD1	2.36	0.60
1:A:285:ALA:CB	1:A:303:LEU:HD21	2.31	0.60
1:H:177:MET:HB2	1:H:179:CYS:SG	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:51:ALA:O	1:L:53:ILE:N	2.32	0.60
1:A:15:ARG:HA	1:A:18:MET:HG3	1.82	0.60
1:A:42:LYS:O	1:L:190:ILE:HG22	2.02	0.60
1:D:118:ASP:HB3	1:D:135:ILE:HB	1.84	0.60
1:D:172:MET:SD	1:D:183:CYS:HB3	2.41	0.60
1:D:302:VAL:HG12	1:D:303:LEU:N	2.17	0.60
1:L:166:LEU:HD12	1:L:167:TYR:H	1.67	0.60
1:A:91:THR:O	1:A:110:ARG:HA	2.02	0.60
1:H:105:VAL:HG12	1:H:106:GLU:O	2.02	0.60
1:A:201:LYS:HA	1:A:291:ALA:O	2.02	0.60
1:H:211:LEU:HD11	1:H:219:PHE:HZ	1.66	0.60
1:A:14:THR:HG23	1:A:35:ASN:HD22	1.67	0.60
1:L:321:PRO:O	1:L:322:ASP:C	2.43	0.60
1:D:44:ILE:HG12	1:D:77:SER:OG	2.02	0.59
1:D:88:SER:O	1:D:89:PHE:HB2	2.01	0.59
1:H:134:THR:O	1:H:164:TYR:HB2	2.02	0.59
1:H:140:ARG:HB2	1:H:160:VAL:HG21	1.83	0.59
1:L:168:GLY:O	1:L:169:SER:C	2.44	0.59
1:L:332:GLU:C	1:L:334:HIS:H	2.08	0.59
1:A:190:ILE:HG22	1:L:43:ALA:HA	1.84	0.59
1:A:266:ALA:HB2	1:A:271:PRO:O	2.01	0.59
1:H:172:MET:SD	1:L:129:LEU:HD11	2.42	0.59
1:L:248:MET:HE2	1:L:252:VAL:HG23	1.83	0.59
1:A:94:LEU:HD23	1:A:115:VAL:HB	1.84	0.59
1:A:120:LEU:HG	1:A:120:LEU:O	2.00	0.59
1:D:242:ALA:O	1:D:243:ARG:CG	2.48	0.59
1:D:286:TYR:O	1:D:287:VAL:C	2.45	0.59
1:A:246:GLY:HA2	1:D:243:ARG:HE	1.66	0.59
1:D:195:LEU:HG	1:D:195:LEU:O	1.98	0.59
1:A:82:MET:HE1	1:A:94:LEU:HB2	1.84	0.59
1:H:49:ARG:HD2	1:H:49:ARG:N	2.17	0.59
1:H:16:PHE:CD1	1:H:16:PHE:C	2.80	0.59
1:H:226:TYR:O	1:H:230:LYS:HG2	2.03	0.59
1:H:243:ARG:HB3	1:H:254:ARG:NH2	2.17	0.59
1:H:78:ASN:OD1	1:H:119:PRO:HG3	2.02	0.59
1:L:223:VAL:O	1:L:225:GLU:N	2.36	0.59
1:L:309:ASP:O	1:L:311:HIS:N	2.35	0.59
1:A:140:ARG:HG3	1:A:141:LYS:O	2.02	0.58
1:H:9:ASP:CG	1:H:10:VAL:N	2.61	0.58
1:L:256:LEU:HD13	1:L:288:MET:CE	2.33	0.58
1:A:81:VAL:O	1:A:82:MET:C	2.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:MET:H	1:A:196:VAL:HG22	1.68	0.58
1:A:322:ASP:O	1:A:326:GLU:HB2	2.04	0.58
1:D:22:ARG:O	1:D:23:LYS:C	2.47	0.58
1:D:79:ASP:O	1:D:82:MET:N	2.36	0.58
1:D:260:GLY:N	1:D:320:SER:OG	2.35	0.58
1:L:120:LEU:HA	1:L:133:GLY:O	2.03	0.58
1:L:215:TYR:CE1	1:L:269:LYS:NZ	2.70	0.58
1:H:112:LYS:O	1:H:141:LYS:HB2	2.03	0.58
1:H:128:CYS:HB2	1:L:254:ARG:HA	1.86	0.58
1:L:80:LEU:O	1:L:81:VAL:C	2.45	0.58
1:A:209:TYR:HA	1:A:261:ILE:HG22	1.86	0.58
1:L:205:LYS:HG2	1:L:206:GLY:N	2.18	0.58
1:L:209:TYR:CB	1:L:261:ILE:HG22	2.34	0.58
1:A:106:GLU:O	1:A:110:ARG:HG3	2.04	0.58
1:D:208:ILE:CD1	1:D:254:ARG:HD3	2.33	0.58
1:L:184:PHE:CB	1:L:193:PHE:HB3	2.34	0.58
1:L:285:ALA:C	1:L:287:VAL:H	2.11	0.58
1:H:130:VAL:HG21	1:H:245:VAL:HG13	1.85	0.58
1:H:222:ALA:HA	1:H:334:HIS:NE2	2.18	0.58
1:L:90:ALA:CA	1:L:111:GLY:HA3	2.32	0.58
1:L:267:ASN:OD1	1:L:269:LYS:HB2	2.03	0.58
1:H:150:LYS:HA	1:H:153:LEU:CD1	2.32	0.57
1:L:221:PRO:CB	1:L:334:HIS:HD2	2.16	0.57
1:A:317:ILE:N	1:A:317:ILE:HD12	2.18	0.57
1:D:15:ARG:NH1	1:H:87:SER:O	2.37	0.57
1:H:125:ASN:O	1:H:130:VAL:HG12	2.04	0.57
1:H:333:LYS:C	1:H:335:SER:H	2.10	0.57
1:L:329:LYS:HZ3	1:L:330:VAL:N	2.02	0.57
1:A:165:ALA:HA	1:A:173:LEU:HA	1.87	0.57
1:A:264:TYR:CD1	1:A:275:LEU:HG	2.38	0.57
1:A:279:TYR:O	1:A:283:PRO:HG2	2.04	0.57
1:D:16:PHE:C	1:D:18:MET:N	2.62	0.57
1:D:294:MET:HB2	1:D:324:VAL:HG11	1.86	0.57
1:L:96:SER:C	1:L:98:GLU:H	2.12	0.57
1:L:112:LYS:HB2	1:L:140:ARG:HH12	1.69	0.57
1:L:210:SER:C	1:L:211:LEU:HD23	2.28	0.57
1:L:332:GLU:C	1:L:334:HIS:N	2.61	0.57
1:A:175:LEU:O	1:A:181:VAL:HG13	2.05	0.57
1:D:82:MET:SD	1:D:103:ILE:HD13	2.44	0.57
1:D:117:PHE:CD1	1:D:117:PHE:N	2.72	0.57
1:H:29:GLU:CD	1:H:112:LYS:NZ	2.62	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:MET:HE2	1:H:94:LEU:HD13	1.86	0.57
1:D:15:ARG:O	1:D:18:MET:HB2	2.03	0.57
1:D:276:ARG:O	1:D:280:GLU:HB2	2.05	0.57
1:L:26:GLY:HA3	2:L:1001:870:HN	1.69	0.57
1:L:230:LYS:HE2	1:L:240:TYR:CE2	2.39	0.57
1:A:278:LEU:HD11	1:A:310:ILE:HA	1.87	0.57
1:D:287:VAL:O	1:D:288:MET:C	2.48	0.57
1:H:82:MET:CG	1:H:86:LYS:HE3	2.34	0.57
1:A:264:TYR:CE1	1:A:275:LEU:HG	2.39	0.57
1:A:331:TYR:CD1	1:A:331:TYR:C	2.83	0.57
1:D:276:ARG:HG2	1:D:279:TYR:CZ	2.40	0.57
1:H:196:VAL:HG23	1:H:197:ASP:N	2.18	0.57
1:A:19:GLU:HB3	1:A:23:LYS:HZ2	1.69	0.57
1:D:13:LEU:O	1:D:14:THR:C	2.46	0.57
1:L:103:ILE:HD12	1:L:103:ILE:N	2.20	0.57
1:A:294:MET:O	1:A:295:ALA:HB2	2.05	0.57
1:D:264:TYR:CD2	1:D:275:LEU:HD21	2.40	0.57
1:H:121:ASP:OD2	1:H:248:MET:HB3	2.05	0.57
1:L:165:ALA:HB2	1:L:173:LEU:HD12	1.87	0.57
1:A:190:ILE:CG2	1:L:43:ALA:HA	2.35	0.56
1:A:228:GLN:HE22	1:A:232:PHE:HE2	1.51	0.56
1:H:273:GLY:HA3	1:H:314:ALA:H	1.70	0.56
1:L:270:SER:C	1:L:272:ASN:N	2.63	0.56
1:A:160:VAL:O	1:A:161:ALA:HB2	2.05	0.56
1:H:155:PRO:O	1:H:158:ASN:HB2	2.04	0.56
1:L:97:GLU:O	1:L:97:GLU:HG2	2.05	0.56
1:A:74:ASP:CG	1:A:123:SER:HG	2.13	0.56
1:A:186:LEU:HD22	1:A:193:PHE:CE1	2.39	0.56
1:A:242:ALA:HB3	1:D:213:GLU:H	1.71	0.56
1:A:282:ASN:O	1:A:283:PRO:C	2.48	0.56
1:D:49:ARG:H	1:D:49:ARG:HD3	1.70	0.56
1:D:245:VAL:HG23	1:D:251:ASP:OD1	2.06	0.56
1:H:80:LEU:O	1:H:81:VAL:C	2.49	0.56
1:H:176:ALA:HB2	1:H:287:VAL:HG22	1.88	0.56
1:L:105:VAL:HG12	1:L:106:GLU:N	2.21	0.56
1:A:224:THR:O	1:A:228:GLN:HG2	2.05	0.56
1:H:288:MET:HE2	1:H:288:MET:HA	1.87	0.56
1:A:31:THR:HG22	1:A:32:GLN:N	2.20	0.56
1:A:96:SER:C	1:A:98:GLU:H	2.12	0.56
1:D:155:PRO:HG2	1:D:158:ASN:HD21	1.70	0.56
1:L:277:LEU:HD11	1:L:282:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:MET:O	1:D:250:ALA:N	2.39	0.56
1:D:282:ASN:CB	1:D:283:PRO:HD3	2.34	0.56
1:H:126:ILE:HG12	1:H:126:ILE:O	2.05	0.56
1:A:53:ILE:HA	1:A:56:LEU:HD21	1.87	0.56
1:D:257:VAL:HG12	1:D:258:TYR:CD2	2.40	0.56
1:D:326:GLU:O	1:D:329:LYS:HB3	2.05	0.56
1:L:247:SER:O	1:L:248:MET:C	2.48	0.56
1:A:28:GLY:O	1:A:31:THR:HB	2.05	0.56
1:A:74:ASP:OD2	1:A:123:SER:OG	2.22	0.56
1:A:146:GLU:HG3	1:A:147:PRO:HD2	1.88	0.56
1:A:310:ILE:O	1:A:310:ILE:HG13	2.03	0.56
1:H:155:PRO:HG2	1:H:158:ASN:HB2	1.87	0.56
1:H:273:GLY:HA3	1:H:314:ALA:N	2.20	0.56
1:H:275:LEU:O	1:H:313:ARG:HA	2.06	0.56
1:D:194:ILE:N	1:D:194:ILE:CD1	2.69	0.56
1:D:278:LEU:O	1:D:283:PRO:HD3	2.06	0.56
1:H:149:GLU:O	1:H:150:LYS:C	2.48	0.56
1:A:256:LEU:HB2	1:A:288:MET:HE1	1.88	0.55
1:L:75:VAL:O	1:L:76:LEU:C	2.49	0.55
1:L:215:TYR:HE1	1:L:269:LYS:HZ1	1.48	0.55
1:L:226:TYR:O	1:L:229:ARG:HB2	2.06	0.55
1:A:25:ARG:HA	2:A:701:870:H18	1.87	0.55
1:A:263:LEU:HD12	1:A:263:LEU:N	2.20	0.55
1:A:296:THR:HG21	1:A:328:LEU:HG	1.87	0.55
1:H:166:LEU:HB2	1:H:249:VAL:CG1	2.36	0.55
1:L:248:MET:O	1:L:249:VAL:C	2.49	0.55
1:A:55:HIS:HA	1:A:59:ILE:HG22	1.89	0.55
1:D:49:ARG:N	1:D:49:ARG:HD2	2.22	0.55
1:H:172:MET:SD	1:H:253:HIS:HE1	2.30	0.55
1:H:222:ALA:HA	1:H:334:HIS:CD2	2.41	0.55
1:A:14:THR:CG2	1:A:35:ASN:HD22	2.19	0.55
1:A:334:HIS:N	1:A:334:HIS:CD2	2.74	0.55
1:H:194:ILE:O	1:H:196:VAL:HG13	2.07	0.55
1:L:53:ILE:HG23	1:L:54:ALA:H	1.70	0.55
1:H:24:ALA:O	1:H:25:ARG:HB2	2.05	0.55
1:L:223:VAL:O	1:L:224:THR:C	2.49	0.55
1:A:78:ASN:C	1:A:80:LEU:N	2.64	0.55
1:D:77:SER:O	1:D:78:ASN:C	2.49	0.55
1:D:118:ASP:CB	1:D:135:ILE:HD12	2.37	0.55
1:L:13:LEU:HA	1:L:184:PHE:CE2	2.41	0.55
1:L:216:ALA:HA	1:L:219:PHE:CD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:325:LEU:HA	1:L:328:LEU:HB2	1.89	0.55
1:L:185:MET:HB2	1:L:196:VAL:HG11	1.87	0.55
1:L:230:LYS:O	1:L:231:LYS:C	2.47	0.55
1:A:147:PRO:HA	1:A:151:ASP:OD2	2.07	0.55
1:H:168:GLY:O	1:H:170:ALA:N	2.39	0.55
1:L:30:LEU:O	1:L:33:LEU:HB3	2.06	0.55
1:L:108:GLU:CD	1:L:108:GLU:H	2.15	0.55
1:A:159:LEU:HD13	1:A:286:TYR:CD2	2.42	0.55
1:H:277:LEU:HB2	1:H:312:GLN:O	2.07	0.55
1:L:77:SER:O	1:L:80:LEU:N	2.40	0.55
1:A:332:GLU:O	1:A:335:SER:N	2.38	0.54
1:H:52:GLY:O	1:H:54:ALA:N	2.40	0.54
1:H:156:GLY:C	1:H:303:LEU:HD22	2.32	0.54
1:H:269:LYS:HZ1	1:H:274:LYS:HE2	1.72	0.54
1:L:52:GLY:O	1:L:56:LEU:CD1	2.52	0.54
1:A:221:PRO:HG2	1:A:222:ALA:H	1.72	0.54
1:A:48:VAL:HG12	1:A:49:ARG:HD2	1.89	0.54
1:A:277:LEU:CD1	1:A:282:ASN:HD21	2.19	0.54
1:D:53:ILE:O	1:D:56:LEU:HD23	2.06	0.54
1:H:165:ALA:HA	1:H:173:LEU:HA	1.89	0.54
1:A:52:GLY:O	1:A:54:ALA:N	2.40	0.54
1:A:158:ASN:O	1:A:159:LEU:C	2.50	0.54
1:H:266:ALA:HB1	1:H:271:PRO:HA	1.87	0.54
1:L:173:LEU:HD23	1:L:173:LEU:O	2.08	0.54
1:A:78:ASN:C	1:A:80:LEU:H	2.14	0.54
1:A:93:VAL:HG22	1:A:104:ILE:CD1	2.36	0.54
1:A:261:ILE:HG23	1:A:261:ILE:O	2.07	0.54
1:H:200:VAL:HG12	1:H:201:LYS:H	1.72	0.54
1:A:173:LEU:C	1:A:173:LEU:HD23	2.32	0.54
1:A:186:LEU:HB2	1:A:193:PHE:CE1	2.43	0.54
1:A:261:ILE:HB	1:A:323:ASP:HB3	1.89	0.54
1:D:253:HIS:O	1:D:256:LEU:N	2.40	0.54
1:H:18:MET:HG2	2:H:901:870:C13	2.37	0.54
1:H:80:LEU:O	1:H:82:MET:N	2.40	0.54
1:L:82:MET:O	1:L:83:ASN:C	2.49	0.54
1:L:171:THR:HB	1:L:186:LEU:HB3	1.89	0.54
1:L:248:MET:HA	1:L:248:MET:HE2	1.89	0.54
1:A:182:ASN:OD1	1:A:199:ASP:N	2.31	0.54
1:D:22:ARG:NH2	1:H:28:GLY:C	2.66	0.54
1:D:117:PHE:HD1	1:D:117:PHE:N	2.04	0.54
1:D:141:LYS:C	1:D:142:LYS:HD2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:SER:O	1:D:238:ALA:C	2.51	0.54
1:D:262:PHE:HE2	1:D:264:TYR:HB2	1.71	0.54
1:D:276:ARG:HG2	1:D:279:TYR:CE1	2.43	0.54
1:D:281:CYS:HB3	1:D:316:VAL:HG21	1.89	0.54
1:L:99:ASP:CB	1:L:103:ILE:HD11	2.30	0.54
1:A:155:PRO:CD	1:A:158:ASN:HD21	2.20	0.54
1:A:252:VAL:O	1:A:255:THR:HB	2.07	0.54
1:D:22:ARG:HH22	1:H:29:GLU:CA	2.20	0.54
1:D:221:PRO:C	1:D:223:VAL:H	2.13	0.54
1:D:286:TYR:HA	1:D:303:LEU:HD11	1.90	0.54
1:H:37:LEU:O	1:H:40:ALA:N	2.41	0.54
1:H:330:VAL:HG12	1:H:330:VAL:O	2.05	0.54
1:L:39:THR:HB	1:L:84:MET:HE2	1.90	0.54
1:L:313:ARG:HG2	1:L:313:ARG:NH1	2.22	0.54
1:D:39:THR:O	1:D:40:ALA:C	2.50	0.54
1:D:79:ASP:O	1:D:81:VAL:N	2.41	0.54
1:D:110:ARG:NH1	1:D:147:PRO:HG3	2.22	0.54
1:H:213:GLU:O	1:H:216:ALA:HB2	2.08	0.54
1:L:17:VAL:HG12	1:L:31:THR:OG1	2.08	0.54
1:L:55:HIS:HA	1:L:59:ILE:HG22	1.90	0.54
1:A:10:VAL:CG2	1:A:11:ASN:H	2.16	0.53
1:A:140:ARG:HG3	1:A:141:LYS:N	2.19	0.53
1:A:176:ALA:CB	1:A:287:VAL:HG22	2.39	0.53
1:H:92:CYS:SG	1:H:93:VAL:N	2.81	0.53
1:H:92:CYS:SG	1:H:114:VAL:HG23	2.48	0.53
1:L:77:SER:O	1:L:78:ASN:C	2.49	0.53
1:L:112:LYS:HE2	1:L:113:TYR:HE2	1.74	0.53
1:L:212:ASN:HA	1:L:244:TYR:CE2	2.43	0.53
1:A:40:ALA:O	1:A:44:ILE:HG13	2.08	0.53
1:D:139:TYR:CE1	1:D:159:LEU:HG	2.42	0.53
1:D:163:GLY:HA3	1:D:174:VAL:O	2.08	0.53
1:H:310:ILE:O	1:H:312:GLN:N	2.39	0.53
1:L:268:LYS:O	1:L:268:LYS:HG2	2.08	0.53
1:D:11:ASN:ND2	1:D:15:ARG:HG2	2.23	0.53
1:D:276:ARG:O	1:D:281:CYS:SG	2.62	0.53
1:H:143:SER:C	1:H:145:ASP:H	2.14	0.53
1:L:20:GLU:HA	1:L:20:GLU:OE1	2.07	0.53
1:L:218:ASP:O	1:L:267:ASN:HB3	2.08	0.53
1:A:49:ARG:NH1	1:D:49:ARG:NH1	2.56	0.53
1:A:153:LEU:HD22	1:A:307:PRO:O	2.09	0.53
1:H:194:ILE:HG12	1:L:54:ALA:CB	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:326:GLU:O	1:H:327:PHE:C	2.52	0.53
1:L:321:PRO:O	1:L:324:VAL:N	2.42	0.53
1:A:34:LEU:O	1:A:37:LEU:HB3	2.07	0.53
1:D:60:ALA:HB2	1:L:80:LEU:HD21	1.91	0.53
1:D:302:VAL:O	1:D:305:VAL:HG23	2.08	0.53
1:H:237:SER:O	1:H:238:ALA:C	2.52	0.53
1:L:166:LEU:HD13	1:L:249:VAL:HG12	1.91	0.53
1:A:141:LYS:HE3	1:A:143:SER:O	2.09	0.53
1:A:251:ASP:O	1:A:252:VAL:C	2.52	0.53
1:A:272:ASN:N	1:A:272:ASN:ND2	2.52	0.53
1:D:193:PHE:C	1:D:194:ILE:HD12	2.34	0.53
1:D:325:LEU:O	1:D:326:GLU:C	2.51	0.53
1:D:332:GLU:C	1:D:334:HIS:H	2.16	0.53
1:H:150:LYS:HD3	1:H:150:LYS:O	2.08	0.53
1:H:156:GLY:O	1:H:159:LEU:HD12	2.09	0.53
1:A:52:GLY:C	1:A:54:ALA:N	2.65	0.53
1:D:198:LYS:O	1:D:199:ASP:C	2.52	0.53
1:D:329:LYS:O	1:D:331:TYR:N	2.42	0.53
1:L:116:CYS:SG	1:L:139:TYR:CE2	3.02	0.53
1:A:125:ASN:O	1:A:130:VAL:HG12	2.08	0.53
1:A:141:LYS:HG3	1:A:151:ASP:OD1	2.08	0.53
1:D:29:GLU:OE1	1:D:112:LYS:HG2	2.09	0.53
1:D:226:TYR:CD1	1:D:327:PHE:HA	2.44	0.53
1:L:53:ILE:O	1:L:56:LEU:HB2	2.09	0.53
1:L:141:LYS:HZ1	1:L:147:PRO:HA	1.73	0.53
1:L:309:ASP:O	1:L:312:GLN:N	2.42	0.53
1:D:53:ILE:HG23	1:D:54:ALA:N	2.23	0.53
1:D:244:TYR:O	1:D:246:GLY:N	2.42	0.53
1:L:36:SER:CB	1:L:88:SER:HB3	2.39	0.53
1:L:203:LYS:O	1:L:320:SER:HB3	2.09	0.53
1:L:286:TYR:CD1	1:L:286:TYR:O	2.62	0.53
1:A:93:VAL:HG23	1:A:147:PRO:HB2	1.90	0.53
1:A:149:GLU:HG2	1:A:310:ILE:HG21	1.91	0.53
1:D:45:SER:HB2	1:D:167:TYR:HE1	1.73	0.53
1:D:191:GLY:HA3	1:H:191:GLY:HA3	1.91	0.53
1:D:49:ARG:N	1:D:49:ARG:HD3	2.25	0.52
1:D:81:VAL:HG11	1:D:117:PHE:CD2	2.43	0.52
1:H:228:GLN:OE1	1:H:228:GLN:HA	2.09	0.52
1:L:41:VAL:O	1:L:44:ILE:HB	2.09	0.52
1:L:219:PHE:HB3	1:L:224:THR:OG1	2.09	0.52
1:L:272:ASN:O	1:L:273:GLY:O	2.26	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:277:LEU:HD11	1:L:282:ASN:HD21	1.73	0.52
1:A:125:ASN:O	1:A:128:CYS:SG	2.67	0.52
1:A:242:ALA:CB	1:D:213:GLU:HB2	2.39	0.52
1:H:165:ALA:HB2	1:H:173:LEU:HG	1.90	0.52
1:H:276:ARG:HE	1:H:313:ARG:NH1	2.06	0.52
1:L:132:VAL:O	1:L:166:LEU:HD12	2.08	0.52
1:L:139:TYR:CD2	1:L:159:LEU:HD21	2.44	0.52
1:A:192:GLU:OE1	1:L:42:LYS:NZ	2.42	0.52
1:D:31:THR:CG2	1:D:31:THR:O	2.57	0.52
1:H:14:THR:HG22	1:H:18:MET:HE3	1.90	0.52
1:H:310:ILE:HG13	1:H:311:HIS:H	1.73	0.52
1:L:14:THR:O	1:L:18:MET:HG3	2.09	0.52
1:A:196:VAL:HG12	1:D:57:TYR:CZ	2.44	0.52
1:D:43:ALA:O	1:D:44:ILE:C	2.50	0.52
1:D:80:LEU:O	1:D:84:MET:HB2	2.09	0.52
1:D:262:PHE:C	1:D:262:PHE:CD2	2.87	0.52
1:D:287:VAL:O	1:D:290:LYS:N	2.39	0.52
1:H:251:ASP:O	1:H:252:VAL:C	2.53	0.52
1:H:310:ILE:C	1:H:312:GLN:H	2.18	0.52
1:A:183:CYS:O	1:A:196:VAL:HG23	2.09	0.52
1:H:91:THR:O	1:H:111:GLY:N	2.42	0.52
1:L:174:VAL:HG22	1:L:183:CYS:SG	2.49	0.52
1:L:181:VAL:C	1:L:182:ASN:CG	2.78	0.52
1:L:252:VAL:CG2	1:L:284:MET:HE3	2.38	0.52
1:A:120:LEU:HD11	1:A:132:VAL:HG11	1.92	0.52
1:L:46:SER:OG	1:L:51:ALA:HB2	2.09	0.52
1:L:51:ALA:C	1:L:53:ILE:H	2.17	0.52
1:L:225:GLU:O	1:L:226:TYR:C	2.53	0.52
1:A:105:VAL:HG11	1:A:109:LYS:O	2.10	0.52
1:A:173:LEU:C	1:A:173:LEU:CD2	2.83	0.52
1:A:261:ILE:CD1	1:A:263:LEU:HD11	2.39	0.52
1:D:317:ILE:HG21	1:D:327:PHE:CD2	2.45	0.52
1:H:13:LEU:CD2	1:H:173:LEU:HD13	2.39	0.52
1:H:48:VAL:C	1:H:50:LYS:H	2.16	0.52
1:H:211:LEU:CD1	1:H:219:PHE:HZ	2.23	0.52
1:L:130:VAL:HG22	1:L:131:SER:N	2.25	0.52
1:L:138:ILE:HG22	1:L:138:ILE:O	2.08	0.52
1:A:93:VAL:O	1:A:114:VAL:HG13	2.09	0.52
1:D:265:PRO:HA	1:D:315:PRO:HB2	1.91	0.52
1:H:44:ILE:O	1:H:48:VAL:HG23	2.10	0.52
1:H:279:TYR:N	1:H:279:TYR:CD2	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLU:O	1:A:23:LYS:HG3	2.10	0.52
1:D:33:LEU:O	1:D:34:LEU:C	2.50	0.52
1:D:120:LEU:HG	1:D:132:VAL:HG21	1.92	0.52
1:L:153:LEU:CD2	1:L:308:THR:O	2.57	0.52
1:A:185:MET:H	1:A:196:VAL:CG2	2.23	0.51
1:D:128:CYS:SG	1:D:130:VAL:HB	2.50	0.51
1:D:142:LYS:O	1:D:143:SER:O	2.27	0.51
1:H:277:LEU:HD23	1:H:312:GLN:NE2	2.25	0.51
1:L:185:MET:HB2	1:L:196:VAL:HG12	1.92	0.51
1:A:103:ILE:HG22	1:A:103:ILE:O	2.10	0.51
1:A:281:CYS:O	1:A:282:ASN:C	2.53	0.51
1:D:263:LEU:CB	1:D:317:ILE:HG13	2.40	0.51
1:H:99:ASP:O	1:H:100:LYS:C	2.53	0.51
1:A:52:GLY:O	1:A:53:ILE:C	2.53	0.51
1:H:13:LEU:HD12	1:H:13:LEU:C	2.34	0.51
1:H:97:GLU:HB2	1:H:279:TYR:CE1	2.45	0.51
1:H:162:ALA:O	1:H:176:ALA:HB3	2.09	0.51
1:L:40:ALA:O	1:L:44:ILE:HG13	2.10	0.51
1:L:288:MET:SD	1:L:318:LEU:HD13	2.50	0.51
1:A:31:THR:HG21	2:L:1001:870:H131	1.92	0.51
1:D:48:VAL:O	1:D:50:LYS:HD2	2.10	0.51
1:D:332:GLU:C	1:D:334:HIS:N	2.69	0.51
1:H:177:MET:HE1	2:H:901:870:CL2	2.48	0.51
1:L:296:THR:CG2	1:L:317:ILE:HB	2.41	0.51
1:A:22:ARG:O	1:A:24:ALA:N	2.43	0.51
1:A:190:ILE:HG13	1:A:191:GLY:N	2.24	0.51
1:A:211:LEU:HD23	1:A:211:LEU:O	2.10	0.51
1:A:248:MET:O	1:A:249:VAL:C	2.54	0.51
1:D:202:ILE:HD13	1:D:320:SER:N	2.25	0.51
1:D:243:ARG:HG2	1:D:243:ARG:HH11	1.75	0.51
1:H:81:VAL:HG12	1:H:85:LEU:HD11	1.92	0.51
1:H:108:GLU:N	1:H:108:GLU:CD	2.68	0.51
1:L:75:VAL:O	1:L:78:ASN:N	2.44	0.51
1:L:164:TYR:HH	1:L:253:HIS:HD1	1.55	0.51
1:L:186:LEU:HB2	1:L:193:PHE:CE1	2.45	0.51
1:A:85:LEU:O	1:A:86:LYS:C	2.53	0.51
1:A:301:ALA:HB3	1:A:304:ASP:OD2	2.10	0.51
1:D:92:CYS:SG	1:D:114:VAL:CG2	2.98	0.51
1:L:270:SER:O	1:L:272:ASN:N	2.43	0.51
1:L:317:ILE:HD12	1:L:317:ILE:N	2.26	0.51
1:A:39:THR:HA	1:A:42:LYS:CE	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LYS:O	1:D:188:PRO:HD2	2.10	0.51
1:A:187:ASP:HB2	1:D:53:ILE:CG2	2.41	0.51
1:A:288:MET:SD	1:A:318:LEU:HD13	2.50	0.51
1:D:122:GLY:HA3	1:D:247:SER:OG	2.11	0.51
1:D:160:VAL:HG12	1:D:160:VAL:O	2.10	0.51
1:H:16:PHE:HD2	1:H:195:LEU:HD13	1.76	0.51
1:H:92:CYS:SG	1:H:114:VAL:CG2	2.99	0.51
1:H:130:VAL:HG22	1:H:131:SER:N	2.26	0.51
1:H:278:LEU:HB2	1:H:279:TYR:CD2	2.46	0.51
1:L:218:ASP:HB3	1:L:267:ASN:HB2	1.92	0.51
1:L:272:ASN:HA	1:L:315:PRO:CD	2.40	0.51
1:A:49:ARG:O	1:A:50:LYS:O	2.29	0.51
1:A:185:MET:CG	1:A:186:LEU:N	2.73	0.51
1:D:317:ILE:HD12	1:D:317:ILE:N	2.24	0.51
1:L:53:ILE:CG2	1:L:54:ALA:N	2.72	0.51
1:A:49:ARG:HG3	1:D:169:SER:O	2.10	0.51
1:A:169:SER:OG	1:D:129:LEU:HA	2.10	0.51
1:D:299:LYS:O	1:D:300:GLU:CB	2.58	0.51
1:D:299:LYS:HE2	1:D:331:TYR:OH	2.11	0.51
1:L:285:ALA:C	1:L:287:VAL:N	2.69	0.51
1:A:31:THR:CG2	1:L:18:MET:HE2	2.41	0.51
1:A:136:PHE:CE1	1:A:162:ALA:HA	2.45	0.51
1:A:222:ALA:O	1:A:223:VAL:C	2.53	0.51
1:D:96:SER:C	1:D:98:GLU:H	2.18	0.51
1:L:156:GLY:C	1:L:303:LEU:HD22	2.36	0.51
1:A:175:LEU:HD11	1:A:177:MET:HG3	1.93	0.50
1:D:22:ARG:NH2	1:H:29:GLU:HG3	2.22	0.50
1:H:93:VAL:HB	1:H:114:VAL:HG22	1.93	0.50
1:H:167:TYR:CD1	1:H:171:THR:HG23	2.46	0.50
1:H:262:PHE:HB3	1:H:318:LEU:CG	2.33	0.50
1:L:58:GLY:O	1:L:60:ALA:N	2.44	0.50
1:L:263:LEU:N	1:L:263:LEU:HD12	2.26	0.50
1:H:13:LEU:HB3	1:H:193:PHE:HB2	1.92	0.50
1:H:98:GLU:HG3	1:H:119:PRO:HG3	1.92	0.50
1:H:221:PRO:O	1:H:224:THR:HB	2.09	0.50
1:H:253:HIS:O	1:H:256:LEU:N	2.44	0.50
1:L:31:THR:HG22	1:L:32:GLN:N	2.26	0.50
1:L:296:THR:HG23	1:L:317:ILE:HB	1.92	0.50
1:D:248:MET:O	1:D:249:VAL:C	2.54	0.50
1:D:288:MET:HG3	1:D:318:LEU:HD22	1.94	0.50
1:H:273:GLY:HA3	1:H:314:ALA:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:81:VAL:O	1:L:85:LEU:HD12	2.11	0.50
1:A:228:GLN:NE2	1:A:232:PHE:HE2	2.10	0.50
1:D:82:MET:CE	1:D:94:LEU:HD12	2.40	0.50
1:D:105:VAL:HG13	1:D:106:GLU:N	2.27	0.50
1:D:107:PRO:CA	1:D:110:ARG:HE	2.24	0.50
1:D:268:LYS:O	1:D:268:LYS:HG2	2.11	0.50
1:D:329:LYS:C	1:D:331:TYR:N	2.68	0.50
1:H:49:ARG:O	1:H:50:LYS:C	2.54	0.50
1:H:81:VAL:HG12	1:H:85:LEU:CD1	2.41	0.50
1:H:239:PRO:O	1:H:240:TYR:O	2.28	0.50
1:A:187:ASP:HB2	1:D:53:ILE:HG22	1.92	0.50
1:D:53:ILE:O	1:D:54:ALA:C	2.54	0.50
1:H:278:LEU:HD11	1:H:310:ILE:HA	1.92	0.50
1:L:73:LEU:O	1:L:73:LEU:HD12	2.12	0.50
1:D:155:PRO:HG2	1:D:158:ASN:ND2	2.27	0.50
1:H:128:CYS:O	1:H:129:LEU:HB2	2.12	0.50
1:H:185:MET:HG2	1:L:50:LYS:HG2	1.93	0.50
1:L:44:ILE:O	1:L:45:SER:C	2.52	0.50
1:L:80:LEU:C	1:L:82:MET:N	2.66	0.50
1:A:13:LEU:HB2	1:A:184:PHE:CD2	2.46	0.50
1:A:227:ILE:CG2	1:A:231:LYS:HE2	2.40	0.50
1:H:44:ILE:HD13	1:H:77:SER:CB	2.42	0.50
1:D:20:GLU:OE1	1:D:23:LYS:NZ	2.24	0.50
1:D:125:ASN:N	1:D:125:ASN:HD22	2.09	0.50
1:D:155:PRO:C	1:D:157:ARG:H	2.20	0.50
1:D:155:PRO:O	1:D:157:ARG:N	2.43	0.50
1:D:166:LEU:C	1:D:166:LEU:HD12	2.36	0.50
1:L:44:ILE:O	1:L:47:ALA:N	2.42	0.50
1:H:171:THR:O	1:H:171:THR:HG22	2.11	0.50
1:H:252:VAL:HG21	1:H:284:MET:HE3	1.94	0.50
1:L:58:GLY:O	1:L:61:GLY:N	2.44	0.50
1:L:81:VAL:HG11	1:L:117:PHE:CD2	2.47	0.50
1:A:41:VAL:CG1	1:A:167:TYR:HE1	2.25	0.49
1:A:88:SER:O	1:A:89:PHE:CB	2.53	0.49
1:D:42:LYS:O	1:D:45:SER:HB3	2.12	0.49
1:L:233:PRO:HG3	1:L:237:SER:O	2.11	0.49
1:L:249:VAL:O	1:L:250:ALA:C	2.54	0.49
1:A:102:ALA:CB	1:A:149:GLU:OE2	2.59	0.49
1:A:152:ALA:O	1:A:154:GLN:N	2.45	0.49
1:A:153:LEU:O	1:A:154:GLN:HG3	2.12	0.49
1:A:176:ALA:HA	1:A:181:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:LYS:HA	1:D:45:SER:HB3	1.93	0.49
1:D:82:MET:HE3	1:D:94:LEU:HD12	1.94	0.49
1:D:209:TYR:OH	1:D:231:LYS:NZ	2.45	0.49
1:D:221:PRO:O	1:D:222:ALA:C	2.53	0.49
1:H:29:GLU:HB2	1:H:112:LYS:HZ3	1.74	0.49
1:H:299:LYS:O	1:H:300:GLU:CB	2.61	0.49
1:A:226:TYR:CE2	1:A:261:ILE:HD13	2.47	0.49
1:D:93:VAL:HG22	1:D:104:ILE:HG23	1.93	0.49
1:H:172:MET:SD	1:H:253:HIS:CE1	3.05	0.49
1:A:155:PRO:HD2	1:A:158:ASN:HD21	1.78	0.49
1:A:262:PHE:C	1:A:263:LEU:HD12	2.38	0.49
1:A:309:ASP:C	1:A:311:HIS:H	2.20	0.49
1:D:17:VAL:HG13	2:D:801:870:CL2	2.48	0.49
1:D:36:SER:OG	1:H:15:ARG:HD3	2.13	0.49
1:D:264:TYR:CZ	1:D:274:LYS:HD2	2.46	0.49
1:H:15:ARG:O	1:H:19:GLU:CG	2.57	0.49
1:H:86:LYS:HG2	1:H:94:LEU:CD1	2.42	0.49
1:H:211:LEU:HD11	1:H:219:PHE:CZ	2.46	0.49
1:H:214:GLY:C	1:H:216:ALA:N	2.58	0.49
1:A:149:GLU:HG3	1:A:310:ILE:HG21	1.91	0.49
1:D:216:ALA:HA	1:D:219:PHE:CD2	2.48	0.49
1:L:20:GLU:O	1:L:21:GLY:C	2.55	0.49
1:L:166:LEU:HD12	1:L:167:TYR:N	2.27	0.49
1:A:51:ALA:O	1:D:187:ASP:OD1	2.31	0.49
1:D:15:ARG:C	1:D:18:MET:HB2	2.37	0.49
1:H:16:PHE:HZ	1:H:182:ASN:ND2	2.11	0.49
1:H:129:LEU:O	1:H:130:VAL:O	2.29	0.49
1:H:200:VAL:HG12	1:H:201:LYS:N	2.26	0.49
1:A:103:ILE:O	1:A:103:ILE:CG2	2.58	0.49
1:A:186:LEU:HD12	1:A:186:LEU:C	2.38	0.49
1:D:270:SER:C	1:D:272:ASN:N	2.51	0.49
1:H:212:ASN:HB2	1:H:244:TYR:CE2	2.47	0.49
1:L:82:MET:HE3	1:L:94:LEU:CD1	2.42	0.49
1:L:221:PRO:O	1:L:222:ALA:C	2.55	0.49
1:A:80:LEU:HD23	1:H:60:ALA:HA	1.94	0.49
1:A:253:HIS:O	1:A:256:LEU:N	2.44	0.49
1:D:132:VAL:HG23	1:D:133:GLY:N	2.28	0.49
1:D:316:VAL:O	1:D:317:ILE:HD12	2.11	0.49
1:H:151:ASP:O	1:H:154:GLN:NE2	2.45	0.49
1:L:59:ILE:HG12	1:L:59:ILE:O	2.13	0.49
1:L:297:THR:OG1	1:L:300:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:CG	1:A:158:ASN:ND2	2.67	0.49
1:D:186:LEU:O	1:D:188:PRO:CD	2.60	0.49
1:D:190:ILE:O	1:D:191:GLY:C	2.55	0.49
1:H:37:LEU:HD21	1:H:136:PHE:CE2	2.47	0.49
1:H:162:ALA:O	1:H:176:ALA:N	2.44	0.49
1:H:173:LEU:HD23	1:H:174:VAL:N	2.27	0.49
1:H:269:LYS:HZ2	1:H:274:LYS:HE2	1.77	0.49
1:D:94:LEU:O	1:D:103:ILE:HB	2.13	0.49
1:D:202:ILE:HD11	1:D:259:GLY:HA2	1.94	0.49
1:D:225:GLU:O	1:D:229:ARG:CG	2.60	0.49
1:D:230:LYS:HE3	1:D:230:LYS:HA	1.94	0.49
1:D:299:LYS:O	1:D:300:GLU:HB3	2.13	0.49
1:H:105:VAL:HG11	1:H:110:ARG:HA	1.95	0.49
1:A:150:LYS:HD2	1:A:153:LEU:HD12	1.94	0.48
1:A:170:ALA:HB3	1:D:129:LEU:CD1	2.43	0.48
2:A:701:870:HN22	1:L:27:THR:HA	1.78	0.48
1:D:244:TYR:O	1:D:244:TYR:CG	2.65	0.48
1:H:139:TYR:CE1	1:H:159:LEU:CG	2.93	0.48
1:H:223:VAL:HG21	1:H:265:PRO:HG3	1.94	0.48
1:L:50:LYS:HD2	1:L:50:LYS:H	1.73	0.48
1:L:123:SER:O	1:L:126:ILE:HB	2.13	0.48
1:L:215:TYR:HE1	1:L:269:LYS:NZ	2.10	0.48
1:L:253:HIS:O	1:L:254:ARG:C	2.56	0.48
1:A:118:ASP:OD2	1:A:280:GLU:OE1	2.31	0.48
1:H:16:PHE:CD2	1:H:195:LEU:HD13	2.48	0.48
1:L:245:VAL:HB	1:L:251:ASP:OD1	2.13	0.48
1:L:256:LEU:HD13	1:L:288:MET:HE1	1.95	0.48
1:L:256:LEU:HD13	1:L:288:MET:HE2	1.94	0.48
1:L:269:LYS:O	1:L:270:SER:OG	2.30	0.48
1:A:91:THR:C	1:A:105:VAL:HG21	2.37	0.48
1:D:16:PHE:O	1:D:18:MET:N	2.45	0.48
1:D:132:VAL:O	1:D:167:TYR:N	2.42	0.48
1:D:153:LEU:O	1:D:307:PRO:HB2	2.13	0.48
1:H:75:VAL:HG12	1:H:79:ASP:OD2	2.14	0.48
1:H:143:SER:OG	1:H:151:ASP:OD1	2.30	0.48
1:H:173:LEU:O	1:H:183:CYS:HA	2.13	0.48
1:H:326:GLU:O	1:H:328:LEU:N	2.46	0.48
1:L:58:GLY:HA2	1:L:62:SER:N	2.23	0.48
1:L:58:GLY:C	1:L:60:ALA:N	2.69	0.48
1:L:195:LEU:HD21	1:L:198:LYS:HG3	1.94	0.48
1:L:266:ALA:C	1:L:267:ASN:ND2	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:327:PHE:O	1:L:328:LEU:C	2.55	0.48
1:D:242:ALA:O	1:D:243:ARG:CB	2.62	0.48
1:H:45:SER:O	1:H:46:SER:C	2.56	0.48
1:H:161:ALA:O	1:H:162:ALA:HB2	2.13	0.48
1:L:79:ASP:O	1:L:82:MET:HB3	2.13	0.48
1:L:317:ILE:O	1:L:318:LEU:HB3	2.13	0.48
1:D:292:GLY:O	1:D:321:PRO:HG2	2.14	0.48
1:L:181:VAL:O	1:L:182:ASN:CG	2.57	0.48
1:A:117:PHE:HB2	1:A:135:ILE:O	2.12	0.48
1:A:159:LEU:HD13	1:A:286:TYR:CG	2.48	0.48
1:A:178:ASP:C	1:A:180:GLY:H	2.21	0.48
1:A:277:LEU:O	1:A:282:ASN:OD1	2.32	0.48
1:A:322:ASP:N	1:A:322:ASP:OD1	2.47	0.48
1:H:44:ILE:O	1:H:47:ALA:HB3	2.14	0.48
1:H:207:LYS:C	1:H:208:ILE:HG13	2.38	0.48
1:H:249:VAL:HG12	1:H:250:ALA:N	2.28	0.48
1:H:308:THR:O	1:H:309:ASP:HB2	2.13	0.48
1:A:53:ILE:HA	1:A:56:LEU:CD2	2.43	0.48
1:A:235:ASP:O	1:A:236:ASN:C	2.56	0.48
1:D:114:VAL:HG21	1:D:151:ASP:O	2.13	0.48
1:D:175:LEU:HD12	1:D:176:ALA:N	2.28	0.48
1:D:201:LYS:HA	1:D:291:ALA:HB1	1.94	0.48
1:D:202:ILE:HD11	1:D:320:SER:OG	2.13	0.48
1:D:262:PHE:O	1:D:317:ILE:HA	2.14	0.48
1:H:153:LEU:O	1:H:154:GLN:HG3	2.14	0.48
1:H:164:TYR:CZ	1:H:174:VAL:HG21	2.49	0.48
1:L:285:ALA:O	1:L:287:VAL:N	2.47	0.48
1:H:37:LEU:O	1:H:38:CYS:C	2.56	0.48
1:H:167:TYR:CE1	1:H:171:THR:HG23	2.48	0.48
1:H:185:MET:O	1:H:194:ILE:HD13	2.13	0.48
1:H:187:ASP:CG	1:L:51:ALA:O	2.57	0.48
1:H:194:ILE:N	1:H:194:ILE:CD1	2.75	0.48
1:H:281:CYS:O	1:H:285:ALA:N	2.41	0.48
1:L:78:ASN:HA	1:L:119:PRO:HB3	1.95	0.48
1:L:153:LEU:HD23	1:L:153:LEU:HA	1.72	0.48
1:L:227:ILE:HG22	1:L:231:LYS:HE2	1.95	0.48
1:A:157:ARG:NH1	1:A:289:GLU:OE2	2.47	0.48
1:A:185:MET:HB2	1:A:196:VAL:HG21	1.96	0.48
1:D:42:LYS:C	1:D:45:SER:HB3	2.38	0.48
1:D:227:ILE:C	1:D:229:ARG:N	2.70	0.48
1:H:248:MET:SD	1:H:275:LEU:CD1	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:141:LYS:HZ3	1:L:147:PRO:HA	1.79	0.48
1:D:54:ALA:O	1:D:56:LEU:N	2.47	0.48
1:D:112:LYS:HG3	1:D:113:TYR:CE1	2.48	0.48
1:L:214:GLY:C	1:L:216:ALA:H	2.22	0.48
1:A:39:THR:HB	1:A:84:MET:CE	2.44	0.47
1:D:150:LYS:C	1:D:152:ALA:H	2.22	0.47
1:D:263:LEU:CA	1:D:317:ILE:HG13	2.44	0.47
1:H:252:VAL:HB	1:H:284:MET:HE3	1.95	0.47
1:H:318:LEU:C	1:H:318:LEU:CD1	2.87	0.47
1:L:76:LEU:O	1:L:77:SER:C	2.57	0.47
1:L:126:ILE:O	1:L:129:LEU:N	2.40	0.47
1:L:223:VAL:C	1:L:225:GLU:N	2.71	0.47
1:A:17:VAL:HG13	2:A:701:870:CL2	2.51	0.47
1:A:185:MET:CG	1:A:186:LEU:H	2.25	0.47
1:D:285:ALA:HB1	1:D:295:ALA:HB3	1.96	0.47
1:H:85:LEU:HB3	1:H:91:THR:HG21	1.95	0.47
1:H:92:CYS:HA	1:H:105:VAL:HB	1.96	0.47
1:H:225:GLU:O	1:H:228:GLN:HB2	2.14	0.47
1:L:82:MET:O	1:L:85:LEU:HB2	2.14	0.47
1:A:105:VAL:HG12	1:A:106:GLU:N	2.29	0.47
1:A:228:GLN:NE2	1:A:232:PHE:CE2	2.82	0.47
1:A:246:GLY:HA2	1:D:243:ARG:NE	2.29	0.47
1:D:209:TYR:HE2	1:D:213:GLU:OE2	1.97	0.47
1:D:224:THR:HG22	1:D:224:THR:O	2.13	0.47
1:D:226:TYR:HA	1:D:229:ARG:HB2	1.96	0.47
1:D:267:ASN:CG	1:D:268:LYS:H	2.21	0.47
1:D:322:ASP:O	1:D:325:LEU:HB2	2.15	0.47
1:H:51:ALA:HA	1:L:188:PRO:HG2	1.96	0.47
1:H:84:MET:HA	1:H:87:SER:HB2	1.94	0.47
1:H:269:LYS:HZ1	1:H:274:LYS:HE3	1.79	0.47
1:L:155:PRO:HB3	1:L:305:VAL:O	2.15	0.47
1:L:277:LEU:HD12	1:L:277:LEU:O	2.14	0.47
1:A:20:GLU:HA	1:A:23:LYS:HD2	1.96	0.47
1:A:41:VAL:HG13	1:A:167:TYR:HE1	1.78	0.47
1:A:49:ARG:HH12	1:D:49:ARG:NH1	2.10	0.47
1:A:136:PHE:O	1:A:162:ALA:HB1	2.14	0.47
1:A:238:ALA:HA	1:A:239:PRO:HD3	1.74	0.47
1:D:274:LYS:O	1:D:275:LEU:O	2.33	0.47
1:H:10:VAL:HG22	1:H:11:ASN:H	1.78	0.47
1:L:97:GLU:HG3	1:L:276:ARG:NH1	2.30	0.47
1:L:149:GLU:O	1:L:152:ALA:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:VAL:CG1	1:D:106:GLU:N	2.75	0.47
1:D:202:ILE:CG1	1:D:203:LYS:N	2.65	0.47
1:H:252:VAL:CB	1:H:284:MET:HE3	2.45	0.47
1:H:258:TYR:O	1:H:259:GLY:O	2.32	0.47
1:L:112:LYS:HE2	1:L:113:TYR:CE2	2.50	0.47
1:L:266:ALA:O	1:L:267:ASN:ND2	2.47	0.47
1:A:31:THR:O	1:A:32:GLN:C	2.56	0.47
1:D:138:ILE:HB	1:D:161:ALA:CB	2.33	0.47
1:L:16:PHE:CD1	1:L:16:PHE:C	2.93	0.47
1:A:56:LEU:H	1:A:56:LEU:HD23	1.79	0.47
1:A:209:TYR:OH	1:A:231:LYS:HE2	2.14	0.47
1:D:16:PHE:C	1:D:16:PHE:CD1	2.92	0.47
1:D:88:SER:C	1:D:89:PHE:HD1	2.23	0.47
1:D:217:LYS:O	1:D:217:LYS:HG2	2.14	0.47
1:D:299:LYS:CG	1:D:331:TYR:OH	2.63	0.47
1:H:49:ARG:NH1	1:H:49:ARG:HG3	2.30	0.47
1:H:138:ILE:O	1:H:160:VAL:HB	2.15	0.47
1:H:149:GLU:O	1:H:153:LEU:HG	2.15	0.47
1:H:226:TYR:HE1	1:H:326:GLU:OE1	1.98	0.47
1:H:268:LYS:O	1:H:269:LYS:C	2.58	0.47
1:L:45:SER:O	1:L:49:ARG:HD3	2.14	0.47
1:L:261:ILE:O	1:L:261:ILE:HG23	2.15	0.47
1:A:15:ARG:NH1	1:L:36:SER:OG	2.45	0.47
1:A:297:THR:HG23	1:A:302:VAL:N	2.29	0.47
1:D:211:LEU:HD23	1:D:211:LEU:O	2.15	0.47
1:H:10:VAL:HG23	1:L:57:TYR:O	2.14	0.47
1:H:81:VAL:O	1:H:85:LEU:HG	2.15	0.47
1:H:92:CYS:O	1:H:105:VAL:HG23	2.13	0.47
1:H:276:ARG:HD2	1:H:276:ARG:H	1.78	0.47
1:A:220:ASP:HB2	1:A:221:PRO:CD	2.35	0.47
1:D:163:GLY:O	1:D:164:TYR:HB3	2.14	0.47
1:D:211:LEU:HD23	1:D:211:LEU:N	2.30	0.47
1:H:104:ILE:O	1:H:105:VAL:C	2.58	0.47
1:H:136:PHE:O	1:H:162:ALA:HB1	2.15	0.47
1:L:227:ILE:C	1:L:229:ARG:H	2.23	0.47
1:A:104:ILE:CD1	1:A:148:SER:HA	2.44	0.47
1:H:52:GLY:C	1:H:54:ALA:H	2.22	0.47
1:H:274:LYS:N	1:H:313:ARG:HB3	2.30	0.47
1:L:324:VAL:O	1:L:327:PHE:N	2.48	0.47
1:H:278:LEU:HB2	1:H:279:TYR:HD2	1.80	0.46
1:L:34:LEU:HD13	1:L:175:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:82:MET:CE	1:L:94:LEU:HD12	2.44	0.46
1:L:194:ILE:N	1:L:194:ILE:HD12	2.29	0.46
1:A:78:ASN:O	1:A:80:LEU:N	2.48	0.46
1:A:221:PRO:HG2	1:A:222:ALA:N	2.31	0.46
1:D:13:LEU:HD12	1:D:184:PHE:CZ	2.50	0.46
1:D:36:SER:O	1:D:84:MET:HE3	2.15	0.46
1:D:227:ILE:C	1:D:229:ARG:H	2.23	0.46
1:D:302:VAL:HG21	1:D:316:VAL:CG1	2.46	0.46
1:H:28:GLY:HA2	2:H:901:870:O1	2.15	0.46
1:H:149:GLU:C	1:H:151:ASP:N	2.71	0.46
1:H:195:LEU:CD2	1:H:198:LYS:HG2	2.44	0.46
1:A:58:GLY:O	1:D:10:VAL:HB	2.15	0.46
1:D:15:ARG:HA	1:D:18:MET:HB2	1.97	0.46
1:D:24:ALA:O	1:D:25:ARG:C	2.58	0.46
1:D:226:TYR:O	1:D:230:LYS:HG2	2.16	0.46
1:L:10:VAL:HG13	1:L:10:VAL:O	2.16	0.46
1:L:81:VAL:HG12	1:L:85:LEU:CD1	2.40	0.46
1:L:184:PHE:HA	1:L:194:ILE:O	2.14	0.46
1:A:141:LYS:HG2	1:A:142:LYS:N	2.30	0.46
1:A:234:PRO:CG	1:A:235:ASP:H	2.27	0.46
1:H:118:ASP:O	1:H:119:PRO:C	2.57	0.46
1:H:130:VAL:HG22	1:H:131:SER:H	1.80	0.46
1:H:185:MET:HB3	1:L:53:ILE:HD13	1.98	0.46
1:H:313:ARG:O	1:H:314:ALA:CB	2.64	0.46
1:L:205:LYS:HE3	1:L:240:TYR:OH	2.16	0.46
1:L:209:TYR:HB2	1:L:261:ILE:CG2	2.46	0.46
1:L:282:ASN:O	1:L:303:LEU:HD21	2.16	0.46
1:D:130:VAL:HG12	1:D:130:VAL:O	2.16	0.46
1:H:29:GLU:OE1	1:H:112:LYS:NZ	2.48	0.46
1:H:148:SER:O	1:H:151:ASP:HB2	2.15	0.46
1:H:230:LYS:C	1:H:232:PHE:N	2.72	0.46
1:L:144:THR:O	1:L:144:THR:HG22	2.16	0.46
1:L:219:PHE:CB	1:L:224:THR:OG1	2.62	0.46
1:A:29:GLU:OE1	1:A:112:LYS:HG2	2.15	0.46
1:A:45:SER:O	1:A:48:VAL:N	2.49	0.46
1:A:73:LEU:C	1:A:75:VAL:H	2.24	0.46
1:H:54:ALA:O	1:H:59:ILE:HG22	2.16	0.46
1:L:101:HIS:O	1:L:103:ILE:HD12	2.15	0.46
1:L:135:ILE:HG22	1:L:283:PRO:HG2	1.98	0.46
1:A:321:PRO:O	1:A:325:LEU:HG	2.16	0.46
1:D:13:LEU:HA	1:D:184:PHE:HE2	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ARG:HH22	1:H:29:GLU:CG	2.25	0.46
1:D:27:THR:C	2:H:901:870:HN22	2.23	0.46
1:L:75:VAL:O	1:L:78:ASN:HB3	2.16	0.46
1:L:201:LYS:O	1:L:202:ILE:CB	2.64	0.46
1:L:227:ILE:CG2	1:L:231:LYS:HE2	2.46	0.46
1:L:276:ARG:H	1:L:276:ARG:HD2	1.78	0.46
1:A:32:GLN:O	1:A:36:SER:N	2.39	0.46
1:A:208:ILE:HA	1:A:241:GLY:H	1.81	0.46
1:A:266:ALA:HB1	1:A:271:PRO:HA	1.98	0.46
1:D:79:ASP:O	1:D:80:LEU:C	2.59	0.46
1:D:81:VAL:HB	1:D:117:PHE:HE2	1.81	0.46
1:D:264:TYR:N	1:D:265:PRO:CD	2.79	0.46
1:H:33:LEU:C	1:H:33:LEU:HD12	2.41	0.46
1:L:130:VAL:CG2	1:L:131:SER:N	2.79	0.46
1:A:22:ARG:HG3	2:A:701:870:C10	2.46	0.46
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.97	0.46
1:D:22:ARG:HH22	1:H:29:GLU:HA	1.81	0.46
1:D:118:ASP:CG	1:D:135:ILE:HD12	2.41	0.46
1:H:106:GLU:OE2	1:H:109:LYS:NZ	2.41	0.46
1:H:135:ILE:HG23	1:H:249:VAL:HG23	1.98	0.46
1:L:198:LYS:O	1:L:199:ASP:C	2.59	0.46
1:L:201:LYS:O	1:L:291:ALA:HB1	2.16	0.46
1:A:95:VAL:O	1:A:96:SER:HB2	2.16	0.46
1:A:140:ARG:HB3	1:A:160:VAL:HG21	1.98	0.46
1:A:245:VAL:HG23	1:A:251:ASP:OD1	2.15	0.46
1:D:104:ILE:CD1	1:D:148:SER:HA	2.44	0.46
1:D:306:ILE:HA	1:D:307:PRO:HD3	1.63	0.46
1:D:329:LYS:O	1:D:330:VAL:C	2.59	0.46
1:H:93:VAL:HG22	1:H:147:PRO:CB	2.45	0.46
1:H:141:LYS:NZ	1:H:151:ASP:OD1	2.49	0.46
1:H:146:GLU:HA	1:H:147:PRO:HD2	1.66	0.46
1:H:330:VAL:O	1:H:330:VAL:CG1	2.64	0.46
1:A:39:THR:HB	1:A:84:MET:HE1	1.98	0.45
1:A:48:VAL:HG21	1:A:167:TYR:CD2	2.52	0.45
1:A:268:LYS:O	1:A:269:LYS:C	2.59	0.45
1:D:184:PHE:HA	1:D:194:ILE:O	2.14	0.45
1:L:205:LYS:HG2	1:L:206:GLY:H	1.81	0.45
1:A:201:LYS:HA	1:A:291:ALA:CA	2.46	0.45
1:A:256:LEU:O	1:A:256:LEU:HG	2.15	0.45
1:D:22:ARG:HH12	1:H:29:GLU:HG3	1.80	0.45
1:D:29:GLU:CG	1:H:22:ARG:NH2	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:SER:O	1:D:211:LEU:HB3	2.16	0.45
1:D:293:GLY:HA2	1:D:321:PRO:CG	2.36	0.45
1:H:29:GLU:CD	1:H:112:LYS:HZ3	2.23	0.45
1:H:122:GLY:O	1:H:126:ILE:HB	2.16	0.45
1:H:264:TYR:HE1	1:H:274:LYS:HG3	1.81	0.45
1:L:222:ALA:O	1:L:225:GLU:HB3	2.15	0.45
1:L:273:GLY:H	1:L:315:PRO:CG	2.19	0.45
1:A:194:ILE:HD12	1:A:194:ILE:N	2.31	0.45
1:A:297:THR:CG2	1:A:302:VAL:HA	2.46	0.45
1:D:219:PHE:HD1	1:D:219:PHE:HA	1.69	0.45
1:D:328:LEU:O	1:D:331:TYR:HB3	2.17	0.45
1:L:49:ARG:HG3	1:L:49:ARG:HH11	1.82	0.45
1:A:284:MET:O	1:A:285:ALA:C	2.59	0.45
1:A:288:MET:O	1:A:293:GLY:N	2.43	0.45
1:D:94:LEU:HD23	1:D:94:LEU:N	2.32	0.45
1:H:44:ILE:HG12	1:H:80:LEU:HD13	1.91	0.45
1:H:253:HIS:O	1:H:254:ARG:C	2.59	0.45
1:H:272:ASN:O	1:H:314:ALA:CA	2.55	0.45
1:A:333:LYS:HG2	1:A:334:HIS:CD2	2.52	0.45
1:H:16:PHE:C	1:H:16:PHE:HD1	2.24	0.45
1:H:42:LYS:O	1:H:45:SER:HB3	2.17	0.45
1:H:52:GLY:C	1:H:54:ALA:N	2.75	0.45
1:H:135:ILE:HD12	1:H:279:TYR:O	2.17	0.45
1:H:320:SER:O	1:H:324:VAL:HG23	2.16	0.45
1:L:125:ASN:O	1:L:130:VAL:HG12	2.17	0.45
1:L:193:PHE:C	1:L:194:ILE:HD12	2.41	0.45
1:L:250:ALA:O	1:L:251:ASP:C	2.59	0.45
1:A:331:TYR:CD1	1:A:331:TYR:O	2.69	0.45
1:D:43:ALA:C	1:D:45:SER:N	2.73	0.45
1:D:238:ALA:HA	1:D:239:PRO:HD3	1.87	0.45
1:H:78:ASN:O	1:H:79:ASP:C	2.60	0.45
1:H:156:GLY:C	1:H:303:LEU:HB3	2.41	0.45
1:H:252:VAL:CG2	1:H:284:MET:HE3	2.47	0.45
1:L:30:LEU:O	1:L:33:LEU:N	2.49	0.45
1:L:262:PHE:C	1:L:263:LEU:HD12	2.42	0.45
1:A:246:GLY:CA	1:D:243:ARG:HE	2.29	0.45
1:A:253:HIS:O	1:A:254:ARG:C	2.60	0.45
1:A:314:ALA:HA	1:A:315:PRO:HD3	1.66	0.45
1:D:99:ASP:OD2	1:D:103:ILE:HD11	2.17	0.45
1:D:160:VAL:O	1:D:160:VAL:CG1	2.65	0.45
1:H:256:LEU:O	1:H:256:LEU:HG	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273:GLY:HA3	1:H:314:ALA:CA	2.47	0.45
1:L:251:ASP:O	1:L:254:ARG:HB3	2.16	0.45
1:L:264:TYR:CG	1:L:275:LEU:HD21	2.50	0.45
1:A:85:LEU:C	1:A:88:SER:H	2.25	0.45
1:A:149:GLU:HG2	1:A:310:ILE:CG2	2.47	0.45
1:A:153:LEU:HD22	1:A:307:PRO:C	2.41	0.45
1:D:123:SER:O	1:D:126:ILE:HB	2.17	0.45
1:D:132:VAL:CG2	1:D:133:GLY:N	2.77	0.45
1:H:83:ASN:O	1:H:87:SER:OG	2.29	0.45
1:H:276:ARG:NE	1:H:313:ARG:NH1	2.65	0.45
1:L:283:PRO:O	1:L:286:TYR:N	2.49	0.45
1:A:18:MET:HE3	1:L:18:MET:HE3	1.98	0.45
1:A:170:ALA:HB3	1:D:129:LEU:HD13	1.98	0.45
1:D:158:ASN:O	1:D:159:LEU:C	2.58	0.45
1:A:30:LEU:O	1:A:33:LEU:CB	2.60	0.45
1:A:120:LEU:HD11	1:A:132:VAL:CG1	2.47	0.45
1:A:187:ASP:OD2	1:D:52:GLY:HA2	2.17	0.45
1:D:279:TYR:CD1	1:D:279:TYR:C	2.95	0.45
1:H:13:LEU:CB	1:H:193:PHE:HB2	2.46	0.45
1:H:76:LEU:HD12	1:H:76:LEU:O	2.17	0.45
1:H:138:ILE:N	1:H:161:ALA:O	2.50	0.45
1:H:194:ILE:H	1:H:194:ILE:CD1	2.25	0.45
1:L:80:LEU:O	1:L:82:MET:N	2.50	0.45
1:A:185:MET:O	1:A:193:PHE:HD1	2.01	0.44
1:D:91:THR:HA	1:D:113:TYR:O	2.17	0.44
1:D:130:VAL:O	1:D:131:SER:C	2.59	0.44
1:A:22:ARG:HD2	1:L:28:GLY:HA3	1.99	0.44
1:A:126:ILE:O	1:A:129:LEU:N	2.48	0.44
1:A:156:GLY:O	1:A:159:LEU:HD12	2.18	0.44
1:A:161:ALA:O	1:A:162:ALA:HB2	2.16	0.44
1:A:190:ILE:CG1	1:A:191:GLY:N	2.79	0.44
1:A:217:LYS:HA	1:D:232:PHE:HE1	1.82	0.44
1:A:223:VAL:O	1:A:224:THR:C	2.58	0.44
1:A:82:MET:HE1	1:A:103:ILE:HG21	1.98	0.44
1:D:55:HIS:HA	1:D:59:ILE:CG2	2.46	0.44
1:H:113:TYR:CE1	1:H:140:ARG:HD3	2.51	0.44
1:H:123:SER:O	1:H:126:ILE:HG22	2.16	0.44
1:H:155:PRO:HG2	1:H:158:ASN:CB	2.47	0.44
1:A:76:LEU:O	1:A:78:ASN:N	2.51	0.44
1:A:98:GLU:HG2	1:A:119:PRO:HG3	1.96	0.44
1:A:133:GLY:HA3	1:A:249:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:CYS:HB2	1:A:197:ASP:CB	2.47	0.44
1:D:48:VAL:C	1:D:50:LYS:N	2.68	0.44
1:H:262:PHE:N	1:H:318:LEU:O	2.37	0.44
1:L:277:LEU:HD21	1:L:307:PRO:HG3	1.99	0.44
1:A:267:ASN:HB2	1:A:268:LYS:H	1.46	0.44
1:H:202:ILE:HD13	1:H:320:SER:HA	2.00	0.44
1:H:279:TYR:HA	1:H:283:PRO:HG2	1.98	0.44
1:L:53:ILE:CG2	1:L:54:ALA:H	2.31	0.44
1:A:203:LYS:O	1:A:320:SER:OG	2.35	0.44
1:A:211:LEU:HD13	1:A:227:ILE:HD11	2.00	0.44
1:D:263:LEU:N	1:D:263:LEU:CD1	2.74	0.44
1:H:196:VAL:CG2	1:H:197:ASP:N	2.81	0.44
1:H:333:LYS:C	1:H:335:SER:N	2.75	0.44
1:L:58:GLY:C	1:L:60:ALA:H	2.26	0.44
1:L:225:GLU:OE2	1:L:330:VAL:CG2	2.66	0.44
1:L:309:ASP:C	1:L:311:HIS:N	2.76	0.44
1:L:330:VAL:O	1:L:331:TYR:C	2.58	0.44
1:A:92:CYS:SG	1:A:113:TYR:O	2.70	0.44
1:A:211:LEU:HB3	1:A:263:LEU:HB2	1.99	0.44
1:A:278:LEU:CD1	1:A:310:ILE:HA	2.47	0.44
1:A:322:ASP:C	1:A:324:VAL:H	2.26	0.44
1:D:50:LYS:HD2	1:D:50:LYS:N	2.33	0.44
1:H:269:LYS:NZ	1:H:274:LYS:CE	2.71	0.44
1:L:25:ARG:HA	2:L:1001:870:C14	2.48	0.44
1:L:36:SER:OG	1:L:88:SER:HB3	2.18	0.44
1:L:75:VAL:HG12	1:L:76:LEU:N	2.32	0.44
1:A:38:CYS:HG	1:A:193:PHE:HD2	1.64	0.44
1:A:120:LEU:CD1	1:A:132:VAL:HB	2.48	0.44
1:D:88:SER:O	1:D:89:PHE:CB	2.66	0.44
1:D:95:VAL:O	1:D:117:PHE:CD1	2.71	0.44
1:D:177:MET:O	1:D:178:ASP:C	2.60	0.44
1:D:245:VAL:N	1:D:251:ASP:OD1	2.51	0.44
1:D:261:ILE:HD13	1:D:263:LEU:HD11	2.00	0.44
1:D:79:ASP:HB3	1:L:60:ALA:O	2.17	0.43
1:L:42:LYS:HG3	1:L:193:PHE:CZ	2.53	0.43
1:L:82:MET:HE3	1:L:94:LEU:HD13	1.99	0.43
1:A:13:LEU:HA	1:A:184:PHE:CE2	2.53	0.43
1:A:97:GLU:HB2	1:A:279:TYR:CE1	2.53	0.43
1:A:148:SER:O	1:A:151:ASP:HB2	2.18	0.43
1:D:22:ARG:O	1:D:25:ARG:N	2.47	0.43
1:H:154:GLN:HG2	1:H:158:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:156:GLY:HA3	1:H:303:LEU:CD2	2.49	0.43
1:L:98:GLU:CG	1:L:119:PRO:HG3	2.48	0.43
1:L:209:TYR:HD1	1:L:240:TYR:HB3	1.83	0.43
1:A:155:PRO:CD	1:A:158:ASN:ND2	2.81	0.43
1:D:53:ILE:HA	1:D:56:LEU:CD2	2.49	0.43
1:D:118:ASP:HB3	1:D:135:ILE:CB	2.48	0.43
1:H:252:VAL:HB	1:H:284:MET:CE	2.48	0.43
1:L:78:ASN:OD1	1:L:98:GLU:HB2	2.18	0.43
1:L:133:GLY:HA3	1:L:249:VAL:HG11	2.00	0.43
1:L:135:ILE:HG22	1:L:136:PHE:N	2.33	0.43
1:L:261:ILE:O	1:L:261:ILE:CG2	2.64	0.43
1:A:234:PRO:C	1:A:236:ASN:N	2.67	0.43
1:A:289:GLU:OE2	1:A:303:LEU:CD1	2.51	0.43
1:D:133:GLY:HA2	1:D:165:ALA:O	2.18	0.43
1:D:262:PHE:CD2	1:D:263:LEU:N	2.86	0.43
1:D:276:ARG:O	1:D:281:CYS:N	2.45	0.43
1:H:164:TYR:OH	1:H:174:VAL:HG21	2.18	0.43
1:H:238:ALA:HA	1:H:239:PRO:HD3	1.69	0.43
1:H:270:SER:HA	1:H:271:PRO:HD3	1.75	0.43
1:L:37:LEU:O	1:L:38:CYS:C	2.61	0.43
1:L:164:TYR:OH	1:L:253:HIS:ND1	2.47	0.43
1:L:186:LEU:HB2	1:L:193:PHE:CD1	2.53	0.43
1:L:276:ARG:HD3	1:L:279:TYR:HE1	1.83	0.43
1:L:283:PRO:O	1:L:284:MET:C	2.60	0.43
1:A:201:LYS:HA	1:A:291:ALA:HB1	2.01	0.43
1:D:146:GLU:HG3	1:D:147:PRO:HD2	2.00	0.43
1:L:97:GLU:CD	1:L:276:ARG:NH1	2.77	0.43
1:L:204:LYS:HB2	1:L:204:LYS:HE3	1.83	0.43
1:L:327:PHE:O	1:L:330:VAL:N	2.51	0.43
1:A:121:ASP:HB3	1:A:249:VAL:HG23	2.00	0.43
1:H:24:ALA:HB1	2:H:901:870:CL1	2.55	0.43
1:H:79:ASP:O	1:H:80:LEU:O	2.37	0.43
1:H:82:MET:C	1:H:84:MET:H	2.25	0.43
1:H:251:ASP:HB2	1:H:262:PHE:CE1	2.54	0.43
1:L:267:ASN:OD1	1:L:269:LYS:CB	2.67	0.43
1:D:13:LEU:CA	1:D:184:PHE:CE2	2.96	0.43
1:D:97:GLU:OE2	1:D:118:ASP:CG	2.62	0.43
1:H:82:MET:O	1:H:85:LEU:N	2.52	0.43
1:H:185:MET:HB2	1:H:196:VAL:HG11	2.00	0.43
1:H:253:HIS:C	1:H:255:THR:N	2.73	0.43
1:L:275:LEU:O	1:L:276:ARG:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:HD2	1:A:158:ASN:ND2	2.34	0.43
1:A:226:TYR:O	1:A:230:LYS:HG3	2.16	0.43
1:D:208:ILE:HG22	1:D:260:GLY:HA3	2.01	0.43
1:D:281:CYS:O	1:D:282:ASN:C	2.60	0.43
1:H:17:VAL:HG13	2:H:901:870:CL2	2.56	0.43
1:H:187:ASP:OD2	1:L:51:ALA:O	2.37	0.43
1:L:81:VAL:O	1:L:82:MET:O	2.37	0.43
1:L:142:LYS:O	1:L:143:SER:O	2.37	0.43
1:L:202:ILE:HG22	1:L:291:ALA:O	2.19	0.43
1:L:267:ASN:HB2	1:L:268:LYS:H	1.59	0.43
1:A:78:ASN:CG	1:A:98:GLU:HG3	2.43	0.43
1:H:34:LEU:O	1:H:35:ASN:C	2.61	0.43
1:H:135:ILE:HG23	1:H:249:VAL:CG2	2.49	0.43
1:H:277:LEU:HD11	1:H:282:ASN:HD21	1.84	0.43
1:L:131:SER:HB2	1:L:250:ALA:HB2	2.00	0.43
1:A:141:LYS:C	1:A:142:LYS:HD2	2.44	0.43
1:A:221:PRO:O	1:A:222:ALA:C	2.61	0.43
1:A:226:TYR:O	1:A:226:TYR:CG	2.72	0.43
1:A:332:GLU:O	1:A:335:SER:O	2.36	0.43
1:D:59:ILE:HD11	1:L:43:ALA:CB	2.49	0.43
1:D:195:LEU:HD11	1:D:198:LYS:HG2	2.00	0.43
1:H:294:MET:HB3	1:H:324:VAL:CG1	2.46	0.43
1:L:160:VAL:O	1:L:161:ALA:HB2	2.18	0.43
1:L:175:LEU:HD12	1:L:175:LEU:C	2.43	0.43
1:D:143:SER:HB2	1:D:145:ASP:OD2	2.18	0.42
1:D:179:CYS:SG	1:D:180:GLY:N	2.92	0.42
1:H:166:LEU:C	1:H:166:LEU:HD12	2.44	0.42
1:D:54:ALA:O	1:D:55:HIS:C	2.63	0.42
1:H:34:LEU:HD11	1:H:177:MET:HE3	2.02	0.42
1:H:93:VAL:HB	1:H:114:VAL:CG2	2.49	0.42
1:H:184:PHE:HA	1:H:194:ILE:O	2.18	0.42
2:A:701:870:HN22	1:L:27:THR:CA	2.32	0.42
1:D:22:ARG:NH2	1:H:29:GLU:N	2.67	0.42
1:D:78:ASN:O	1:D:79:ASP:C	2.62	0.42
1:D:118:ASP:OD1	1:D:118:ASP:C	2.62	0.42
1:A:13:LEU:O	1:A:17:VAL:HG23	2.20	0.42
1:A:317:ILE:HG12	1:A:327:PHE:CZ	2.54	0.42
1:D:118:ASP:HB3	1:D:135:ILE:HD12	2.00	0.42
1:D:302:VAL:CG2	1:D:316:VAL:HG13	2.49	0.42
1:D:304:ASP:O	1:D:305:VAL:C	2.62	0.42
1:D:327:PHE:C	1:D:329:LYS:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:HA	1:A:48:VAL:HB	2.02	0.42
1:A:53:ILE:HD11	1:A:57:TYR:CE1	2.55	0.42
1:A:162:ALA:O	1:A:176:ALA:N	2.50	0.42
1:A:186:LEU:HD22	1:A:193:PHE:CZ	2.55	0.42
1:D:81:VAL:HB	1:D:117:PHE:CE2	2.55	0.42
1:D:82:MET:O	1:D:83:ASN:C	2.62	0.42
1:H:50:LYS:O	1:L:188:PRO:HD2	2.19	0.42
1:L:83:ASN:C	1:L:85:LEU:N	2.78	0.42
1:L:135:ILE:HG22	1:L:136:PHE:H	1.84	0.42
1:L:240:TYR:OH	1:L:323:ASP:OD1	2.28	0.42
1:L:322:ASP:O	1:L:326:GLU:HB2	2.20	0.42
1:A:96:SER:C	1:A:98:GLU:N	2.76	0.42
2:A:701:870:N2	1:L:27:THR:HA	2.34	0.42
1:D:286:TYR:CE1	1:D:290:LYS:HG3	2.55	0.42
1:H:86:LYS:HE2	1:H:94:LEU:HD12	2.01	0.42
1:H:263:LEU:HD12	1:H:263:LEU:N	2.34	0.42
1:L:203:LYS:HB3	1:L:205:LYS:O	2.20	0.42
1:L:333:LYS:C	1:L:334:HIS:ND1	2.78	0.42
1:A:43:ALA:HA	1:L:190:ILE:CG2	2.49	0.42
1:D:31:THR:O	1:D:31:THR:HG22	2.19	0.42
1:D:205:LYS:HA	1:D:322:ASP:HB2	2.00	0.42
1:L:50:LYS:CB	1:L:53:ILE:HD12	2.50	0.42
1:L:183:CYS:CB	1:L:196:VAL:HG22	2.46	0.42
1:L:276:ARG:CB	1:L:279:TYR:CE1	2.98	0.42
1:D:280:GLU:O	1:D:284:MET:HG2	2.19	0.42
1:D:302:VAL:HG21	1:D:316:VAL:HG11	2.01	0.42
1:H:112:LYS:HG3	1:H:113:TYR:N	2.35	0.42
1:H:115:VAL:HG13	1:H:138:ILE:HG12	2.02	0.42
1:H:331:TYR:C	1:H:331:TYR:CD1	2.98	0.42
1:L:51:ALA:C	1:L:53:ILE:N	2.77	0.42
1:L:91:THR:C	1:L:111:GLY:H	2.28	0.42
1:A:20:GLU:OE2	1:A:179:CYS:SG	2.77	0.42
1:A:107:PRO:HA	1:A:110:ARG:HD2	2.01	0.42
1:A:261:ILE:CD1	1:A:323:ASP:O	2.59	0.42
1:D:123:SER:C	1:D:125:ASN:H	2.27	0.42
1:D:134:THR:O	1:D:164:TYR:HB2	2.19	0.42
1:D:150:LYS:C	1:D:152:ALA:N	2.77	0.42
1:D:173:LEU:HG	1:D:174:VAL:N	2.34	0.42
1:H:45:SER:O	1:H:48:VAL:HG23	2.19	0.42
1:H:104:ILE:H	1:H:104:ILE:HG12	1.76	0.42
1:H:135:ILE:CD1	1:H:279:TYR:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:222:ALA:O	1:H:223:VAL:C	2.63	0.42
1:L:274:LYS:C	1:L:275:LEU:HD23	2.45	0.42
1:D:56:LEU:HG	1:D:57:TYR:HD1	1.85	0.42
1:D:75:VAL:O	1:D:76:LEU:C	2.60	0.42
1:D:321:PRO:O	1:D:324:VAL:HB	2.20	0.42
1:L:82:MET:CE	1:L:94:LEU:CD1	2.97	0.42
1:A:159:LEU:HD13	1:A:286:TYR:HB2	2.02	0.41
1:L:54:ALA:C	1:L:56:LEU:N	2.75	0.41
1:A:327:PHE:O	1:A:328:LEU:C	2.62	0.41
1:D:73:LEU:HD12	1:D:73:LEU:HA	1.83	0.41
1:D:131:SER:C	1:D:132:VAL:HG12	2.44	0.41
1:D:186:LEU:HB2	1:D:193:PHE:HE1	1.85	0.41
1:D:201:LYS:HE2	1:D:291:ALA:C	2.44	0.41
1:D:263:LEU:HB3	1:D:317:ILE:HG13	2.02	0.41
1:H:42:LYS:HZ3	1:H:192:GLU:HA	1.85	0.41
1:H:139:TYR:CE1	1:H:159:LEU:CD2	3.03	0.41
1:L:50:LYS:HG2	1:L:53:ILE:HD12	2.02	0.41
1:L:56:LEU:C	1:L:58:GLY:H	2.28	0.41
1:L:151:ASP:C	1:L:153:LEU:N	2.77	0.41
1:L:230:LYS:HE2	1:L:240:TYR:CD2	2.55	0.41
1:A:22:ARG:HD2	1:L:28:GLY:O	2.20	0.41
1:A:211:LEU:O	1:A:211:LEU:CG	2.68	0.41
1:A:230:LYS:C	1:A:233:PRO:HD3	2.41	0.41
1:A:243:ARG:O	1:A:244:TYR:HB2	2.20	0.41
1:A:252:VAL:CG1	1:A:284:MET:HE3	2.50	0.41
1:A:281:CYS:C	1:A:283:PRO:HD2	2.46	0.41
1:D:126:ILE:C	1:D:128:CYS:N	2.77	0.41
1:D:275:LEU:HD23	1:D:275:LEU:N	2.27	0.41
1:D:314:ALA:HA	1:D:315:PRO:HD3	1.88	0.41
1:H:82:MET:HE2	1:H:94:LEU:CD1	2.49	0.41
1:A:98:GLU:CD	1:A:119:PRO:HG3	2.44	0.41
1:A:173:LEU:HD12	1:A:193:PHE:CZ	2.55	0.41
1:A:277:LEU:O	1:A:278:LEU:C	2.62	0.41
1:D:42:LYS:CA	1:D:45:SER:HB3	2.50	0.41
1:D:134:THR:OG1	1:D:167:TYR:HE2	2.03	0.41
1:H:16:PHE:CD1	1:H:16:PHE:O	2.72	0.41
1:H:218:ASP:CG	1:H:268:LYS:HB2	2.45	0.41
1:L:14:THR:O	1:L:18:MET:SD	2.79	0.41
1:L:333:LYS:O	1:L:333:LYS:HG2	2.19	0.41
1:A:102:ALA:HB2	1:A:149:GLU:CD	2.45	0.41
1:A:211:LEU:HD21	1:A:213:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:C	1:A:318:LEU:CD1	2.93	0.41
1:D:22:ARG:NH2	1:H:29:GLU:CA	2.84	0.41
1:D:225:GLU:CD	1:D:333:LYS:HZ3	2.27	0.41
1:D:255:THR:O	1:D:259:GLY:HA2	2.20	0.41
1:H:166:LEU:HD12	1:H:167:TYR:N	2.36	0.41
1:H:187:ASP:C	1:H:189:ALA:H	2.28	0.41
1:H:239:PRO:O	1:H:240:TYR:C	2.63	0.41
1:L:37:LEU:HD21	1:L:136:PHE:CE2	2.56	0.41
1:L:50:LYS:HB3	1:L:53:ILE:HD12	2.02	0.41
1:L:77:SER:O	1:L:80:LEU:HB2	2.20	0.41
1:L:115:VAL:HG22	1:L:138:ILE:HG12	2.02	0.41
1:L:248:MET:CE	1:L:248:MET:CA	2.92	0.41
1:A:76:LEU:C	1:A:78:ASN:N	2.78	0.41
1:A:324:VAL:CA	1:A:327:PHE:HB3	2.49	0.41
1:H:96:SER:C	1:H:98:GLU:H	2.28	0.41
1:H:154:GLN:C	1:H:307:PRO:HG2	2.45	0.41
1:H:306:ILE:HA	1:H:307:PRO:HD3	1.81	0.41
1:L:91:THR:HG21	1:L:94:LEU:CD2	2.33	0.41
1:L:317:ILE:HG12	1:L:327:PHE:HE2	1.80	0.41
1:D:39:THR:CG2	1:D:84:MET:HE2	2.50	0.41
1:D:50:LYS:O	1:D:51:ALA:C	2.63	0.41
1:D:240:TYR:HB3	1:D:241:GLY:H	1.65	0.41
1:D:277:LEU:HB3	1:D:278:LEU:H	1.60	0.41
1:D:297:THR:HG21	1:D:305:VAL:HG21	2.02	0.41
1:D:317:ILE:N	1:D:317:ILE:CD1	2.82	0.41
1:H:30:LEU:HB2	1:H:113:TYR:CE2	2.56	0.41
1:L:276:ARG:HD3	1:L:279:TYR:CE1	2.55	0.41
1:H:127:ASP:C	1:H:129:LEU:H	2.27	0.41
1:H:274:LYS:HA	1:H:313:ARG:HD3	2.02	0.41
1:L:96:SER:C	1:L:98:GLU:N	2.76	0.41
1:L:114:VAL:HG12	1:L:115:VAL:N	2.36	0.41
1:L:149:GLU:O	1:L:150:LYS:C	2.63	0.41
1:L:297:THR:HA	1:L:315:PRO:O	2.21	0.41
1:A:32:GLN:HE22	1:L:22:ARG:HH21	1.69	0.41
1:A:36:SER:O	1:A:37:LEU:C	2.63	0.41
1:A:41:VAL:CG1	1:A:167:TYR:CE1	3.02	0.41
1:A:43:ALA:HA	1:L:190:ILE:HG21	2.03	0.41
1:A:91:THR:O	1:A:105:VAL:HG11	2.21	0.41
1:A:126:ILE:O	1:A:127:ASP:C	2.61	0.41
1:A:182:ASN:HB3	1:A:195:LEU:HD11	2.02	0.41
1:D:88:SER:C	1:D:89:PHE:CD1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:LEU:HD13	1:D:193:PHE:CD1	2.54	0.41
1:D:254:ARG:O	1:D:255:THR:C	2.64	0.41
1:H:13:LEU:O	1:H:16:PHE:HB3	2.21	0.41
1:H:58:GLY:C	1:H:60:ALA:N	2.79	0.41
1:H:143:SER:C	1:H:145:ASP:N	2.76	0.41
1:H:156:GLY:O	1:H:159:LEU:HB2	2.21	0.41
1:H:252:VAL:CG2	1:H:318:LEU:HD21	2.50	0.41
1:L:105:VAL:CG1	1:L:106:GLU:N	2.84	0.41
1:L:149:GLU:OE1	1:L:310:ILE:CD1	2.68	0.41
1:L:180:GLY:O	1:L:182:ASN:ND2	2.53	0.41
1:L:273:GLY:N	1:L:315:PRO:HG3	2.21	0.41
1:L:302:VAL:HG21	1:L:316:VAL:HG13	2.02	0.41
1:A:150:LYS:O	1:A:153:LEU:HB2	2.21	0.41
1:A:225:GLU:C	1:A:227:ILE:N	2.79	0.41
1:A:225:GLU:HA	1:A:228:GLN:HB2	2.02	0.41
1:D:309:ASP:C	1:D:311:HIS:N	2.78	0.41
1:H:277:LEU:HD11	1:H:282:ASN:ND2	2.35	0.41
1:H:318:LEU:HD12	1:H:319:GLY:N	2.36	0.41
1:L:138:ILE:HB	1:L:161:ALA:O	2.20	0.41
1:L:208:ILE:O	1:L:260:GLY:CA	2.69	0.41
1:L:277:LEU:CD1	1:L:282:ASN:ND2	2.84	0.41
1:A:318:LEU:HD12	1:A:318:LEU:O	2.21	0.40
1:D:226:TYR:CE1	1:D:327:PHE:HB2	2.56	0.40
1:D:332:GLU:O	1:D:334:HIS:N	2.54	0.40
1:L:24:ALA:O	1:L:25:ARG:C	2.61	0.40
1:L:73:LEU:O	1:L:74:ASP:C	2.64	0.40
1:L:223:VAL:HG12	1:L:224:THR:N	2.36	0.40
1:L:279:TYR:CD1	1:L:279:TYR:C	2.99	0.40
1:D:32:GLN:HE21	1:H:15:ARG:HG3	1.86	0.40
1:D:39:THR:HB	1:D:84:MET:HE2	2.03	0.40
1:D:49:ARG:HH11	1:D:49:ARG:HG3	1.86	0.40
1:D:81:VAL:O	1:D:85:LEU:HG	2.21	0.40
1:D:91:THR:HB	1:D:94:LEU:CD2	2.28	0.40
1:D:235:ASP:O	1:D:237:SER:N	2.54	0.40
1:D:292:GLY:O	1:D:321:PRO:CG	2.70	0.40
1:H:12:THR:O	1:H:13:LEU:C	2.64	0.40
1:H:45:SER:HA	1:H:167:TYR:CE1	2.56	0.40
1:H:130:VAL:CG2	1:H:245:VAL:HG13	2.50	0.40
1:H:142:LYS:HB2	1:H:154:GLN:NE2	2.36	0.40
1:H:227:ILE:HG22	1:H:231:LYS:CD	2.51	0.40
1:L:164:TYR:CD1	1:L:164:TYR:C	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:209:TYR:CB	1:L:261:ILE:CG2	2.99	0.40
1:D:39:THR:C	1:D:41:VAL:N	2.78	0.40
1:D:295:ALA:CB	1:D:318:LEU:HB3	2.52	0.40
1:H:49:ARG:N	1:H:49:ARG:CD	2.84	0.40
1:H:82:MET:C	1:H:84:MET:N	2.78	0.40
1:H:129:LEU:O	1:H:130:VAL:C	2.64	0.40
1:H:149:GLU:O	1:H:152:ALA:N	2.55	0.40
1:A:84:MET:O	1:A:88:SER:HB3	2.22	0.40
1:D:85:LEU:HD13	1:D:115:VAL:HG21	2.02	0.40
1:H:16:PHE:CZ	1:H:182:ASN:ND2	2.88	0.40
1:L:122:GLY:O	1:L:123:SER:C	2.63	0.40
1:L:246:GLY:O	1:L:247:SER:CB	2.69	0.40
1:A:28:GLY:O	1:A:29:GLU:C	2.65	0.40
1:A:73:LEU:C	1:A:75:VAL:N	2.80	0.40
1:A:186:LEU:O	1:A:188:PRO:CD	2.61	0.40
1:D:102:ALA:HB3	1:D:104:ILE:HD11	2.04	0.40
1:D:324:VAL:O	1:D:328:LEU:HB2	2.21	0.40
1:H:128:CYS:HA	1:L:257:VAL:HG21	2.03	0.40
1:H:209:TYR:CE1	1:H:242:ALA:HB2	2.57	0.40
1:H:313:ARG:HG2	1:H:313:ARG:HH11	1.87	0.40
1:L:141:LYS:NZ	1:L:151:ASP:OD2	2.53	0.40
1:L:266:ALA:O	1:L:267:ASN:CB	2.69	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	315/338 (93%)	207 (66%)	72 (23%)	36 (11%)	<b>0</b>   <b>5</b>
1	D	315/338 (93%)	192 (61%)	74 (24%)	49 (16%)	<b>0</b>   <b>2</b>
1	H	315/338 (93%)	211 (67%)	62 (20%)	42 (13%)	<b>0</b>   <b>3</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	315/338 (93%)	196 (62%)	73 (23%)	46 (15%)	0	3
All	All	1260/1352 (93%)	806 (64%)	281 (22%)	173 (14%)	0	3

All (173) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	51	ALA
1	A	123	SER
1	A	199	ASP
1	A	222	ALA
1	A	235	ASP
1	A	237	SER
1	A	295	ALA
1	D	10	VAL
1	D	51	ALA
1	D	80	LEU
1	D	82	MET
1	D	100	LYS
1	D	143	SER
1	D	178	ASP
1	D	236	ASN
1	D	240	TYR
1	D	243	ARG
1	D	245	VAL
1	D	249	VAL
1	D	267	ASN
1	D	270	SER
1	D	275	LEU
1	D	277	LEU
1	D	287	VAL
1	D	300	GLU
1	D	303	LEU
1	D	310	ILE
1	H	59	ILE
1	H	80	LEU
1	H	81	VAL
1	H	82	MET
1	H	83	ASN
1	H	100	LYS
1	H	130	VAL
1	H	236	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	240	TYR
1	H	244	TYR
1	H	300	GLU
1	H	310	ILE
1	H	311	HIS
1	L	51	ALA
1	L	82	MET
1	L	112	LYS
1	L	143	SER
1	L	199	ASP
1	L	202	ILE
1	L	221	PRO
1	L	223	VAL
1	L	247	SER
1	L	248	MET
1	L	249	VAL
1	L	267	ASN
1	L	273	GLY
1	L	310	ILE
1	L	314	ALA
1	A	50	LYS
1	A	77	SER
1	A	105	VAL
1	A	153	LEU
1	A	236	ASN
1	A	244	TYR
1	A	252	VAL
1	A	267	ASN
1	A	282	ASN
1	D	55	HIS
1	D	74	ASP
1	D	79	ASP
1	D	101	HIS
1	D	119	PRO
1	D	131	SER
1	D	156	GLY
1	D	222	ALA
1	D	248	MET
1	D	331	TYR
1	H	53	ILE
1	H	92	CYS
1	H	198	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	199	ASP
1	H	259	GLY
1	H	267	ASN
1	H	274	LYS
1	H	302	VAL
1	H	327	PHE
1	L	58	GLY
1	L	75	VAL
1	L	83	ASN
1	L	90	ALA
1	L	100	LYS
1	L	120	LEU
1	L	123	SER
1	L	124	SER
1	L	224	THR
1	L	286	TYR
1	L	302	VAL
1	L	321	PRO
1	L	322	ASP
1	L	324	VAL
1	A	117	PHE
1	A	129	LEU
1	A	161	ALA
1	A	203	LYS
1	A	331	TYR
1	D	17	VAL
1	D	54	ALA
1	D	124	SER
1	D	286	TYR
1	D	330	VAL
1	H	74	ASP
1	H	313	ARG
1	L	108	GLU
1	L	303	LEU
1	A	89	PHE
1	A	120	LEU
1	A	162	ALA
1	A	234	PRO
1	A	300	GLU
1	D	25	ARG
1	D	199	ASP
1	D	242	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	271	PRO
1	H	22	ARG
1	H	61	GLY
1	H	101	HIS
1	H	147	PRO
1	H	203	LYS
1	H	238	ALA
1	H	271	PRO
1	H	292	GLY
1	H	321	PRO
1	L	76	LEU
1	L	110	ARG
1	L	246	GLY
1	L	283	PRO
1	A	38	CYS
1	A	53	ILE
1	A	60	ALA
1	A	79	ASP
1	A	201	LYS
1	A	269	LYS
1	A	283	PRO
1	D	59	ILE
1	D	83	ASN
1	D	211	LEU
1	H	141	LYS
1	H	169	SER
1	H	211	LEU
1	H	222	ALA
1	H	309	ASP
1	L	77	SER
1	L	251	ASP
1	L	328	LEU
1	A	310	ILE
1	D	105	VAL
1	D	151	ASP
1	D	164	TYR
1	D	238	ALA
1	H	105	VAL
1	L	52	GLY
1	L	252	VAL
1	L	325	LEU
1	A	265	PRO

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Mol	Chain	Res	Type
1	D	315	PRO
1	H	119	PRO
1	L	59	ILE
1	L	61	GLY
1	L	200	VAL
1	L	270	SER
1	H	314	ALA
1	D	305	VAL
1	H	188	PRO
1	L	271	PRO
1	D	190	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	265/281 (94%)	240 (91%)	25 (9%)	8	31
1	D	265/281 (94%)	221 (83%)	44 (17%)	2	13
1	H	265/281 (94%)	234 (88%)	31 (12%)	5	24
1	L	265/281 (94%)	226 (85%)	39 (15%)	3	17
All	All	1060/1124 (94%)	921 (87%)	139 (13%)	4	20

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	33	LEU
1	A	49	ARG
1	A	50	LYS
1	A	74	ASP
1	A	79	ASP
1	A	89	PHE
1	A	103	ILE
1	A	107	PRO
1	A	123	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	130	VAL
1	A	131	SER
1	A	132	VAL
1	A	140	ARG
1	A	173	LEU
1	A	196	VAL
1	A	200	VAL
1	A	201	LYS
1	A	204	LYS
1	A	225	GLU
1	A	243	ARG
1	A	272	ASN
1	A	278	LEU
1	A	310	ILE
1	A	334	HIS
1	D	9	ASP
1	D	14	THR
1	D	18	MET
1	D	27	THR
1	D	31	THR
1	D	33	LEU
1	D	49	ARG
1	D	50	LYS
1	D	53	ILE
1	D	73	LEU
1	D	94	LEU
1	D	105	VAL
1	D	117	PHE
1	D	120	LEU
1	D	123	SER
1	D	124	SER
1	D	125	ASN
1	D	126	ILE
1	D	127	ASP
1	D	130	VAL
1	D	132	VAL
1	D	145	ASP
1	D	171	THR
1	D	173	LEU
1	D	194	ILE
1	D	195	LEU
1	D	196	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	199	ASP
1	D	208	ILE
1	D	219	PHE
1	D	220	ASP
1	D	236	ASN
1	D	261	ILE
1	D	263	LEU
1	D	272	ASN
1	D	275	LEU
1	D	305	VAL
1	D	308	THR
1	D	309	ASP
1	D	310	ILE
1	D	316	VAL
1	D	318	LEU
1	D	328	LEU
1	D	332	GLU
1	H	12	THR
1	H	13	LEU
1	H	16	PHE
1	H	17	VAL
1	H	27	THR
1	H	33	LEU
1	H	35	ASN
1	H	48	VAL
1	H	49	ARG
1	H	82	MET
1	H	103	ILE
1	H	104	ILE
1	H	115	VAL
1	H	126	ILE
1	H	135	ILE
1	H	166	LEU
1	H	178	ASP
1	H	194	ILE
1	H	197	ASP
1	H	200	VAL
1	H	219	PHE
1	H	220	ASP
1	H	224	THR
1	H	249	VAL
1	H	263	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	277	LEU
1	H	288	MET
1	H	294	MET
1	H	306	ILE
1	H	310	ILE
1	H	311	HIS
1	L	12	THR
1	L	13	LEU
1	L	27	THR
1	L	31	THR
1	L	32	GLN
1	L	33	LEU
1	L	50	LYS
1	L	56	LEU
1	L	62	SER
1	L	79	ASP
1	L	91	THR
1	L	106	GLU
1	L	108	GLU
1	L	123	SER
1	L	124	SER
1	L	126	ILE
1	L	145	ASP
1	L	146	GLU
1	L	149	GLU
1	L	181	VAL
1	L	196	VAL
1	L	197	ASP
1	L	217	LYS
1	L	220	ASP
1	L	245	VAL
1	L	248	MET
1	L	249	VAL
1	L	255	THR
1	L	263	LEU
1	L	272	ASN
1	L	275	LEU
1	L	277	LEU
1	L	279	TYR
1	L	310	ILE
1	L	316	VAL
1	L	320	SER

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Mol	Chain	Res	Type
1	L	329	LYS
1	L	330	VAL
1	L	335	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	35	ASN
1	A	154	GLN
1	A	158	ASN
1	A	228	GLN
1	A	272	ASN
1	A	282	ASN
1	A	334	HIS
1	D	101	HIS
1	D	125	ASN
1	D	158	ASN
1	D	212	ASN
1	D	272	ASN
1	H	158	ASN
1	H	212	ASN
1	H	272	ASN
1	H	282	ASN
1	H	334	HIS
1	L	35	ASN
1	L	55	HIS
1	L	228	GLN
1	L	282	ASN
1	L	334	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	870	H	901	-	33,33,33	2.64	13 (39%)	45,49,49	1.61	7 (15%)
2	870	A	701	-	33,33,33	2.42	11 (33%)	45,49,49	1.45	6 (13%)
2	870	D	801	-	33,33,33	2.46	15 (45%)	45,49,49	1.50	8 (17%)
2	870	L	1001	-	33,33,33	2.36	11 (33%)	45,49,49	1.71	7 (15%)

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	870	H	901	-	-	6/15/17/17	0/4/4/4
2	870	A	701	-	-	4/15/17/17	0/4/4/4
2	870	D	801	-	-	6/15/17/17	0/4/4/4
2	870	L	1001	-	-	9/15/17/17	0/4/4/4

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	901	870	C6-N	8.57	1.52	1.36
2	A	701	870	C6-N	6.99	1.49	1.36
2	L	1001	870	C6-N	6.46	1.48	1.36
2	D	801	870	C11-C12	5.65	1.51	1.41
2	H	901	870	C10-C9	5.34	1.47	1.39
2	A	701	870	C11-C12	5.16	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1001	870	C11-C12	5.16	1.50	1.41
2	H	901	870	C6-N1	5.10	1.39	1.30
2	A	701	870	C6-N1	4.92	1.38	1.30
2	H	901	870	C11-C12	4.69	1.49	1.41
2	D	801	870	C6-N	4.66	1.45	1.36
2	L	1001	870	C6-N1	4.28	1.37	1.30
2	D	801	870	C11-C17	4.28	1.57	1.49
2	A	701	870	C11-C17	4.12	1.56	1.49
2	D	801	870	C16-C17	4.12	1.46	1.39
2	L	1001	870	C5-C4	3.96	1.45	1.40
2	D	801	870	C6-N1	3.86	1.36	1.30
2	D	801	870	C16-C19	3.78	1.45	1.39
2	H	901	870	C5-C4	3.40	1.44	1.40
2	L	1001	870	C8-C9	3.17	1.44	1.39
2	D	801	870	O3-C12	-3.17	1.33	1.38
2	A	701	870	C5-C4	3.16	1.44	1.40
2	D	801	870	C10-C9	3.04	1.44	1.39
2	D	801	870	C12-C7	3.04	1.41	1.38
2	H	901	870	C1-C2	2.94	1.43	1.38
2	A	701	870	C10-C9	2.75	1.43	1.39
2	D	801	870	C14-C15	2.75	1.43	1.38
2	A	701	870	O3-C12	-2.73	1.34	1.38
2	L	1001	870	C3-C4	2.70	1.43	1.39
2	L	1001	870	C1-C2	2.61	1.42	1.38
2	H	901	870	C10-C11	2.54	1.43	1.39
2	A	701	870	C16-C17	2.50	1.44	1.39
2	D	801	870	C18-C17	2.49	1.44	1.39
2	L	1001	870	C16-C17	2.42	1.44	1.39
2	L	1001	870	C11-C17	2.41	1.53	1.49
2	L	1001	870	C4-S	2.39	1.80	1.77
2	H	901	870	C8-C9	2.27	1.42	1.39
2	H	901	870	C11-C17	2.25	1.53	1.49
2	A	701	870	C1-C	2.22	1.42	1.38
2	L	1001	870	C12-C7	2.19	1.40	1.38
2	H	901	870	C18-C17	2.16	1.43	1.39
2	A	701	870	C16-C19	2.14	1.43	1.39
2	D	801	870	C-C5	2.12	1.43	1.38
2	H	901	870	C14-C18	2.11	1.42	1.38
2	A	701	870	C-C5	2.08	1.43	1.38
2	D	801	870	C3-C2	2.07	1.41	1.38
2	D	801	870	O2-S	2.05	1.45	1.43
2	H	901	870	C12-C7	2.03	1.40	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	870	C5-C4	2.02	1.42	1.40
2	H	901	870	C2-CL2	-2.01	1.69	1.74

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	901	870	C8-C7-C12	5.71	125.37	120.81
2	A	701	870	C8-C7-C12	5.19	124.95	120.81
2	L	1001	870	O2-S-O1	-5.18	113.22	119.52
2	L	1001	870	C8-C7-C12	4.81	124.65	120.81
2	D	801	870	C8-C7-C12	4.59	124.47	120.81
2	L	1001	870	O1-S-C4	3.85	114.03	107.68
2	A	701	870	O3-C12-C11	3.82	133.47	125.93
2	H	901	870	O3-C12-C7	3.80	111.87	107.69
2	D	801	870	O2-S-O1	-3.66	115.08	119.52
2	L	1001	870	O3-C12-C7	3.31	111.33	107.69
2	L	1001	870	C-C5-C4	3.17	122.11	120.04
2	D	801	870	C-C5-C4	3.13	122.08	120.04
2	L	1001	870	C4-S-N	3.01	109.70	105.96
2	D	801	870	O3-C12-C7	2.84	110.81	107.69
2	A	701	870	O2-S-O1	-2.72	116.21	119.52
2	D	801	870	O3-C12-C11	2.72	131.28	125.93
2	H	901	870	O2-S-O1	-2.63	116.32	119.52
2	H	901	870	C12-C7-N1	-2.60	106.34	108.73
2	A	701	870	C4-S-N	2.55	109.13	105.96
2	H	901	870	O3-C6-N1	-2.54	111.01	115.57
2	L	1001	870	O3-C12-C11	2.50	130.87	125.93
2	A	701	870	O3-C6-N1	-2.50	111.07	115.57
2	D	801	870	C12-C7-N1	-2.35	106.57	108.73
2	A	701	870	O3-C12-C7	2.16	110.07	107.69
2	D	801	870	C4-S-N	2.15	108.64	105.96
2	H	901	870	C14-C18-C17	2.15	122.99	120.54
2	H	901	870	C5-C4-S	2.11	124.65	123.19
2	D	801	870	C5-C4-S	2.08	124.63	123.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	801	870	C8-C9-O4-C13
2	D	801	870	C10-C9-O4-C13
2	D	801	870	C10-C11-C17-C18

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Mol	Chain	Res	Type	Atoms
2	L	1001	870	C10-C9-O4-C13
2	A	701	870	C10-C11-C17-C18
2	H	901	870	C10-C11-C17-C18
2	L	1001	870	C10-C11-C17-C18
2	L	1001	870	C8-C9-O4-C13
2	D	801	870	C10-C11-C17-C16
2	L	1001	870	C10-C11-C17-C16
2	A	701	870	C10-C11-C17-C16
2	H	901	870	C10-C11-C17-C16
2	H	901	870	C12-C11-C17-C18
2	L	1001	870	C12-C11-C17-C18
2	D	801	870	C12-C11-C17-C18
2	H	901	870	C8-C9-O4-C13
2	A	701	870	C12-C11-C17-C18
2	L	1001	870	C12-C11-C17-C16
2	H	901	870	C10-C9-O4-C13
2	H	901	870	C12-C11-C17-C16
2	D	801	870	C12-C11-C17-C16
2	A	701	870	C12-C11-C17-C16
2	L	1001	870	C6-N-S-O2
2	L	1001	870	C6-N-S-C4
2	L	1001	870	C6-N-S-O1

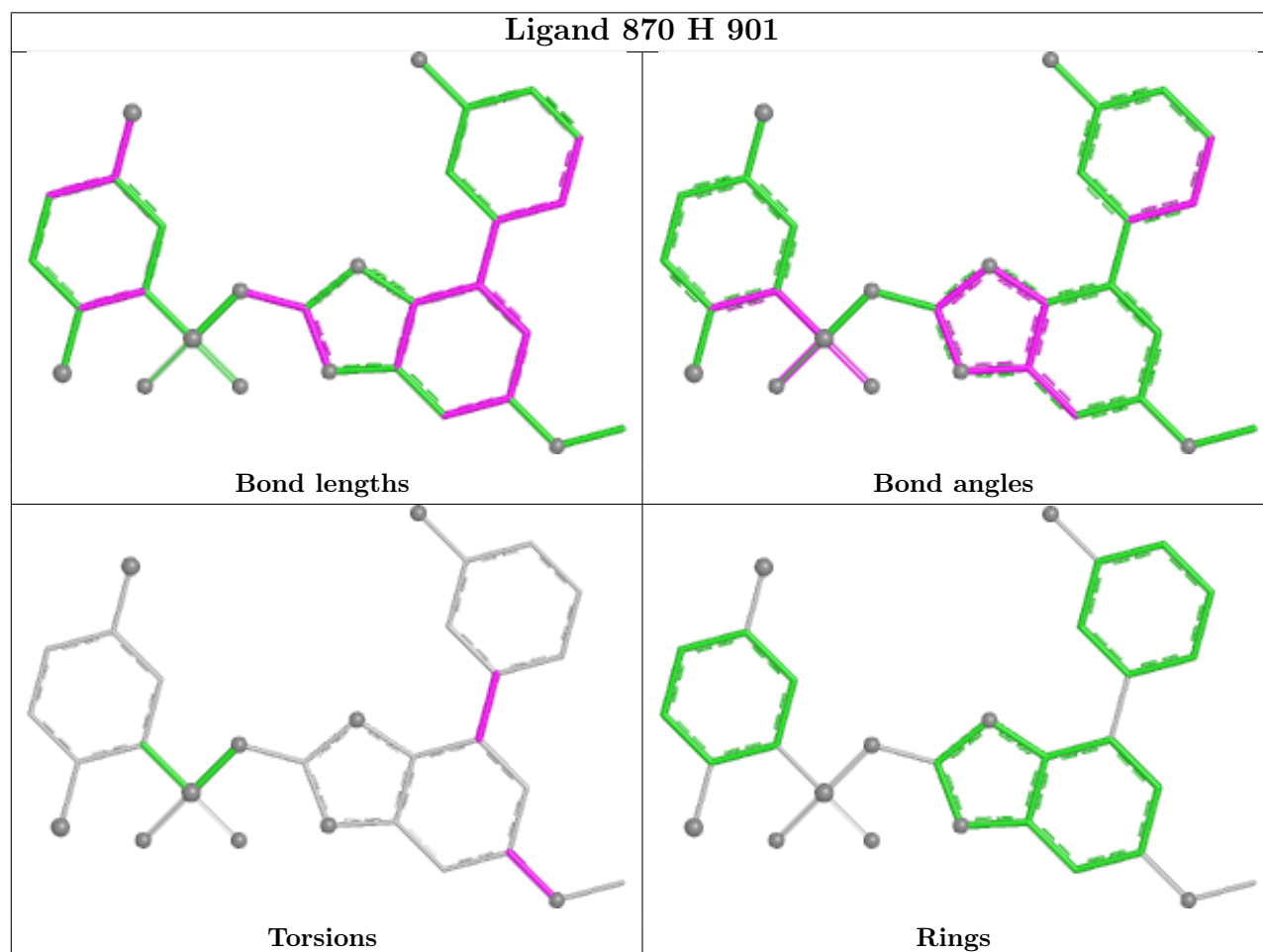
There are no ring outliers.

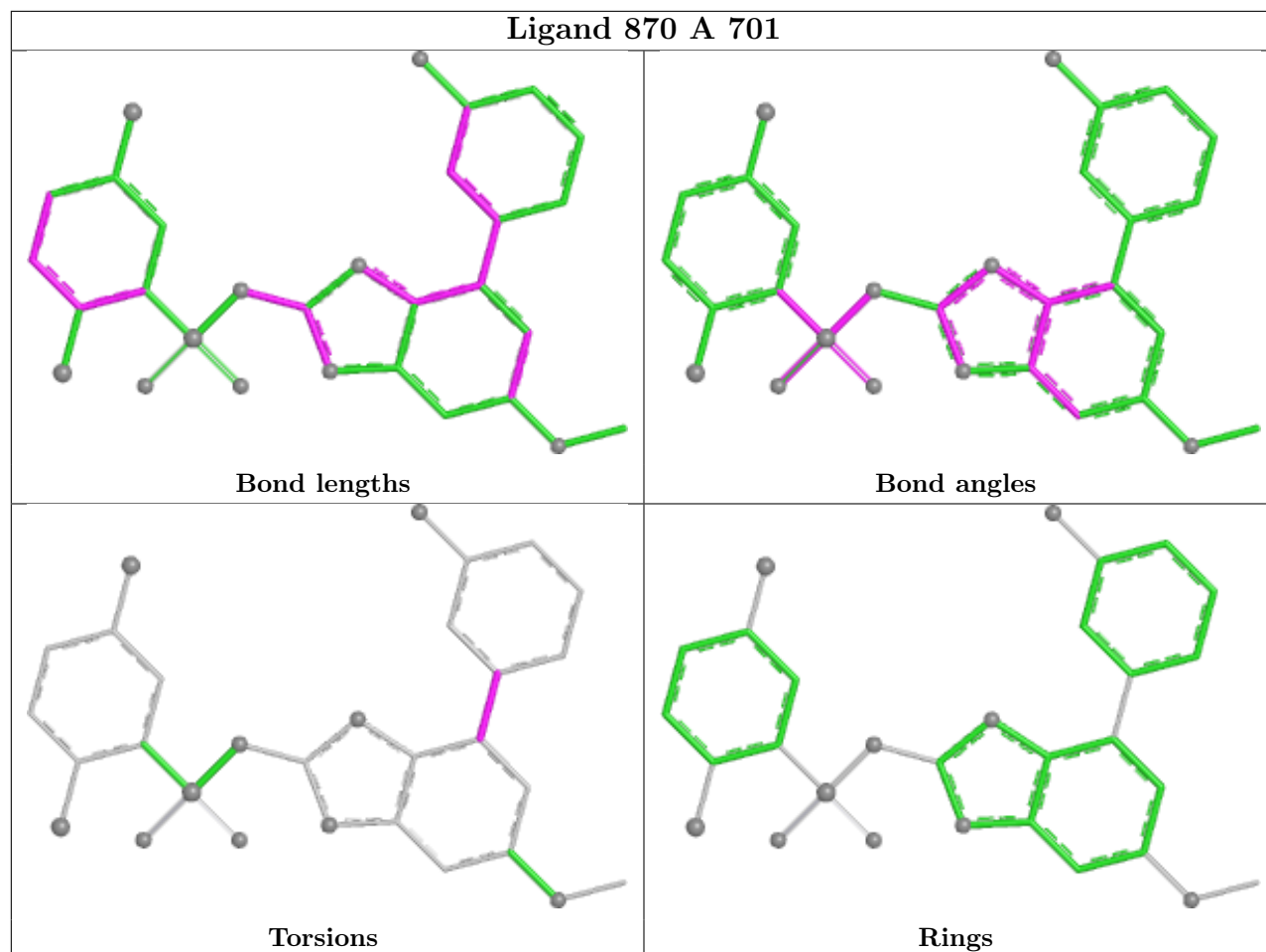
4 monomers are involved in 20 short contacts:

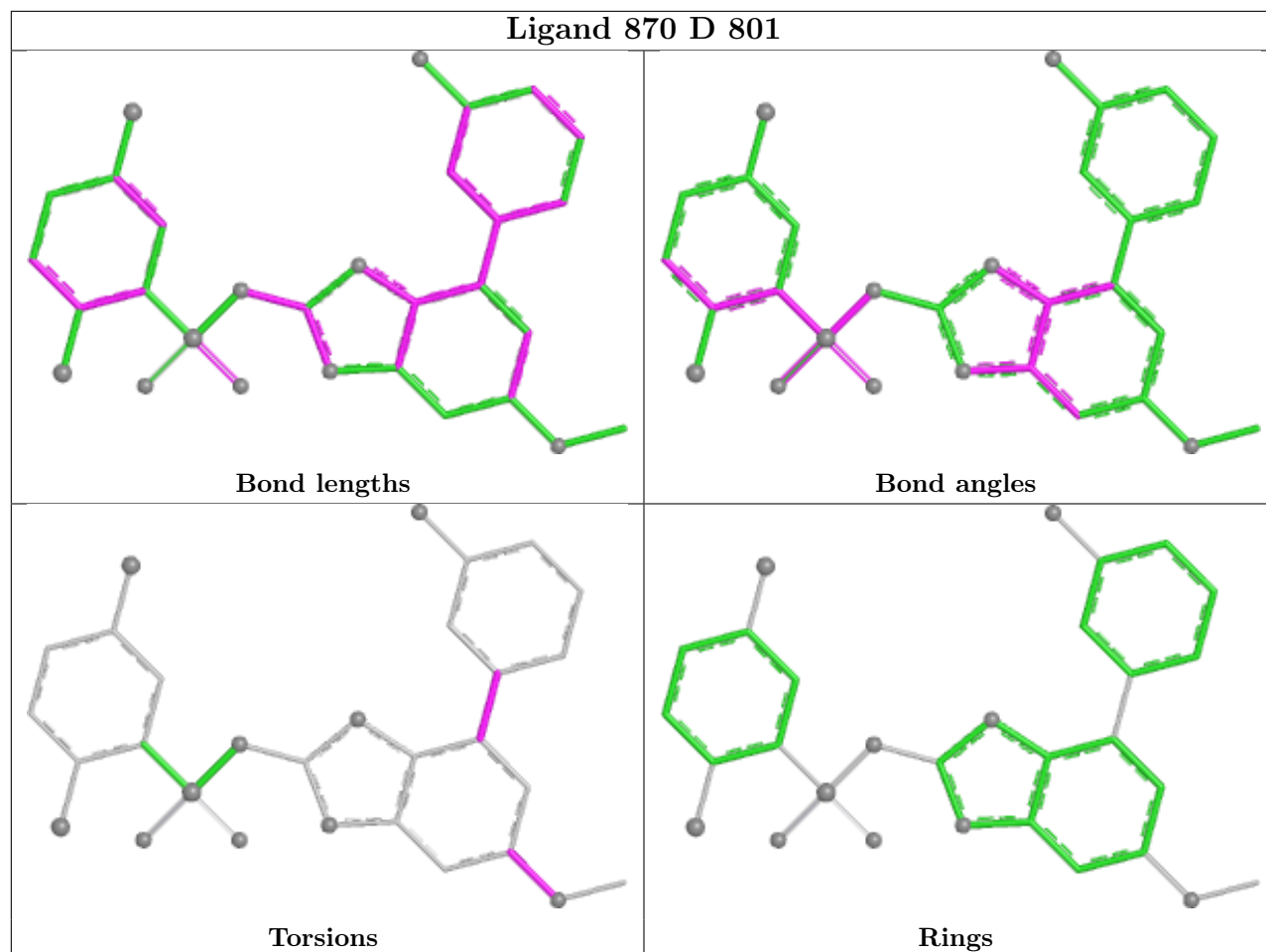
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	901	870	9	0
2	A	701	870	7	0
2	D	801	870	1	0
2	L	1001	870	3	0

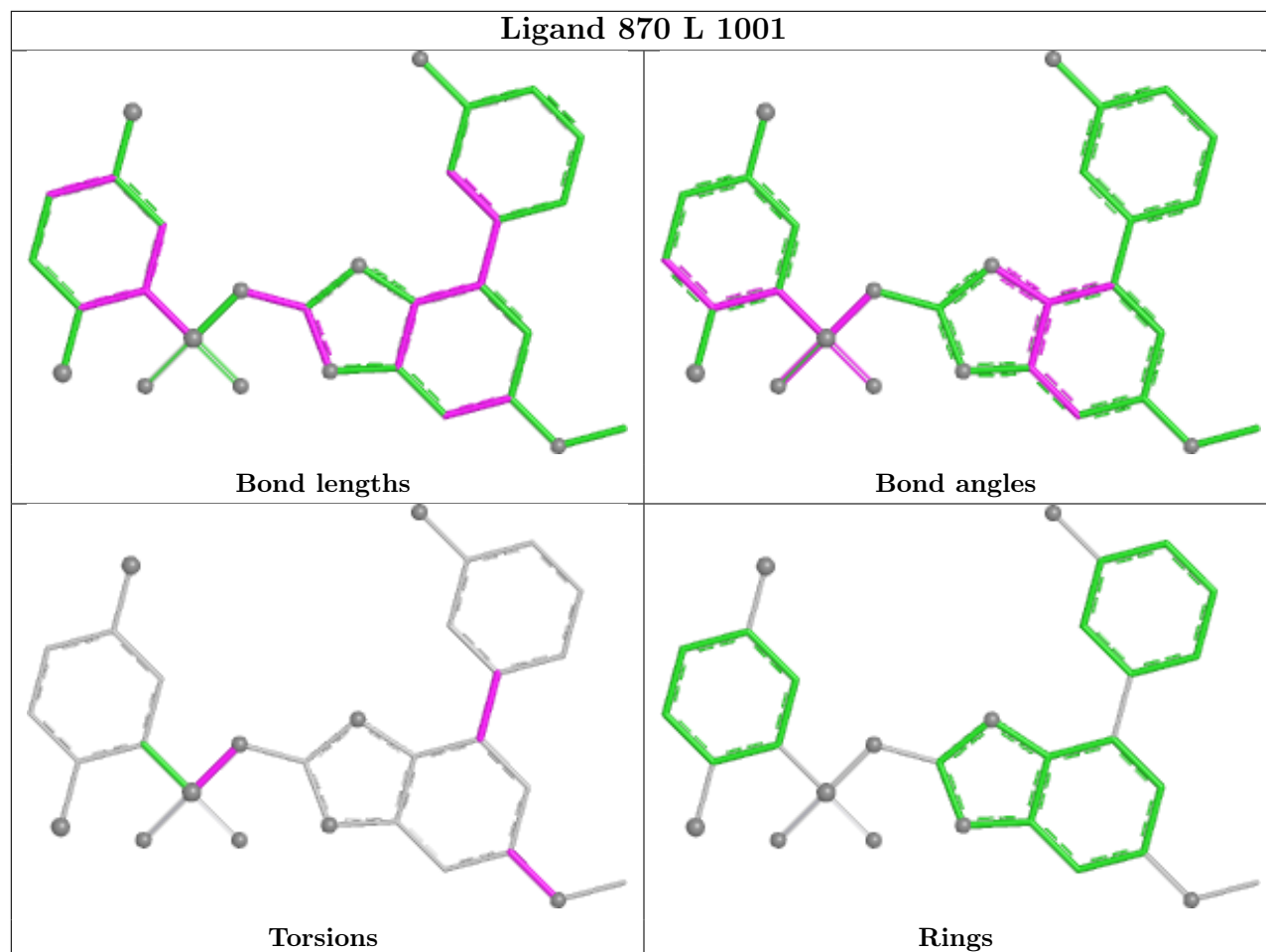
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.