



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 01:57 AM EDT

PDB ID : 1JRP  
Title : Crystal Structure of Xanthine Dehydrogenase inhibited by alloxanthine from Rhodobacter capsulatus  
Authors : Truglio, J.J.; Theis, K.; Leimkuhler, S.; Rappa, R.; Rajagopalan, K.V.; Kisker, C.  
Deposited on : 2001-08-14  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

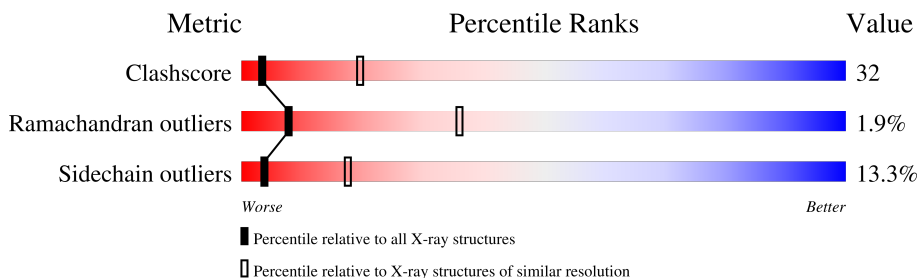
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	462	44% 43% 10% ..
1	C	462	55% 33% 9% ..
1	E	462	39% 46% 11% ..
1	G	462	38% 46% 12% ..
2	B	777	48% 39% 9% ..
2	D	777	48% 37% 11% ..
2	F	777	44% 40% 12% ..
2	H	777	44% 43% 8% ..

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
3	FES	E	3002	-	-	X	-
3	FES	G	3001	-	-	X	-
6	MTE	F	3003	-	-	X	-
6	MTE	H	3003	-	-	X	-
7	MOS	B	3004	-	-	X	-
7	MOS	D	3004	-	-	X	-
7	MOS	F	3004	-	-	X	-
7	MOS	H	3004	-	-	X	-
8	141	B	4000	-	-	X	-
8	141	D	4000	-	-	X	-
8	141	F	4000	-	-	X	-
8	141	H	4000	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 36748 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 xanthine dehydrogenase, chain A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3370	2110	607	628	25	0	0	0
1	C	450	3370	2110	607	628	25	0	0	0
1	E	450	3370	2110	607	628	25	0	0	0
1	G	450	3370	2110	607	628	25	0	0	0

- Molecule 2 is a protein called xanthine dehydrogenase, chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	760	5717	3581	1056	1054	26	0	0	0
2	D	760	5717	3581	1056	1054	26	0	0	0
2	F	760	5717	3581	1056	1054	26	0	0	0
2	H	760	5717	3581	1056	1054	26	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	772	ARG	GLY	conflict	EMBL 13397863
D	772	ARG	GLY	conflict	EMBL 13397863
F	772	ARG	GLY	conflict	EMBL 13397863
H	772	ARG	GLY	conflict	EMBL 13397863

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		
3	G	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).

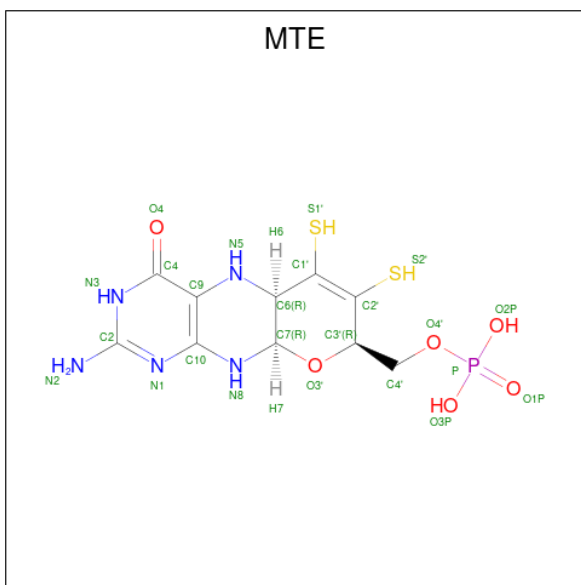


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

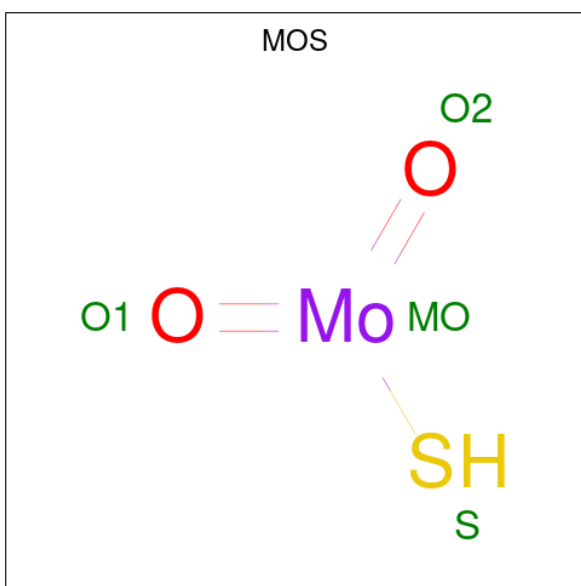
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		

- Molecule 6 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>6</sub>PS<sub>2</sub>).



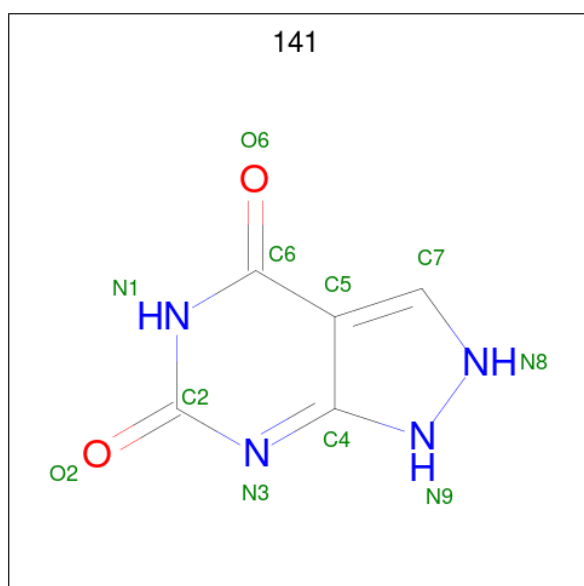
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
6	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
6	D	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
6	F	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
6	H	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 7 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula:  $\text{HMoO}_2\text{S}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Mo	O	S		
7	B	1	Total 3	Mo 1	O 1	S 1	0	0
7	D	1	Total 3	Mo 1	O 1	S 1	0	0
7	F	1	Total 3	Mo 1	O 1	S 1	0	0
7	H	1	Total 3	Mo 1	O 1	S 1	0	0

- Molecule 8 is Oxypurinol (three-letter code: 141) (formula: C<sub>5</sub>H<sub>4</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
8	B	1	Total 11	C 5	N 4	O 2	0	0
8	D	1	Total 11	C 5	N 4	O 2	0	0
8	F	1	Total 11	C 5	N 4	O 2	0	0
8	H	1	Total 11	C 5	N 4	O 2	0	0

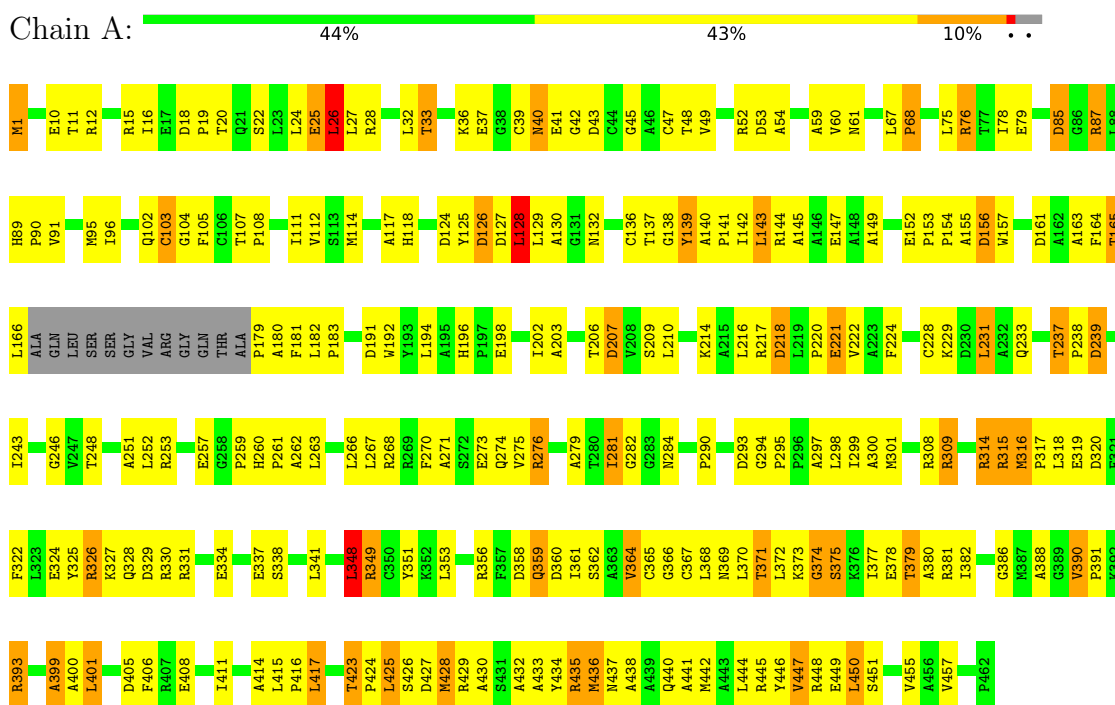


### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: xanthine dehydrogenase, chain A



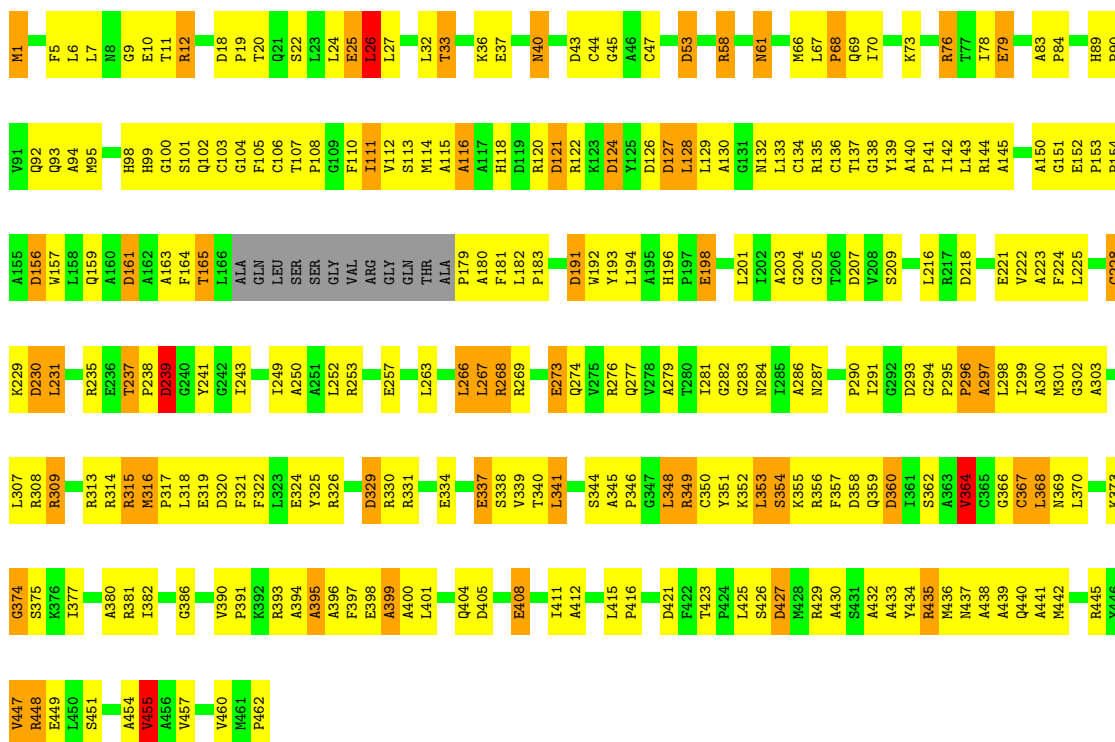
- Molecule 1: xanthine dehydrogenase, chain A





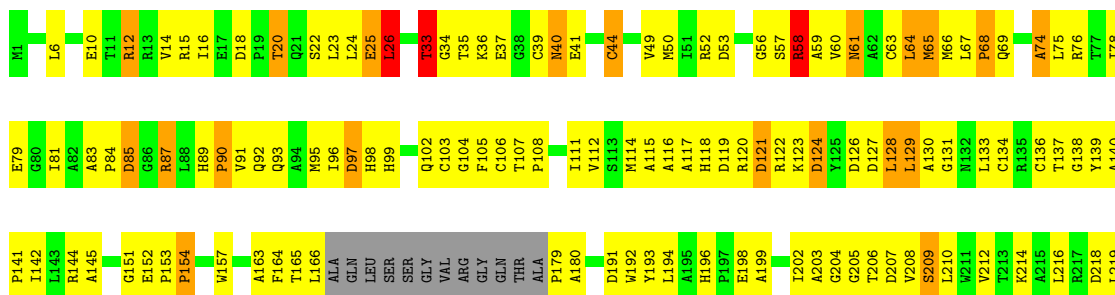
- Molecule 1: xanthine dehydrogenase, chain A

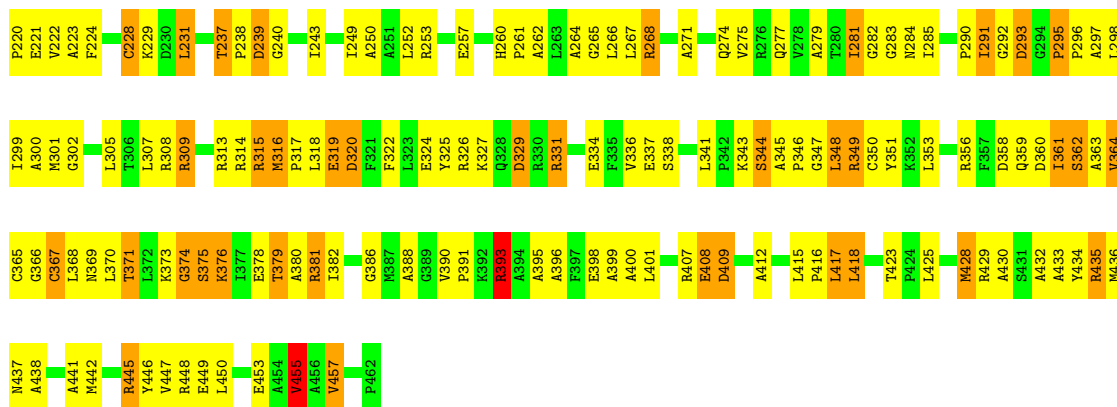
Chain E: 39% 46% 11% ..



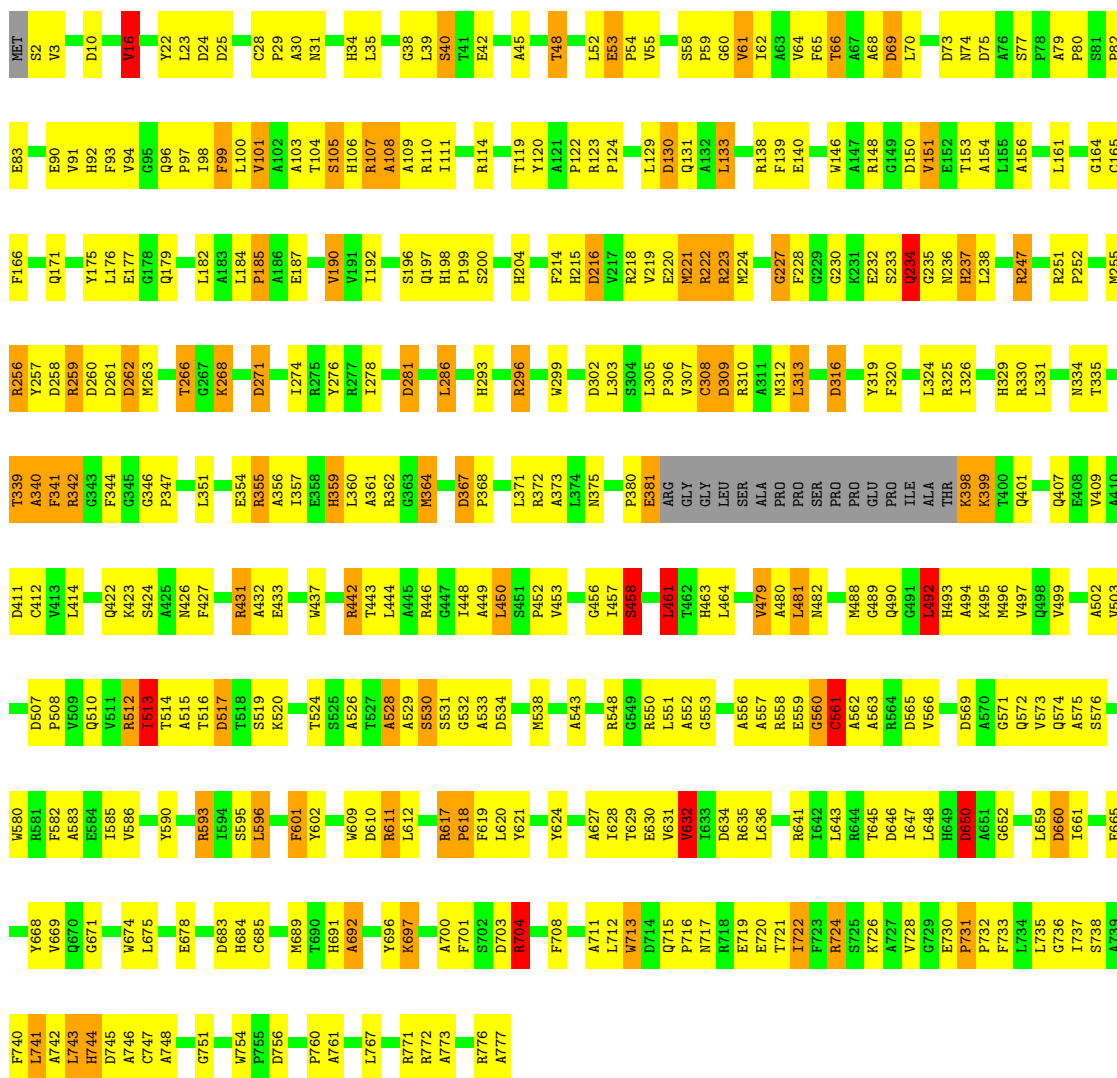
- Molecule 1: xanthine dehydrogenase, chain A

Chain G: 38% 46% 12% ..



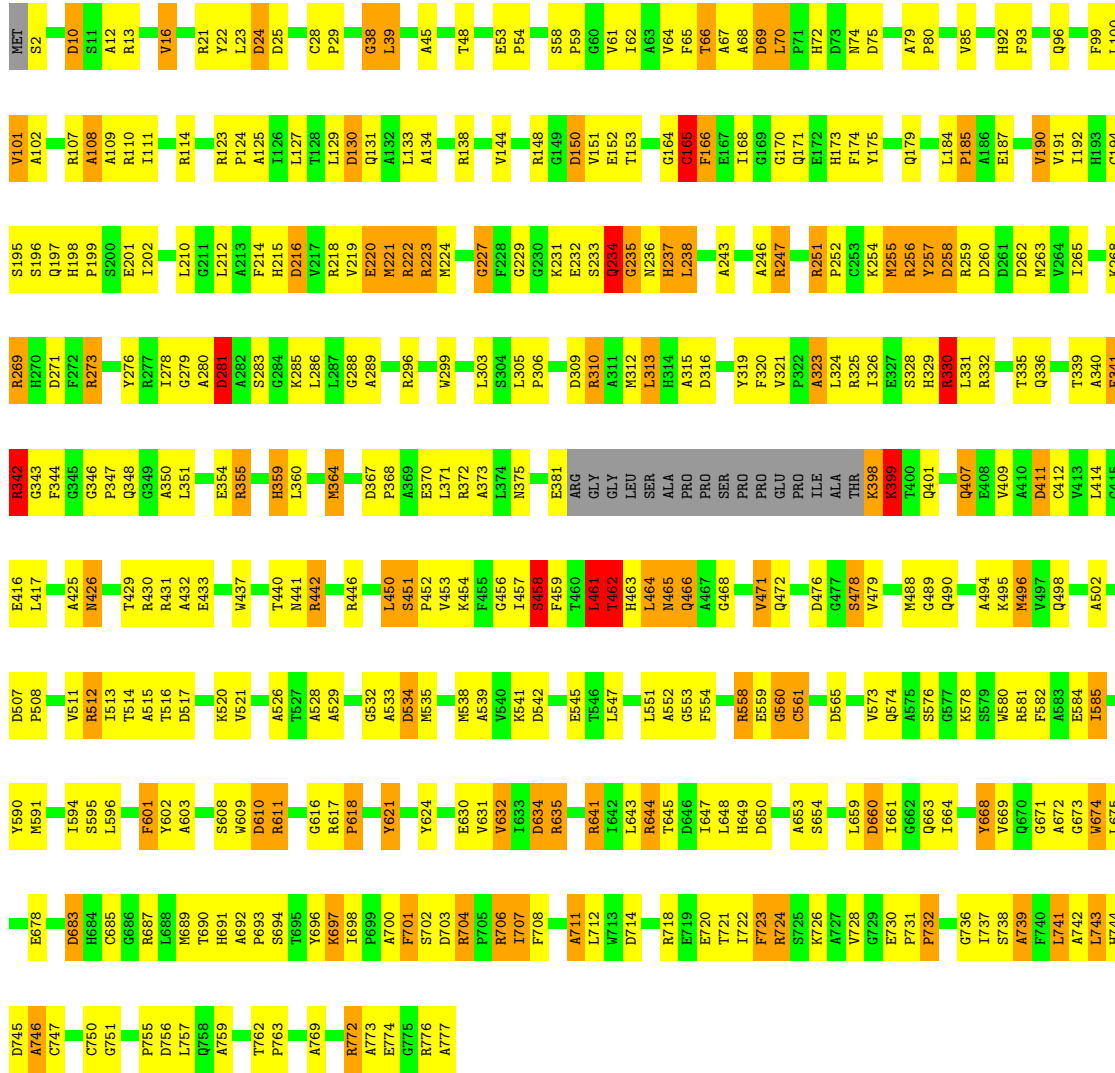


• Molecule 2: xanthine dehydrogenase, chain B



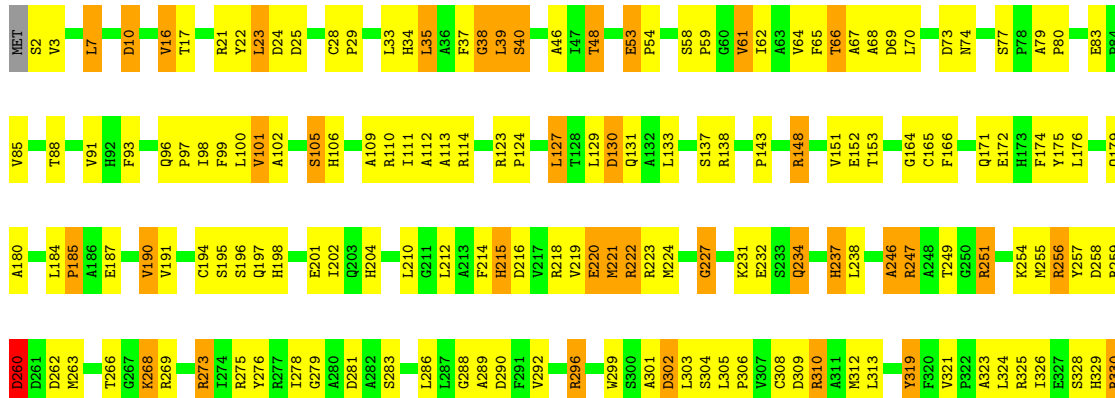
• Molecule 2: xanthine dehydrogenase, chain B

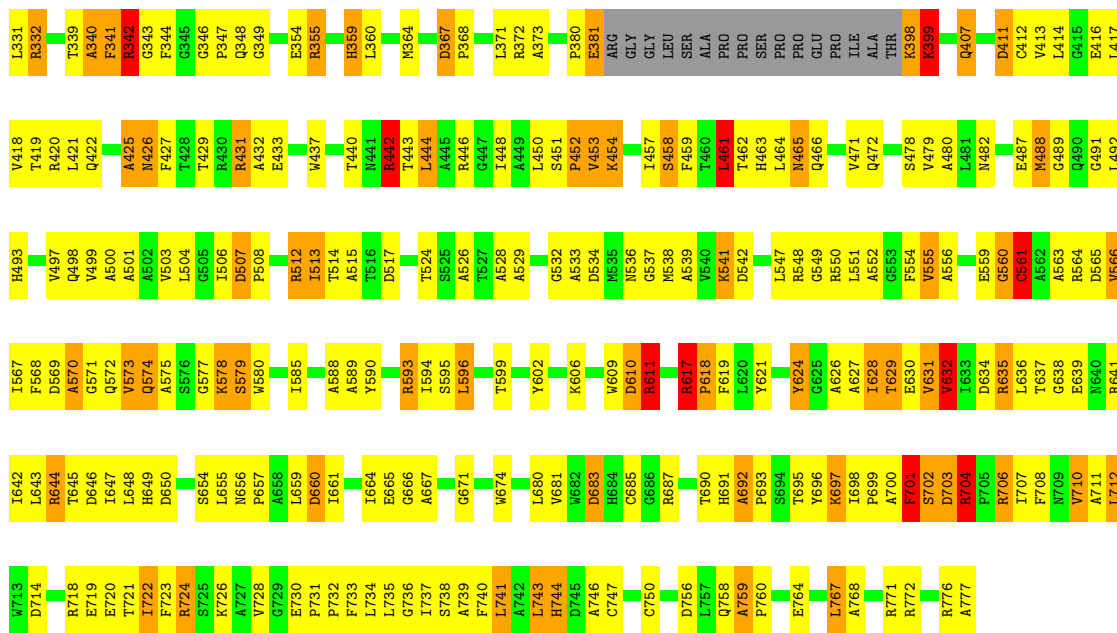
Chain D:  48% 37% 11% ..



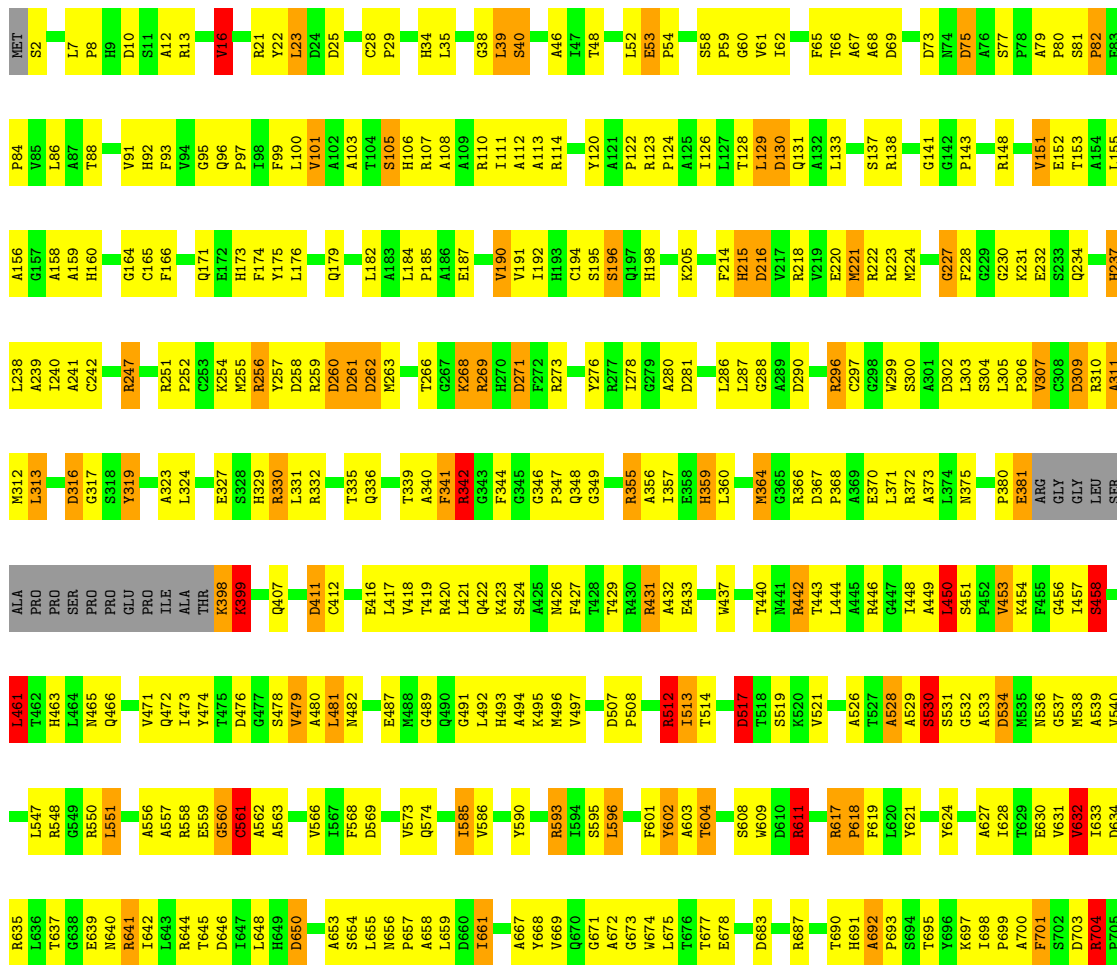
• Molecule 2: xanthine dehydrogenase, chain B

Chain F:  44% 40% 12% ..





• Molecule 2: xanthine dehydrogenase, chain B



R706  
I707  
F708  
A711  
L712  
W713  
N717  
R718  
E719  
E720  
T721  
I722  
F723  
R724  
S725  
K726  
A727  
V728  
G729  
E730  
P731  
P732  
F733  
L734  
L735  
G736  
I737  
S738  
A739  
F740  
L741  
A742  
L743  
H744  
D745  
A746  
C747  
C750  
H753  
V754  
F755  
D756  
L757  
Q758  
A759  
P760  
A761  
I762  
P763  
E764  
A765  
V766  
L767  
V770  
R771

R772  
A773  
R776  
A777

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.62Å 140.73Å 157.66Å 109.59° 105.84° 101.25°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.1 (30.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.193 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	36748	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	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: MOS, CA, 141, FAD, MTE, FES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.17	3/3431 (0.1%)	1.34	28/4647 (0.6%)
1	C	1.44	15/3431 (0.4%)	1.37	31/4647 (0.7%)
1	E	1.23	6/3431 (0.2%)	1.40	35/4647 (0.8%)
1	G	1.16	4/3431 (0.1%)	1.38	29/4647 (0.6%)
2	B	1.41	22/5845 (0.4%)	1.46	65/7942 (0.8%)
2	D	1.50	37/5845 (0.6%)	1.49	78/7942 (1.0%)
2	F	1.39	18/5845 (0.3%)	1.48	70/7942 (0.9%)
2	H	1.34	20/5845 (0.3%)	1.43	54/7942 (0.7%)
All	All	1.35	125/37104 (0.3%)	1.43	390/50356 (0.8%)

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	674	TRP	CB-CG	-8.75	1.34	1.50
2	F	220	GLU	CD-OE2	8.40	1.34	1.25
1	C	116	ALA	CA-CB	-8.12	1.35	1.52
2	D	759	ALA	CA-CB	-7.75	1.36	1.52
1	C	103	CYS	CB-SG	-7.70	1.69	1.82
2	B	220	GLU	CD-OE2	7.69	1.34	1.25
2	H	220	GLU	CD-OE2	7.56	1.33	1.25
2	D	220	GLU	CD-OE2	7.39	1.33	1.25
2	F	219	VAL	CB-CG2	-7.15	1.37	1.52
2	D	258	ASP	CB-CG	-7.09	1.36	1.51
2	D	108	ALA	CA-CB	-7.06	1.37	1.52
2	F	64	VAL	CA-CB	-6.95	1.40	1.54
2	B	16	VAL	CA-CB	-6.84	1.40	1.54
2	B	515	ALA	CA-CB	-6.66	1.38	1.52
2	D	590	TYR	CE2-CZ	-6.63	1.29	1.38
2	D	191	VAL	CB-CG2	-6.58	1.39	1.52
1	G	44	CYS	CB-SG	-6.53	1.71	1.82
2	D	515	ALA	CA-CB	-6.45	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	190	VAL	CB-CG1	-6.44	1.39	1.52
2	D	669	VAL	CA-CB	-6.43	1.41	1.54
2	H	528	ALA	CA-CB	-6.43	1.39	1.52
2	D	257	TYR	CD1-CE1	-6.36	1.29	1.39
2	B	3	VAL	CB-CG1	-6.34	1.39	1.52
2	H	713	TRP	CB-CG	-6.34	1.38	1.50
2	F	191	VAL	CB-CG2	-6.31	1.39	1.52
2	H	521	VAL	CA-CB	-6.26	1.41	1.54
2	D	545	GLU	CD-OE1	6.24	1.32	1.25
2	B	409	VAL	CB-CG2	-6.20	1.39	1.52
2	H	701	PHE	CB-CG	-6.13	1.41	1.51
2	D	769	ALA	CA-CB	-6.11	1.39	1.52
1	G	63	CYS	CB-SG	-6.03	1.72	1.82
2	F	61	VAL	CA-CB	-6.01	1.42	1.54
2	F	573	VAL	CB-CG2	-5.97	1.40	1.52
1	C	74	ALA	CA-CB	-5.97	1.40	1.52
2	D	219	VAL	CA-CB	-5.96	1.42	1.54
2	B	99	PHE	CE2-CZ	-5.96	1.26	1.37
2	H	16	VAL	CA-CB	-5.91	1.42	1.54
2	B	220	GLU	CD-OE1	5.89	1.32	1.25
2	B	340	ALA	CA-CB	-5.89	1.40	1.52
2	D	12	ALA	CA-CB	-5.89	1.40	1.52
2	D	323	ALA	CA-CB	-5.87	1.40	1.52
2	H	604	THR	CA-CB	-5.87	1.38	1.53
1	E	150	ALA	CA-CB	-5.84	1.40	1.52
2	D	109	ALA	CA-CB	-5.83	1.40	1.52
2	B	573	VAL	CB-CG2	-5.82	1.40	1.52
2	B	590	TYR	CD2-CE2	-5.81	1.30	1.39
1	C	105	PHE	CB-CG	-5.81	1.41	1.51
2	B	108	ALA	CA-CB	-5.80	1.40	1.52
2	F	685	CYS	CB-SG	-5.79	1.72	1.81
1	E	426	SER	CA-CB	-5.77	1.44	1.52
2	D	471	VAL	CA-CB	-5.76	1.42	1.54
1	C	262	ALA	CA-CB	-5.72	1.40	1.52
1	C	390	VAL	CB-CG2	-5.72	1.40	1.52
1	C	228	CYS	CB-SG	-5.71	1.72	1.81
2	B	713	TRP	CB-CG	-5.70	1.40	1.50
2	H	497	VAL	CB-CG2	-5.70	1.40	1.52
2	F	626	ALA	CA-CB	-5.68	1.40	1.52
2	D	260	ASP	CB-CG	5.68	1.63	1.51
1	C	457	VAL	CB-CG1	-5.59	1.41	1.52
2	F	220	GLU	CD-OE1	5.58	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	746	ALA	CA-CB	-5.57	1.40	1.52
2	B	528	ALA	CA-CB	-5.55	1.40	1.52
2	B	601	PHE	CB-CG	-5.54	1.42	1.51
2	F	759	ALA	CA-CB	-5.50	1.40	1.52
2	B	611	ARG	CB-CG	-5.50	1.37	1.52
2	D	711	ALA	CA-CB	-5.47	1.41	1.52
2	F	340	ALA	CA-CB	-5.45	1.41	1.52
2	H	611	ARG	CB-CG	-5.45	1.37	1.52
1	C	390	VAL	CB-CG1	-5.45	1.41	1.52
1	C	150	ALA	CA-CB	-5.43	1.41	1.52
2	D	668	TYR	CE2-CZ	-5.43	1.31	1.38
1	G	10	GLU	CG-CD	5.39	1.60	1.51
2	H	311	ALA	CA-CB	-5.38	1.41	1.52
2	D	621	TYR	CG-CD1	-5.38	1.32	1.39
2	D	246	ALA	CA-CB	-5.38	1.41	1.52
2	D	466	GLN	CB-CG	-5.37	1.38	1.52
2	D	573	VAL	CB-CG2	-5.34	1.41	1.52
2	F	246	ALA	CA-CB	-5.34	1.41	1.52
2	D	591	MET	C-O	-5.33	1.13	1.23
2	F	37	PHE	CB-CG	-5.31	1.42	1.51
1	A	103	CYS	CB-SG	-5.30	1.73	1.81
2	H	590	TYR	CE1-CZ	-5.29	1.31	1.38
2	D	739	ALA	CA-CB	-5.27	1.41	1.52
1	E	282	GLY	C-O	5.27	1.32	1.23
2	H	300	SER	CA-CB	-5.26	1.45	1.52
2	H	191	VAL	CB-CG1	-5.26	1.41	1.52
1	C	48	THR	C-O	-5.24	1.13	1.23
1	A	107	THR	CA-CB	-5.23	1.39	1.53
1	E	457	VAL	CB-CG1	-5.22	1.41	1.52
1	A	149	ALA	CA-CB	-5.22	1.41	1.52
2	B	502	ALA	CA-CB	-5.21	1.41	1.52
1	C	63	CYS	CB-SG	-5.21	1.73	1.81
2	H	126	ILE	CA-CB	-5.20	1.42	1.54
2	H	764	GLU	CG-CD	5.20	1.59	1.51
2	H	260	ASP	CB-CG	5.20	1.62	1.51
2	F	555	VAL	CA-CB	-5.19	1.43	1.54
2	D	125	ALA	CA-CB	-5.18	1.41	1.52
2	F	46	ALA	CA-CB	-5.18	1.41	1.52
2	F	701	PHE	CB-CG	-5.17	1.42	1.51
2	H	602	TYR	CB-CG	-5.17	1.43	1.51
2	D	409	VAL	CB-CG2	-5.16	1.42	1.52
2	B	30	ALA	CA-CB	-5.15	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	561	CYS	CB-SG	-5.14	1.73	1.81
2	H	479	VAL	CB-CG1	-5.13	1.42	1.52
2	D	64	VAL	CB-CG1	-5.13	1.42	1.52
1	E	111	ILE	CA-CB	-5.12	1.43	1.54
1	C	441	ALA	CA-CB	-5.12	1.41	1.52
2	D	10	ASP	C-O	-5.11	1.13	1.23
2	D	243	ALA	CA-CB	-5.10	1.41	1.52
2	D	364	MET	CG-SD	5.10	1.94	1.81
1	C	359	GLN	CB-CG	-5.10	1.38	1.52
2	D	601	PHE	CB-CG	-5.09	1.42	1.51
2	F	425	ALA	CA-CB	-5.08	1.41	1.52
2	B	497	VAL	CB-CG2	-5.07	1.42	1.52
2	D	502	ALA	CA-CB	-5.06	1.41	1.52
1	E	116	ALA	CA-CB	-5.05	1.41	1.52
2	B	156	ALA	CA-CB	-5.04	1.41	1.52
2	B	711	ALA	CA-CB	-5.04	1.41	1.52
2	B	543	ALA	CA-CB	-5.03	1.41	1.52
1	G	74	ALA	CA-CB	-5.03	1.41	1.52
2	H	474	TYR	CD2-CE2	-5.01	1.31	1.39
2	D	701	PHE	CB-CG	-5.00	1.42	1.51
2	H	307	VAL	CA-CB	-5.00	1.44	1.54
1	C	202	ILE	CA-CB	-5.00	1.43	1.54
2	D	468	GLY	C-O	-5.00	1.15	1.23

All (390) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	704	ARG	NE-CZ-NH1	-12.32	114.14	120.30
2	D	542	ASP	CB-CG-OD2	12.01	129.11	118.30
2	D	635	ARG	NE-CZ-NH2	-11.81	114.39	120.30
2	D	273	ARG	NE-CZ-NH1	-11.38	114.61	120.30
2	B	660	ASP	CB-CG-OD2	11.14	128.33	118.30
2	B	309	ASP	CB-CG-OD2	10.48	127.73	118.30
2	F	260	ASP	CB-CG-OD2	10.48	127.73	118.30
2	D	660	ASP	CB-CG-OD2	10.47	127.72	118.30
1	E	127	ASP	CB-CG-OD2	10.36	127.62	118.30
2	D	703	ASP	CB-CG-OD2	10.31	127.58	118.30
2	F	683	ASP	CB-CG-OD2	10.30	127.57	118.30
2	F	542	ASP	CB-CG-OD2	10.10	127.39	118.30
2	H	309	ASP	CB-CG-OD2	9.90	127.21	118.30
2	F	632	VAL	CB-CA-C	-9.78	92.82	111.40
2	H	411	ASP	CB-CG-OD2	9.75	127.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	632	VAL	CB-CA-C	-9.69	92.99	111.40
2	D	25	ASP	CB-CG-OD2	9.65	126.99	118.30
1	G	127	ASP	CB-CG-OD2	9.64	126.97	118.30
1	G	97	ASP	CB-CG-OD2	9.59	126.93	118.30
2	B	262	ASP	CB-CG-OD2	9.58	126.92	118.30
2	D	262	ASP	CB-CG-OD2	9.46	126.82	118.30
1	E	161	ASP	CB-CG-OD2	9.40	126.76	118.30
1	C	135	ARG	NE-CZ-NH2	9.35	124.98	120.30
2	F	10	ASP	CB-CG-OD2	9.29	126.66	118.30
1	C	135	ARG	NE-CZ-NH1	-9.19	115.71	120.30
1	G	126	ASP	CB-CG-OD2	9.02	126.42	118.30
1	C	26	LEU	CB-CG-CD2	9.02	126.33	111.00
2	F	342	ARG	NE-CZ-NH1	-8.91	115.84	120.30
2	B	316	ASP	CB-CG-OD2	8.89	126.31	118.30
2	F	332	ARG	NE-CZ-NH1	-8.81	115.90	120.30
1	E	126	ASP	CB-CG-OD2	8.73	126.16	118.30
2	D	10	ASP	CB-CG-OD2	8.71	126.14	118.30
2	F	411	ASP	CB-CG-OD2	8.71	126.14	118.30
2	B	182	LEU	CB-CG-CD1	-8.70	96.21	111.00
1	C	58	ARG	NE-CZ-NH2	-8.66	115.97	120.30
1	C	276	ARG	NE-CZ-NH1	-8.59	116.00	120.30
2	B	745	ASP	CB-CG-OD2	8.59	126.03	118.30
2	B	632	VAL	CB-CA-C	-8.57	95.12	111.40
2	D	199	PRO	N-CD-CG	-8.55	90.37	103.20
1	C	320	ASP	CB-CG-OD2	8.54	125.98	118.30
2	D	757	LEU	CB-CG-CD2	-8.49	96.57	111.00
2	D	310	ARG	NE-CZ-NH2	-8.43	116.08	120.30
2	D	260	ASP	CB-CG-OD2	8.42	125.88	118.30
2	D	610	ASP	CB-CG-OD2	8.42	125.88	118.30
1	E	207	ASP	CB-CG-OD2	8.42	125.87	118.30
1	E	356	ARG	NE-CZ-NH1	-8.39	116.10	120.30
2	F	273	ARG	NE-CZ-NH1	-8.38	116.11	120.30
2	H	262	ASP	CB-CG-OD2	8.38	125.84	118.30
2	H	261	ASP	CB-CG-OD2	8.28	125.75	118.30
1	G	207	ASP	CB-CG-OD2	8.24	125.71	118.30
1	C	207	ASP	CB-CG-OD2	8.23	125.70	118.30
1	A	26	LEU	CB-CG-CD2	8.20	124.94	111.00
2	D	461	LEU	CA-CB-CG	8.20	134.16	115.30
2	H	741	LEU	CA-CB-CG	-8.19	96.46	115.30
2	B	190	VAL	CB-CA-C	-8.18	95.86	111.40
2	F	596	LEU	CB-CG-CD2	-8.17	97.12	111.00
2	H	704	ARG	NE-CZ-NH1	-8.13	116.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	417	LEU	CA-CB-CG	-8.11	96.65	115.30
2	H	260	ASP	CB-CG-OD2	8.10	125.59	118.30
2	F	185	PRO	N-CD-CG	-8.01	91.18	103.20
1	A	161	ASP	CB-CG-OD2	8.00	125.50	118.30
2	H	593	ARG	NE-CZ-NH2	-7.97	116.31	120.30
2	B	756	ASP	CB-CG-OD2	7.97	125.48	118.30
2	F	660	ASP	CB-CG-OD2	7.84	125.36	118.30
1	E	320	ASP	CB-CG-OD2	7.81	125.33	118.30
2	H	703	ASP	CB-CG-OD2	7.80	125.32	118.30
2	B	223	ARG	NE-CZ-NH1	-7.78	116.41	120.30
2	F	262	ASP	CB-CG-OD2	7.71	125.23	118.30
2	H	534	ASP	CB-CG-OD1	7.66	125.19	118.30
2	B	260	ASP	CB-CG-OD2	7.63	125.17	118.30
2	H	479	VAL	CB-CA-C	-7.63	96.91	111.40
2	B	223	ARG	NE-CZ-NH2	7.62	124.11	120.30
2	B	517	ASP	CB-CG-OD2	7.62	125.15	118.30
1	G	320	ASP	CB-CG-OD2	7.50	125.05	118.30
2	H	269	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	B	216	ASP	CB-CG-OD2	7.49	125.04	118.30
2	F	453	VAL	CB-CA-C	-7.48	97.20	111.40
2	B	316	ASP	CB-CG-OD1	-7.47	111.57	118.30
2	F	309	ASP	CB-CG-OD2	7.45	125.01	118.30
1	A	127	ASP	CB-CG-OD2	7.42	124.98	118.30
2	D	683	ASP	CB-CG-OD2	7.41	124.97	118.30
2	F	127	LEU	CB-CG-CD2	-7.37	98.48	111.00
2	H	269	ARG	NE-CZ-NH1	-7.37	116.62	120.30
2	B	492	LEU	CB-CG-CD2	-7.35	98.50	111.00
2	D	332	ARG	NE-CZ-NH1	-7.34	116.63	120.30
2	H	190	VAL	CB-CA-C	-7.33	97.48	111.40
2	F	492	LEU	CB-CG-CD2	-7.26	98.67	111.00
2	F	310	ARG	NE-CZ-NH2	-7.21	116.69	120.30
2	D	216	ASP	CB-CG-OD2	7.21	124.78	118.30
2	B	479	VAL	CB-CA-C	-7.20	97.72	111.40
2	B	704	ARG	NE-CZ-NH1	-7.18	116.71	120.30
2	F	641	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	E	448	ARG	NE-CZ-NH1	-7.18	116.71	120.30
2	H	481	LEU	CB-CG-CD1	-7.13	98.88	111.00
2	D	756	ASP	CB-CG-OD2	7.11	124.70	118.30
2	D	316	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	330	ARG	NE-CZ-NH1	-7.10	116.75	120.30
2	F	635	ARG	NE-CZ-NH2	-7.08	116.76	120.30
2	D	21	ARG	NE-CZ-NH2	-7.08	116.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ASP	CB-CG-OD2	7.07	124.66	118.30
2	F	695	THR	OG1-CB-CG2	-7.05	93.78	110.00
1	E	329	ASP	CB-CG-OD2	7.04	124.63	118.30
2	H	25	ASP	CB-CG-OD2	7.04	124.63	118.30
1	C	58	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	126	ASP	CB-CG-OD2	6.99	124.59	118.30
2	D	223	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	E	228	CYS	CA-CB-SG	-6.94	101.50	114.00
1	A	364	VAL	CB-CA-C	-6.94	98.22	111.40
1	E	427	ASP	CB-CG-OD1	-6.92	112.07	118.30
2	H	25	ASP	CB-CG-OD1	-6.92	112.08	118.30
2	D	238	LEU	CB-CG-CD2	-6.86	99.34	111.00
1	E	126	ASP	CB-CG-OD1	-6.85	112.14	118.30
2	D	521	VAL	CB-CA-C	-6.82	98.44	111.40
2	F	165	CYS	CA-CB-SG	-6.82	101.72	114.00
2	B	271	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	76	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	C	187	ASP	CB-CG-OD2	6.72	124.35	118.30
2	F	444	LEU	CA-CB-CG	-6.72	99.84	115.30
2	B	185	PRO	N-CD-CG	-6.72	93.12	103.20
1	C	119	ASP	CB-CG-OD1	6.69	124.32	118.30
1	E	364	VAL	CB-CA-C	-6.67	98.72	111.40
2	F	712	LEU	CA-CB-CG	6.66	130.62	115.30
1	C	330	ARG	NE-CZ-NH1	-6.65	116.97	120.30
2	B	151	VAL	CB-CA-C	-6.65	98.77	111.40
2	B	261	ASP	CB-CG-OD2	6.64	124.28	118.30
2	F	685	CYS	CB-CA-C	-6.64	97.13	110.40
1	E	427	ASP	CB-CG-OD2	6.63	124.27	118.30
1	C	76	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	G	44	CYS	CA-CB-SG	-6.59	102.13	114.00
2	B	69	ASP	CB-CG-OD2	6.58	124.23	118.30
2	H	73	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	276	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	C	230	ASP	CB-CG-OD2	6.55	124.19	118.30
2	B	703	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	239	ASP	CB-CG-OD2	6.54	124.19	118.30
2	H	271	ASP	CB-CG-OD2	6.51	124.16	118.30
2	B	565	ASP	CB-CG-OD2	6.49	124.14	118.30
2	H	151	VAL	CB-CA-C	-6.46	99.13	111.40
2	H	216	ASP	CB-CG-OD2	6.45	124.10	118.30
1	A	207	ASP	CB-CG-OD2	6.44	124.09	118.30
2	D	687	ARG	NE-CZ-NH1	6.43	123.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	714	ASP	CB-CG-OD2	6.43	124.09	118.30
1	G	26	LEU	CB-CG-CD1	6.42	121.92	111.00
2	B	107	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	E	124	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	329	ASP	CB-CG-OD2	6.38	124.04	118.30
1	E	348	LEU	CB-CG-CD1	-6.38	100.15	111.00
2	B	712	LEU	CB-CG-CD1	-6.38	100.16	111.00
2	D	685	CYS	CB-CA-C	-6.38	97.65	110.40
2	B	660	ASP	CB-CG-OD1	-6.37	112.57	118.30
2	H	569	ASP	CB-CG-OD2	6.37	124.03	118.30
2	F	561	CYS	CA-CB-SG	-6.35	102.57	114.00
2	F	342	ARG	NE-CZ-NH2	6.33	123.47	120.30
2	D	411	ASP	CB-CG-OD2	6.32	123.99	118.30
2	D	534	ASP	CB-CG-OD2	6.32	123.99	118.30
2	D	511	VAL	CB-CA-C	-6.31	99.42	111.40
2	F	290	ASP	CB-CG-OD2	6.29	123.97	118.30
2	D	13	ARG	NE-CZ-NH1	-6.29	117.16	120.30
2	D	150	ASP	CB-CG-OD2	6.29	123.96	118.30
2	F	25	ASP	CB-CG-OD2	6.29	123.96	118.30
2	D	634	ASP	CB-CG-OD2	6.28	123.95	118.30
2	D	585	ILE	CG1-CB-CG2	-6.26	97.62	111.40
1	E	360	ASP	CB-CG-OD2	6.26	123.93	118.30
2	F	710	VAL	CB-CA-C	-6.25	99.53	111.40
2	D	192	ILE	CB-CA-C	-6.23	99.14	111.60
2	F	38	GLY	N-CA-C	-6.23	97.53	113.10
2	D	516	THR	OG1-CB-CG2	-6.23	95.68	110.00
2	B	550	ARG	NE-CZ-NH1	-6.22	117.19	120.30
2	B	222	ARG	NE-CZ-NH2	6.21	123.41	120.30
2	B	24	ASP	CB-CG-OD2	6.21	123.89	118.30
2	H	192	ILE	CB-CA-C	-6.20	99.19	111.60
2	D	133	LEU	CB-CG-CD1	-6.17	100.51	111.00
1	C	85	ASP	CB-CG-OD2	6.16	123.84	118.30
2	H	281	ASP	N-CA-CB	-6.15	99.53	110.60
2	F	644	ARG	NE-CZ-NH1	-6.13	117.24	120.30
1	A	314	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	F	712	LEU	CB-CG-CD1	-6.12	100.60	111.00
1	G	445	ARG	NE-CZ-NH2	-6.11	117.25	120.30
2	D	255	MET	CG-SD-CE	6.09	109.95	100.20
2	D	309	ASP	CB-CG-OD2	6.09	123.78	118.30
2	D	281	ASP	N-CA-CB	-6.07	99.68	110.60
2	F	367	ASP	CB-CG-OD2	6.07	123.76	118.30
2	D	281	ASP	CB-CG-OD2	6.06	123.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	ASP	CB-CG-OD2	6.05	123.75	118.30
2	D	133	LEU	CA-CB-CG	-6.05	101.38	115.30
2	D	745	ASP	CB-CG-OD2	6.05	123.75	118.30
1	G	129	LEU	CA-CB-CG	-6.05	101.39	115.30
2	H	646	ASP	CB-CG-OD2	6.05	123.74	118.30
1	G	121	ASP	CB-CG-OD2	6.03	123.73	118.30
2	F	101	VAL	CB-CA-C	-6.03	99.95	111.40
1	A	348	LEU	CB-CG-CD1	-6.02	100.76	111.00
2	B	73	ASP	CB-CG-OD2	6.02	123.72	118.30
2	B	611	ARG	CG-CD-NE	-6.02	99.16	111.80
1	E	405	ASP	CB-CG-OD2	6.01	123.70	118.30
2	H	316	ASP	CB-CG-OD2	5.98	123.68	118.30
1	C	183	PRO	N-CD-CG	-5.97	94.24	103.20
1	E	135	ARG	NE-CZ-NH2	5.95	123.28	120.30
1	A	436	MET	CG-SD-CE	-5.95	90.69	100.20
2	H	461	LEU	CA-CB-CG	5.94	128.96	115.30
2	H	650	ASP	CB-CG-OD1	5.92	123.63	118.30
2	H	512	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	F	302	ASP	CB-CG-OD2	5.91	123.62	118.30
2	H	641	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	B	646	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	156	ASP	CB-CG-OD2	5.89	123.60	118.30
2	F	7	LEU	CB-CG-CD2	-5.89	100.99	111.00
2	B	266	THR	OG1-CB-CG2	-5.88	96.47	110.00
2	B	411	ASP	CB-CG-OD2	5.87	123.58	118.30
2	D	772	ARG	NE-CZ-NH1	-5.87	117.37	120.30
2	F	21	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	H	743	LEU	CB-CG-CD2	5.84	120.93	111.00
1	C	124	ASP	CB-CG-OD2	5.84	123.55	118.30
2	D	535	MET	CG-SD-CE	5.83	109.53	100.20
2	F	690	THR	OG1-CB-CG2	-5.83	96.58	110.00
1	G	293	ASP	CB-CG-OD2	5.82	123.54	118.30
1	G	348	LEU	CB-CG-CD1	-5.82	101.11	111.00
2	B	650	ASP	CB-CG-OD2	5.80	123.52	118.30
2	H	290	ASP	CB-CG-OD2	5.80	123.52	118.30
2	B	513	ILE	CG1-CB-CG2	-5.79	98.66	111.40
2	F	442	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	E	273	GLU	OE1-CD-OE2	-5.78	116.36	123.30
2	D	714	ASP	CB-CG-OD2	5.78	123.50	118.30
2	D	190	VAL	CB-CA-C	-5.76	100.45	111.40
1	C	364	VAL	CB-CA-C	-5.76	100.46	111.40
2	B	308	CYS	CA-CB-SG	-5.74	103.67	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	551	LEU	CA-CB-CG	-5.74	102.09	115.30
1	A	417	LEU	CA-CB-CG	-5.74	102.11	115.30
2	B	192	ILE	CB-CA-C	-5.74	100.13	111.60
2	B	453	VAL	CB-CA-C	-5.73	100.51	111.40
1	C	348	LEU	CB-CG-CD1	-5.73	101.25	111.00
2	H	585	ILE	CG1-CB-CG2	-5.73	98.80	111.40
1	C	405	ASP	CB-CG-OD2	5.73	123.45	118.30
2	B	261	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	C	134	CYS	CA-CB-SG	5.71	124.28	114.00
2	B	367	ASP	CB-CG-OD2	5.71	123.44	118.30
2	D	69	ASP	CB-CG-OD2	5.71	123.44	118.30
2	F	73	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	450	LEU	CA-CB-CG	-5.70	102.19	115.30
2	F	683	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	A	293	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	122	ARG	NE-CZ-NH1	5.69	123.14	120.30
2	D	165	CYS	CA-CB-SG	-5.69	103.76	114.00
2	H	687	ARG	NE-CZ-NH2	-5.69	117.46	120.30
2	F	610	ASP	CB-CG-OD2	5.68	123.42	118.30
1	E	183	PRO	N-CD-CG	-5.68	94.68	103.20
1	E	53	ASP	CB-CG-OD2	5.68	123.41	118.30
2	B	516	THR	OG1-CB-CG2	-5.67	96.95	110.00
1	C	137	THR	CB-CA-C	-5.67	96.29	111.60
2	D	342	ARG	NE-CZ-NH1	-5.66	117.47	120.30
2	B	281	ASP	N-CA-CB	-5.66	100.41	110.60
1	G	393	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	E	368	LEU	CA-CB-CG	-5.65	102.31	115.30
1	E	353	LEU	CB-CG-CD1	-5.64	101.42	111.00
2	F	596	LEU	CA-CB-CG	-5.63	102.36	115.30
1	E	191	ASP	CB-CG-OD2	5.62	123.36	118.30
2	H	596	LEU	CA-CB-CG	-5.62	102.36	115.30
2	D	75	ASP	CB-CG-OD2	5.61	123.35	118.30
2	D	610	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	E	263	LEU	CB-CG-CD2	5.59	120.51	111.00
1	G	124	ASP	CB-CG-OD2	5.59	123.33	118.30
2	B	524	THR	CA-CB-CG2	-5.57	104.60	112.40
2	H	632	VAL	CB-CA-C	-5.57	100.82	111.40
1	G	364	VAL	CB-CA-C	-5.56	100.83	111.40
2	F	461	LEU	CA-CB-CG	5.56	128.09	115.30
1	C	252	LEU	CB-CG-CD1	-5.56	101.56	111.00
1	G	329	ASP	CB-CG-OD2	5.54	123.29	118.30
1	G	207	ASP	OD1-CG-OD2	-5.54	112.77	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	308	CYS	CA-CB-SG	-5.54	104.03	114.00
1	A	32	LEU	CA-CB-CG	-5.53	102.59	115.30
2	D	732	PRO	N-CD-CG	-5.53	94.91	103.20
1	C	421	ASP	CB-CG-OD2	5.52	123.27	118.30
2	D	281	ASP	CB-CA-C	-5.50	99.39	110.40
2	B	255	MET	CG-SD-CE	5.50	108.99	100.20
2	H	513	ILE	CG1-CB-CG2	-5.50	99.31	111.40
2	H	82	PRO	N-CD-CG	-5.49	94.96	103.20
1	G	365	CYS	CA-CB-SG	-5.49	104.13	114.00
2	F	767	LEU	CB-CG-CD1	-5.48	101.68	111.00
2	F	191	VAL	CB-CA-C	-5.48	100.99	111.40
1	G	64	LEU	CA-CB-CG	-5.47	102.71	115.30
2	D	462	THR	N-CA-C	5.47	125.78	111.00
2	D	281	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	A	270	PHE	N-CA-C	-5.47	96.24	111.00
1	E	421	ASP	CB-CG-OD2	5.46	123.22	118.30
2	F	596	LEU	CB-CG-CD1	-5.46	101.72	111.00
2	F	599	THR	CB-CA-C	-5.45	96.89	111.60
2	F	703	ASP	CB-CG-OD2	5.45	123.20	118.30
2	B	101	VAL	CB-CA-C	-5.44	101.06	111.40
2	D	10	ASP	CB-CG-OD1	-5.43	113.42	118.30
2	B	461	LEU	CA-CB-CG	5.42	127.77	115.30
2	H	604	THR	CA-CB-CG2	-5.41	104.82	112.40
2	H	21	ARG	CB-CA-C	-5.41	99.59	110.40
2	F	513	ILE	CG1-CB-CG2	-5.40	99.53	111.40
2	D	707	ILE	N-CA-C	-5.39	96.45	111.00
1	E	156	ASP	CB-CG-OD2	5.38	123.14	118.30
2	D	101	VAL	CB-CA-C	-5.37	101.19	111.40
1	E	268	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	G	307	LEU	CA-CB-CG	-5.37	102.95	115.30
2	F	507	ASP	CB-CG-OD2	5.36	123.13	118.30
1	G	58	ARG	NE-CZ-NH2	-5.35	117.63	120.30
2	D	235	GLY	N-CA-C	-5.34	99.74	113.10
1	A	217	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	D	310	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	F	570	ALA	C-N-CA	-5.33	111.12	122.30
1	C	126	ASP	CB-CG-OD2	5.32	123.09	118.30
2	D	70	LEU	CB-CG-CD1	-5.32	101.95	111.00
2	D	644	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	276	ARG	NE-CZ-NH2	5.31	122.96	120.30
1	E	448	ARG	NE-CZ-NH2	5.30	122.95	120.30
2	F	666	GLY	C-N-CA	-5.30	108.44	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	THR	OG1-CB-CG2	-5.30	97.81	110.00
2	F	249	THR	CB-CA-C	-5.29	97.31	111.60
2	D	185	PRO	N-CD-CG	-5.29	95.26	103.20
1	G	418	LEU	CA-CB-CG	-5.29	103.14	115.30
2	B	634	ASP	CB-CG-OD2	5.28	123.06	118.30
2	H	21	ARG	NE-CZ-NH1	-5.28	117.66	120.30
2	H	756	ASP	CB-CG-OD2	5.27	123.05	118.30
2	H	342	ARG	NE-CZ-NH1	-5.27	117.67	120.30
2	F	631	VAL	CB-CA-C	-5.26	101.41	111.40
2	B	593	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	H	316	ASP	CB-CG-OD1	-5.26	113.57	118.30
2	D	127	LEU	CB-CG-CD2	-5.25	102.08	111.00
2	F	629	THR	OG1-CB-CG2	-5.24	97.95	110.00
2	D	38	GLY	N-CA-C	-5.23	100.02	113.10
2	D	260	ASP	OD1-CG-OD2	-5.23	113.36	123.30
1	E	230	ASP	CB-CG-OD2	5.23	123.01	118.30
2	F	646	ASP	CB-CG-OD2	5.22	123.00	118.30
2	F	127	LEU	CA-CB-CG	-5.21	103.32	115.30
2	B	94	VAL	CB-CA-C	-5.18	101.57	111.40
2	D	683	ASP	CB-CG-OD1	-5.17	113.65	118.30
2	F	88	THR	OG1-CB-CG2	-5.16	98.14	110.00
2	H	182	LEU	CB-CG-CD1	-5.16	102.23	111.00
2	B	569	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	447	VAL	CB-CA-C	-5.15	101.62	111.40
2	H	677	THR	CA-CB-CG2	-5.15	105.19	112.40
1	A	218	ASP	CB-CG-OD2	5.14	122.93	118.30
1	E	26	LEU	CB-CG-CD1	5.14	119.75	111.00
1	G	268	ARG	NE-CZ-NH2	5.13	122.87	120.30
2	B	510	GLN	CB-CA-C	-5.12	100.16	110.40
1	C	296	PRO	N-CD-CG	-5.12	95.52	103.20
2	H	521	VAL	CB-CA-C	-5.12	101.68	111.40
2	H	101	VAL	CB-CA-C	-5.12	101.68	111.40
2	D	330	ARG	CG-CD-NE	-5.11	101.06	111.80
2	D	580	TRP	CB-CA-C	-5.11	100.18	110.40
2	B	580	TRP	CB-CA-C	-5.11	100.18	110.40
1	A	124	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	342	PRO	N-CD-CG	-5.10	95.56	103.20
2	D	25	ASP	CB-CG-OD1	-5.09	113.72	118.30
2	B	82	PRO	N-CD-CG	-5.08	95.58	103.20
2	F	190	VAL	CB-CA-C	-5.08	101.75	111.40
1	G	360	ASP	CB-CG-OD2	5.08	122.87	118.30
2	F	687	ARG	NE-CZ-NH1	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	LEU	CB-CG-CD1	-5.08	102.37	111.00
2	F	524	THR	CA-CB-CG2	-5.08	105.30	112.40
1	A	33	THR	N-CA-CB	-5.07	100.67	110.30
2	B	635	ARG	NE-CZ-NH2	-5.07	117.77	120.30
2	B	610	ASP	CB-CG-OD2	5.07	122.86	118.30
2	B	309	ASP	CB-CG-OD1	-5.06	113.74	118.30
2	H	88	THR	OG1-CB-CG2	-5.06	98.36	110.00
1	E	460	VAL	CB-CA-C	-5.06	101.79	111.40
2	D	219	VAL	CB-CA-C	-5.05	101.80	111.40
2	D	453	VAL	CB-CA-C	-5.05	101.80	111.40
1	A	10	GLU	CA-CB-CG	5.05	124.51	113.40
2	D	330	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	G	239	ASP	CB-CG-OD2	5.05	122.84	118.30
2	B	286	LEU	CB-CG-CD1	-5.05	102.42	111.00
2	H	517	ASP	CB-CG-OD2	5.04	122.84	118.30
1	E	296	PRO	N-CD-CG	-5.04	95.64	103.20
1	G	33	THR	N-CA-CB	-5.04	100.72	110.30
2	B	259	ARG	CB-CA-C	-5.04	100.32	110.40
2	H	453	VAL	CB-CA-C	-5.04	101.83	111.40
1	A	128	LEU	CA-CB-CG	5.03	126.88	115.30
2	B	61	VAL	CB-CA-C	-5.03	101.83	111.40
2	D	534	ASP	OD1-CG-OD2	-5.03	113.74	123.30
2	D	24	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	E	239	ASP	CB-CG-OD2	5.02	122.82	118.30
2	D	565	ASP	CB-CG-OD1	5.02	122.82	118.30
2	F	35	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	E	367	CYS	CA-CB-SG	-5.01	104.97	114.00
2	F	593	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	H	75	ASP	CB-CG-OD2	5.01	122.81	118.30
2	B	492	LEU	CB-CG-CD1	-5.01	102.48	111.00
2	B	596	LEU	CA-CB-CG	-5.01	103.78	115.30
1	G	228	CYS	CA-CB-SG	-5.01	104.98	114.00
1	G	367	CYS	CA-CB-SG	-5.01	104.98	114.00
2	H	450	LEU	CB-CG-CD1	-5.01	102.48	111.00
2	B	339	THR	CA-CB-CG2	-5.01	105.39	112.40
2	D	464	LEU	CB-CG-CD1	5.01	119.51	111.00
2	F	273	ARG	N-CA-C	-5.00	97.49	111.00
2	F	617	ARG	NE-CZ-NH1	5.00	122.80	120.30
2	D	269	ARG	NE-CZ-NH2	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3370	0	3368	249	0
1	C	3370	0	3368	158	0
1	E	3370	0	3370	293	1
1	G	3370	0	3370	299	1
2	B	5717	0	5630	326	0
2	D	5717	0	5631	309	0
2	F	5717	0	5631	368	0
2	H	5717	0	5630	409	0
3	A	8	0	0	1	0
3	C	8	0	0	0	0
3	E	8	0	0	4	0
3	G	8	0	0	3	0
4	A	53	0	31	10	0
4	C	53	0	30	3	0
4	E	53	0	30	11	0
4	G	53	0	31	8	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	B	24	0	10	4	0
6	D	24	0	10	4	0
6	F	24	0	11	7	0
6	H	24	0	10	7	0
7	B	3	0	0	4	0
7	D	3	0	0	7	0
7	F	3	0	0	8	0
7	H	3	0	0	5	0
8	B	11	0	3	9	0
8	D	11	0	3	5	0
8	F	11	0	3	5	0
8	H	11	0	3	4	0
All	All	36748	0	36173	2352	1

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 32.

All (2352) 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)
2:D:689:MET:CE	2:D:689:MET:SD	2.04	1.46
1:E:381:ARG:HH21	1:E:393:ARG:NH2	1.30	1.28
1:A:425:LEU:CD1	2:F:579:SER:HB3	1.62	1.27
2:D:496:MET:HE2	2:D:496:MET:HA	1.18	1.17
1:A:425:LEU:HD12	2:F:579:SER:HB3	1.22	1.14
1:A:348:LEU:HD12	1:A:349:ARG:N	1.62	1.13
2:D:339:THR:HG23	2:D:340:ALA:N	1.56	1.12
2:B:339:THR:HG23	2:B:340:ALA:N	1.59	1.10
1:G:325:TYR:O	1:G:326:ARG:HB2	1.52	1.09
2:D:496:MET:HA	2:D:496:MET:CE	1.83	1.08
1:A:348:LEU:HD12	1:A:349:ARG:H	1.10	1.07
2:B:560:GLY:O	2:B:561:CYS:HB3	1.48	1.07
2:D:507:ASP:OD1	2:D:508:PRO:HD2	1.55	1.07
2:B:704:ARG:HG2	2:B:704:ARG:HH11	0.98	1.06
1:A:138:GLY:O	1:A:139:TYR:HB2	1.53	1.06
1:C:133:LEU:HD13	2:D:698:ILE:HD11	1.37	1.06
1:E:301:MET:HE2	1:E:341:LEU:HB3	1.38	1.05
2:F:657:PRO:O	2:F:661:ILE:HG12	1.56	1.05
2:B:704:ARG:HH11	2:B:704:ARG:CG	1.65	1.04
2:H:631:VAL:HG12	2:H:642:ILE:HA	1.33	1.04
1:E:95:MET:SD	1:E:114:MET:HE3	1.98	1.04
1:G:455:VAL:HG22	2:H:443:THR:HG21	1.38	1.04
1:G:390:VAL:HG22	1:G:391:PRO:HD2	1.38	1.03
2:F:621:TYR:CE1	2:F:726:LYS:HG2	1.95	1.02
2:H:446:ARG:HG2	2:H:632:VAL:CG1	1.91	1.01
1:G:353:LEU:HD21	1:G:434:TYR:OH	1.62	1.00
2:H:296:ARG:HG3	2:H:296:ARG:NH1	1.74	0.99
2:H:138:ARG:NH2	2:H:329:HIS:ND1	2.07	0.99
1:G:50:MET:CE	1:G:116:ALA:HA	1.93	0.98
1:E:325:TYR:O	1:E:326:ARG:HB2	1.61	0.98
1:G:408:GLU:OE1	2:H:442:ARG:NH2	1.96	0.98
2:H:339:THR:HG23	2:H:340:ALA:N	1.73	0.98
1:E:381:ARG:HH21	1:E:393:ARG:CZ	1.78	0.97
2:H:560:GLY:O	2:H:561:CYS:HB3	1.63	0.97
2:H:621:TYR:HE1	2:H:726:LYS:HG2	1.27	0.96
2:B:558:ARG:HD3	2:B:559:GLU:OE2	1.64	0.96
2:B:704:ARG:HG2	2:B:704:ARG:NH1	1.78	0.95
2:D:138:ARG:NH2	2:D:329:HIS:ND1	2.14	0.95
1:G:237:THR:HG23	1:G:238:PRO:CD	1.96	0.95
1:E:301:MET:CE	1:E:341:LEU:HB3	1.95	0.95
1:E:381:ARG:NH2	1:E:393:ARG:NH2	2.14	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:305:LEU:HB3	2:F:306:PRO:HD3	1.49	0.94
2:F:197:GLN:HG2	2:F:488:MET:HE1	1.50	0.94
2:H:731:PRO:N	2:H:732:PRO:HD2	1.79	0.94
1:E:368:LEU:HD12	1:E:368:LEU:N	1.81	0.94
2:H:66:THR:HG22	2:H:68:ALA:H	1.31	0.93
1:G:368:LEU:N	1:G:368:LEU:HD12	1.81	0.93
1:A:390:VAL:HG22	1:A:391:PRO:HD2	1.49	0.93
2:H:561:CYS:SG	2:H:562:ALA:N	2.42	0.93
2:D:496:MET:CE	2:D:496:MET:CA	2.46	0.93
1:E:102:GLN:HB3	2:F:489:GLY:O	1.68	0.93
2:H:198:HIS:CG	2:H:526:ALA:HB2	2.02	0.92
1:E:95:MET:SD	1:E:114:MET:CE	2.58	0.92
1:G:210:LEU:N	1:G:210:LEU:HD23	1.83	0.92
2:B:446:ARG:HG2	2:B:632:VAL:HG13	1.50	0.92
2:F:538:MET:HG3	2:F:602:TYR:CE1	2.05	0.92
1:G:50:MET:HE3	1:G:116:ALA:HA	1.52	0.92
2:F:339:THR:HG23	2:F:340:ALA:N	1.84	0.91
1:E:266:LEU:O	1:E:268:ARG:N	2.04	0.91
2:H:303:LEU:O	2:H:306:PRO:HD2	1.70	0.91
2:B:319:TYR:OH	2:B:372:ARG:HD3	1.70	0.91
1:E:6:LEU:HD12	1:E:10:GLU:O	1.70	0.91
1:E:314:ARG:HD3	1:E:334:GLU:OE1	1.71	0.91
2:H:312:MET:CE	2:H:330:ARG:HH12	1.84	0.90
2:D:528:ALA:O	2:D:529:ALA:HB3	1.68	0.90
2:F:66:THR:HG22	2:F:68:ALA:H	1.34	0.90
2:F:621:TYR:HE1	2:F:726:LYS:HG2	1.35	0.90
2:H:296:ARG:HG3	2:H:296:ARG:HH11	1.28	0.90
1:G:301:MET:CE	1:G:341:LEU:HB3	2.01	0.90
1:C:237:THR:HG23	1:C:238:PRO:CD	2.01	0.90
2:H:621:TYR:CE1	2:H:726:LYS:HG2	2.06	0.90
1:G:106:CYS:HG	3:G:3001:FES:FE2	0.68	0.89
1:C:314:ARG:O	1:C:315:ARG:HB2	1.70	0.89
1:E:225:LEU:N	1:E:225:LEU:HD23	1.87	0.89
1:G:138:GLY:O	1:G:139:TYR:HB2	1.73	0.89
1:G:50:MET:HE3	1:G:116:ALA:CA	2.02	0.88
2:B:560:GLY:O	2:B:561:CYS:CB	2.21	0.88
2:H:319:TYR:OH	2:H:372:ARG:HD3	1.72	0.88
2:D:58:SER:OG	2:D:59:PRO:HD2	1.72	0.88
2:H:457:ILE:O	2:H:458:SER:HB2	1.72	0.88
1:A:425:LEU:HD12	2:F:579:SER:CB	2.02	0.88
2:B:731:PRO:HB2	2:B:732:PRO:HD3	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:364:VAL:CG2	1:G:435:ARG:HG2	2.03	0.88
1:C:41:GLU:HG3	1:C:214:LYS:HE3	1.55	0.87
2:H:496:MET:HE2	2:H:496:MET:HA	1.56	0.87
2:D:538:MET:HG3	2:D:602:TYR:CE1	2.09	0.87
1:A:325:TYR:O	1:A:326:ARG:HB2	1.73	0.87
2:B:66:THR:HG22	2:B:68:ALA:H	1.40	0.87
2:H:517:ASP:OD2	2:H:519:SER:N	2.07	0.87
1:A:237:THR:HG23	1:A:238:PRO:CD	2.04	0.87
2:D:560:GLY:O	2:D:561:CYS:HB3	1.73	0.87
2:H:446:ARG:HG2	2:H:632:VAL:HG12	1.56	0.87
1:E:399:ALA:O	1:E:401:LEU:N	2.07	0.86
2:F:247:ARG:HG2	2:F:247:ARG:HH11	1.38	0.86
2:F:507:ASP:OD1	2:F:508:PRO:HD2	1.75	0.86
2:H:195:SER:O	2:H:231:LYS:HD3	1.75	0.86
2:F:218:ARG:NE	2:F:220:GLU:OE2	2.06	0.86
1:E:237:THR:HG23	1:E:238:PRO:CD	2.06	0.86
2:D:247:ARG:HG2	2:D:247:ARG:HH11	1.39	0.86
1:G:58:ARG:HD3	1:G:277:GLN:OE1	1.76	0.86
1:G:348:LEU:HD12	1:G:349:ARG:H	1.40	0.86
1:G:322:PHE:HB3	1:G:390:VAL:CG2	2.05	0.85
1:A:26:LEU:HD13	1:A:67:LEU:HD11	1.57	0.85
1:G:364:VAL:HG22	1:G:435:ARG:HG2	1.59	0.84
2:H:538:MET:HG3	2:H:602:TYR:CE1	2.12	0.84
2:D:339:THR:CG2	2:D:340:ALA:N	2.35	0.84
2:H:247:ARG:HG2	2:H:247:ARG:HH11	1.42	0.84
1:C:301:MET:CE	1:C:341:LEU:HB3	2.08	0.84
1:E:44:CYS:HG	3:E:3002:FES:FE2	0.55	0.84
1:E:349:ARG:HD3	1:E:449:GLU:OE2	1.76	0.84
2:F:138:ARG:NH2	2:F:329:HIS:ND1	2.26	0.84
2:D:528:ALA:HB1	8:D:4000:141:C7	2.08	0.83
1:C:237:THR:HG23	1:C:238:PRO:HD2	1.60	0.83
2:D:24:ASP:OD2	2:D:254:LYS:NZ	2.10	0.83
2:F:559:GLU:OE1	2:F:578:LYS:NZ	2.11	0.83
1:G:390:VAL:HG22	1:G:391:PRO:CD	2.07	0.83
6:H:3003:MTE:S1'	7:H:3004:MOS:S	2.77	0.83
1:E:6:LEU:HD12	1:E:10:GLU:C	1.98	0.83
2:D:496:MET:N	2:D:496:MET:HE3	1.94	0.83
2:F:319:TYR:OH	2:F:372:ARG:HD3	1.77	0.83
2:D:731:PRO:N	2:D:732:PRO:HD2	1.92	0.83
1:G:348:LEU:HD12	1:G:349:ARG:N	1.93	0.83
1:A:18:ASP:OD2	1:A:19:PRO:HD2	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:79:ALA:HB1	2:H:80:PRO:HD2	1.60	0.82
2:H:731:PRO:CD	2:H:732:PRO:HD2	2.09	0.82
2:F:58:SER:OG	2:F:59:PRO:HD2	1.77	0.82
2:B:138:ARG:NH2	2:B:329:HIS:ND1	2.26	0.82
2:B:704:ARG:CG	2:B:704:ARG:NH1	2.28	0.82
1:E:367:CYS:C	1:E:368:LEU:HD12	1.99	0.82
2:H:60:GLY:O	2:H:103:ALA:HB1	1.80	0.82
2:B:684:HIS:CE1	2:F:567:ILE:HD11	2.15	0.82
2:D:179:GLN:HB3	2:D:238:LEU:HD13	1.61	0.82
1:A:425:LEU:HD11	2:F:579:SER:HB3	1.58	0.82
1:G:390:VAL:CG2	1:G:391:PRO:HD2	2.10	0.82
1:G:314:ARG:HD3	1:G:334:GLU:OE1	1.80	0.82
2:F:528:ALA:HB1	8:F:4000:141:C7	2.10	0.82
1:G:102:GLN:HB3	2:H:489:GLY:O	1.80	0.81
1:A:368:LEU:N	1:A:368:LEU:HD12	1.94	0.81
1:E:83:ALA:HB2	1:E:157:TRP:CD2	2.15	0.81
2:F:573:VAL:HG21	2:F:585:ILE:HG13	1.60	0.81
2:D:507:ASP:OD1	2:D:508:PRO:CD	2.27	0.81
1:A:24:LEU:HD21	1:A:37:GLU:HB2	1.62	0.81
2:H:198:HIS:ND1	2:H:526:ALA:HB2	1.96	0.81
1:G:349:ARG:HD3	1:G:449:GLU:OE2	1.81	0.81
1:G:373:LYS:HB2	1:G:378:GLU:HG2	1.62	0.81
4:A:3005:FAD:H8A	4:A:3005:FAD:H51A	1.63	0.80
2:F:632:VAL:HG22	2:F:643:LEU:HD11	1.63	0.80
1:A:399:ALA:O	1:A:401:LEU:N	2.13	0.80
2:B:558:ARG:CD	2:B:559:GLU:OE2	2.29	0.80
2:D:513:ILE:HG13	2:D:514:THR:N	1.97	0.80
1:E:22:SER:OG	1:E:25:GLU:HG2	1.80	0.80
2:B:513:ILE:HG13	2:B:514:THR:N	1.97	0.80
2:B:684:HIS:ND1	2:F:567:ILE:HD11	1.97	0.80
2:F:216:ASP:OD1	2:H:512:ARG:HD2	1.81	0.80
1:E:366:GLY:HA3	1:E:442:MET:SD	2.22	0.79
1:G:134:CYS:SG	1:G:137:THR:HG23	2.22	0.79
1:G:237:THR:CG2	1:G:239:ASP:H	1.95	0.79
2:F:665:GLU:HG2	2:F:710:VAL:HG21	1.64	0.79
2:F:720:GLU:HG2	2:F:724:ARG:NH2	1.96	0.79
1:C:349:ARG:HD3	1:C:449:GLU:OE2	1.82	0.79
2:D:621:TYR:CE1	2:D:726:LYS:HG2	2.18	0.79
1:A:252:LEU:CD2	1:A:281:ILE:HD13	2.13	0.78
1:A:390:VAL:HG22	1:A:391:PRO:CD	2.13	0.78
6:F:3003:MTE:S1'	7:F:3004:MOS:O2	2.42	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:278:ILE:HD11	2:D:286:LEU:HD22	1.64	0.78
1:A:390:VAL:HG13	1:A:391:PRO:O	1.84	0.78
1:C:314:ARG:HD3	1:C:334:GLU:OE1	1.84	0.78
2:D:635:ARG:HD3	2:D:750:CYS:SG	2.23	0.78
1:E:237:THR:CG2	1:E:239:ASP:H	1.96	0.78
1:E:127:ASP:OD2	1:E:268:ARG:HD2	1.84	0.77
1:A:301:MET:CE	1:A:341:LEU:HB3	2.15	0.77
2:B:731:PRO:HB2	2:B:732:PRO:CD	2.15	0.77
1:E:302:GLY:HA2	1:E:381:ARG:HH11	1.48	0.77
2:H:635:ARG:HD3	2:H:750:CYS:SG	2.24	0.77
2:D:319:TYR:OH	2:D:372:ARG:HD3	1.84	0.77
1:C:316:MET:HB2	1:C:317:PRO:HD2	1.66	0.77
2:D:632:VAL:HG22	2:D:643:LEU:HD11	1.67	0.77
1:E:381:ARG:NH2	1:E:393:ARG:CZ	2.46	0.77
2:F:563:ALA:O	2:F:566:VAL:HG23	1.83	0.77
2:D:621:TYR:HE1	2:D:726:LYS:HG2	1.49	0.77
1:E:316:MET:HB2	1:E:317:PRO:HD2	1.66	0.77
2:B:221:MET:O	2:B:221:MET:HG3	1.81	0.76
4:C:3005:FAD:N1	4:C:3005:FAD:H2'	1.99	0.76
2:F:720:GLU:HG2	2:F:724:ARG:HH21	1.48	0.76
1:E:32:LEU:HD22	1:E:79:GLU:HG3	1.66	0.76
1:G:373:LYS:O	1:G:374:GLY:O	2.04	0.76
2:H:312:MET:HE1	2:H:330:ARG:HH12	1.51	0.76
2:H:496:MET:HA	2:H:496:MET:CE	2.14	0.76
1:E:399:ALA:C	1:E:401:LEU:H	1.88	0.76
2:F:65:PHE:HB2	2:F:100:LEU:HB3	1.67	0.76
1:C:301:MET:HE3	1:C:341:LEU:HB3	1.66	0.76
2:H:691:HIS:O	2:H:692:ALA:HB2	1.84	0.76
1:G:237:THR:HG23	1:G:238:PRO:HD2	1.68	0.76
1:E:192:TRP:O	1:E:196:HIS:HD2	1.69	0.76
2:H:305:LEU:HD23	2:H:305:LEU:C	2.06	0.76
2:B:40:SER:HB2	2:B:91:VAL:HG11	1.67	0.75
2:F:538:MET:HG3	2:F:602:TYR:CD1	2.20	0.75
2:B:674:TRP:CE3	2:B:675:LEU:HD21	2.21	0.75
4:A:3005:FAD:H51A	4:A:3005:FAD:C8A	2.16	0.75
2:H:123:ARG:HB3	2:H:124:PRO:HD2	1.68	0.75
2:B:42:GLU:OE1	2:F:564:ARG:NH2	2.19	0.75
2:H:559:GLU:O	2:H:560:GLY:O	2.03	0.75
1:A:301:MET:CE	1:A:341:LEU:HD22	2.17	0.74
2:D:303:LEU:O	2:D:306:PRO:HD2	1.87	0.74
1:E:381:ARG:HH21	1:E:393:ARG:HH21	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:TYR:O	1:C:326:ARG:HB2	1.85	0.74
1:A:367:CYS:C	1:A:368:LEU:HD12	2.06	0.74
2:B:517:ASP:OD2	2:B:519:SER:OG	2.05	0.74
2:D:407:GLN:OE1	2:D:618:PRO:HD2	1.87	0.74
2:B:530:SER:OG	2:B:730:GLU:HG3	1.87	0.74
1:E:83:ALA:HB2	1:E:157:TRP:CE3	2.23	0.74
2:F:296:ARG:HG3	2:F:296:ARG:NH1	2.03	0.74
6:F:3003:MTE:S1'	7:F:3004:MOS:S	2.83	0.74
2:H:674:TRP:CE3	2:H:675:LEU:HD21	2.23	0.74
2:H:701:PHE:O	2:H:704:ARG:HG2	1.88	0.73
1:G:237:THR:HG23	1:G:238:PRO:CG	2.18	0.73
2:H:247:ARG:HG2	2:H:247:ARG:NH1	2.01	0.73
1:A:233:GLN:OE1	1:A:233:GLN:HA	1.87	0.73
2:B:728:VAL:O	2:B:728:VAL:HG22	1.88	0.73
1:G:41:GLU:HG3	1:G:214:LYS:HE3	1.68	0.73
2:H:367:ASP:OD2	2:H:431:ARG:NH1	2.17	0.73
2:D:247:ARG:HG2	2:D:247:ARG:NH1	2.01	0.73
1:E:133:LEU:HD13	2:F:698:ILE:HD11	1.71	0.73
1:A:314:ARG:HD3	1:A:334:GLU:OE1	1.88	0.73
1:G:366:GLY:HA3	1:G:442:MET:SD	2.28	0.73
1:G:301:MET:HE3	1:G:341:LEU:HB3	1.69	0.73
2:H:296:ARG:HH11	2:H:296:ARG:CG	1.96	0.73
1:C:279:ALA:HB1	4:C:3005:FAD:H4'	1.69	0.73
1:C:360:ASP:OD1	2:D:697:LYS:HE3	1.88	0.73
1:E:337:GLU:O	1:E:338:SER:HB3	1.87	0.73
2:H:58:SER:OG	2:H:59:PRO:HD2	1.88	0.73
2:H:412:CYS:HA	2:H:624:TYR:CZ	2.24	0.73
1:A:432:ALA:O	1:A:433:ALA:C	2.24	0.72
2:F:720:GLU:CG	2:F:724:ARG:HH21	2.01	0.72
2:H:312:MET:HE2	2:H:330:ARG:HH12	1.51	0.72
2:B:492:LEU:C	2:B:492:LEU:HD12	2.07	0.72
2:H:507:ASP:OD1	2:H:508:PRO:CD	2.37	0.72
1:A:128:LEU:O	1:A:129:LEU:HD23	1.89	0.72
1:A:271:ALA:HA	1:A:359:GLN:NE2	2.05	0.72
2:B:621:TYR:CE1	2:B:726:LYS:HG2	2.24	0.72
1:C:12:ARG:NH2	1:C:30:GLU:OE1	2.20	0.72
1:E:319:GLU:OE2	1:E:319:GLU:N	2.22	0.72
1:A:237:THR:HG23	1:A:238:PRO:HD2	1.72	0.72
1:E:83:ALA:HB2	1:E:157:TRP:CE2	2.25	0.72
7:B:3004:MOS:MO	7:B:3004:MOS:S	2.01	0.72
2:D:232:GLU:OE2	8:D:4000:141:H1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:631:VAL:HG21	2:D:743:LEU:CD1	2.20	0.72
1:E:390:VAL:HG23	1:E:391:PRO:HD2	1.70	0.72
1:G:271:ALA:HA	1:G:359:GLN:NE2	2.05	0.72
2:H:417:LEU:HG	2:H:648:LEU:HD23	1.71	0.72
2:F:221:MET:HE1	2:F:224:MET:HG3	1.70	0.72
2:B:303:LEU:O	2:B:306:PRO:HD2	1.89	0.71
2:H:731:PRO:HB2	2:H:732:PRO:CD	2.20	0.71
2:B:561:CYS:SG	2:B:562:ALA:N	2.63	0.71
1:E:58:ARG:HG2	1:E:277:GLN:OE1	1.90	0.71
1:E:358:ASP:OD2	2:F:702:SER:HB3	1.90	0.71
1:A:41:GLU:HG3	1:A:214:LYS:HE3	1.72	0.71
1:C:301:MET:HE2	1:C:341:LEU:HD13	1.72	0.71
2:D:731:PRO:CD	2:D:732:PRO:HD2	2.19	0.71
1:C:165:THR:C	1:C:166:LEU:HD23	2.09	0.71
1:C:319:GLU:N	1:C:319:GLU:OE2	2.22	0.71
2:D:329:HIS:HB3	2:D:331:LEU:HD21	1.71	0.71
2:F:221:MET:CE	2:F:224:MET:HG3	2.20	0.71
1:A:373:LYS:HB2	1:A:378:GLU:HG2	1.72	0.71
1:G:115:ALA:O	1:G:116:ALA:C	2.27	0.71
1:E:360:ASP:OD1	2:F:697:LYS:HE3	1.91	0.71
1:G:115:ALA:O	1:G:118:HIS:N	2.24	0.71
1:G:252:LEU:CD2	1:G:281:ILE:HD13	2.19	0.71
2:H:673:GLY:O	2:H:678:GLU:HB2	1.91	0.71
1:A:322:PHE:HB3	1:A:390:VAL:CG2	2.21	0.71
2:D:198:HIS:CG	2:D:526:ALA:HB2	2.26	0.71
1:G:301:MET:HE2	1:G:341:LEU:HB3	1.72	0.70
2:H:595:SER:O	2:H:596:LEU:HD23	1.91	0.70
2:B:691:HIS:O	2:B:692:ALA:HB2	1.91	0.70
2:F:635:ARG:HD3	2:F:750:CYS:SG	2.31	0.70
2:H:671:GLY:O	2:H:674:TRP:HB3	1.90	0.70
2:H:448:ILE:HG13	2:H:630:GLU:HB2	1.73	0.70
2:D:325:ARG:C	2:D:326:ILE:HG13	2.11	0.70
7:D:3004:MOS:S	7:D:3004:MOS:MO	2.03	0.70
7:F:3004:MOS:S	7:F:3004:MOS:MO	2.01	0.70
1:G:367:CYS:C	1:G:368:LEU:HD12	2.11	0.70
1:A:399:ALA:C	1:A:401:LEU:H	1.95	0.70
1:C:373:LYS:O	1:C:374:GLY:O	2.10	0.70
1:E:237:THR:HG22	1:E:239:ASP:H	1.57	0.70
2:F:367:ASP:OD2	2:F:431:ARG:NH1	2.21	0.70
2:B:617:ARG:HD3	2:B:619:PHE:O	1.92	0.69
1:G:37:GLU:OE1	2:H:256:ARG:NH2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:776:ARG:O	2:H:777:ALA:HB3	1.92	0.69
2:D:559:GLU:OE1	2:D:578:LYS:NZ	2.15	0.69
1:E:243:ILE:CD1	1:E:341:LEU:HD11	2.21	0.69
2:B:457:ILE:O	2:B:458:SER:HB2	1.93	0.69
2:F:303:LEU:O	2:F:306:PRO:HD2	1.93	0.69
2:H:507:ASP:OD1	2:H:508:PRO:HD2	1.92	0.69
2:F:66:THR:HG22	2:F:68:ALA:N	2.08	0.69
2:D:496:MET:CA	2:D:496:MET:HE3	2.19	0.69
1:A:359:GLN:HG3	1:A:359:GLN:O	1.93	0.69
2:B:296:ARG:HG3	2:B:296:ARG:NH1	2.08	0.69
2:B:367:ASP:OD1	2:B:368:PRO:HD2	1.93	0.69
1:E:445:ARG:NH2	2:F:634:ASP:OD2	2.26	0.69
2:F:247:ARG:HG2	2:F:247:ARG:NH1	2.05	0.69
2:H:757:LEU:HD12	2:H:758:GLN:N	2.07	0.69
1:A:446:TYR:CE2	1:A:450:LEU:HD12	2.28	0.69
2:D:496:MET:HE2	2:D:496:MET:CA	2.06	0.69
1:C:367:CYS:C	1:C:368:LEU:HD12	2.14	0.68
1:E:349:ARG:HG2	1:E:351:TYR:OH	1.93	0.68
2:F:221:MET:HE1	2:F:223:ARG:C	2.13	0.68
1:C:368:LEU:HD12	1:C:368:LEU:N	2.08	0.68
2:D:631:VAL:HG21	2:D:743:LEU:HD13	1.74	0.68
1:G:237:THR:HG23	1:G:238:PRO:HG2	1.76	0.68
2:H:65:PHE:HB2	2:H:100:LEU:HB3	1.74	0.68
2:D:310:ARG:HD2	2:D:344:PHE:O	1.93	0.68
2:D:728:VAL:O	2:D:728:VAL:HG22	1.93	0.68
2:F:728:VAL:O	2:F:728:VAL:HG22	1.91	0.68
1:G:50:MET:CE	1:G:116:ALA:CA	2.65	0.68
2:H:105:SER:O	2:H:106:HIS:C	2.30	0.68
2:H:276:TYR:OH	2:H:359:HIS:HD2	1.76	0.68
2:H:457:ILE:O	2:H:458:SER:CB	2.42	0.68
1:A:103:CYS:HB3	1:A:136:CYS:SG	2.33	0.68
2:F:422:GLN:HG2	2:F:427:PHE:CD2	2.28	0.68
2:F:446:ARG:NH1	2:F:630:GLU:OE2	2.25	0.68
1:E:302:GLY:CA	1:E:381:ARG:HH11	2.05	0.68
2:H:528:ALA:HB1	8:H:4000:141:C7	2.23	0.68
2:H:656:ASN:ND2	2:H:659:LEU:HD12	2.09	0.68
2:D:360:LEU:HD11	2:D:364:MET:CE	2.23	0.68
1:E:299:ILE:HG13	1:E:318:LEU:HD23	1.75	0.68
1:G:432:ALA:O	1:G:433:ALA:C	2.27	0.68
2:H:171:GLN:HG3	2:H:678:GLU:OE1	1.94	0.68
1:A:301:MET:HE2	1:A:341:LEU:HD22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:VAL:HG12	2:D:62:ILE:N	2.09	0.68
2:F:310:ARG:HD2	2:F:344:PHE:O	1.93	0.68
1:G:415:LEU:HB2	1:G:416:PRO:HD3	1.75	0.68
2:B:448:ILE:HG13	2:B:630:GLU:HB2	1.75	0.67
2:B:461:LEU:HD12	2:B:463:HIS:CE1	2.29	0.67
2:B:563:ALA:O	2:B:566:VAL:HG23	1.94	0.67
2:D:730:GLU:C	2:D:732:PRO:HD2	2.13	0.67
2:F:195:SER:O	2:F:231:LYS:HD3	1.94	0.67
1:A:361:ILE:HD12	1:A:429:ARG:NH2	2.09	0.67
1:A:128:LEU:C	1:A:129:LEU:HD23	2.14	0.67
1:A:297:ALA:HA	1:A:367:CYS:SG	2.34	0.67
1:E:314:ARG:HH22	1:E:329:ASP:CG	1.97	0.67
2:F:179:GLN:HB3	2:F:238:LEU:HD13	1.75	0.67
1:G:237:THR:OG1	1:G:238:PRO:HD2	1.94	0.67
2:D:360:LEU:HG	2:D:364:MET:HE3	1.75	0.67
2:D:678:GLU:HB3	2:D:696:TYR:CZ	2.29	0.67
1:E:352:LYS:HE3	1:E:362:SER:OG	1.93	0.67
1:G:24:LEU:HD21	1:G:37:GLU:HB2	1.77	0.67
2:D:312:MET:HE1	2:D:330:ARG:HH12	1.60	0.67
1:E:273:GLU:OE1	1:E:276:ARG:NH1	2.27	0.67
2:D:471:VAL:HG12	2:D:472:GLN:N	2.10	0.67
4:A:3005:FAD:N1	4:A:3005:FAD:H2'	2.10	0.67
2:B:538:MET:HG3	2:B:602:TYR:CE1	2.29	0.67
1:E:266:LEU:O	1:E:267:LEU:C	2.32	0.67
1:G:337:GLU:HG3	1:G:337:GLU:O	1.94	0.67
2:H:347:PRO:HG3	2:H:734:LEU:HD11	1.75	0.67
2:B:776:ARG:O	2:B:777:ALA:HB3	1.95	0.67
1:A:445:ARG:HG3	1:A:455:VAL:HG11	1.76	0.67
1:E:89:HIS:O	1:E:90:PRO:C	2.29	0.67
2:H:644:ARG:HB2	2:H:707:ILE:HB	1.77	0.67
1:A:301:MET:HE3	1:A:341:LEU:HB3	1.77	0.66
1:C:60:VAL:HG21	1:C:65:MET:HE1	1.76	0.66
2:D:678:GLU:OE1	2:D:696:TYR:OH	2.13	0.66
2:B:422:GLN:HG2	2:B:427:PHE:CD2	2.30	0.66
2:D:660:ASP:O	2:D:664:ILE:HG13	1.95	0.66
2:H:263:MET:HE3	2:H:692:ALA:HA	1.77	0.66
2:H:633:ILE:HD13	2:H:746:ALA:CB	2.26	0.66
6:H:3003:MTE:S2'	7:H:3004:MOS:S	2.92	0.66
2:B:61:VAL:CG1	2:B:62:ILE:N	2.55	0.66
1:E:37:GLU:CD	2:F:256:ARG:NH2	2.49	0.66
1:E:68:PRO:HG2	1:E:224:PHE:CE1	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:23:LEU:HD13	2:F:194:CYS:HA	1.76	0.66
2:F:281:ASP:OD1	2:F:283:SER:OG	2.12	0.66
2:H:280:ALA:C	2:H:287:LEU:HD12	2.16	0.66
1:E:237:THR:HG23	1:E:238:PRO:HD2	1.75	0.66
1:C:390:VAL:CG2	1:C:391:PRO:HD2	2.25	0.66
2:F:70:LEU:HD12	2:F:74:ASN:HB2	1.76	0.66
2:H:558:ARG:CD	2:H:559:GLU:OE2	2.43	0.66
2:B:446:ARG:HG2	2:B:632:VAL:CG1	2.25	0.66
1:E:302:GLY:HA2	1:E:381:ARG:NH1	2.11	0.66
1:G:337:GLU:O	1:G:338:SER:HB3	1.95	0.66
2:H:296:ARG:NH1	2:H:296:ARG:CG	2.51	0.66
2:D:446:ARG:NH1	2:D:630:GLU:OE2	2.28	0.66
4:E:3005:FAD:H2'	4:E:3005:FAD:N1	2.11	0.66
7:F:3004:MOS:S	8:F:4000:141:N8	2.69	0.66
2:B:744:HIS:C	2:B:744:HIS:CD2	2.70	0.66
2:D:671:GLY:O	2:D:674:TRP:HB3	1.96	0.66
1:E:106:CYS:SG	1:E:134:CYS:HB2	2.35	0.66
2:H:173:HIS:HA	2:H:341:PHE:CE1	2.31	0.65
2:B:310:ARG:HD2	2:B:344:PHE:O	1.96	0.65
1:C:316:MET:HB2	1:C:317:PRO:CD	2.25	0.65
1:E:237:THR:HG23	1:E:238:PRO:CG	2.27	0.65
1:G:141:PRO:HG2	1:G:142:ILE:N	2.12	0.65
2:H:558:ARG:HD3	2:H:559:GLU:OE2	1.96	0.65
1:A:237:THR:CG2	1:A:239:ASP:H	2.08	0.65
1:G:325:TYR:CE1	1:G:326:ARG:HG2	2.32	0.65
1:E:76:ARG:NH1	1:E:161:ASP:OD2	2.24	0.65
2:F:40:SER:HB2	2:F:91:VAL:HG11	1.78	0.65
2:F:346:GLY:N	2:F:347:PRO:CD	2.59	0.65
2:H:179:GLN:HB3	2:H:238:LEU:HD13	1.79	0.65
2:F:367:ASP:OD1	2:F:368:PRO:HD2	1.96	0.65
1:E:129:LEU:O	1:E:130:ALA:C	2.32	0.65
2:F:644:ARG:HB2	2:F:707:ILE:HB	1.78	0.65
2:H:53:GLU:N	2:H:54:PRO:CD	2.59	0.65
2:B:34:HIS:C	2:B:35:LEU:HD23	2.16	0.65
2:B:218:ARG:HH22	2:D:218:ARG:HH22	1.44	0.65
2:D:168:ILE:HD13	2:D:351:LEU:HD23	1.78	0.65
2:F:568:PHE:CD2	2:F:573:VAL:HG22	2.31	0.65
1:G:314:ARG:HH22	1:G:329:ASP:CG	2.00	0.65
4:G:3005:FAD:N1	4:G:3005:FAD:H2'	2.12	0.65
1:A:316:MET:HB2	1:A:317:PRO:CD	2.27	0.65
2:B:325:ARG:C	2:B:326:ILE:HG13	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:TYR:O	2:H:122:PRO:HD3	1.97	0.65
1:A:425:LEU:HD21	2:F:577:GLY:O	1.96	0.65
2:B:262:ASP:O	2:B:266:THR:HG23	1.96	0.64
1:E:205:GLY:N	4:E:3005:FAD:O2A	2.30	0.64
1:G:164:PHE:O	1:G:166:LEU:HG	1.97	0.64
1:G:299:ILE:HG13	1:G:318:LEU:HD23	1.78	0.64
1:C:102:GLN:HB3	2:D:489:GLY:O	1.97	0.64
7:D:3004:MOS:MO	7:D:3004:MOS:O2	1.68	0.64
2:F:296:ARG:HG3	2:F:296:ARG:HH11	1.60	0.64
1:G:390:VAL:CG2	1:G:391:PRO:CD	2.72	0.64
2:H:198:HIS:CG	2:H:526:ALA:CB	2.79	0.64
2:H:221:MET:HG3	2:H:221:MET:O	1.96	0.64
1:A:349:ARG:HD3	1:A:449:GLU:OE2	1.97	0.64
2:F:498:GLN:O	2:F:499:VAL:C	2.35	0.64
2:H:329:HIS:HB3	2:H:331:LEU:HD21	1.78	0.64
1:A:28:ARG:NH2	2:B:25:ASP:OD1	2.25	0.64
1:A:231:LEU:CD2	1:A:231:LEU:O	2.46	0.64
7:F:3004:MOS:O2	7:F:3004:MOS:MO	1.69	0.64
2:H:538:MET:HG3	2:H:602:TYR:CD1	2.33	0.64
2:B:107:ARG:O	2:B:108:ALA:C	2.33	0.64
2:B:344:PHE:CZ	8:B:4000:141:C6	2.81	0.64
2:F:222:ARG:HB2	2:F:515:ALA:HB2	1.80	0.64
2:H:481:LEU:HD12	2:H:482:ASN:N	2.12	0.64
2:B:150:ASP:C	2:B:150:ASP:OD1	2.35	0.64
2:F:166:PHE:CZ	2:F:355:ARG:HG3	2.32	0.64
1:G:237:THR:HG23	1:G:238:PRO:N	2.11	0.64
1:C:390:VAL:HG23	1:C:391:PRO:HD2	1.80	0.64
1:E:237:THR:HG23	1:E:238:PRO:HG2	1.80	0.64
1:E:243:ILE:HD12	1:E:341:LEU:HD11	1.79	0.64
1:C:349:ARG:CD	1:C:449:GLU:OE2	2.45	0.63
2:D:558:ARG:HD3	2:D:559:GLU:OE2	1.98	0.63
2:F:513:ILE:HG23	2:F:513:ILE:O	1.98	0.63
1:G:92:GLN:HG2	2:H:16:VAL:HG13	1.79	0.63
1:A:252:LEU:HD22	1:A:281:ILE:HD13	1.79	0.63
1:C:408:GLU:OE1	2:D:442:ARG:NH2	2.24	0.63
2:F:407:GLN:OE1	2:F:618:PRO:HD2	1.98	0.63
2:H:417:LEU:HG	2:H:648:LEU:CD2	2.27	0.63
6:H:3003:MTE:S1'	7:H:3004:MOS:O2	2.56	0.63
2:B:40:SER:HB2	2:B:98:ILE:HD11	1.79	0.63
2:B:647:ILE:HD13	2:B:735:LEU:HD13	1.79	0.63
2:D:66:THR:HG22	2:D:68:ALA:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:674:TRP:CE3	2:D:675:LEU:HD21	2.34	0.63
1:E:377:ILE:HG13	1:E:404:GLN:O	1.98	0.63
1:G:203:ALA:HB3	4:G:3005:FAD:O1P	1.98	0.63
1:G:316:MET:HB2	1:G:317:PRO:HD2	1.81	0.63
2:H:93:PHE:CE2	2:H:299:TRP:NE1	2.67	0.63
2:B:717:ASN:OD1	2:B:719:GLU:N	2.31	0.63
2:F:324:LEU:HD23	2:F:324:LEU:C	2.19	0.63
2:F:497:VAL:O	2:F:500:ALA:HB3	1.98	0.63
1:G:231:LEU:O	1:G:231:LEU:HD23	1.99	0.63
2:H:143:PRO:HB3	2:H:329:HIS:ND1	2.13	0.63
1:A:206:THR:HG21	1:A:275:VAL:HG13	1.79	0.63
2:F:593:ARG:NH1	2:H:604:THR:O	2.27	0.63
2:F:595:SER:HB2	2:H:601:PHE:CD1	2.33	0.63
2:H:731:PRO:N	2:H:732:PRO:CD	2.57	0.63
1:A:337:GLU:O	1:A:338:SER:HB3	1.96	0.63
1:A:366:GLY:HA3	1:A:442:MET:SD	2.39	0.63
2:B:166:PHE:CZ	2:B:355:ARG:HG3	2.34	0.63
2:B:496:MET:HE2	2:B:496:MET:HA	1.81	0.63
2:F:730:GLU:C	2:F:732:PRO:HD2	2.18	0.63
2:H:733:PHE:HD2	2:H:734:LEU:HD12	1.64	0.63
7:H:3004:MOS:S	7:H:3004:MOS:MO	2.09	0.63
2:B:218:ARG:HH22	2:D:218:ARG:NH2	1.97	0.63
1:E:399:ALA:C	1:E:401:LEU:N	2.48	0.63
1:G:103:CYS:HB3	1:G:136:CYS:SG	2.39	0.63
1:G:283:GLY:O	1:G:284:ASN:C	2.34	0.63
2:B:776:ARG:O	2:B:777:ALA:CB	2.47	0.63
1:C:37:GLU:OE1	2:D:256:ARG:NH2	2.31	0.63
2:D:674:TRP:CD2	2:D:675:LEU:HD21	2.34	0.63
2:D:731:PRO:N	2:D:732:PRO:CD	2.60	0.63
1:E:390:VAL:CG2	1:E:391:PRO:HD2	2.28	0.63
2:F:61:VAL:HG12	2:F:62:ILE:N	2.10	0.63
2:H:262:ASP:O	2:H:266:THR:HG23	1.99	0.63
2:H:507:ASP:OD1	2:H:508:PRO:N	2.32	0.63
2:H:634:ASP:OD2	2:H:637:THR:OG1	2.17	0.63
1:A:408:GLU:CD	2:B:442:ARG:HH22	2.02	0.63
1:C:216:LEU:HD12	2:D:114:ARG:NH1	2.14	0.63
2:H:247:ARG:HH11	2:H:247:ARG:CG	2.11	0.63
2:D:645:THR:HG21	2:D:668:TYR:CZ	2.34	0.62
1:E:95:MET:SD	1:E:114:MET:HE1	2.38	0.62
2:F:305:LEU:HB3	2:F:306:PRO:CD	2.28	0.62
1:G:237:THR:HG23	1:G:239:ASP:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:TYR:O	1:G:326:ARG:CB	2.35	0.62
2:D:53:GLU:HA	2:D:53:GLU:OE1	1.98	0.62
1:E:36:LYS:HD3	1:E:105:PHE:CE1	2.35	0.62
1:E:297:ALA:O	1:E:300:ALA:N	2.31	0.62
2:F:214:PHE:CD1	2:F:214:PHE:N	2.64	0.62
2:F:325:ARG:C	2:F:326:ILE:HG13	2.20	0.62
1:G:322:PHE:HB3	1:G:390:VAL:HG21	1.80	0.62
2:H:563:ALA:O	2:H:566:VAL:HG23	1.98	0.62
1:A:301:MET:HE2	1:A:341:LEU:HB3	1.82	0.62
2:F:218:ARG:NH2	2:F:517:ASP:OD1	2.32	0.62
2:F:446:ARG:HG2	2:F:632:VAL:HG13	1.81	0.62
1:G:85:ASP:OD2	1:G:87:ARG:HD3	1.99	0.62
1:E:283:GLY:O	1:E:284:ASN:C	2.36	0.62
1:E:298:LEU:O	1:E:299:ILE:C	2.34	0.62
2:H:312:MET:HE1	2:H:330:ARG:NH1	2.13	0.62
1:C:322:PHE:HB3	1:C:390:VAL:HG23	1.80	0.62
1:E:151:GLY:O	1:E:152:GLU:HG2	2.00	0.62
7:H:3004:MOS:O2	7:H:3004:MOS:MO	1.69	0.62
2:F:461:LEU:HD12	2:F:463:HIS:CE1	2.34	0.62
2:H:476:ASP:OD2	2:H:478:SER:OG	2.13	0.62
2:D:61:VAL:CG1	2:D:62:ILE:N	2.63	0.62
2:F:459:PHE:N	2:F:465:ASN:OD1	2.33	0.62
1:G:237:THR:CG2	1:G:238:PRO:HD2	2.30	0.62
1:E:241:TYR:O	1:E:340:THR:HG23	1.99	0.62
1:G:61:ASN:ND2	1:G:61:ASN:H	1.98	0.62
1:G:237:THR:CB	1:G:238:PRO:HD2	2.30	0.62
2:H:38:GLY:C	2:H:39:LEU:HD23	2.20	0.62
2:H:668:TYR:O	2:H:669:VAL:C	2.35	0.62
2:B:61:VAL:HG12	2:B:62:ILE:N	2.12	0.61
2:B:457:ILE:O	2:B:458:SER:CB	2.48	0.61
1:C:92:GLN:HG2	2:D:16:VAL:HG13	1.82	0.61
1:E:104:GLY:HA3	2:F:22:TYR:OH	2.00	0.61
1:G:237:THR:HG22	1:G:239:ASP:H	1.63	0.61
2:B:324:LEU:HD23	2:B:324:LEU:C	2.20	0.61
2:B:360:LEU:HG	2:B:364:MET:HE2	1.83	0.61
2:B:22:TYR:CD1	2:B:22:TYR:N	2.68	0.61
1:A:53:ASP:C	1:A:53:ASP:OD1	2.37	0.61
1:A:237:THR:OG1	1:A:238:PRO:HD2	1.99	0.61
1:A:316:MET:HB2	1:A:317:PRO:HD2	1.81	0.61
2:B:730:GLU:C	2:B:732:PRO:HD2	2.20	0.61
1:C:301:MET:CE	1:C:341:LEU:HD13	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:305:LEU:HB3	2:D:306:PRO:HD3	1.81	0.61
2:D:312:MET:CE	2:D:330:ARG:HH12	2.13	0.61
2:B:512:ARG:HD2	2:D:216:ASP:OD1	2.00	0.61
2:D:339:THR:HG23	2:D:340:ALA:H	1.61	0.61
1:G:237:THR:CG2	1:G:238:PRO:CD	2.77	0.61
2:B:305:LEU:HD23	2:B:305:LEU:C	2.21	0.61
1:C:85:ASP:OD1	1:C:87:ARG:NH1	2.34	0.61
2:B:443:THR:O	2:B:444:LEU:HD23	2.01	0.61
2:F:24:ASP:OD2	2:F:254:LYS:NZ	2.31	0.61
2:F:443:THR:O	2:F:444:LEU:HD23	2.00	0.61
1:G:359:GLN:HG3	1:G:359:GLN:O	2.00	0.61
2:H:107:ARG:O	2:H:108:ALA:C	2.39	0.61
2:H:633:ILE:HD13	2:H:746:ALA:HB1	1.81	0.61
2:H:737:ILE:O	2:H:738:SER:C	2.37	0.61
1:A:231:LEU:O	1:A:231:LEU:HD23	1.99	0.61
1:C:50:MET:HE1	1:C:116:ALA:HA	1.82	0.61
2:D:70:LEU:HD12	2:D:74:ASN:HB2	1.83	0.61
1:E:78:ILE:HG23	1:E:79:GLU:N	2.15	0.61
2:F:560:GLY:O	2:F:561:CYS:HB3	1.99	0.61
2:H:762:THR:O	2:H:766:VAL:HG23	2.00	0.61
2:F:453:VAL:HG12	2:F:454:LYS:N	2.16	0.61
2:F:595:SER:HB2	2:H:601:PHE:CG	2.36	0.61
1:G:423:THR:O	1:G:423:THR:HG22	2.01	0.61
1:A:237:THR:HG23	1:A:239:ASP:H	1.66	0.61
1:G:59:ALA:C	1:G:60:VAL:CG1	2.68	0.61
1:E:18:ASP:OD2	1:E:19:PRO:HD2	2.01	0.60
1:G:83:ALA:HB2	1:G:157:TRP:CE3	2.36	0.60
2:H:46:ALA:HB2	2:H:123:ARG:HH21	1.65	0.60
2:B:171:GLN:HG3	2:B:678:GLU:OE1	2.00	0.60
1:E:228:CYS:O	1:E:229:LYS:C	2.37	0.60
1:G:81:ILE:HG22	1:G:81:ILE:O	2.00	0.60
2:B:691:HIS:O	2:B:691:HIS:CG	2.52	0.60
2:D:440:THR:HG22	2:D:440:THR:O	2.02	0.60
2:D:731:PRO:HD2	2:D:732:PRO:HD2	1.83	0.60
2:F:329:HIS:HB3	2:F:331:LEU:HD21	1.82	0.60
2:H:730:GLU:N	2:H:731:PRO:CD	2.65	0.60
2:H:741:LEU:N	2:H:741:LEU:CD1	2.55	0.60
1:A:237:THR:HG23	1:A:238:PRO:CG	2.31	0.60
2:B:58:SER:OG	2:B:59:PRO:HD2	2.00	0.60
2:B:737:ILE:O	2:B:738:SER:C	2.38	0.60
2:F:237:HIS:ND1	2:F:237:HIS:N	2.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:37:GLU:CD	2:H:256:ARG:NH2	2.55	0.60
1:G:271:ALA:HA	1:G:359:GLN:HE22	1.66	0.60
2:B:93:PHE:CE2	2:B:299:TRP:NE1	2.70	0.60
2:B:631:VAL:HG21	2:B:743:LEU:HD13	1.83	0.60
2:F:61:VAL:CG1	2:F:62:ILE:N	2.62	0.60
2:F:269:ARG:NH2	2:F:341:PHE:CD2	2.69	0.60
2:H:372:ARG:O	2:H:373:ALA:C	2.39	0.60
2:B:528:ALA:O	2:B:529:ALA:HB3	2.02	0.60
1:C:369:ASN:O	1:C:370:LEU:HD23	2.01	0.60
2:F:197:GLN:CG	2:F:488:MET:HE1	2.28	0.60
1:A:370:LEU:CD2	1:A:380:ALA:HA	2.32	0.60
2:B:490:GLN:O	2:B:490:GLN:HG2	2.02	0.60
1:C:165:THR:O	1:C:166:LEU:HD23	2.00	0.60
1:E:67:LEU:O	1:E:69:GLN:N	2.34	0.60
2:H:479:VAL:HG12	2:H:480:ALA:N	2.16	0.60
2:H:661:ILE:HD11	2:H:712:LEU:HG	1.82	0.60
1:C:28:ARG:O	1:C:31:GLY:N	2.28	0.60
1:G:349:ARG:CD	1:G:449:GLU:OE2	2.50	0.60
2:H:440:THR:O	2:H:440:THR:HG22	2.02	0.60
1:A:22:SER:OG	1:A:25:GLU:HG2	2.02	0.60
1:A:444:LEU:O	1:A:448:ARG:HG3	2.02	0.60
1:E:427:ASP:OD1	1:E:435:ARG:NH2	2.35	0.60
1:G:240:GLY:HA2	1:G:343:LYS:HG2	1.83	0.60
2:B:66:THR:HG22	2:B:68:ALA:N	2.13	0.59
2:F:594:ILE:O	2:F:596:LEU:HG	2.02	0.59
2:F:647:ILE:HG22	2:F:648:LEU:N	2.17	0.59
1:G:252:LEU:HD22	1:G:281:ILE:HD13	1.84	0.59
2:H:251:ARG:HB2	2:H:252:PRO:CD	2.32	0.59
1:A:337:GLU:O	1:A:337:GLU:HG3	2.02	0.59
1:A:351:TYR:CE2	1:A:445:ARG:HD3	2.36	0.59
2:B:412:CYS:HA	2:B:624:TYR:CZ	2.38	0.59
2:D:731:PRO:HB2	2:D:732:PRO:CD	2.31	0.59
2:B:507:ASP:OD1	2:B:508:PRO:HD2	2.01	0.59
2:D:678:GLU:HB3	2:D:696:TYR:OH	2.02	0.59
2:H:731:PRO:HD2	2:H:732:PRO:HD2	1.82	0.59
1:A:165:THR:O	1:A:165:THR:HG23	2.01	0.59
2:F:637:THR:OG1	2:F:639:GLU:HG3	2.03	0.59
2:H:731:PRO:CB	2:H:732:PRO:CD	2.79	0.59
2:D:360:LEU:CG	2:D:364:MET:HE3	2.33	0.59
1:E:181:PHE:C	1:E:182:LEU:HD12	2.23	0.59
1:G:59:ALA:C	1:G:60:VAL:HG13	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:263:MET:CE	2:H:692:ALA:HA	2.33	0.59
2:D:58:SER:OG	2:D:59:PRO:CD	2.49	0.59
2:F:123:ARG:HB3	2:F:124:PRO:HD2	1.85	0.59
2:F:606:LYS:NZ	2:F:719:GLU:OE1	2.33	0.59
1:G:192:TRP:O	1:G:196:HIS:HD2	1.85	0.59
2:H:66:THR:HG22	2:H:68:ALA:N	2.09	0.59
2:H:372:ARG:HG3	2:H:372:ARG:HH11	1.67	0.59
2:H:700:ALA:O	2:H:701:PHE:C	2.40	0.59
1:C:237:THR:HG23	1:C:238:PRO:N	2.17	0.59
2:D:367:ASP:OD1	2:D:368:PRO:HD2	2.02	0.59
1:E:216:LEU:HD12	2:F:114:ARG:NH1	2.18	0.59
2:H:450:LEU:HG	2:H:451:SER:N	2.14	0.59
2:B:65:PHE:HB2	2:B:100:LEU:HB3	1.85	0.59
2:D:179:GLN:HB3	2:D:238:LEU:CD1	2.32	0.59
2:F:275:ARG:HB3	2:F:292:VAL:HB	1.85	0.59
2:F:650:ASP:OD2	2:F:726:LYS:NZ	2.29	0.59
2:H:251:ARG:HB2	2:H:252:PRO:HD2	1.85	0.59
1:A:78:ILE:HG23	1:A:79:GLU:N	2.16	0.59
2:D:263:MET:CE	2:D:692:ALA:HA	2.32	0.59
2:D:320:PHE:CD2	2:D:401:GLN:NE2	2.71	0.59
1:E:53:ASP:C	1:E:53:ASP:OD1	2.41	0.59
1:E:138:GLY:O	1:E:139:TYR:HB2	2.02	0.59
1:C:53:ASP:OD2	1:C:58:ARG:NH2	2.36	0.58
2:D:221:MET:HG3	2:D:221:MET:O	2.01	0.58
1:E:373:LYS:O	1:E:374:GLY:O	2.21	0.58
1:E:447:VAL:O	1:E:448:ARG:C	2.37	0.58
2:F:462:THR:O	2:F:465:ASN:ND2	2.35	0.58
2:H:372:ARG:O	2:H:375:ASN:N	2.31	0.58
2:B:232:GLU:OE2	8:B:4000:141:H1	2.03	0.58
2:D:38:GLY:C	2:D:39:LEU:HD23	2.24	0.58
1:E:58:ARG:HD3	1:E:277:GLN:OE1	2.02	0.58
2:F:573:VAL:CG2	2:F:585:ILE:HG13	2.30	0.58
2:F:629:THR:OG1	2:F:645:THR:HG23	2.03	0.58
2:F:736:GLY:O	2:F:737:ILE:C	2.40	0.58
2:H:16:VAL:HG13	2:H:16:VAL:O	2.03	0.58
2:B:305:LEU:HB3	2:B:306:PRO:HD3	1.83	0.58
2:B:481:LEU:HD12	2:B:482:ASN:N	2.19	0.58
1:G:34:GLY:O	1:G:36:LYS:HE3	2.04	0.58
1:G:210:LEU:HD23	1:G:210:LEU:H	1.62	0.58
2:B:296:ARG:HG3	2:B:296:ARG:HH11	1.66	0.58
2:D:730:GLU:N	2:D:731:PRO:CD	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:CE	1:E:180:ALA:O	2.51	0.58
2:F:221:MET:HG3	2:F:221:MET:O	2.01	0.58
2:F:691:HIS:CD2	2:F:691:HIS:O	2.57	0.58
2:H:46:ALA:HB2	2:H:123:ARG:NH2	2.18	0.58
2:H:166:PHE:CZ	2:H:355:ARG:HG3	2.39	0.58
2:H:310:ARG:HD2	2:H:344:PHE:O	2.03	0.58
2:D:45:ALA:HA	2:D:123:ARG:HG3	1.86	0.58
2:D:166:PHE:CZ	2:D:355:ARG:HG3	2.39	0.58
2:D:661:ILE:HD11	2:D:712:LEU:HG	1.84	0.58
1:G:98:HIS:O	1:G:99:HIS:HB2	2.01	0.58
2:B:571:GLY:C	2:B:572:GLN:HG2	2.22	0.58
2:B:730:GLU:N	2:B:731:PRO:HD2	2.18	0.58
2:D:269:ARG:NH2	2:D:341:PHE:CD2	2.71	0.58
1:E:58:ARG:CG	1:E:277:GLN:OE1	2.51	0.58
1:E:354:SER:HB2	1:E:360:ASP:OD2	2.03	0.58
2:D:398:LYS:O	2:D:399:LYS:HD2	2.04	0.58
2:F:174:PHE:CZ	2:F:693:PRO:HG3	2.38	0.58
2:F:507:ASP:OD1	2:F:508:PRO:CD	2.51	0.58
2:H:130:ASP:O	2:H:131:GLN:C	2.41	0.58
2:H:269:ARG:NH2	2:H:341:PHE:CD2	2.72	0.58
1:A:455:VAL:HG22	2:B:443:THR:HG21	1.85	0.58
2:D:471:VAL:CG1	2:D:472:GLN:N	2.64	0.58
1:E:297:ALA:O	1:E:298:LEU:C	2.41	0.58
1:E:322:PHE:HB3	1:E:390:VAL:HG23	1.84	0.58
2:F:360:LEU:HD11	2:F:364:MET:CE	2.33	0.58
1:G:138:GLY:HA2	2:H:669:VAL:HG21	1.85	0.58
1:G:243:ILE:CD1	1:G:341:LEU:HD11	2.33	0.58
1:A:399:ALA:C	1:A:401:LEU:N	2.56	0.58
1:C:216:LEU:HD12	2:D:114:ARG:HH11	1.69	0.58
1:C:390:VAL:CG2	1:C:391:PRO:CD	2.81	0.58
2:D:451:SER:HB3	2:D:738:SER:HB3	1.85	0.58
1:G:22:SER:OG	1:G:25:GLU:HG2	2.03	0.58
2:D:324:LEU:HD23	2:D:324:LEU:C	2.24	0.58
2:H:648:LEU:HD12	2:H:711:ALA:O	2.03	0.58
2:H:730:GLU:O	2:H:731:PRO:C	2.41	0.58
2:B:276:TYR:OH	2:B:359:HIS:HD2	1.86	0.57
2:D:238:LEU:HD11	2:D:257:TYR:CE1	2.39	0.57
2:F:731:PRO:N	2:F:732:PRO:HD2	2.19	0.57
1:G:351:TYR:CZ	1:G:445:ARG:HG2	2.38	0.57
2:B:120:TYR:O	2:B:122:PRO:HD3	2.05	0.57
2:B:227:GLY:O	2:B:230:GLY:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:650:ASP:OD2	2:D:726:LYS:NZ	2.29	0.57
1:G:41:GLU:HG3	1:G:214:LYS:CE	2.33	0.57
1:G:61:ASN:H	1:G:61:ASN:HD22	1.49	0.57
1:G:106:CYS:SG	1:G:134:CYS:HB2	2.44	0.57
1:A:434:TYR:O	1:A:435:ARG:C	2.40	0.57
1:A:436:MET:O	1:A:438:ALA:N	2.37	0.57
2:B:528:ALA:HB1	8:B:4000:141:C7	2.34	0.57
2:B:632:VAL:HG22	2:B:643:LEU:HD11	1.86	0.57
1:C:446:TYR:CE2	1:C:450:LEU:HD12	2.39	0.57
2:H:446:ARG:HG2	2:H:632:VAL:HG13	1.82	0.57
1:C:138:GLY:O	1:C:139:TYR:HB2	2.04	0.57
2:D:324:LEU:HD21	2:D:326:ILE:HD11	1.86	0.57
2:D:683:ASP:C	2:D:683:ASP:OD1	2.40	0.57
1:E:237:THR:HG23	1:E:238:PRO:N	2.19	0.57
2:F:664:ILE:O	2:F:665:GLU:C	2.41	0.57
1:G:231:LEU:O	1:G:231:LEU:CD2	2.52	0.57
2:H:446:ARG:NH1	2:H:630:GLU:OE2	2.37	0.57
1:A:138:GLY:O	1:A:139:TYR:CB	2.32	0.57
1:A:237:THR:HG23	1:A:238:PRO:N	2.17	0.57
1:A:237:THR:CG2	1:A:238:PRO:HD2	2.35	0.57
2:D:107:ARG:O	2:D:108:ALA:C	2.42	0.57
1:G:318:LEU:O	1:G:320:ASP:N	2.37	0.57
1:G:322:PHE:HB3	1:G:390:VAL:HG23	1.85	0.57
1:G:438:ALA:O	1:G:441:ALA:N	2.38	0.57
2:H:645:THR:HG21	2:H:668:TYR:CZ	2.39	0.57
1:C:215:ALA:O	1:C:216:LEU:HB2	2.05	0.57
1:G:69:GLN:NE2	1:G:203:ALA:O	2.37	0.57
1:G:243:ILE:HD12	1:G:341:LEU:HD11	1.86	0.57
2:H:258:ASP:O	2:H:259:ARG:C	2.41	0.57
2:H:305:LEU:HD23	2:H:305:LEU:O	2.04	0.57
2:H:380:PRO:O	2:H:381:GLU:HB2	2.04	0.57
2:H:757:LEU:HD12	2:H:758:GLN:H	1.69	0.57
1:A:203:ALA:HB3	4:A:3005:FAD:O1P	2.05	0.57
1:A:228:CYS:O	1:A:229:LYS:C	2.43	0.57
2:B:339:THR:HG23	2:B:340:ALA:H	1.63	0.57
1:E:321:PHE:CG	1:E:321:PHE:O	2.58	0.57
1:C:393:ARG:HD2	1:C:398:GLU:OE1	2.05	0.57
2:F:443:THR:C	2:F:444:LEU:HD23	2.25	0.57
2:F:671:GLY:O	2:F:674:TRP:HB3	2.04	0.57
1:G:393:ARG:HB3	1:G:398:GLU:OE1	2.05	0.57
1:E:83:ALA:HB2	1:E:157:TRP:CZ3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:MET:CE	1:E:341:LEU:HD22	2.34	0.57
2:F:513:ILE:O	2:F:513:ILE:CG2	2.53	0.57
1:A:408:GLU:OE1	2:B:442:ARG:NH2	2.27	0.56
2:B:407:GLN:CD	2:B:617:ARG:HG2	2.26	0.56
1:C:301:MET:CE	1:C:341:LEU:HD22	2.34	0.56
2:F:197:GLN:HA	2:F:224:MET:HE1	1.86	0.56
1:G:436:MET:O	1:G:438:ALA:N	2.38	0.56
2:H:741:LEU:N	2:H:741:LEU:HD13	2.20	0.56
2:H:776:ARG:O	2:H:777:ALA:CB	2.53	0.56
1:E:250:ALA:O	1:E:253:ARG:N	2.38	0.56
1:G:83:ALA:HB2	1:G:157:TRP:CD2	2.40	0.56
1:A:314:ARG:O	1:A:315:ARG:HB2	2.05	0.56
1:A:368:LEU:HB2	1:A:446:TYR:CD1	2.39	0.56
1:A:426:SER:O	1:A:427:ASP:HB3	2.06	0.56
1:A:442:MET:O	1:A:445:ARG:HB3	2.06	0.56
1:A:446:TYR:CE2	1:A:450:LEU:CD1	2.88	0.56
2:B:247:ARG:HG2	2:B:247:ARG:HH11	1.70	0.56
6:D:3003:MTE:SI'	7:D:3004:MOS:S	3.04	0.56
2:F:776:ARG:O	2:F:777:ALA:HB3	2.06	0.56
1:G:350:CYS:HG	1:G:367:CYS:HG	1.53	0.56
2:H:79:ALA:HB1	2:H:80:PRO:CD	2.32	0.56
2:H:309:ASP:O	2:H:313:LEU:HB2	2.05	0.56
2:H:496:MET:CE	2:H:496:MET:CA	2.82	0.56
1:A:26:LEU:HD13	1:A:67:LEU:CD1	2.34	0.56
2:B:360:LEU:HG	2:B:364:MET:CE	2.35	0.56
1:C:164:PHE:O	1:C:166:LEU:HG	2.05	0.56
2:D:346:GLY:N	2:D:347:PRO:CD	2.68	0.56
2:D:645:THR:HG21	2:D:668:TYR:CE1	2.40	0.56
2:F:648:LEU:HA	2:F:711:ALA:O	2.06	0.56
2:H:672:ALA:O	2:H:675:LEU:N	2.35	0.56
1:C:59:ALA:C	1:C:60:VAL:HG13	2.25	0.56
1:E:191:ASP:O	1:E:194:LEU:HB3	2.05	0.56
2:H:93:PHE:CE1	2:H:96:GLN:N	2.74	0.56
2:H:276:TYR:OH	2:H:359:HIS:CD2	2.57	0.56
1:C:301:MET:HE2	1:C:341:LEU:HD22	1.87	0.56
2:D:305:LEU:HD21	2:D:611:ARG:NE	2.21	0.56
1:E:68:PRO:HG2	1:E:224:PHE:HE1	1.67	0.56
2:F:278:ILE:HD11	2:F:286:LEU:HD22	1.87	0.56
1:G:139:TYR:C	1:G:141:PRO:HD2	2.26	0.56
1:G:299:ILE:O	1:G:302:GLY:N	2.33	0.56
2:H:533:ALA:O	2:H:534:ASP:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ILE:HD12	1:A:429:ARG:HH22	1.71	0.56
2:B:730:GLU:H	2:B:731:PRO:HD2	1.70	0.56
1:E:237:THR:HG22	1:E:239:ASP:N	2.19	0.56
2:F:238:LEU:HD11	2:F:257:TYR:CE1	2.41	0.56
1:G:370:LEU:CD2	1:G:380:ALA:HA	2.36	0.56
2:H:721:THR:O	2:H:722:ILE:C	2.44	0.56
2:H:760:PRO:O	2:H:762:THR:N	2.38	0.56
2:H:763:PRO:O	2:H:764:GLU:C	2.43	0.56
1:A:237:THR:CB	1:A:238:PRO:HD2	2.35	0.56
1:C:427:ASP:OD1	1:C:435:ARG:NH2	2.39	0.56
2:D:221:MET:HE1	2:D:223:ARG:C	2.26	0.56
1:E:61:ASN:H	1:E:61:ASN:ND2	2.03	0.56
1:G:91:VAL:CG1	1:G:111:ILE:HD12	2.36	0.56
1:G:301:MET:HG3	1:G:301:MET:O	2.05	0.56
2:D:198:HIS:ND1	2:D:526:ALA:HB2	2.21	0.56
2:D:263:MET:HE3	2:D:692:ALA:HA	1.87	0.56
1:E:12:ARG:HH11	1:E:12:ARG:HG3	1.70	0.56
1:E:67:LEU:O	1:E:68:PRO:C	2.40	0.56
2:F:66:THR:HB	2:F:69:ASP:OD2	2.06	0.56
2:F:720:GLU:CG	2:F:724:ARG:NH2	2.64	0.56
1:G:50:MET:CE	1:G:116:ALA:CB	2.84	0.56
1:A:75:LEU:HD12	1:A:76:ARG:H	1.71	0.56
1:A:243:ILE:O	1:A:338:SER:HB2	2.06	0.56
1:C:60:VAL:HG21	1:C:65:MET:CE	2.36	0.56
1:C:314:ARG:HH22	1:C:329:ASP:CG	2.10	0.56
2:D:93:PHE:CE2	2:D:96:GLN:HB2	2.41	0.56
2:F:79:ALA:HB1	2:F:80:PRO:CD	2.34	0.56
2:H:66:THR:HB	2:H:69:ASP:OD2	2.06	0.56
1:A:143:LEU:HD22	1:A:147:GLU:CD	2.26	0.55
1:C:78:ILE:HG23	1:C:79:GLU:N	2.20	0.55
2:D:635:ARG:NH1	2:D:774:GLU:OE2	2.32	0.55
2:F:736:GLY:O	2:F:739:ALA:N	2.39	0.55
2:F:776:ARG:O	2:F:777:ALA:CB	2.55	0.55
2:B:247:ARG:HG2	2:B:247:ARG:NH1	2.21	0.55
2:D:360:LEU:HD11	2:D:364:MET:HE2	1.86	0.55
2:D:674:TRP:CD2	2:D:675:LEU:CD2	2.89	0.55
1:E:301:MET:HB3	1:E:348:LEU:HD22	1.88	0.55
2:F:704:ARG:HG3	2:F:704:ARG:O	2.04	0.55
2:H:316:ASP:N	2:H:316:ASP:OD1	2.39	0.55
1:A:423:THR:O	1:A:423:THR:HG22	2.06	0.55
2:B:271:ASP:OD2	2:B:296:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:VAL:HG12	2:B:480:ALA:N	2.19	0.55
2:B:618:PRO:HG2	2:B:619:PHE:N	2.20	0.55
2:F:634:ASP:C	2:F:634:ASP:OD1	2.44	0.55
2:H:728:VAL:O	2:H:732:PRO:HG3	2.06	0.55
1:A:39:CYS:O	1:A:40:ASN:CB	2.53	0.55
1:A:319:GLU:N	1:A:319:GLU:OE2	2.39	0.55
2:B:437:TRP:CZ3	2:B:446:ARG:HG3	2.42	0.55
2:B:730:GLU:O	2:B:731:PRO:C	2.43	0.55
2:H:196:SER:HG	2:H:198:HIS:H	1.51	0.55
2:B:344:PHE:CE1	8:B:4000:141:C6	2.90	0.55
2:B:513:ILE:HG13	2:B:514:THR:H	1.69	0.55
1:E:218:ASP:C	1:E:218:ASP:OD1	2.44	0.55
1:G:67:LEU:O	1:G:69:GLN:N	2.40	0.55
1:G:140:ALA:N	1:G:141:PRO:HD2	2.21	0.55
4:G:3005:FAD:N1	4:G:3005:FAD:C2'	2.65	0.55
2:H:251:ARG:O	2:H:252:PRO:C	2.43	0.55
2:H:517:ASP:OD2	2:H:517:ASP:C	2.45	0.55
1:A:237:THR:HG23	1:A:238:PRO:HG2	1.88	0.55
1:E:37:GLU:OE1	2:F:256:ARG:NH2	2.39	0.55
1:G:382:ILE:O	1:G:382:ILE:HG22	2.06	0.55
2:H:143:PRO:HB3	2:H:329:HIS:CE1	2.42	0.55
1:C:24:LEU:HD21	1:C:37:GLU:HB2	1.88	0.55
2:D:286:LEU:HG	2:D:375:ASN:OD1	2.06	0.55
2:D:723:PHE:O	2:D:724:ARG:HB2	2.07	0.55
1:E:390:VAL:CG2	1:E:391:PRO:CD	2.84	0.55
2:F:499:VAL:O	2:F:503:VAL:HG23	2.07	0.55
1:G:369:ASN:O	1:G:370:LEU:HD23	2.07	0.55
2:H:730:GLU:C	2:H:732:PRO:HD2	2.26	0.55
2:H:767:LEU:HD12	2:H:767:LEU:O	2.06	0.55
1:C:356:ARG:CZ	2:D:697:LYS:NZ	2.70	0.55
2:F:289:ALA:O	2:F:324:LEU:HA	2.06	0.55
2:F:721:THR:O	2:F:722:ILE:C	2.43	0.55
2:H:179:GLN:HB3	2:H:238:LEU:CD1	2.36	0.55
2:H:528:ALA:O	2:H:529:ALA:HB3	2.06	0.55
2:H:558:ARG:HD2	2:H:559:GLU:OE2	2.07	0.55
2:H:674:TRP:CD2	2:H:675:LEU:HD21	2.41	0.55
2:B:278:ILE:HD11	2:B:286:LEU:HD22	1.89	0.55
1:E:144:ARG:O	1:E:145:ALA:C	2.42	0.55
1:E:237:THR:HG23	1:E:239:ASP:H	1.69	0.55
4:E:3005:FAD:H2B	4:E:3005:FAD:O5B	2.07	0.55
2:F:321:VAL:HG12	2:F:323:ALA:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:237:THR:CG2	1:G:238:PRO:N	2.70	0.55
1:A:18:ASP:OD2	1:A:19:PRO:CD	2.52	0.55
2:B:16:VAL:O	2:B:16:VAL:HG13	2.06	0.55
2:D:412:CYS:HA	2:D:624:TYR:CZ	2.42	0.55
1:G:44:CYS:N	3:G:3002:FES:S1	2.78	0.55
2:H:529:ALA:O	2:H:530:SER:C	2.46	0.55
2:B:106:HIS:O	2:B:107:ARG:C	2.42	0.54
2:D:164:GLY:HA3	2:D:276:TYR:CZ	2.42	0.54
2:D:224:MET:HE3	2:D:488:MET:HB3	1.89	0.54
1:E:351:TYR:CE1	1:E:445:ARG:HG2	2.43	0.54
2:F:533:ALA:O	2:F:534:ASP:C	2.44	0.54
2:F:744:HIS:C	2:F:744:HIS:CD2	2.81	0.54
1:E:107:THR:HB	1:E:108:PRO:HD3	1.89	0.54
1:E:293:ASP:O	1:E:296:PRO:HD2	2.06	0.54
1:E:348:LEU:HD12	1:E:349:ARG:N	2.23	0.54
1:E:368:LEU:N	1:E:368:LEU:CD1	2.59	0.54
1:G:301:MET:CE	1:G:341:LEU:HD22	2.37	0.54
1:A:301:MET:HB3	1:A:348:LEU:HD22	1.90	0.54
1:A:368:LEU:CB	1:A:446:TYR:CD1	2.90	0.54
2:B:443:THR:C	2:B:444:LEU:HD23	2.28	0.54
1:C:399:ALA:C	1:C:401:LEU:H	2.11	0.54
1:E:432:ALA:O	1:E:433:ALA:C	2.43	0.54
1:G:136:CYS:HB2	3:G:3001:FES:S1	2.46	0.54
2:H:407:GLN:OE1	2:H:618:PRO:HD2	2.07	0.54
2:H:656:ASN:CG	2:H:659:LEU:HD12	2.27	0.54
2:B:629:THR:OG1	2:B:668:TYR:OH	2.19	0.54
1:E:7:LEU:HD21	1:E:32:LEU:HD11	1.88	0.54
2:B:61:VAL:HA	2:B:103:ALA:CB	2.37	0.54
2:B:683:ASP:C	2:B:683:ASP:OD1	2.45	0.54
1:E:369:ASN:O	1:E:370:LEU:HD23	2.07	0.54
1:G:281:ILE:HG23	1:G:282:GLY:N	2.22	0.54
2:H:39:LEU:HB3	2:H:95:GLY:O	2.07	0.54
2:H:650:ASP:OD2	2:H:726:LYS:NZ	2.30	0.54
1:C:228:CYS:O	1:C:229:LYS:C	2.45	0.54
2:D:736:GLY:O	2:D:737:ILE:C	2.46	0.54
1:E:395:ALA:O	1:E:396:ALA:C	2.44	0.54
2:F:683:ASP:C	2:F:683:ASP:OD1	2.45	0.54
1:G:151:GLY:O	1:G:152:GLU:HG2	2.07	0.54
1:A:216:LEU:HD12	2:B:114:ARG:NH1	2.22	0.54
2:B:517:ASP:OD2	2:B:519:SER:N	2.35	0.54
2:D:150:ASP:OD2	2:D:153:THR:OG1	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:661:ILE:CD1	2:F:712:LEU:HG	2.37	0.54
2:H:128:THR:O	2:H:129:LEU:C	2.46	0.54
2:H:621:TYR:CE1	2:H:726:LYS:CG	2.85	0.54
1:A:267:LEU:O	1:A:268:ARG:C	2.46	0.54
2:D:691:HIS:CD2	2:D:691:HIS:O	2.61	0.54
1:E:318:LEU:O	1:E:319:GLU:C	2.45	0.54
2:F:466:GLN:NE2	2:H:593:ARG:HG2	2.22	0.54
1:G:81:ILE:O	1:G:81:ILE:CG2	2.55	0.54
1:G:237:THR:HG22	1:G:239:ASP:N	2.22	0.54
1:G:281:ILE:O	1:G:282:GLY:C	2.45	0.54
1:G:316:MET:HB2	1:G:317:PRO:CD	2.37	0.54
2:D:171:GLN:HG3	2:D:678:GLU:OE1	2.08	0.54
2:D:720:GLU:CG	2:D:724:ARG:HH21	2.20	0.54
2:F:655:LEU:HD21	2:F:722:ILE:HG23	1.90	0.54
2:H:432:ALA:O	2:H:433:GLU:C	2.43	0.54
1:A:324:GLU:O	1:A:325:TYR:C	2.45	0.54
1:G:291:ILE:O	1:G:292:GLY:C	2.44	0.54
2:H:740:PHE:O	2:H:741:LEU:C	2.44	0.54
1:A:75:LEU:HD12	1:A:76:ARG:N	2.23	0.53
1:A:78:ILE:HD13	1:A:108:PRO:HA	1.90	0.53
1:C:374:GLY:O	1:C:376:LYS:N	2.41	0.53
2:F:238:LEU:HD11	2:F:257:TYR:CZ	2.43	0.53
2:H:330:ARG:NH2	2:H:611:ARG:NH2	2.56	0.53
2:H:730:GLU:H	2:H:731:PRO:CD	2.21	0.53
2:B:496:MET:HA	2:B:496:MET:CE	2.38	0.53
1:E:301:MET:CE	1:E:341:LEU:CB	2.79	0.53
2:F:105:SER:O	2:F:106:HIS:C	2.46	0.53
2:F:171:GLN:HG2	2:F:341:PHE:CE1	2.43	0.53
2:F:344:PHE:CD2	8:F:4000:141:C2	2.92	0.53
2:F:411:ASP:OD1	2:F:411:ASP:N	2.39	0.53
2:F:432:ALA:O	2:F:433:GLU:C	2.46	0.53
2:F:627:ALA:HB2	2:F:735:LEU:HD22	1.89	0.53
1:G:260:HIS:O	1:G:261:PRO:C	2.47	0.53
2:H:61:VAL:HA	2:H:103:ALA:CB	2.38	0.53
2:H:346:GLY:N	2:H:347:PRO:CD	2.70	0.53
2:D:247:ARG:HH11	2:D:247:ARG:CG	2.18	0.53
1:E:118:HIS:HE1	1:E:154:PRO:HA	1.74	0.53
2:F:312:MET:CE	2:F:330:ARG:HH12	2.22	0.53
2:F:412:CYS:HA	2:F:624:TYR:CZ	2.42	0.53
2:H:456:GLY:O	2:H:457:ILE:HD13	2.07	0.53
2:H:617:ARG:HD3	2:H:619:PHE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ALA:CA	1:A:367:CYS:SG	2.96	0.53
6:B:3003:MTE:S1'	7:B:3004:MOS:S	3.07	0.53
1:E:390:VAL:HG23	1:E:391:PRO:CD	2.35	0.53
1:G:218:ASP:C	1:G:218:ASP:OD1	2.46	0.53
1:A:360:ASP:OD1	2:B:697:LYS:HE3	2.08	0.53
2:B:351:LEU:HD13	2:B:737:ILE:HG12	1.89	0.53
2:B:481:LEU:HD12	2:B:482:ASN:H	1.74	0.53
2:B:595:SER:HB2	2:D:601:PHE:CD1	2.43	0.53
2:B:650:ASP:HB2	2:B:713:TRP:CD1	2.43	0.53
1:G:428:MET:SD	1:G:429:ARG:N	2.81	0.53
2:H:536:ASN:O	2:H:540:VAL:HG23	2.09	0.53
2:F:96:GLN:HG3	2:F:97:PRO:HD2	1.89	0.53
1:G:202:ILE:HD12	1:G:222:VAL:HG13	1.91	0.53
2:H:278:ILE:HD11	2:H:286:LEU:HD22	1.91	0.53
1:A:102:GLN:NE2	1:A:137:THR:HA	2.24	0.53
2:D:341:PHE:O	2:D:342:ARG:C	2.47	0.53
1:E:61:ASN:H	1:E:61:ASN:HD22	1.57	0.53
1:E:266:LEU:C	1:E:268:ARG:N	2.62	0.53
2:F:730:GLU:O	2:F:731:PRO:C	2.47	0.53
1:G:353:LEU:O	1:G:363:ALA:N	2.30	0.53
1:G:436:MET:C	1:G:438:ALA:N	2.62	0.53
1:E:92:GLN:NE2	2:F:17:THR:HG22	2.24	0.53
2:F:164:GLY:HA3	2:F:276:TYR:CZ	2.44	0.53
2:F:341:PHE:O	2:F:342:ARG:C	2.47	0.53
2:H:359:HIS:O	2:H:360:LEU:C	2.47	0.53
1:A:271:ALA:HB2	4:A:3005:FAD:N5	2.24	0.53
1:C:369:ASN:C	1:C:370:LEU:HD23	2.30	0.53
1:C:423:THR:HG22	1:C:423:THR:O	2.09	0.53
1:E:237:THR:CG2	1:E:238:PRO:N	2.72	0.53
2:F:35:LEU:N	2:F:35:LEU:HD23	2.24	0.53
2:H:422:GLN:HG2	2:H:427:PHE:CD2	2.43	0.53
2:H:746:ALA:O	2:H:747:CYS:C	2.47	0.53
1:C:36:LYS:HD3	1:C:105:PHE:CE1	2.43	0.53
1:E:92:GLN:HE22	2:F:17:THR:HG22	1.74	0.53
2:F:198:HIS:ND1	2:F:526:ALA:HB2	2.24	0.53
2:F:448:ILE:HG23	2:F:448:ILE:O	2.09	0.53
2:F:704:ARG:HG2	2:F:704:ARG:HH11	1.74	0.53
1:G:295:PRO:HB2	1:G:296:PRO:HD3	1.89	0.53
2:H:341:PHE:O	2:H:342:ARG:C	2.46	0.53
2:B:380:PRO:O	2:B:381:GLU:HB2	2.09	0.52
1:C:50:MET:CE	1:C:116:ALA:HA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ASP:O	1:C:128:LEU:HD22	2.08	0.52
2:D:372:ARG:O	2:D:373:ALA:C	2.45	0.52
2:D:457:ILE:O	2:D:458:SER:HB2	2.09	0.52
2:F:276:TYR:OH	2:F:359:HIS:HD2	1.92	0.52
1:G:191:ASP:O	1:G:194:LEU:HB3	2.10	0.52
2:H:573:VAL:HG11	2:H:585:ILE:HG13	1.91	0.52
2:H:631:VAL:HG21	2:H:743:LEU:HD13	1.90	0.52
1:A:356:ARG:CZ	2:B:697:LYS:NZ	2.73	0.52
2:B:661:ILE:O	2:B:665:GLU:HG3	2.09	0.52
2:B:668:TYR:O	2:B:669:VAL:C	2.44	0.52
1:C:237:THR:CG2	1:C:239:ASP:H	2.22	0.52
1:E:369:ASN:C	1:E:369:ASN:OD1	2.45	0.52
1:G:447:VAL:O	1:G:448:ARG:C	2.48	0.52
2:H:348:GLN:O	2:H:349:GLY:C	2.46	0.52
2:B:251:ARG:HB2	2:B:252:PRO:HD2	1.91	0.52
1:C:129:LEU:O	1:C:130:ALA:C	2.47	0.52
2:F:618:PRO:HG2	2:F:619:PHE:CD1	2.45	0.52
2:H:23:LEU:HD13	2:H:194:CYS:HA	1.91	0.52
1:C:192:TRP:O	1:C:196:HIS:HD2	1.92	0.52
2:F:700:ALA:O	2:F:701:PHE:C	2.48	0.52
2:B:28:CYS:HB2	2:B:29:PRO:CD	2.39	0.52
1:E:111:ILE:O	1:E:112:VAL:C	2.47	0.52
1:G:120:ARG:O	1:G:121:ASP:C	2.47	0.52
1:G:368:LEU:N	1:G:368:LEU:CD1	2.60	0.52
2:H:166:PHE:HB3	2:H:355:ARG:NH2	2.24	0.52
2:H:411:ASP:OD1	2:H:411:ASP:N	2.42	0.52
2:B:339:THR:CG2	2:B:340:ALA:N	2.37	0.52
2:B:528:ALA:O	2:B:531:SER:OG	2.16	0.52
2:F:568:PHE:CE2	2:F:573:VAL:HG22	2.45	0.52
1:G:409:ASP:OD2	1:G:409:ASP:N	2.42	0.52
2:H:196:SER:OG	2:H:198:HIS:N	2.27	0.52
2:H:214:PHE:N	2:H:214:PHE:CD1	2.71	0.52
2:B:601:PHE:CG	2:D:595:SER:HB2	2.44	0.52
2:F:210:LEU:HD12	2:F:212:LEU:HD12	1.92	0.52
1:G:282:GLY:O	1:G:285:ILE:HB	2.10	0.52
1:G:373:LYS:O	1:G:374:GLY:C	2.48	0.52
2:H:602:TYR:C	2:H:602:TYR:CD2	2.83	0.52
2:D:74:ASN:OD1	2:D:85:VAL:N	2.38	0.52
1:E:1:MET:HE1	1:E:180:ALA:O	2.09	0.52
1:E:22:SER:HG	1:E:25:GLU:HG2	1.74	0.52
2:F:566:VAL:HG13	2:F:575:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:721:THR:O	2:F:724:ARG:N	2.39	0.52
2:F:746:ALA:O	2:F:747:CYS:C	2.47	0.52
2:H:347:PRO:HG3	2:H:734:LEU:CD1	2.39	0.52
2:B:28:CYS:HB2	2:B:29:PRO:HD2	1.91	0.52
2:B:45:ALA:HA	2:B:123:ARG:HG3	1.91	0.52
2:B:98:ILE:O	2:B:98:ILE:CG2	2.58	0.52
2:B:214:PHE:N	2:B:214:PHE:CD1	2.74	0.52
2:B:367:ASP:OD1	2:B:368:PRO:CD	2.58	0.52
1:E:78:ILE:CG2	1:E:79:GLU:N	2.72	0.52
1:E:110:PHE:O	1:E:111:ILE:C	2.48	0.52
2:F:569:ASP:O	2:F:570:ALA:HB3	2.10	0.52
2:F:617:ARG:HD3	2:F:619:PHE:O	2.09	0.52
1:G:50:MET:HE3	1:G:116:ALA:N	2.25	0.52
2:H:360:LEU:HG	2:H:364:MET:HE2	1.92	0.52
1:A:132:ASN:OD1	1:A:274:GLN:NE2	2.35	0.52
1:C:301:MET:HE1	1:C:341:LEU:HB3	1.91	0.52
1:E:296:PRO:O	1:E:297:ALA:C	2.47	0.52
2:F:328:SER:OG	2:F:330:ARG:NH1	2.39	0.52
1:G:141:PRO:HA	1:G:144:ARG:HH11	1.75	0.52
2:H:513:ILE:HG13	2:H:514:THR:N	2.25	0.52
2:D:351:LEU:HD13	2:D:737:ILE:HG12	1.92	0.51
1:E:165:THR:HG23	1:E:165:THR:O	2.10	0.51
1:E:382:ILE:O	1:E:393:ARG:HA	2.10	0.51
1:G:141:PRO:CG	1:G:142:ILE:N	2.73	0.51
2:H:92:HIS:O	2:H:93:PHE:HB3	2.10	0.51
1:A:202:ILE:HD12	1:A:222:VAL:HG13	1.93	0.51
1:C:237:THR:CG2	1:C:238:PRO:N	2.72	0.51
1:E:68:PRO:CB	1:E:224:PHE:CE1	2.92	0.51
1:E:423:THR:HG22	1:E:423:THR:O	2.10	0.51
2:F:347:PRO:O	2:F:348:GLN:C	2.48	0.51
2:F:453:VAL:CG1	2:F:454:LYS:N	2.69	0.51
2:F:621:TYR:CE1	2:F:726:LYS:CG	2.83	0.51
1:G:296:PRO:O	1:G:297:ALA:C	2.46	0.51
2:H:691:HIS:O	2:H:692:ALA:CB	2.54	0.51
1:A:95:MET:SD	1:A:114:MET:CE	2.99	0.51
1:A:301:MET:HE1	1:A:341:LEU:HD22	1.90	0.51
1:C:237:THR:CG2	1:C:238:PRO:HD2	2.35	0.51
2:D:185:PRO:O	2:D:185:PRO:HG2	2.10	0.51
2:F:482:ASN:ND2	2:F:514:THR:OG1	2.32	0.51
1:G:118:HIS:O	1:G:120:ARG:N	2.44	0.51
2:H:221:MET:HE1	2:H:223:ARG:C	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:733:PHE:C	2:H:733:PHE:CD2	2.83	0.51
2:B:218:ARG:NH2	2:D:218:ARG:HH22	2.08	0.51
2:B:237:HIS:ND1	2:B:237:HIS:N	2.58	0.51
1:E:381:ARG:NH2	1:E:393:ARG:HH21	1.98	0.51
2:F:296:ARG:HH11	2:F:296:ARG:CG	2.18	0.51
2:F:305:LEU:HD21	2:F:611:ARG:NE	2.24	0.51
2:F:448:ILE:HG13	2:F:630:GLU:HB2	1.91	0.51
1:C:106:CYS:SG	1:C:134:CYS:HB2	2.51	0.51
2:D:360:LEU:CD1	2:D:364:MET:CE	2.89	0.51
1:G:359:GLN:HA	1:G:359:GLN:HE21	1.75	0.51
2:H:305:LEU:HB3	2:H:306:PRO:HD3	1.91	0.51
2:B:652:GLY:N	2:B:726:LYS:HB2	2.26	0.51
1:C:331:ARG:HG3	1:C:331:ARG:HH11	1.76	0.51
2:D:528:ALA:O	2:D:529:ALA:CB	2.41	0.51
2:D:648:LEU:HA	2:D:711:ALA:O	2.11	0.51
2:D:776:ARG:O	2:D:777:ALA:HB3	2.10	0.51
1:E:201:LEU:O	4:E:3005:FAD:O2B	2.27	0.51
1:E:249:ILE:O	1:E:250:ALA:C	2.47	0.51
1:E:348:LEU:HD12	1:E:349:ARG:H	1.75	0.51
2:F:631:VAL:HG12	2:F:642:ILE:HA	1.92	0.51
2:H:547:LEU:O	2:H:550:ARG:N	2.43	0.51
1:A:370:LEU:HD23	1:A:380:ALA:HA	1.93	0.51
2:B:52:LEU:O	2:B:55:VAL:N	2.43	0.51
2:B:93:PHE:CE2	2:B:299:TRP:CE2	2.99	0.51
1:C:37:GLU:CD	2:D:256:ARG:NH2	2.64	0.51
1:E:6:LEU:HA	1:E:10:GLU:O	2.10	0.51
1:E:279:ALA:HB1	4:E:3005:FAD:H4'	1.92	0.51
1:G:141:PRO:HG2	1:G:142:ILE:H	1.75	0.51
1:G:368:LEU:HB2	1:G:446:TYR:CD1	2.45	0.51
2:H:324:LEU:C	2:H:324:LEU:HD23	2.31	0.51
2:H:449:ALA:CB	2:H:741:LEU:HB3	2.41	0.51
2:H:595:SER:C	2:H:596:LEU:HD23	2.31	0.51
1:A:271:ALA:CA	1:A:359:GLN:NE2	2.74	0.51
1:A:373:LYS:O	1:A:374:GLY:O	2.29	0.51
2:B:660:ASP:O	2:B:661:ILE:C	2.48	0.51
2:B:760:PRO:O	2:B:760:PRO:HG2	2.11	0.51
1:C:322:PHE:HB3	1:C:390:VAL:CG2	2.40	0.51
2:D:398:LYS:N	2:D:398:LYS:HE3	2.25	0.51
2:F:130:ASP:O	2:F:131:GLN:C	2.44	0.51
2:H:760:PRO:O	2:H:760:PRO:HG2	2.11	0.51
1:A:16:ILE:HD13	1:A:68:PRO:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ASP:OD2	1:A:87:ARG:HD3	2.11	0.51
2:D:201:GLU:O	2:D:202:ILE:C	2.45	0.51
2:D:320:PHE:CG	2:D:401:GLN:NE2	2.78	0.51
1:E:83:ALA:HB2	1:E:157:TRP:CZ2	2.46	0.51
2:F:354:GLU:OE1	2:F:372:ARG:NE	2.43	0.51
2:H:683:ASP:C	2:H:683:ASP:OD1	2.48	0.51
1:A:95:MET:SD	1:A:114:MET:HE3	2.51	0.51
1:A:194:LEU:HD12	1:A:194:LEU:O	2.11	0.51
1:A:314:ARG:HH22	1:A:329:ASP:CG	2.14	0.51
1:A:415:LEU:HB2	1:A:416:PRO:HD3	1.93	0.51
2:B:171:GLN:O	2:B:268:LYS:HB3	2.11	0.51
2:D:218:ARG:NE	2:D:220:GLU:OE2	2.44	0.51
2:D:532:GLY:N	6:D:3003:MTE:O1P	2.30	0.51
1:E:237:THR:CG2	1:E:238:PRO:CD	2.86	0.51
1:E:370:LEU:HD22	1:E:380:ALA:CB	2.41	0.51
1:E:390:VAL:HG22	1:E:391:PRO:N	2.26	0.51
1:E:436:MET:O	1:E:437:ASN:C	2.48	0.51
2:F:66:THR:CG2	2:F:67:ALA:N	2.74	0.51
2:F:343:GLY:O	2:F:344:PHE:C	2.47	0.51
1:G:370:LEU:HD21	1:G:380:ALA:HB1	1.92	0.51
1:A:102:GLN:HB3	2:B:489:GLY:O	2.11	0.50
1:A:140:ALA:N	1:A:141:PRO:HD2	2.27	0.50
2:B:105:SER:O	2:B:106:HIS:C	2.49	0.50
2:D:554:PHE:HB2	2:D:594:ILE:HD12	1.93	0.50
1:E:439:ALA:O	1:E:440:GLN:C	2.43	0.50
2:F:33:LEU:HD21	2:F:251:ARG:NH1	2.25	0.50
2:F:471:VAL:HG12	2:F:472:GLN:N	2.26	0.50
2:F:649:HIS:HB3	2:F:664:ILE:HD13	1.93	0.50
2:H:7:LEU:HB3	2:H:8:PRO:HD2	1.94	0.50
2:H:198:HIS:CD2	2:H:526:ALA:HA	2.46	0.50
2:H:690:THR:HA	2:H:695:THR:OG1	2.11	0.50
1:A:191:ASP:O	1:A:194:LEU:HB3	2.11	0.50
2:B:556:ALA:O	2:B:557:ALA:C	2.48	0.50
2:B:621:TYR:HE1	2:B:726:LYS:HG2	1.74	0.50
1:E:266:LEU:C	1:E:268:ARG:H	2.14	0.50
1:E:316:MET:HB2	1:E:317:PRO:CD	2.38	0.50
1:G:50:MET:HE2	1:G:116:ALA:CB	2.42	0.50
2:H:28:CYS:HB2	2:H:29:PRO:HD2	1.93	0.50
2:H:106:HIS:O	2:H:107:ARG:C	2.48	0.50
1:A:89:HIS:ND1	1:A:90:PRO:HD2	2.27	0.50
1:A:388:ALA:C	1:A:390:VAL:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:359:HIS:O	2:B:360:LEU:C	2.49	0.50
2:B:398:LYS:N	2:B:398:LYS:HE3	2.27	0.50
2:B:492:LEU:O	2:B:493:HIS:C	2.50	0.50
2:D:459:PHE:N	2:D:465:ASN:OD1	2.44	0.50
1:E:37:GLU:OE2	2:F:256:ARG:NH2	2.44	0.50
1:E:58:ARG:CD	1:E:277:GLN:OE1	2.60	0.50
2:F:278:ILE:HG12	2:F:279:GLY:N	2.27	0.50
2:F:704:ARG:HH11	2:F:704:ARG:CG	2.24	0.50
2:H:633:ILE:CD1	2:H:746:ALA:HB1	2.42	0.50
1:A:210:LEU:HD23	1:A:210:LEU:N	2.25	0.50
2:B:166:PHE:CE1	2:B:355:ARG:HG3	2.47	0.50
2:B:329:HIS:HB3	2:B:331:LEU:HD21	1.93	0.50
2:B:674:TRP:CD2	2:B:675:LEU:HD21	2.45	0.50
2:B:742:ALA:O	2:B:743:LEU:C	2.49	0.50
1:C:374:GLY:C	1:C:376:LYS:H	2.15	0.50
1:G:18:ASP:OD2	1:G:20:THR:N	2.32	0.50
1:C:349:ARG:HG2	1:C:351:TYR:OH	2.11	0.50
1:C:390:VAL:HG22	1:C:391:PRO:HD2	1.93	0.50
2:D:721:THR:O	2:D:722:ILE:C	2.49	0.50
2:D:731:PRO:CB	2:D:732:PRO:CD	2.85	0.50
2:F:730:GLU:N	2:F:731:PRO:CD	2.74	0.50
1:G:144:ARG:O	1:G:145:ALA:C	2.46	0.50
1:G:314:ARG:O	1:G:315:ARG:HB2	2.10	0.50
2:H:448:ILE:HG23	2:H:448:ILE:O	2.11	0.50
2:H:586:VAL:HG13	2:H:596:LEU:HD13	1.94	0.50
2:H:722:ILE:HG13	2:H:723:PHE:CD1	2.46	0.50
1:A:105:PHE:CD1	2:B:177:GLU:HB2	2.46	0.50
1:A:414:ALA:O	1:A:415:LEU:C	2.48	0.50
2:B:123:ARG:HB3	2:B:124:PRO:HD2	1.93	0.50
2:B:582:PHE:O	2:B:586:VAL:HG23	2.11	0.50
2:B:731:PRO:CB	2:B:732:PRO:CD	2.81	0.50
1:C:305:LEU:HD21	1:C:307:LEU:HD21	1.94	0.50
1:C:350:CYS:HG	1:C:367:CYS:HG	1.60	0.50
2:D:450:LEU:HG	2:D:451:SER:N	2.24	0.50
1:E:231:LEU:O	1:E:231:LEU:HD23	2.11	0.50
2:F:571:GLY:C	2:F:572:GLN:HG2	2.31	0.50
2:D:672:ALA:O	2:D:673:GLY:C	2.50	0.50
1:E:5:PHE:CG	1:E:70:ILE:HD12	2.47	0.50
1:E:100:GLY:HA2	1:E:141:PRO:HB2	1.94	0.50
2:F:201:GLU:O	2:F:202:ILE:C	2.50	0.50
2:F:210:LEU:HD12	2:F:212:LEU:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:528:ALA:O	2:F:529:ALA:HB3	2.12	0.50
1:G:134:CYS:SG	1:G:136:CYS:HB2	2.52	0.50
2:H:93:PHE:CD2	2:H:299:TRP:NE1	2.79	0.50
1:A:129:LEU:O	1:A:130:ALA:C	2.46	0.50
1:A:294:GLY:N	1:A:295:PRO:CD	2.74	0.50
2:B:70:LEU:HD12	2:B:74:ASN:HB2	1.92	0.50
2:D:28:CYS:HB2	2:D:29:PRO:CD	2.42	0.50
1:E:103:CYS:HA	2:F:489:GLY:CA	2.42	0.50
1:E:111:ILE:HD11	2:F:16:VAL:HG22	1.93	0.50
1:E:118:HIS:CE1	1:E:154:PRO:HA	2.47	0.50
1:G:50:MET:CE	1:G:116:ALA:HB2	2.41	0.50
1:G:344:SER:OG	1:G:346:PRO:HD3	2.11	0.50
1:A:207:ASP:OD2	4:A:3005:FAD:H3'	2.12	0.50
2:D:195:SER:O	2:D:231:LYS:HD3	2.11	0.50
2:F:310:ARG:HD2	2:F:344:PHE:HB3	1.94	0.50
2:H:120:TYR:C	2:H:122:PRO:HD3	2.31	0.50
1:A:37:GLU:OE1	2:B:256:ARG:NH2	2.45	0.49
2:B:164:GLY:HA3	2:B:276:TYR:CZ	2.45	0.49
1:E:110:PHE:O	1:E:114:MET:N	2.35	0.49
1:E:115:ALA:O	1:E:116:ALA:C	2.50	0.49
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.12	0.49
6:F:3003:MTE:S2'	7:F:3004:MOS:S	3.10	0.49
2:H:461:LEU:HD12	2:H:463:HIS:CE1	2.47	0.49
1:A:181:PHE:CD2	1:A:183:PRO:HD3	2.46	0.49
1:A:260:HIS:O	1:A:261:PRO:C	2.50	0.49
1:A:408:GLU:CD	2:B:442:ARG:NH2	2.65	0.49
4:A:3005:FAD:N1	4:A:3005:FAD:C2'	2.74	0.49
2:B:674:TRP:CZ3	2:B:675:LEU:HD21	2.48	0.49
1:C:283:GLY:O	1:C:284:ASN:C	2.49	0.49
1:C:359:GLN:O	1:C:359:GLN:CG	2.58	0.49
2:D:131:GLN:O	2:D:134:ALA:HB3	2.12	0.49
2:D:152:GLU:O	2:D:153:THR:C	2.48	0.49
2:D:229:GLY:HA2	7:D:3004:MOS:S	2.53	0.49
1:E:205:GLY:N	4:E:3005:FAD:O2P	2.44	0.49
2:F:319:TYR:N	2:F:319:TYR:CD1	2.80	0.49
2:F:698:ILE:HB	2:F:699:PRO:CD	2.41	0.49
1:G:165:THR:O	1:G:166:LEU:HD23	2.12	0.49
2:H:633:ILE:HD13	2:H:746:ALA:HB3	1.94	0.49
1:A:237:THR:CG2	1:A:238:PRO:CD	2.85	0.49
1:C:165:THR:O	1:C:165:THR:HG23	2.12	0.49
1:C:205:GLY:O	1:C:209:SER:OG	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:GLU:O	1:C:338:SER:HB3	2.12	0.49
2:D:265:ILE:O	2:D:265:ILE:HG22	2.11	0.49
2:D:281:ASP:OD1	2:D:283:SER:OG	2.20	0.49
2:D:720:GLU:HG2	2:D:724:ARG:NH2	2.27	0.49
2:D:731:PRO:CD	2:D:732:PRO:CD	2.90	0.49
1:E:139:TYR:O	1:E:140:ALA:C	2.51	0.49
1:G:95:MET:HG3	1:G:111:ILE:HD11	1.94	0.49
1:G:118:HIS:O	1:G:121:ASP:N	2.35	0.49
2:H:536:ASN:O	2:H:537:GLY:C	2.50	0.49
1:A:144:ARG:O	1:A:145:ALA:C	2.48	0.49
2:B:251:ARG:O	2:B:252:PRO:C	2.50	0.49
2:B:296:ARG:HH11	2:B:296:ARG:CG	2.25	0.49
2:B:492:LEU:HD12	2:B:492:LEU:O	2.12	0.49
2:D:214:PHE:N	2:D:214:PHE:CD1	2.75	0.49
2:D:238:LEU:HD23	2:D:255:MET:HG2	1.95	0.49
2:F:574:GLN:HG3	2:F:579:SER:HB2	1.94	0.49
2:F:647:ILE:HD13	2:F:735:LEU:HD13	1.94	0.49
1:A:78:ILE:CG2	1:A:79:GLU:N	2.76	0.49
2:B:341:PHE:O	2:B:342:ARG:C	2.49	0.49
2:B:507:ASP:OD1	2:B:508:PRO:CD	2.61	0.49
2:B:566:VAL:HG13	2:B:575:ALA:HB2	1.95	0.49
2:B:671:GLY:O	2:B:674:TRP:HB3	2.12	0.49
1:C:25:GLU:O	1:C:26:LEU:C	2.48	0.49
1:C:237:THR:HG23	1:C:238:PRO:CG	2.40	0.49
1:E:12:ARG:HH11	1:E:12:ARG:CG	2.23	0.49
1:G:52:ARG:NH1	1:G:57:SER:HB3	2.27	0.49
1:G:61:ASN:ND2	1:G:61:ASN:N	2.60	0.49
2:H:492:LEU:O	2:H:493:HIS:C	2.51	0.49
1:A:261:PRO:O	1:A:262:ALA:C	2.48	0.49
2:B:331:LEU:N	2:B:331:LEU:HD23	2.25	0.49
1:E:102:GLN:NE2	1:E:137:THR:HA	2.27	0.49
2:F:288:GLY:HA2	2:F:323:ALA:O	2.13	0.49
1:G:318:LEU:O	1:G:319:GLU:C	2.51	0.49
1:G:356:ARG:NH2	1:G:359:GLN:O	2.45	0.49
2:H:466:GLN:HA	2:H:602:TYR:O	2.13	0.49
1:A:139:TYR:C	1:A:141:PRO:HD2	2.32	0.49
1:A:165:THR:O	1:A:165:THR:CG2	2.61	0.49
1:A:271:ALA:HA	1:A:359:GLN:HE21	1.75	0.49
2:B:407:GLN:OE1	2:B:617:ARG:HG2	2.12	0.49
2:B:674:TRP:CD2	2:B:675:LEU:CD2	2.96	0.49
1:E:198:GLU:HA	1:E:198:GLU:OE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:429:ARG:O	1:E:430:ALA:HB2	2.12	0.49
1:E:434:TYR:O	1:E:435:ARG:C	2.49	0.49
2:F:407:GLN:OE1	2:F:617:ARG:HG2	2.13	0.49
1:G:111:ILE:HD13	1:G:114:MET:HE3	1.95	0.49
1:G:301:MET:HE1	1:G:341:LEU:HD22	1.95	0.49
1:G:370:LEU:HD21	1:G:380:ALA:CB	2.42	0.49
1:A:415:LEU:O	1:A:417:LEU:N	2.45	0.49
1:C:139:TYR:O	1:C:140:ALA:C	2.50	0.49
1:C:368:LEU:HB2	1:C:446:TYR:CD1	2.47	0.49
2:D:720:GLU:CG	2:D:724:ARG:NH2	2.76	0.49
2:F:512:ARG:NH1	2:H:216:ASP:OD2	2.45	0.49
2:F:556:ALA:HB1	2:F:561:CYS:O	2.12	0.49
2:H:494:ALA:O	2:H:495:LYS:C	2.49	0.49
1:A:41:GLU:HG2	1:A:210:LEU:HD13	1.95	0.49
2:B:79:ALA:HB1	2:B:80:PRO:CD	2.43	0.49
2:B:650:ASP:HA	2:B:713:TRP:HB3	1.94	0.49
1:E:394:ALA:O	1:E:397:PHE:N	2.41	0.49
2:F:448:ILE:O	2:F:448:ILE:CG2	2.60	0.49
1:G:75:LEU:HD12	1:G:76:ARG:N	2.27	0.49
1:G:105:PHE:HD2	2:H:176:LEU:HB3	1.77	0.49
1:G:418:LEU:HD23	1:G:418:LEU:HA	1.63	0.49
2:H:448:ILE:O	2:H:448:ILE:CG2	2.61	0.49
2:B:53:GLU:N	2:B:54:PRO:CD	2.76	0.49
1:C:390:VAL:HG23	1:C:391:PRO:CD	2.42	0.49
1:E:301:MET:HE1	1:E:341:LEU:HD22	1.94	0.49
1:G:370:LEU:CD2	1:G:380:ALA:CB	2.91	0.49
1:G:429:ARG:O	1:G:430:ALA:HB2	2.13	0.49
2:H:35:LEU:HA	2:H:101:VAL:O	2.13	0.49
2:H:93:PHE:CD2	2:H:299:TRP:CD1	3.01	0.49
2:H:238:LEU:HD11	2:H:257:TYR:CE1	2.47	0.49
1:A:165:THR:O	1:A:166:LEU:HD23	2.12	0.48
1:A:252:LEU:HD23	1:A:281:ILE:CD1	2.43	0.48
2:D:65:PHE:O	2:D:99:PHE:HB2	2.12	0.48
4:E:3005:FAD:O5B	4:E:3005:FAD:C2B	2.58	0.48
2:F:198:HIS:CG	2:F:526:ALA:HB2	2.48	0.48
2:F:232:GLU:OE2	8:F:4000:141:H1	2.13	0.48
1:G:50:MET:HE3	1:G:116:ALA:CB	2.42	0.48
1:G:194:LEU:HD12	1:G:194:LEU:O	2.11	0.48
2:H:12:ALA:O	2:H:13:ARG:C	2.49	0.48
2:H:339:THR:HG23	2:H:340:ALA:H	1.73	0.48
2:H:635:ARG:CD	2:H:750:CYS:SG	2.98	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HD21	1:A:434:TYR:OH	2.13	0.48
1:A:359:GLN:HE21	1:A:359:GLN:HA	1.78	0.48
1:A:430:ALA:HB1	1:A:434:TYR:HD2	1.78	0.48
1:E:98:HIS:O	1:E:99:HIS:HB2	2.13	0.48
2:F:152:GLU:O	2:F:153:THR:C	2.51	0.48
2:F:218:ARG:HE	2:F:220:GLU:CD	2.14	0.48
2:F:452:PRO:O	2:F:452:PRO:HG2	2.13	0.48
7:F:3004:MOS:S	8:F:4000:141:C7	3.01	0.48
1:G:271:ALA:CA	1:G:359:GLN:HE22	2.26	0.48
2:H:744:HIS:CD2	2:H:744:HIS:C	2.86	0.48
2:D:227:GLY:N	6:D:3003:MTE:O4	2.37	0.48
2:D:661:ILE:CD1	2:D:712:LEU:HG	2.44	0.48
7:D:3004:MOS:S	8:D:4000:141:N8	2.86	0.48
1:E:231:LEU:O	1:E:231:LEU:CD2	2.61	0.48
2:F:34:HIS:C	2:F:35:LEU:HD23	2.33	0.48
2:F:419:THR:O	2:F:420:ARG:C	2.51	0.48
2:F:756:ASP:O	2:F:758:GLN:NE2	2.39	0.48
2:H:319:TYR:N	2:H:319:TYR:CD1	2.81	0.48
1:A:436:MET:O	1:A:437:ASN:C	2.49	0.48
1:A:447:VAL:O	1:A:448:ARG:C	2.50	0.48
2:B:150:ASP:OD1	2:B:150:ASP:O	2.30	0.48
2:B:346:GLY:N	2:B:347:PRO:CD	2.77	0.48
2:D:110:ARG:O	2:D:111:ILE:C	2.52	0.48
2:D:528:ALA:HB1	8:D:4000:141:H1	1.93	0.48
1:G:319:GLU:N	1:G:319:GLU:OE2	2.46	0.48
1:G:412:ALA:O	1:G:415:LEU:HG	2.13	0.48
2:H:205:LYS:HB3	2:H:240:ILE:HD11	1.95	0.48
2:H:307:VAL:O	2:H:310:ARG:N	2.45	0.48
2:B:751:GLY:HA3	2:B:773:ALA:O	2.14	0.48
2:D:197:GLN:HG3	2:D:231:LYS:HB2	1.96	0.48
2:D:328:SER:OG	2:D:330:ARG:NH1	2.42	0.48
2:D:347:PRO:O	2:D:348:GLN:C	2.46	0.48
2:D:722:ILE:HG23	2:D:722:ILE:O	2.12	0.48
1:G:78:ILE:HG21	1:G:108:PRO:HB3	1.94	0.48
2:H:443:THR:O	2:H:444:LEU:HD23	2.13	0.48
1:A:252:LEU:CD2	1:A:281:ILE:CD1	2.88	0.48
2:B:216:ASP:OD2	2:D:512:ARG:NH1	2.46	0.48
2:B:221:MET:HE1	2:B:223:ARG:C	2.34	0.48
2:D:237:HIS:ND1	2:D:237:HIS:N	2.55	0.48
2:D:731:PRO:HB2	2:D:732:PRO:HD3	1.95	0.48
1:E:61:ASN:ND2	1:E:61:ASN:N	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:364:VAL:CG2	1:E:435:ARG:HG2	2.44	0.48
2:F:214:PHE:N	2:F:214:PHE:HD1	2.08	0.48
2:H:107:ARG:O	2:H:110:ARG:N	2.47	0.48
2:H:330:ARG:NH2	2:H:611:ARG:HH21	2.10	0.48
2:H:481:LEU:HD12	2:H:482:ASN:H	1.77	0.48
2:H:487:GLU:OE2	2:H:489:GLY:CA	2.61	0.48
2:H:641:ARG:HH21	2:H:706:ARG:NE	2.12	0.48
1:A:45:GLY:O	1:A:48:THR:OG1	2.19	0.48
1:A:52:ARG:HG2	1:A:53:ASP:N	2.28	0.48
2:B:65:PHE:O	2:B:99:PHE:HB2	2.13	0.48
2:D:130:ASP:O	2:D:131:GLN:C	2.47	0.48
2:D:457:ILE:O	2:D:458:SER:CB	2.62	0.48
2:D:755:PRO:O	2:D:772:ARG:HD2	2.14	0.48
1:E:408:GLU:OE1	2:F:442:ARG:NH2	2.31	0.48
2:H:722:ILE:HG13	2:H:723:PHE:HD1	1.77	0.48
1:A:105:PHE:CE1	2:B:177:GLU:HB2	2.48	0.48
1:C:53:ASP:C	1:C:53:ASP:OD1	2.51	0.48
2:D:39:LEU:HD23	2:D:39:LEU:N	2.29	0.48
2:D:65:PHE:HB2	2:D:100:LEU:HB3	1.95	0.48
2:D:360:LEU:CD1	2:D:364:MET:HE2	2.43	0.48
2:D:691:HIS:O	2:D:692:ALA:HB2	2.14	0.48
1:E:68:PRO:HB2	1:E:224:PHE:CE1	2.48	0.48
1:E:107:THR:HG21	2:F:16:VAL:HA	1.96	0.48
1:E:192:TRP:O	1:E:196:HIS:CD2	2.59	0.48
1:E:295:PRO:HB2	1:E:296:PRO:HD3	1.95	0.48
1:E:324:GLU:O	1:E:325:TYR:C	2.52	0.48
2:H:453:VAL:CG1	2:H:454:LYS:N	2.72	0.48
2:B:696:TYR:C	2:B:697:LYS:HD2	2.34	0.48
1:C:399:ALA:O	1:C:401:LEU:N	2.47	0.48
2:D:737:ILE:O	2:D:738:SER:C	2.49	0.48
1:E:301:MET:HE2	1:E:341:LEU:HD22	1.96	0.48
1:E:331:ARG:O	1:E:334:GLU:HB2	2.14	0.48
1:G:37:GLU:CD	2:H:256:ARG:HH22	2.15	0.48
2:H:731:PRO:O	2:H:732:PRO:C	2.51	0.48
1:A:237:THR:CG2	1:A:238:PRO:N	2.77	0.48
2:B:198:HIS:CG	2:B:526:ALA:HB2	2.49	0.48
2:B:216:ASP:OD1	2:D:512:ARG:HD2	2.14	0.48
2:D:66:THR:HB	2:D:69:ASP:OD2	2.13	0.48
2:D:464:LEU:HA	2:D:464:LEU:HD23	1.64	0.48
2:D:746:ALA:O	2:D:747:CYS:C	2.48	0.48
1:E:353:LEU:HD12	1:E:353:LEU:HA	1.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:166:PHE:CE1	2:F:355:ARG:HG3	2.49	0.48
1:G:67:LEU:O	1:G:68:PRO:C	2.50	0.48
1:G:78:ILE:HD13	1:G:108:PRO:HA	1.95	0.48
1:A:42:GLY:HA3	4:A:3005:FAD:HM71	1.96	0.47
2:B:166:PHE:HB3	2:B:355:ARG:NH2	2.28	0.47
2:B:274:ILE:HG12	2:B:293:HIS:HD2	1.78	0.47
1:C:324:GLU:O	1:C:325:TYR:C	2.51	0.47
2:D:560:GLY:O	2:D:561:CYS:CB	2.44	0.47
2:D:644:ARG:HB2	2:D:707:ILE:HB	1.96	0.47
1:E:120:ARG:O	1:E:121:ASP:C	2.53	0.47
1:E:314:ARG:NH1	1:E:334:GLU:OE2	2.47	0.47
1:E:314:ARG:O	1:E:315:ARG:HB2	2.12	0.47
1:G:331:ARG:HH11	1:G:331:ARG:HG3	1.78	0.47
1:A:95:MET:CG	1:A:114:MET:HE3	2.44	0.47
1:A:141:PRO:HG2	1:A:142:ILE:N	2.29	0.47
2:B:556:ALA:HB1	2:B:561:CYS:O	2.14	0.47
2:D:66:THR:O	2:D:67:ALA:C	2.49	0.47
2:F:437:TRP:CZ3	2:F:446:ARG:HG3	2.50	0.47
1:G:205:GLY:O	1:G:209:SER:OG	2.31	0.47
1:G:266:LEU:O	1:G:267:LEU:C	2.51	0.47
1:G:317:PRO:O	1:G:320:ASP:HB2	2.14	0.47
1:G:399:ALA:C	1:G:401:LEU:H	2.17	0.47
2:H:556:ALA:O	2:H:557:ALA:C	2.53	0.47
2:H:560:GLY:O	2:H:561:CYS:CB	2.45	0.47
1:C:102:GLN:NE2	1:C:137:THR:HA	2.28	0.47
1:C:193:TYR:O	1:C:196:HIS:N	2.47	0.47
2:D:741:LEU:HD12	2:D:741:LEU:HA	1.60	0.47
2:F:179:GLN:HB3	2:F:238:LEU:CD1	2.41	0.47
1:G:297:ALA:HA	1:G:367:CYS:SG	2.55	0.47
2:H:58:SER:OG	2:H:59:PRO:CD	2.61	0.47
2:H:701:PHE:HE2	2:H:704:ARG:NH1	2.13	0.47
1:A:415:LEU:O	1:A:416:PRO:C	2.49	0.47
1:A:440:GLN:O	1:A:441:ALA:C	2.52	0.47
2:B:344:PHE:CD1	8:B:4000:141:C5	2.97	0.47
2:B:744:HIS:HE1	2:B:754:TRP:CZ3	2.33	0.47
1:C:191:ASP:O	1:C:194:LEU:HB3	2.14	0.47
1:C:252:LEU:O	1:C:252:LEU:HD12	2.14	0.47
2:F:77:SER:HB2	2:F:83:GLU:HB3	1.96	0.47
1:G:78:ILE:HG23	1:G:79:GLU:N	2.30	0.47
1:G:267:LEU:O	1:G:268:ARG:C	2.50	0.47
1:G:290:PRO:O	1:G:386:GLY:N	2.36	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:302:GLY:HA2	1:G:381:ARG:NH1	2.29	0.47
2:H:330:ARG:HH21	2:H:611:ARG:NH2	2.13	0.47
2:H:398:LYS:O	2:H:399:LYS:O	2.32	0.47
2:H:450:LEU:HD12	2:H:628:ILE:HG13	1.96	0.47
2:H:487:GLU:OE2	2:H:489:GLY:N	2.46	0.47
2:H:730:GLU:O	2:H:733:PHE:N	2.42	0.47
2:B:218:ARG:NH2	2:B:517:ASP:OD1	2.48	0.47
2:D:69:ASP:O	2:D:70:LEU:C	2.51	0.47
2:D:166:PHE:CE1	2:D:355:ARG:HG3	2.49	0.47
2:D:673:GLY:O	2:D:678:GLU:HG3	2.15	0.47
1:E:411:ILE:O	1:E:412:ALA:C	2.51	0.47
2:F:174:PHE:CE1	2:F:693:PRO:HG3	2.49	0.47
2:D:648:LEU:HD12	2:D:711:ALA:O	2.15	0.47
2:D:701:PHE:O	2:D:704:ARG:HG2	2.15	0.47
1:E:92:GLN:HB3	2:F:16:VAL:CG1	2.45	0.47
1:E:95:MET:CG	1:E:114:MET:HE3	2.44	0.47
2:F:278:ILE:CG1	2:F:279:GLY:N	2.77	0.47
2:B:31:ASN:HB2	2:B:251:ARG:HH11	1.79	0.47
2:B:179:GLN:HB3	2:B:238:LEU:HD13	1.95	0.47
2:B:627:ALA:HB2	2:B:735:LEU:HD22	1.96	0.47
2:B:647:ILE:HG22	2:B:648:LEU:N	2.30	0.47
1:C:281:ILE:HG13	1:C:281:ILE:O	2.15	0.47
2:D:609:TRP:HA	2:D:616:GLY:HA3	1.95	0.47
2:D:649:HIS:HB3	2:D:664:ILE:HD13	1.96	0.47
1:E:237:THR:CG2	1:E:238:PRO:HD2	2.41	0.47
1:E:237:THR:CB	1:E:238:PRO:HD2	2.45	0.47
1:E:241:TYR:N	1:E:341:LEU:O	2.42	0.47
1:E:366:GLY:CA	1:E:442:MET:SD	3.00	0.47
1:E:415:LEU:N	1:E:416:PRO:CD	2.78	0.47
2:F:28:CYS:HB2	2:F:29:PRO:CD	2.44	0.47
2:F:74:ASN:OD1	2:F:85:VAL:N	2.44	0.47
2:F:414:LEU:HG	2:F:624:TYR:CD2	2.50	0.47
1:G:39:CYS:SG	1:G:40:ASN:N	2.87	0.47
1:G:89:HIS:ND1	1:G:91:VAL:HB	2.29	0.47
1:G:353:LEU:HD21	1:G:434:TYR:CZ	2.49	0.47
1:G:436:MET:C	1:G:438:ALA:H	2.16	0.47
2:H:674:TRP:O	2:H:675:LEU:HD23	2.14	0.47
1:A:143:LEU:HD22	1:A:147:GLU:OE2	2.15	0.47
2:B:238:LEU:HD11	2:B:257:TYR:CE1	2.50	0.47
2:B:731:PRO:N	2:B:732:PRO:HD2	2.30	0.47
2:D:609:TRP:HB2	2:D:616:GLY:HA3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:342:ARG:CZ	2:F:667:ALA:HB2	2.45	0.47
2:F:367:ASP:OD1	2:F:368:PRO:CD	2.63	0.47
2:F:706:ARG:HD3	2:F:706:ARG:HA	1.65	0.47
1:G:115:ALA:O	1:G:117:ALA:N	2.46	0.47
2:H:137:SER:OG	2:H:332:ARG:HB3	2.15	0.47
2:H:198:HIS:CD2	2:H:526:ALA:CA	2.97	0.47
2:H:227:GLY:N	6:H:3003:MTE:O4	2.43	0.47
2:H:355:ARG:O	2:H:356:ALA:C	2.48	0.47
2:H:731:PRO:HB2	2:H:732:PRO:HD3	1.95	0.47
2:H:771:ARG:O	2:H:772:ARG:C	2.51	0.47
1:A:91:VAL:HG12	1:A:111:ILE:HD13	1.96	0.47
1:A:351:TYR:OH	1:A:449:GLU:OE1	2.29	0.47
1:A:361:ILE:HG21	1:A:429:ARG:CZ	2.45	0.47
2:B:496:MET:CE	2:B:496:MET:CA	2.92	0.47
2:B:683:ASP:HB3	2:B:689:MET:SD	2.55	0.47
1:C:256:ALA:HB1	1:C:260:HIS:HB2	1.97	0.47
1:C:273:GLU:OE1	1:C:276:ARG:NH1	2.47	0.47
2:D:456:GLY:O	2:D:457:ILE:HD13	2.15	0.47
2:D:559:GLU:O	2:D:560:GLY:O	2.33	0.47
1:E:401:LEU:HA	1:E:401:LEU:HD12	1.50	0.47
2:F:221:MET:HE1	2:F:224:MET:N	2.28	0.47
2:F:691:HIS:O	2:F:692:ALA:HB2	2.15	0.47
1:G:81:ILE:HA	1:G:81:ILE:HD13	1.44	0.47
1:G:361:ILE:HG21	1:G:429:ARG:CZ	2.45	0.47
2:H:418:VAL:O	2:H:419:THR:C	2.52	0.47
1:A:273:GLU:OE1	1:A:276:ARG:NH1	2.48	0.47
1:A:348:LEU:CD1	1:A:349:ARG:H	2.02	0.47
1:A:368:LEU:HB3	1:A:446:TYR:CE1	2.50	0.47
1:A:441:ALA:HB1	2:B:636:LEU:HB3	1.97	0.47
2:B:446:ARG:NH1	2:B:630:GLU:OE2	2.42	0.47
2:B:720:GLU:HG3	2:B:724:ARG:NH2	2.29	0.47
2:D:398:LYS:C	2:D:399:LYS:HD2	2.35	0.47
4:E:3005:FAD:N1	4:E:3005:FAD:C2'	2.78	0.47
2:F:464:LEU:HD23	2:F:464:LEU:HA	1.69	0.47
2:F:661:ILE:HD13	2:F:712:LEU:HG	1.97	0.47
1:G:121:ASP:OD1	1:G:123:LYS:HE2	2.15	0.47
2:H:164:GLY:HA3	2:H:276:TYR:CZ	2.50	0.47
2:H:280:ALA:C	2:H:287:LEU:CD1	2.83	0.47
2:B:344:PHE:CE1	8:B:4000:141:C5	2.98	0.46
1:G:281:ILE:CG2	1:G:282:GLY:N	2.78	0.46
1:G:453:GLU:OE1	2:H:442:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:717:ASN:OD1	2:H:719:GLU:N	2.48	0.46
1:A:25:GLU:O	1:A:26:LEU:C	2.53	0.46
1:A:67:LEU:CB	1:A:68:PRO:HD3	2.45	0.46
1:A:382:ILE:O	1:A:393:ARG:HA	2.14	0.46
1:C:373:LYS:HB2	1:C:378:GLU:HG2	1.97	0.46
1:E:241:TYR:O	1:E:340:THR:CG2	2.63	0.46
1:E:241:TYR:O	1:E:340:THR:HA	2.15	0.46
2:F:321:VAL:CG1	2:F:323:ALA:O	2.63	0.46
2:F:348:GLN:OE1	2:F:348:GLN:N	2.40	0.46
1:G:104:GLY:O	1:G:107:THR:HB	2.15	0.46
1:G:131:GLY:HA3	1:G:274:GLN:OE1	2.15	0.46
1:A:371:THR:C	1:A:372:LEU:HD23	2.35	0.46
1:C:67:LEU:HD23	1:C:67:LEU:HA	1.59	0.46
1:C:390:VAL:HG22	1:C:391:PRO:N	2.31	0.46
1:E:45:GLY:O	1:E:47:CYS:N	2.48	0.46
2:F:133:LEU:HA	2:F:133:LEU:HD12	1.27	0.46
2:F:312:MET:HE1	2:F:330:ARG:HH12	1.81	0.46
2:F:691:HIS:O	2:F:691:HIS:CG	2.66	0.46
1:G:293:ASP:OD1	1:G:362:SER:OG	2.31	0.46
2:H:628:ILE:O	2:H:628:ILE:HG22	2.16	0.46
1:A:284:ASN:OD1	1:A:295:PRO:HD3	2.16	0.46
1:A:322:PHE:HB3	1:A:390:VAL:HG22	1.97	0.46
2:B:133:LEU:HA	2:B:133:LEU:HD12	1.32	0.46
2:B:334:ASN:C	2:B:335:THR:HG23	2.35	0.46
2:D:312:MET:HE1	2:D:330:ARG:NH1	2.28	0.46
1:E:12:ARG:CG	1:E:12:ARG:NH1	2.76	0.46
2:F:101:VAL:HG12	2:F:102:ALA:N	2.30	0.46
2:F:457:ILE:O	2:F:458:SER:CB	2.64	0.46
1:G:275:VAL:HG21	4:G:3005:FAD:HM73	1.96	0.46
1:G:322:PHE:CB	1:G:390:VAL:CG2	2.86	0.46
1:A:327:LYS:N	1:A:328:GLN:NE2	2.64	0.46
2:B:60:GLY:O	2:B:103:ALA:HB1	2.16	0.46
2:B:493:HIS:ND1	2:B:513:ILE:HD13	2.31	0.46
1:C:390:VAL:HG22	1:C:391:PRO:CD	2.44	0.46
2:D:101:VAL:HG12	2:D:102:ALA:N	2.30	0.46
2:F:417:LEU:O	2:F:418:VAL:C	2.53	0.46
1:G:418:LEU:HB3	1:G:436:MET:HE1	1.98	0.46
2:H:627:ALA:HB2	2:H:735:LEU:HD22	1.97	0.46
1:A:349:ARG:CD	1:A:449:GLU:OE2	2.63	0.46
2:B:31:ASN:HB2	2:B:251:ARG:NH1	2.31	0.46
2:B:66:THR:HB	2:B:69:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:PRO:HB3	2:B:219:VAL:CG1	2.46	0.46
1:C:21:GLN:HG2	1:C:22:SER:N	2.29	0.46
1:C:41:GLU:HG3	1:C:214:LYS:CE	2.38	0.46
1:C:83:ALA:HB1	1:C:84:PRO:CD	2.45	0.46
1:C:181:PHE:CD2	1:C:183:PRO:HD3	2.51	0.46
1:C:231:LEU:O	1:C:231:LEU:HD22	2.15	0.46
2:D:310:ARG:HD2	2:D:344:PHE:HB3	1.97	0.46
2:D:507:ASP:OD1	2:D:508:PRO:N	2.47	0.46
2:D:552:ALA:O	2:D:553:GLY:C	2.54	0.46
1:E:252:LEU:HD22	1:E:281:ILE:HD13	1.98	0.46
2:F:656:ASN:O	2:F:657:PRO:C	2.52	0.46
2:F:767:LEU:O	2:F:768:ALA:C	2.52	0.46
1:G:369:ASN:HB3	1:G:381:ARG:HB2	1.96	0.46
2:H:61:VAL:HA	2:H:103:ALA:HB2	1.97	0.46
1:A:153:PRO:HA	1:A:154:PRO:HD3	1.81	0.46
1:A:231:LEU:O	1:A:231:LEU:HD22	2.15	0.46
1:A:425:LEU:O	1:A:432:ALA:HB2	2.16	0.46
2:B:645:THR:HG21	2:B:668:TYR:CZ	2.50	0.46
1:C:399:ALA:C	1:C:401:LEU:N	2.66	0.46
2:D:53:GLU:N	2:D:54:PRO:CD	2.78	0.46
2:D:343:GLY:O	2:D:344:PHE:C	2.53	0.46
2:D:533:ALA:O	2:D:534:ASP:C	2.53	0.46
1:E:103:CYS:HA	2:F:489:GLY:HA3	1.98	0.46
2:F:380:PRO:O	2:F:381:GLU:HB2	2.16	0.46
2:F:414:LEU:HG	2:F:624:TYR:HD2	1.81	0.46
2:F:425:ALA:O	2:F:426:ASN:CB	2.64	0.46
2:H:302:ASP:OD1	2:H:303:LEU:N	2.48	0.46
2:B:697:LYS:HD2	2:B:697:LYS:N	2.31	0.46
1:C:446:TYR:CE2	1:C:450:LEU:CD1	2.98	0.46
2:D:425:ALA:O	2:D:426:ASN:CB	2.63	0.46
2:D:496:MET:CE	2:D:496:MET:N	2.66	0.46
2:H:173:HIS:HA	2:H:341:PHE:CZ	2.51	0.46
2:H:734:LEU:CD1	2:H:734:LEU:N	2.77	0.46
2:H:753:HIS:O	2:H:755:PRO:HD3	2.16	0.46
1:A:206:THR:OG1	4:A:3005:FAD:O3'	2.27	0.46
1:A:368:LEU:HB3	1:A:446:TYR:CD1	2.51	0.46
2:D:23:LEU:HD13	2:D:194:CYS:HA	1.98	0.46
2:D:123:ARG:HB3	2:D:124:PRO:HD2	1.98	0.46
2:D:461:LEU:HD12	2:D:463:HIS:CE1	2.50	0.46
2:F:222:ARG:HB2	2:F:515:ALA:CB	2.46	0.46
2:F:740:PHE:O	2:F:741:LEU:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:450:LEU:HA	1:G:450:LEU:HD23	1.54	0.46
2:H:367:ASP:OD1	2:H:368:PRO:HD2	2.15	0.46
2:D:197:GLN:HG2	2:D:488:MET:HE2	1.98	0.46
2:D:776:ARG:O	2:D:777:ALA:CB	2.63	0.46
1:E:222:VAL:HG12	1:E:223:ALA:N	2.31	0.46
1:E:364:VAL:HG22	1:E:435:ARG:HG2	1.98	0.46
1:G:298:LEU:O	1:G:299:ILE:C	2.53	0.46
2:H:95:GLY:O	2:H:96:GLN:C	2.54	0.46
2:H:568:PHE:CD2	2:H:573:VAL:HG22	2.50	0.46
1:A:428:MET:HG2	1:A:429:ARG:N	2.30	0.45
2:B:488:MET:HG3	6:B:3003:MTE:C4	2.46	0.45
2:B:659:LEU:HD23	2:B:659:LEU:HA	1.73	0.45
2:D:609:TRP:CB	2:D:616:GLY:HA3	2.46	0.45
4:E:3005:FAD:H2B	4:E:3005:FAD:H8A	1.54	0.45
2:F:65:PHE:O	2:F:99:PHE:HB2	2.16	0.45
2:F:260:ASP:OD1	2:F:691:HIS:CD2	2.70	0.45
2:F:339:THR:HG23	2:F:340:ALA:O	2.16	0.45
2:F:767:LEU:HA	2:F:767:LEU:HD12	1.60	0.45
1:G:261:PRO:O	1:G:262:ALA:C	2.52	0.45
2:H:158:ALA:O	2:H:159:ALA:C	2.52	0.45
2:H:639:GLU:O	2:H:640:ASN:HB3	2.15	0.45
2:H:641:ARG:NH2	2:H:706:ARG:NE	2.64	0.45
1:A:41:GLU:HG3	1:A:214:LYS:CE	2.44	0.45
1:A:371:THR:OG1	1:A:379:THR:HB	2.16	0.45
2:B:93:PHE:CD2	2:B:299:TRP:NE1	2.84	0.45
2:B:258:ASP:O	2:B:259:ARG:C	2.53	0.45
2:B:372:ARG:O	2:B:373:ALA:C	2.51	0.45
2:D:321:VAL:HG12	2:D:323:ALA:O	2.16	0.45
2:D:411:ASP:N	2:D:411:ASP:OD1	2.48	0.45
2:F:644:ARG:HG3	2:F:707:ILE:HG22	1.97	0.45
2:F:722:ILE:HD12	2:F:722:ILE:HA	1.65	0.45
1:A:49:VAL:HA	1:A:112:VAL:HG11	1.99	0.45
2:B:38:GLY:C	2:B:39:LEU:HD23	2.37	0.45
2:B:344:PHE:CE2	8:B:4000:141:N1	2.84	0.45
2:B:356:ALA:O	2:B:357:ILE:C	2.53	0.45
2:D:23:LEU:O	2:D:23:LEU:HG	2.17	0.45
2:D:218:ARG:NH2	2:D:517:ASP:OD1	2.49	0.45
2:D:258:ASP:O	2:D:259:ARG:C	2.52	0.45
2:D:751:GLY:HA3	2:D:773:ALA:O	2.16	0.45
1:E:67:LEU:HA	1:E:67:LEU:HD23	1.52	0.45
2:F:551:LEU:HD23	2:F:551:LEU:HA	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:LEU:O	1:G:130:ALA:C	2.54	0.45
2:H:547:LEU:O	2:H:548:ARG:C	2.55	0.45
2:H:551:LEU:HD23	2:H:551:LEU:HA	1.49	0.45
1:A:271:ALA:HA	1:A:359:GLN:HE22	1.81	0.45
1:C:27:LEU:HD23	1:C:27:LEU:HA	1.80	0.45
2:D:360:LEU:CG	2:D:364:MET:CE	2.95	0.45
1:E:68:PRO:CG	1:E:224:PHE:CE1	2.98	0.45
1:E:83:ALA:HB2	1:E:157:TRP:CH2	2.51	0.45
1:E:269:ARG:NH2	1:E:357:PHE:HA	2.32	0.45
2:F:137:SER:OG	2:F:332:ARG:HB3	2.16	0.45
2:F:771:ARG:O	2:F:772:ARG:C	2.53	0.45
1:G:103:CYS:CB	1:G:136:CYS:SG	3.02	0.45
1:G:104:GLY:HA3	2:H:22:TYR:OH	2.17	0.45
2:H:61:VAL:HG12	2:H:62:ILE:N	2.31	0.45
2:H:263:MET:CE	2:H:692:ALA:CA	2.94	0.45
1:A:237:THR:HG22	1:A:239:ASP:H	1.80	0.45
2:B:93:PHE:CD2	2:B:299:TRP:CD1	3.05	0.45
2:B:558:ARG:HD2	2:B:559:GLU:OE2	2.15	0.45
1:E:53:ASP:HB3	1:E:73:LYS:HD3	1.97	0.45
1:E:308:ARG:HD3	1:E:337:GLU:OE1	2.16	0.45
1:E:337:GLU:O	1:E:337:GLU:HG3	2.17	0.45
2:F:143:PRO:HB3	2:F:329:HIS:ND1	2.32	0.45
2:F:440:THR:O	2:F:440:THR:HG22	2.16	0.45
2:F:536:ASN:O	2:F:537:GLY:C	2.55	0.45
1:G:12:ARG:HH11	1:G:12:ARG:CG	2.29	0.45
1:G:53:ASP:C	1:G:53:ASP:OD1	2.55	0.45
1:G:202:ILE:HG12	1:G:208:VAL:HG11	1.98	0.45
2:H:297:CYS:HB3	2:H:304:SER:OG	2.16	0.45
2:H:306:PRO:HB2	2:H:344:PHE:CE2	2.52	0.45
2:H:532:GLY:N	6:H:3003:MTE:O1P	2.48	0.45
2:H:656:ASN:HA	2:H:657:PRO:HD3	1.86	0.45
2:H:674:TRP:C	2:H:675:LEU:HD23	2.36	0.45
1:A:220:PRO:O	1:A:221:GLU:O	2.35	0.45
1:A:260:HIS:O	1:A:263:LEU:N	2.50	0.45
2:B:361:ALA:HB2	2:B:371:LEU:HD23	1.99	0.45
2:B:683:ASP:OD1	2:B:685:CYS:N	2.50	0.45
2:B:743:LEU:HD12	2:B:743:LEU:HA	1.61	0.45
1:C:89:HIS:O	1:C:90:PRO:C	2.53	0.45
2:D:288:GLY:HA2	2:D:323:ALA:O	2.16	0.45
2:D:476:ASP:OD2	2:D:478:SER:OG	2.34	0.45
1:E:124:ASP:O	1:E:128:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:PRO:O	1:E:386:GLY:N	2.50	0.45
2:F:731:PRO:N	2:F:732:PRO:CD	2.80	0.45
1:G:122:ARG:NH2	1:G:124:ASP:OD2	2.49	0.45
2:H:39:LEU:HD23	2:H:39:LEU:N	2.32	0.45
2:H:232:GLU:OE2	8:H:4000:141:H1	2.16	0.45
2:B:730:GLU:O	2:B:733:PHE:N	2.44	0.45
1:C:432:ALA:O	1:C:433:ALA:C	2.51	0.45
1:G:25:GLU:O	1:G:26:LEU:C	2.53	0.45
1:G:129:LEU:HA	1:G:129:LEU:HD23	1.49	0.45
2:H:227:GLY:O	2:H:230:GLY:N	2.46	0.45
2:H:344:PHE:CE1	8:H:4000:141:C6	3.00	0.45
1:A:40:ASN:N	3:A:3002:FES:S2	2.75	0.45
2:B:551:LEU:HA	2:B:551:LEU:HD23	1.55	0.45
2:D:659:LEU:HD23	2:D:659:LEU:HA	1.59	0.45
2:F:478:SER:C	2:F:479:VAL:CG2	2.85	0.45
1:G:264:ALA:O	1:G:265:GLY:C	2.55	0.45
2:H:173:HIS:N	2:H:341:PHE:HE1	2.14	0.45
2:H:507:ASP:OD1	2:H:507:ASP:C	2.54	0.45
2:B:596:LEU:HA	2:B:596:LEU:HD23	1.72	0.45
2:D:79:ALA:HB1	2:D:80:PRO:CD	2.47	0.45
2:D:210:LEU:HD12	2:D:212:LEU:HD12	1.97	0.45
2:D:478:SER:C	2:D:479:VAL:HG23	2.36	0.45
6:D:3003:MTE:S1'	7:D:3004:MOS:O2	2.75	0.45
2:F:547:LEU:O	2:F:548:ARG:C	2.53	0.45
1:G:299:ILE:O	1:G:300:ALA:C	2.52	0.45
2:H:93:PHE:CZ	2:H:96:GLN:N	2.85	0.45
2:B:354:GLU:O	2:B:357:ILE:HG22	2.17	0.45
1:E:103:CYS:HB3	1:E:136:CYS:SG	2.56	0.45
1:E:151:GLY:C	1:E:152:GLU:HG2	2.37	0.45
1:E:194:LEU:O	1:E:194:LEU:HD12	2.17	0.45
2:F:93:PHE:CE2	2:F:299:TRP:NE1	2.85	0.45
2:F:532:GLY:N	6:F:3003:MTE:O1P	2.31	0.45
1:G:279:ALA:HB1	4:G:3005:FAD:H4'	1.97	0.45
1:G:393:ARG:NH1	1:G:398:GLU:OE2	2.50	0.45
1:A:371:THR:O	1:A:372:LEU:HD23	2.16	0.44
2:B:139:PHE:O	2:B:140:GLU:HB2	2.16	0.44
2:B:184:LEU:HA	2:B:185:PRO:HD2	1.81	0.44
2:B:233:SER:C	2:B:235:GLY:H	2.20	0.44
2:B:309:ASP:O	2:B:313:LEU:HB2	2.17	0.44
2:B:736:GLY:O	2:B:737:ILE:C	2.55	0.44
1:C:104:GLY:HA3	2:D:22:TYR:OH	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ARG:HH11	1:C:276:ARG:HD2	1.50	0.44
2:D:53:GLU:HB3	2:D:54:PRO:HD3	1.99	0.44
2:D:276:TYR:OH	2:D:359:HIS:CD2	2.70	0.44
1:E:40:ASN:HD22	1:E:40:ASN:HA	1.56	0.44
1:E:398:GLU:O	1:E:401:LEU:HB2	2.17	0.44
2:F:555:VAL:O	2:F:555:VAL:CG1	2.62	0.44
2:H:123:ARG:CB	2:H:124:PRO:HD2	2.38	0.44
2:H:174:PHE:CZ	2:H:693:PRO:HG3	2.52	0.44
1:A:125:TYR:O	1:A:126:ASP:C	2.55	0.44
1:A:231:LEU:HD22	1:A:246:GLY:H	1.82	0.44
1:A:276:ARG:HH11	1:A:276:ARG:HD2	1.63	0.44
2:B:444:LEU:HD23	2:B:444:LEU:HA	1.63	0.44
1:C:83:ALA:HB2	1:C:157:TRP:CD2	2.52	0.44
2:D:273:ARG:HH11	2:D:273:ARG:HD2	1.44	0.44
2:D:321:VAL:CG1	2:D:323:ALA:O	2.65	0.44
2:D:700:ALA:O	2:D:701:PHE:C	2.55	0.44
1:G:253:ARG:NH2	1:G:268:ARG:HG3	2.32	0.44
2:H:66:THR:HG22	2:H:67:ALA:N	2.32	0.44
2:H:66:THR:CG2	2:H:67:ALA:N	2.79	0.44
2:H:133:LEU:HD12	2:H:133:LEU:HA	1.26	0.44
1:A:18:ASP:OD2	1:A:18:ASP:C	2.55	0.44
2:B:130:ASP:O	2:B:131:GLN:C	2.54	0.44
2:B:334:ASN:O	2:B:335:THR:CG2	2.65	0.44
1:C:439:ALA:O	1:C:440:GLN:C	2.50	0.44
1:E:252:LEU:CD2	1:E:281:ILE:HD13	2.47	0.44
1:E:434:TYR:CD1	2:F:764:GLU:HG3	2.52	0.44
2:F:444:LEU:HD23	2:F:444:LEU:HA	1.33	0.44
2:F:547:LEU:O	2:F:550:ARG:N	2.50	0.44
1:G:271:ALA:CA	1:G:359:GLN:NE2	2.77	0.44
1:G:399:ALA:O	1:G:401:LEU:N	2.51	0.44
2:H:79:ALA:O	2:H:80:PRO:C	2.56	0.44
2:H:110:ARG:O	2:H:111:ILE:C	2.56	0.44
2:H:419:THR:O	2:H:420:ARG:C	2.53	0.44
2:H:556:ALA:O	2:H:560:GLY:N	2.50	0.44
2:B:316:ASP:N	2:B:316:ASP:OD1	2.43	0.44
2:B:517:ASP:O	2:B:519:SER:N	2.51	0.44
1:C:139:TYR:C	1:C:141:PRO:HD2	2.38	0.44
1:C:271:ALA:HB2	4:C:3005:FAD:N5	2.33	0.44
2:D:354:GLU:OE1	2:D:372:ARG:NE	2.47	0.44
1:E:44:CYS:N	3:E:3002:FES:S1	2.89	0.44
2:F:227:GLY:N	6:F:3003:MTE:O4	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:421:LEU:HG	2:F:628:ILE:HD12	1.98	0.44
2:F:555:VAL:O	2:F:555:VAL:HG12	2.15	0.44
2:F:588:ALA:O	2:F:589:ALA:C	2.56	0.44
2:F:590:TYR:CE1	2:H:466:GLN:NE2	2.86	0.44
2:F:671:GLY:HA2	2:F:733:PHE:CE1	2.52	0.44
1:G:117:ALA:O	1:G:118:HIS:C	2.54	0.44
2:H:96:GLN:HG3	2:H:97:PRO:HD2	1.97	0.44
2:H:273:ARG:HH11	2:H:273:ARG:HD2	1.63	0.44
2:B:236:ASN:N	2:B:236:ASN:ND2	2.65	0.44
2:B:449:ALA:CB	2:B:741:LEU:HB3	2.47	0.44
2:D:360:LEU:HG	2:D:364:MET:CE	2.43	0.44
2:D:691:HIS:O	2:D:691:HIS:CG	2.70	0.44
2:F:654:SER:OG	2:F:656:ASN:N	2.50	0.44
1:G:301:MET:O	1:G:301:MET:CG	2.65	0.44
1:G:455:VAL:O	1:G:455:VAL:HG13	2.16	0.44
2:H:112:ALA:O	2:H:113:ALA:C	2.52	0.44
1:A:327:LYS:H	1:A:328:GLN:NE2	2.14	0.44
2:B:75:ASP:HA	2:B:83:GLU:O	2.17	0.44
2:B:407:GLN:OE1	2:B:618:PRO:HD2	2.17	0.44
2:B:456:GLY:O	2:B:457:ILE:HD13	2.16	0.44
2:B:586:VAL:HG23	2:B:586:VAL:H	1.59	0.44
2:B:700:ALA:O	2:B:701:PHE:C	2.55	0.44
2:D:335:THR:O	2:D:336:GLN:C	2.55	0.44
1:E:222:VAL:CG1	1:E:223:ALA:N	2.79	0.44
2:F:91:VAL:HG11	2:F:98:ILE:HD11	1.98	0.44
2:F:221:MET:CE	2:F:223:ARG:C	2.84	0.44
1:G:331:ARG:O	1:G:334:GLU:CB	2.66	0.44
1:G:345:ALA:O	1:G:347:GLY:N	2.51	0.44
1:G:358:ASP:O	1:G:359:GLN:C	2.55	0.44
2:H:112:ALA:C	2:H:114:ARG:N	2.68	0.44
2:H:228:PHE:O	2:H:341:PHE:HA	2.17	0.44
2:H:335:THR:O	2:H:336:GLN:C	2.55	0.44
2:B:146:TRP:CH2	2:B:312:MET:HE3	2.52	0.44
2:B:238:LEU:HD11	2:B:257:TYR:CZ	2.53	0.44
2:B:612:LEU:HD23	2:B:612:LEU:HA	1.81	0.44
1:C:194:LEU:HD12	1:C:194:LEU:O	2.18	0.44
2:D:93:PHE:CE2	2:D:299:TRP:NE1	2.86	0.44
2:D:276:TYR:OH	2:D:359:HIS:HD2	2.01	0.44
2:D:370:GLU:O	2:D:371:LEU:C	2.54	0.44
2:D:414:LEU:HG	2:D:624:TYR:CD2	2.53	0.44
2:D:641:ARG:HH11	2:D:641:ARG:HD3	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:398:LYS:O	2:F:399:LYS:HD2	2.17	0.44
2:H:96:GLN:HA	2:H:97:PRO:HD3	1.66	0.44
2:H:112:ALA:O	2:H:114:ARG:N	2.51	0.44
1:A:181:PHE:CE2	1:A:183:PRO:HD3	2.53	0.44
1:A:266:LEU:O	1:A:268:ARG:N	2.51	0.44
1:E:436:MET:O	1:E:438:ALA:N	2.51	0.44
1:G:216:LEU:HA	1:G:216:LEU:HD23	1.74	0.44
1:G:228:CYS:O	1:G:229:LYS:C	2.55	0.44
1:G:266:LEU:O	1:G:268:ARG:N	2.51	0.44
1:G:407:ARG:HB3	1:G:409:ASP:OD2	2.18	0.44
2:H:367:ASP:CG	2:H:431:ARG:HH12	2.12	0.44
2:H:491:GLY:O	2:H:495:LYS:HG3	2.17	0.44
2:H:556:ALA:HB1	2:H:561:CYS:O	2.17	0.44
1:A:368:LEU:N	1:A:368:LEU:CD1	2.71	0.44
1:A:450:LEU:HA	1:A:450:LEU:HD23	1.40	0.44
2:B:146:TRP:CE2	2:B:312:MET:HE1	2.52	0.44
2:B:674:TRP:CE3	2:B:675:LEU:CD2	2.98	0.44
1:C:252:LEU:CD2	1:C:281:ILE:HD13	2.48	0.44
2:D:66:THR:HG22	2:D:68:ALA:N	2.31	0.44
1:E:321:PHE:O	1:E:321:PHE:CD1	2.71	0.44
2:F:7:LEU:HA	2:F:7:LEU:HD23	1.77	0.44
2:F:79:ALA:HB1	2:F:80:PRO:HD2	2.00	0.44
2:F:302:ASP:OD1	2:F:303:LEU:N	2.49	0.44
2:F:647:ILE:CG2	2:F:648:LEU:N	2.80	0.44
6:F:3003:MTE:H1S	7:F:3004:MOS:MO	1.54	0.44
1:G:153:PRO:HA	1:G:154:PRO:HD2	1.67	0.44
2:H:370:GLU:O	2:H:371:LEU:C	2.53	0.44
1:A:59:ALA:C	1:A:60:VAL:CG1	2.86	0.43
2:B:64:VAL:HG12	2:B:65:PHE:N	2.33	0.43
2:B:532:GLY:HA3	6:B:3003:MTE:O3P	2.17	0.43
2:D:462:THR:O	2:D:465:ASN:ND2	2.45	0.43
2:D:581:ARG:O	2:D:582:PHE:C	2.56	0.43
2:D:653:ALA:O	2:D:654:SER:C	2.54	0.43
1:E:44:CYS:SG	3:E:3002:FES:S2	3.16	0.43
1:E:300:ALA:C	1:E:302:GLY:H	2.21	0.43
1:E:436:MET:O	1:E:439:ALA:N	2.50	0.43
1:G:33:THR:O	1:G:36:LYS:NZ	2.44	0.43
2:H:60:GLY:O	2:H:103:ALA:CB	2.60	0.43
2:H:319:TYR:HE2	2:H:372:ARG:HB3	1.83	0.43
1:A:26:LEU:O	1:A:27:LEU:C	2.56	0.43
1:A:36:LYS:HD3	1:A:36:LYS:HA	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:CD1	1:A:349:ARG:N	2.56	0.43
1:A:369:ASN:HB3	1:A:381:ARG:HB2	2.00	0.43
2:B:53:GLU:OE1	2:B:53:GLU:HA	2.19	0.43
2:D:174:PHE:CZ	2:D:693:PRO:HG3	2.53	0.43
2:D:251:ARG:CB	2:D:252:PRO:CD	2.96	0.43
2:D:432:ALA:O	2:D:433:GLU:C	2.55	0.43
2:D:490:GLN:HA	2:D:663:GLN:NE2	2.32	0.43
2:D:736:GLY:O	2:D:739:ALA:N	2.50	0.43
1:E:139:TYR:O	1:E:142:ILE:N	2.46	0.43
1:E:152:GLU:HA	1:E:153:PRO:HD3	1.81	0.43
1:E:249:ILE:HG23	1:E:267:LEU:HD22	1.99	0.43
1:E:330:ARG:HH11	1:E:330:ARG:HD3	1.61	0.43
1:E:390:VAL:HG22	1:E:391:PRO:O	2.17	0.43
2:F:319:TYR:OH	2:F:354:GLU:OE2	2.29	0.43
2:F:585:ILE:HD12	2:F:585:ILE:HG23	1.57	0.43
1:G:206:THR:HG1	4:G:3005:FAD:C3'	2.28	0.43
1:G:305:LEU:HD11	1:G:336:VAL:HG13	1.99	0.43
2:H:730:GLU:N	2:H:731:PRO:HD2	2.32	0.43
2:H:766:VAL:O	2:H:770:VAL:HG23	2.18	0.43
2:B:367:ASP:CG	2:B:431:ARG:HH12	2.16	0.43
2:D:168:ILE:CD1	2:D:351:LEU:HD23	2.48	0.43
2:D:265:ILE:O	2:D:265:ILE:CG2	2.63	0.43
2:D:742:ALA:O	2:D:743:LEU:C	2.55	0.43
2:F:38:GLY:C	2:F:39:LEU:HD23	2.38	0.43
2:H:457:ILE:HD13	2:H:457:ILE:HA	1.65	0.43
1:A:117:ALA:O	1:A:118:HIS:C	2.56	0.43
1:A:218:ASP:C	1:A:218:ASP:OD1	2.56	0.43
2:B:214:PHE:N	2:B:214:PHE:HD1	2.15	0.43
2:B:499:VAL:O	2:B:503:VAL:HG23	2.19	0.43
2:B:552:ALA:O	2:B:553:GLY:C	2.54	0.43
2:B:731:PRO:CB	2:B:732:PRO:HD3	2.35	0.43
2:D:238:LEU:HD11	2:D:257:TYR:CZ	2.53	0.43
2:D:609:TRP:CD2	2:D:618:PRO:HB3	2.54	0.43
1:E:139:TYR:C	1:E:141:PRO:HD2	2.38	0.43
2:F:123:ARG:HB3	2:F:124:PRO:CD	2.48	0.43
2:F:273:ARG:HH11	2:F:273:ARG:HD2	1.53	0.43
2:F:657:PRO:O	2:F:661:ILE:CG1	2.47	0.43
1:G:206:THR:HG21	1:G:275:VAL:HG13	2.01	0.43
2:H:528:ALA:HA	6:H:3003:MTE:S2'	2.59	0.43
2:H:645:THR:CG2	2:H:668:TYR:CZ	3.01	0.43
1:C:231:LEU:O	1:C:231:LEU:CD2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ILE:O	1:C:292:GLY:C	2.52	0.43
1:C:295:PRO:HB2	1:C:296:PRO:HD3	1.99	0.43
1:E:303:ALA:CB	1:E:341:LEU:HD23	2.48	0.43
1:E:454:ALA:O	1:E:455:VAL:HG23	2.18	0.43
2:F:266:THR:O	2:F:268:LYS:HE2	2.19	0.43
2:F:348:GLN:O	2:F:349:GLY:C	2.51	0.43
2:F:636:LEU:HD23	2:F:636:LEU:HA	1.55	0.43
1:G:61:ASN:ND2	1:G:274:GLN:HB3	2.33	0.43
1:G:64:LEU:HA	1:G:64:LEU:HD23	1.47	0.43
1:G:301:MET:HB3	1:G:348:LEU:HD22	1.99	0.43
2:H:93:PHE:CE2	2:H:299:TRP:CE2	3.07	0.43
2:H:93:PHE:CE2	2:H:96:GLN:HB2	2.53	0.43
2:H:254:LYS:HG2	2:H:255:MET:N	2.34	0.43
1:C:126:ASP:OD1	2:D:704:ARG:NH1	2.48	0.43
4:E:3005:FAD:O2'	4:E:3005:FAD:O4'	2.34	0.43
2:F:360:LEU:CG	2:F:364:MET:HE3	2.49	0.43
2:F:491:GLY:HA3	2:F:659:LEU:HD13	2.01	0.43
1:G:34:GLY:C	1:G:36:LYS:HE3	2.39	0.43
1:G:151:GLY:C	1:G:152:GLU:HG2	2.38	0.43
1:G:324:GLU:O	1:G:325:TYR:C	2.56	0.43
1:G:388:ALA:C	1:G:390:VAL:N	2.72	0.43
2:H:99:PHE:N	2:H:99:PHE:CD2	2.86	0.43
2:H:237:HIS:ND1	2:H:237:HIS:N	2.65	0.43
1:A:179:PRO:O	1:A:180:ALA:HB2	2.19	0.43
1:A:388:ALA:C	1:A:390:VAL:N	2.71	0.43
1:A:425:LEU:HD12	1:A:425:LEU:HA	1.78	0.43
2:B:35:LEU:HA	2:B:101:VAL:O	2.19	0.43
2:B:39:LEU:HD23	2:B:39:LEU:N	2.34	0.43
2:B:432:ALA:O	2:B:433:GLU:C	2.55	0.43
2:B:747:CYS:O	2:B:748:ALA:C	2.56	0.43
2:B:771:ARG:O	2:B:772:ARG:C	2.56	0.43
1:C:59:ALA:C	1:C:60:VAL:CG1	2.86	0.43
1:C:83:ALA:HB2	1:C:157:TRP:CE3	2.53	0.43
1:C:388:ALA:C	1:C:390:VAL:H	2.21	0.43
1:E:286:ALA:O	1:E:287:ASN:C	2.51	0.43
2:F:551:LEU:O	2:F:552:ALA:C	2.56	0.43
1:G:363:ALA:O	1:G:435:ARG:HD3	2.18	0.43
2:H:173:HIS:CD2	2:H:341:PHE:CD1	3.06	0.43
2:H:344:PHE:CD1	8:H:4000:141:C5	3.02	0.43
2:H:448:ILE:CG1	2:H:630:GLU:HB2	2.47	0.43
2:H:457:ILE:HG21	2:H:621:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:THR:O	1:A:251:ALA:N	2.51	0.43
2:B:48:THR:HG22	2:B:119:THR:OG1	2.17	0.43
2:B:286:LEU:HA	2:B:286:LEU:HD23	1.81	0.43
2:B:737:ILE:O	2:B:740:PHE:N	2.51	0.43
2:D:222:ARG:O	2:D:222:ARG:HG3	2.16	0.43
2:F:127:LEU:HA	2:F:127:LEU:HD23	1.71	0.43
2:F:143:PRO:HB3	2:F:329:HIS:CE1	2.53	0.43
2:F:197:GLN:HG2	2:F:224:MET:HE3	2.00	0.43
1:G:139:TYR:O	1:G:142:ILE:N	2.52	0.43
2:H:418:VAL:O	2:H:421:LEU:N	2.51	0.43
1:A:192:TRP:O	1:A:196:HIS:HD2	2.01	0.43
1:A:279:ALA:HB1	4:A:3005:FAD:H4'	2.01	0.43
2:B:324:LEU:HD21	2:B:326:ILE:HD11	2.01	0.43
2:B:334:ASN:O	2:B:335:THR:HG23	2.18	0.43
2:D:280:ALA:HB1	2:D:285:LYS:O	2.18	0.43
2:D:312:MET:O	2:D:313:LEU:C	2.57	0.43
2:D:430:ARG:NH1	2:D:630:GLU:OE1	2.51	0.43
1:E:83:ALA:CB	1:E:157:TRP:CD2	2.95	0.43
1:E:92:GLN:HB3	2:F:16:VAL:HG11	2.00	0.43
1:E:317:PRO:O	1:E:318:LEU:C	2.57	0.43
1:E:381:ARG:NH2	1:E:393:ARG:NE	2.67	0.43
2:F:493:HIS:CG	2:F:513:ILE:HG12	2.54	0.43
1:G:6:LEU:HB3	1:G:74:ALA:HA	2.01	0.43
1:G:371:THR:CB	1:G:379:THR:HG1	2.32	0.43
2:H:701:PHE:CE2	2:H:704:ARG:NH1	2.86	0.43
1:A:253:ARG:HH11	1:A:253:ARG:HD3	1.72	0.43
1:A:436:MET:C	1:A:438:ALA:N	2.72	0.43
2:B:233:SER:O	2:B:235:GLY:N	2.52	0.43
2:B:234:GLN:H	2:B:234:GLN:HG2	1.67	0.43
2:B:236:ASN:N	2:B:236:ASN:HD22	2.16	0.43
6:B:3003:MTE:S2'	7:B:3004:MOS:S	3.17	0.43
1:C:238:PRO:HG2	1:C:239:ASP:CG	2.39	0.43
2:D:278:ILE:HD11	2:D:286:LEU:CD2	2.42	0.43
2:D:722:ILE:HG13	2:D:723:PHE:CD1	2.54	0.43
1:E:6:LEU:HD11	1:E:9:GLY:C	2.39	0.43
1:E:69:GLN:NE2	1:E:203:ALA:O	2.52	0.43
2:F:62:ILE:O	2:F:62:ILE:CG2	2.65	0.43
1:G:237:THR:CG2	1:G:239:ASP:OD2	2.67	0.43
1:G:430:ALA:HB1	1:G:434:TYR:HD2	1.84	0.43
2:H:288:GLY:HA2	2:H:323:ALA:O	2.19	0.43
2:H:360:LEU:HG	2:H:364:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:731:PRO:O	2:H:733:PHE:N	2.52	0.43
2:H:763:PRO:O	2:H:766:VAL:N	2.52	0.43
2:B:494:ALA:O	2:B:495:LYS:C	2.55	0.42
2:B:533:ALA:O	2:B:534:ASP:C	2.54	0.42
1:E:83:ALA:HB1	1:E:84:PRO:HD2	2.01	0.42
2:F:148:ARG:HH11	2:F:148:ARG:HD2	1.65	0.42
2:F:372:ARG:O	2:F:373:ALA:C	2.56	0.42
2:F:722:ILE:HG23	2:F:722:ILE:O	2.19	0.42
1:G:12:ARG:CG	1:G:12:ARG:NH1	2.81	0.42
1:G:364:VAL:HG23	1:G:435:ARG:HG2	1.92	0.42
1:A:1:MET:CE	1:A:182:LEU:HD13	2.49	0.42
1:A:358:ASP:O	1:A:359:GLN:C	2.57	0.42
2:D:278:ILE:CG1	2:D:279:GLY:N	2.82	0.42
2:D:584:GLU:O	2:D:585:ILE:C	2.54	0.42
1:E:24:LEU:HA	1:E:24:LEU:HD12	1.86	0.42
1:E:37:GLU:CD	2:F:256:ARG:HH21	2.21	0.42
1:E:438:ALA:O	1:E:441:ALA:N	2.52	0.42
2:F:301:ALA:O	2:F:302:ASP:C	2.58	0.42
1:G:81:ILE:HG23	1:G:81:ILE:HD12	1.70	0.42
1:G:193:TYR:O	1:G:196:HIS:N	2.48	0.42
2:B:153:THR:O	2:B:154:ALA:C	2.57	0.42
2:B:197:GLN:HG2	2:B:224:MET:HE3	2.01	0.42
2:B:361:ALA:O	2:B:362:ARG:C	2.58	0.42
2:B:741:LEU:HD12	2:B:741:LEU:HA	1.43	0.42
2:B:746:ALA:O	2:B:747:CYS:C	2.53	0.42
2:D:417:LEU:HG	2:D:648:LEU:HD23	2.00	0.42
1:E:351:TYR:CD2	1:E:351:TYR:N	2.85	0.42
2:F:472:GLN:O	2:F:479:VAL:HG13	2.19	0.42
1:G:49:VAL:HA	1:G:112:VAL:HG11	2.01	0.42
1:G:67:LEU:HA	1:G:67:LEU:HD23	1.36	0.42
2:H:221:MET:HE1	2:H:224:MET:N	2.34	0.42
2:H:261:ASP:O	2:H:262:ASP:C	2.58	0.42
2:H:303:LEU:C	2:H:306:PRO:HD2	2.38	0.42
2:H:367:ASP:OD1	2:H:367:ASP:C	2.57	0.42
2:B:233:SER:C	2:B:235:GLY:N	2.73	0.42
1:C:237:THR:HG23	1:C:238:PRO:HG2	2.01	0.42
2:F:166:PHE:CE2	2:F:355:ARG:HG3	2.54	0.42
2:F:197:GLN:HG3	2:F:231:LYS:HB2	2.01	0.42
2:F:286:LEU:HA	2:F:286:LEU:HD23	1.81	0.42
2:B:274:ILE:HG12	2:B:293:HIS:CD2	2.54	0.42
2:B:503:VAL:O	2:B:548:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:585:ILE:HG23	2:B:585:ILE:HD12	1.64	0.42
1:C:83:ALA:HB1	1:C:84:PRO:HD2	2.01	0.42
1:C:198:GLU:OE2	1:C:198:GLU:HA	2.20	0.42
2:D:234:GLN:H	2:D:234:GLN:HG2	1.44	0.42
2:D:289:ALA:O	2:D:324:LEU:HA	2.19	0.42
2:D:581:ARG:O	2:D:584:GLU:N	2.52	0.42
2:D:641:ARG:HH21	2:D:706:ARG:CZ	2.33	0.42
1:E:68:PRO:HB2	1:E:224:PHE:CD1	2.55	0.42
1:E:103:CYS:N	3:E:3001:FES:S1	2.90	0.42
1:E:440:GLN:O	1:E:441:ALA:C	2.57	0.42
2:F:341:PHE:HD2	2:F:342:ARG:N	2.18	0.42
2:F:680:LEU:C	2:F:681:VAL:HG23	2.39	0.42
1:G:124:ASP:O	1:G:128:LEU:N	2.44	0.42
1:G:209:SER:O	1:G:212:VAL:N	2.52	0.42
2:H:160:HIS:CD2	2:H:364:MET:HB3	2.55	0.42
2:H:214:PHE:N	2:H:214:PHE:HD1	2.14	0.42
2:H:347:PRO:O	2:H:348:GLN:C	2.57	0.42
2:H:473:ILE:HB	2:H:596:LEU:HB3	2.01	0.42
1:A:68:PRO:HB2	1:A:224:PHE:CE1	2.55	0.42
1:A:155:ALA:HB1	1:A:157:TRP:CE2	2.55	0.42
1:C:426:SER:OG	1:C:432:ALA:N	2.42	0.42
2:D:233:SER:C	2:D:235:GLY:H	2.22	0.42
2:D:263:MET:HE1	2:D:692:ALA:HA	1.99	0.42
2:D:609:TRP:CG	2:D:618:PRO:HB3	2.54	0.42
1:E:105:PHE:HD2	2:F:176:LEU:HB3	1.83	0.42
1:E:303:ALA:HB2	1:E:341:LEU:HD23	2.01	0.42
1:E:394:ALA:O	1:E:395:ALA:C	2.58	0.42
2:F:110:ARG:O	2:F:111:ILE:C	2.56	0.42
1:G:417:LEU:HD23	1:G:417:LEU:HA	1.69	0.42
1:A:39:CYS:SG	1:A:40:ASN:N	2.93	0.42
1:A:164:PHE:CG	1:A:165:THR:N	2.87	0.42
1:A:281:ILE:O	1:A:282:GLY:C	2.57	0.42
2:B:307:VAL:O	2:B:308:CYS:C	2.57	0.42
2:B:520:LYS:HZ2	2:D:218:ARG:HH12	1.68	0.42
1:C:64:LEU:HA	1:C:64:LEU:HD23	1.66	0.42
1:C:248:THR:O	1:C:251:ALA:N	2.53	0.42
2:D:494:ALA:O	2:D:495:LYS:C	2.57	0.42
2:D:762:THR:HB	2:D:763:PRO:CD	2.49	0.42
1:E:7:LEU:HD21	1:E:32:LEU:CD1	2.50	0.42
1:E:314:ARG:NH2	1:E:329:ASP:CG	2.70	0.42
1:E:348:LEU:HD12	1:E:348:LEU:HA	1.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:172:GLU:HB3	2:F:696:TYR:CZ	2.54	0.42
2:F:487:GLU:HB2	2:F:493:HIS:CD2	2.55	0.42
2:F:500:ALA:O	2:F:501:ALA:C	2.57	0.42
2:F:638:GLY:O	2:F:639:GLU:C	2.57	0.42
1:G:23:LEU:HD12	1:G:23:LEU:HA	1.69	0.42
1:G:297:ALA:HB2	1:G:350:CYS:HG	1.84	0.42
2:H:91:VAL:H	2:H:91:VAL:HG22	1.57	0.42
2:H:437:TRP:CZ3	2:H:446:ARG:HG3	2.54	0.42
2:H:471:VAL:HG12	2:H:472:GLN:N	2.32	0.42
2:H:657:PRO:O	2:H:658:ALA:C	2.56	0.42
2:D:174:PHE:HZ	2:D:693:PRO:HG3	1.84	0.42
1:E:122:ARG:HD2	1:E:122:ARG:HA	1.89	0.42
1:E:224:PHE:C	1:E:225:LEU:HD23	2.39	0.42
2:F:736:GLY:C	2:F:738:SER:N	2.70	0.42
1:G:83:ALA:HB2	1:G:157:TRP:CZ3	2.55	0.42
1:G:89:HIS:C	1:G:91:VAL:N	2.72	0.42
1:G:204:GLY:HA3	4:G:3005:FAD:O2P	2.18	0.42
2:H:34:HIS:C	2:H:35:LEU:HD23	2.41	0.42
2:H:655:LEU:HA	2:H:655:LEU:HD23	1.84	0.42
1:A:266:LEU:O	1:A:267:LEU:C	2.59	0.42
1:C:78:ILE:CG2	1:C:79:GLU:N	2.82	0.42
2:D:170:GLY:N	2:D:271:ASP:HB3	2.35	0.42
2:D:202:ILE:HD12	2:D:202:ILE:HG23	1.76	0.42
1:E:390:VAL:CG2	1:E:391:PRO:N	2.83	0.42
1:E:462:PRO:HG2	2:F:706:ARG:HB2	2.02	0.42
2:F:185:PRO:O	2:F:185:PRO:HG2	2.19	0.42
2:F:303:LEU:O	2:F:304:SER:C	2.58	0.42
2:F:660:ASP:O	2:F:664:ILE:HG13	2.20	0.42
2:F:734:LEU:N	2:F:734:LEU:HD12	2.35	0.42
1:G:89:HIS:O	1:G:90:PRO:C	2.57	0.42
4:G:3005:FAD:H9	4:G:3005:FAD:H1'2	1.84	0.42
2:H:316:ASP:O	2:H:317:GLY:C	2.56	0.42
2:H:398:LYS:N	2:H:398:LYS:HE3	2.35	0.42
1:A:290:PRO:O	1:A:386:GLY:N	2.53	0.42
2:B:367:ASP:OD1	2:B:367:ASP:C	2.58	0.42
1:C:272:SER:O	1:C:273:GLU:C	2.58	0.42
2:D:720:GLU:HG3	2:D:724:ARG:HH21	1.83	0.42
1:E:102:GLN:O	2:F:489:GLY:HA2	2.19	0.42
2:F:278:ILE:HD11	2:F:286:LEU:CD2	2.50	0.42
2:F:610:ASP:C	2:F:610:ASP:OD2	2.58	0.42
1:G:345:ALA:C	1:G:347:GLY:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:457:VAL:HG22	2:H:632:VAL:CG2	2.50	0.42
2:H:66:THR:O	2:H:67:ALA:C	2.54	0.42
2:H:241:ALA:O	2:H:242:CYS:C	2.57	0.42
2:H:251:ARG:CB	2:H:252:PRO:CD	2.95	0.42
2:H:305:LEU:C	2:H:305:LEU:CD2	2.78	0.42
2:H:631:VAL:HG12	2:H:642:ILE:CA	2.25	0.42
2:B:107:ARG:O	2:B:110:ARG:N	2.52	0.41
2:B:593:ARG:HD2	2:D:603:ALA:HB1	2.02	0.41
1:C:103:CYS:HA	2:D:489:GLY:CA	2.50	0.41
1:C:248:THR:O	1:C:251:ALA:HB3	2.20	0.41
1:C:356:ARG:NH1	2:D:697:LYS:HZ3	2.18	0.41
2:D:538:MET:O	2:D:539:ALA:C	2.58	0.41
1:E:276:ARG:HH11	1:E:276:ARG:HD2	1.69	0.41
1:E:370:LEU:CD2	1:E:380:ALA:CB	2.98	0.41
2:F:305:LEU:CB	2:F:306:PRO:HD3	2.31	0.41
2:H:52:LEU:O	2:H:53:GLU:C	2.58	0.41
2:H:667:ALA:O	2:H:668:TYR:C	2.57	0.41
2:B:70:LEU:HD23	2:B:70:LEU:HA	1.67	0.41
2:B:92:HIS:O	2:B:93:PHE:HB3	2.21	0.41
2:B:251:ARG:CB	2:B:252:PRO:HD2	2.49	0.41
2:B:464:LEU:HA	2:B:464:LEU:HD23	1.80	0.41
2:B:620:LEU:HD12	2:B:620:LEU:HA	1.77	0.41
2:B:767:LEU:HD12	2:B:767:LEU:HA	1.80	0.41
1:C:434:TYR:O	1:C:435:ARG:C	2.55	0.41
2:D:144:VAL:HG11	2:D:312:MET:CE	2.50	0.41
2:D:202:ILE:HD13	2:D:236:ASN:HD22	1.85	0.41
1:E:381:ARG:HA	1:E:398:GLU:OE1	2.20	0.41
2:F:96:GLN:HA	2:F:97:PRO:HD3	1.84	0.41
2:F:258:ASP:O	2:F:259:ARG:C	2.53	0.41
1:G:133:LEU:HA	1:G:139:TYR:OH	2.20	0.41
2:H:75:ASP:OD1	2:H:75:ASP:C	2.57	0.41
2:H:81:SER:HA	2:H:82:PRO:HD3	1.72	0.41
1:A:259:PRO:O	1:A:260:HIS:CG	2.73	0.41
1:A:364:VAL:HG23	1:A:435:ARG:HG2	2.02	0.41
2:B:35:LEU:HD23	2:B:35:LEU:N	2.32	0.41
2:B:98:ILE:O	2:B:98:ILE:HG22	2.17	0.41
2:B:227:GLY:O	2:B:228:PHE:C	2.59	0.41
1:C:81:ILE:HD12	1:C:81:ILE:HG23	1.82	0.41
1:C:368:LEU:N	1:C:368:LEU:CD1	2.77	0.41
1:C:446:TYR:O	1:C:447:VAL:C	2.53	0.41
2:D:367:ASP:OD1	2:D:367:ASP:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:538:MET:HG3	2:D:602:TYR:CD1	2.50	0.41
1:E:94:ALA:HB1	1:E:145:ALA:HB1	2.02	0.41
1:E:370:LEU:CD2	1:E:380:ALA:HA	2.50	0.41
2:F:697:LYS:HA	2:F:697:LYS:HD2	1.93	0.41
2:H:28:CYS:HB2	2:H:29:PRO:CD	2.49	0.41
2:H:138:ARG:HH11	2:H:138:ARG:HD2	1.73	0.41
2:H:152:GLU:O	2:H:153:THR:C	2.58	0.41
2:H:184:LEU:HA	2:H:185:PRO:HD2	1.85	0.41
2:H:311:ALA:O	2:H:312:MET:C	2.54	0.41
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.57	0.41
1:A:67:LEU:O	1:A:68:PRO:C	2.58	0.41
1:A:364:VAL:CG1	1:A:365:CYS:N	2.81	0.41
2:B:60:GLY:O	2:B:104:THR:N	2.53	0.41
2:B:110:ARG:O	2:B:111:ILE:C	2.57	0.41
2:B:450:LEU:HD12	2:B:628:ILE:HG13	2.01	0.41
2:B:730:GLU:N	2:B:731:PRO:CD	2.83	0.41
1:C:295:PRO:O	1:C:296:PRO:C	2.52	0.41
2:D:730:GLU:O	2:D:731:PRO:C	2.57	0.41
1:E:26:LEU:O	1:E:27:LEU:C	2.58	0.41
1:E:164:PHE:CG	1:E:165:THR:N	2.88	0.41
2:F:722:ILE:O	2:F:722:ILE:CG2	2.69	0.41
1:G:14:VAL:HG12	1:G:15:ARG:N	2.35	0.41
1:G:89:HIS:CE1	1:G:91:VAL:HB	2.55	0.41
1:G:164:PHE:CG	1:G:165:THR:N	2.88	0.41
1:G:301:MET:HE2	1:G:341:LEU:HD22	2.02	0.41
1:G:308:ARG:HG3	1:G:309:ARG:N	2.35	0.41
2:H:654:SER:OG	2:H:656:ASN:N	2.53	0.41
1:A:104:GLY:HA3	2:B:22:TYR:OH	2.20	0.41
1:A:298:LEU:HD23	1:A:298:LEU:HA	1.71	0.41
2:B:34:HIS:O	2:B:35:LEU:HD23	2.20	0.41
2:B:176:LEU:HD13	2:B:176:LEU:HA	1.86	0.41
1:C:153:PRO:HA	1:C:154:PRO:HD3	1.75	0.41
1:C:237:THR:CB	1:C:238:PRO:HD2	2.51	0.41
2:D:437:TRP:CZ3	2:D:446:ARG:HG3	2.56	0.41
2:D:495:LYS:C	2:D:496:MET:HE3	2.40	0.41
1:E:110:PHE:CE2	1:E:132:ASN:HB2	2.55	0.41
1:E:181:PHE:CD2	1:E:192:TRP:CD2	3.09	0.41
1:E:294:GLY:O	1:E:295:PRO:C	2.58	0.41
1:E:415:LEU:HB3	1:E:440:GLN:HG2	2.03	0.41
2:F:218:ARG:HH22	2:H:218:ARG:HH22	1.67	0.41
2:F:457:ILE:O	2:F:458:SER:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:536:ASN:O	2:F:539:ALA:N	2.53	0.41
2:F:563:ALA:C	2:F:565:ASP:H	2.23	0.41
1:G:353:LEU:HA	1:G:353:LEU:HD12	1.77	0.41
2:H:38:GLY:HA3	2:H:99:PHE:CZ	2.55	0.41
2:H:228:PHE:H	6:H:3003:MTE:HN5	1.69	0.41
2:H:239:ALA:O	2:H:240:ILE:C	2.55	0.41
2:H:446:ARG:HA	2:H:631:VAL:O	2.21	0.41
2:B:414:LEU:HA	2:B:414:LEU:HD23	1.66	0.41
1:C:89:HIS:ND1	1:C:90:PRO:HD2	2.36	0.41
2:D:184:LEU:HD23	2:D:252:PRO:HB3	2.03	0.41
2:D:221:MET:HE3	2:D:223:ARG:N	2.35	0.41
1:E:307:LEU:HD23	1:E:307:LEU:HA	1.74	0.41
1:E:345:ALA:N	1:E:346:PRO:HD3	2.35	0.41
1:E:408:GLU:CD	2:F:442:ARG:HH22	2.19	0.41
2:F:48:THR:O	2:F:48:THR:HG23	2.20	0.41
2:F:413:VAL:O	2:F:413:VAL:HG23	2.21	0.41
2:F:538:MET:O	2:F:541:LYS:HB3	2.21	0.41
1:G:133:LEU:HD13	2:H:698:ILE:HD11	2.02	0.41
1:G:219:LEU:HA	1:G:220:PRO:HD3	1.86	0.41
1:G:395:ALA:O	1:G:396:ALA:C	2.58	0.41
2:H:327:GLU:OE2	2:H:329:HIS:NE2	2.52	0.41
2:H:372:ARG:HG3	2:H:372:ARG:NH1	2.35	0.41
2:H:641:ARG:HH21	2:H:706:ARG:CZ	2.33	0.41
2:B:40:SER:HB2	2:B:91:VAL:CG1	2.44	0.41
2:B:251:ARG:CB	2:B:252:PRO:CD	2.99	0.41
2:B:582:PHE:O	2:B:583:ALA:C	2.58	0.41
7:B:3004:MOS:S	8:B:4000:141:N8	2.93	0.41
1:C:370:LEU:HD22	1:C:380:ALA:HA	2.01	0.41
2:D:28:CYS:HB2	2:D:29:PRO:HD2	2.01	0.41
2:D:79:ALA:HB1	2:D:80:PRO:HD2	2.03	0.41
2:D:414:LEU:HA	2:D:414:LEU:HD23	1.76	0.41
1:E:5:PHE:CD2	1:E:70:ILE:HD12	2.56	0.41
1:E:110:PHE:HB3	1:E:114:MET:HE2	2.02	0.41
1:E:301:MET:HE3	1:E:341:LEU:HB3	1.91	0.41
1:E:350:CYS:C	1:E:351:TYR:CD2	2.94	0.41
2:F:53:GLU:N	2:F:54:PRO:CD	2.83	0.41
2:F:547:LEU:C	2:F:549:GLY:N	2.73	0.41
2:F:740:PHE:O	2:F:743:LEU:N	2.53	0.41
1:G:374:GLY:C	1:G:376:LYS:H	2.24	0.41
2:H:86:LEU:HD23	2:H:86:LEU:HA	1.80	0.41
2:H:93:PHE:CD1	2:H:93:PHE:C	2.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:531:SER:O	2:H:532:GLY:C	2.58	0.41
2:H:608:SER:O	2:H:609:TRP:HB3	2.19	0.41
2:H:631:VAL:CG1	2:H:642:ILE:HA	2.25	0.41
2:H:701:PHE:C	2:H:701:PHE:CD2	2.93	0.41
1:A:47:CYS:O	1:A:49:VAL:HG13	2.20	0.41
1:A:271:ALA:CA	1:A:359:GLN:HE22	2.33	0.41
1:A:356:ARG:NH2	1:A:359:GLN:O	2.52	0.41
1:A:401:LEU:HD11	1:A:411:ILE:HD13	2.02	0.41
1:A:423:THR:HA	1:A:424:PRO:HD3	1.61	0.41
2:B:320:PHE:CG	2:B:401:GLN:NE2	2.89	0.41
2:B:715:GLN:HA	2:B:716:PRO:HD3	1.82	0.41
2:B:731:PRO:N	2:B:732:PRO:CD	2.83	0.41
1:C:301:MET:HB3	1:C:348:LEU:HD22	2.02	0.41
1:E:322:PHE:CB	1:E:390:VAL:HG23	2.51	0.41
2:F:215:HIS:CG	2:H:478:SER:HB2	2.56	0.41
2:F:263:MET:HE3	2:F:692:ALA:HA	2.03	0.41
2:F:504:LEU:HD23	2:F:504:LEU:HA	1.92	0.41
2:F:554:PHE:O	2:F:555:VAL:C	2.53	0.41
1:G:249:ILE:O	1:G:250:ALA:C	2.59	0.41
2:H:280:ALA:CA	2:H:287:LEU:HD12	2.50	0.41
1:A:59:ALA:C	1:A:60:VAL:HG13	2.38	0.41
1:A:95:MET:HG3	1:A:111:ILE:HD11	2.03	0.41
1:A:331:ARG:HG2	1:A:334:GLU:OE2	2.21	0.41
2:B:61:VAL:HA	2:B:103:ALA:HB2	2.03	0.41
2:B:302:ASP:OD1	2:B:303:LEU:N	2.50	0.41
2:B:344:PHE:CD2	8:B:4000:141:C2	3.04	0.41
2:B:367:ASP:HA	2:B:368:PRO:HD3	1.96	0.41
1:C:134:CYS:SG	1:C:137:THR:HG23	2.61	0.41
1:C:370:LEU:HD22	1:C:380:ALA:CB	2.51	0.41
2:F:28:CYS:HB2	2:F:29:PRO:HD2	2.03	0.41
2:F:109:ALA:O	2:F:110:ARG:C	2.57	0.41
2:F:201:GLU:O	2:F:204:HIS:N	2.54	0.41
2:F:234:GLN:H	2:F:234:GLN:HG2	1.58	0.41
2:F:247:ARG:HH11	2:F:247:ARG:CG	2.20	0.41
2:F:479:VAL:HG12	2:F:480:ALA:N	2.36	0.41
2:F:528:ALA:HA	6:F:3003:MTE:S2'	2.60	0.41
1:G:93:GLN:O	1:G:97:ASP:N	2.37	0.41
1:G:359:GLN:O	1:G:359:GLN:CG	2.58	0.41
2:H:537:GLY:O	2:H:538:MET:C	2.59	0.41
2:H:538:MET:O	2:H:539:ALA:C	2.59	0.41
2:H:734:LEU:HD12	2:H:734:LEU:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:MET:HB3	1:A:348:LEU:CD2	2.51	0.41
1:C:61:ASN:H	1:C:61:ASN:ND2	2.19	0.41
1:C:219:LEU:HA	1:C:220:PRO:HD3	1.90	0.41
4:E:3005:FAD:H9	4:E:3005:FAD:H1'2	1.61	0.41
2:F:512:ARG:HD2	2:H:216:ASP:OD1	2.20	0.41
1:G:16:ILE:HD13	1:G:68:PRO:HG3	2.03	0.41
1:G:65:MET:HE2	1:G:65:MET:HB2	1.96	0.41
1:G:68:PRO:HG2	1:G:224:PHE:CE1	2.55	0.41
1:G:91:VAL:CG2	1:G:114:MET:HB3	2.50	0.41
1:G:91:VAL:HG21	1:G:114:MET:HB3	2.03	0.41
2:H:40:SER:HB2	2:H:91:VAL:HG11	2.03	0.41
2:H:84:PRO:HB2	2:H:86:LEU:O	2.21	0.41
2:H:166:PHE:CE1	2:H:355:ARG:HG3	2.56	0.41
2:H:171:GLN:O	2:H:268:LYS:HB3	2.21	0.41
2:H:214:PHE:O	2:H:215:HIS:C	2.58	0.41
2:H:602:TYR:CG	2:H:603:ALA:N	2.89	0.41
1:A:53:ASP:OD1	1:A:54:ALA:N	2.54	0.40
1:A:140:ALA:HB3	1:A:141:PRO:CD	2.51	0.40
1:A:152:GLU:HA	1:A:153:PRO:HD2	1.67	0.40
1:C:299:ILE:O	1:C:300:ALA:C	2.57	0.40
2:D:325:ARG:C	2:D:326:ILE:CG1	2.86	0.40
2:D:350:ALA:O	2:D:351:LEU:C	2.55	0.40
2:D:551:LEU:HA	2:D:551:LEU:HD23	1.73	0.40
2:D:596:LEU:HD23	2:D:596:LEU:HA	1.67	0.40
2:D:647:ILE:HG22	2:D:648:LEU:N	2.35	0.40
1:E:351:TYR:HB2	1:E:442:MET:SD	2.62	0.40
2:F:184:LEU:O	2:F:185:PRO:C	2.55	0.40
2:F:367:ASP:OD1	2:F:367:ASP:C	2.58	0.40
2:F:517:ASP:OD2	2:F:517:ASP:C	2.60	0.40
1:G:40:ASN:HD22	1:G:40:ASN:HA	1.42	0.40
1:G:102:GLN:NE2	1:G:137:THR:HA	2.36	0.40
2:H:155:LEU:O	2:H:156:ALA:C	2.59	0.40
2:H:271:ASP:OD2	2:H:296:ARG:NH1	2.54	0.40
1:A:299:ILE:O	1:A:300:ALA:C	2.58	0.40
1:A:300:ALA:HB2	1:A:367:CYS:HB3	2.02	0.40
2:B:96:GLN:HA	2:B:97:PRO:HD3	1.78	0.40
2:B:372:ARG:O	2:B:375:ASN:N	2.53	0.40
2:B:721:THR:O	2:B:722:ILE:C	2.59	0.40
1:C:444:LEU:HD23	1:C:444:LEU:HA	1.90	0.40
1:E:115:ALA:O	1:E:118:HIS:N	2.53	0.40
1:E:203:ALA:HB3	1:E:204:GLY:H	1.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:THR:CG2	1:E:239:ASP:OD2	2.69	0.40
1:E:253:ARG:NH2	1:E:268:ARG:HG3	2.36	0.40
1:E:296:PRO:O	1:E:297:ALA:O	2.40	0.40
1:E:358:ASP:OD2	2:F:702:SER:CB	2.65	0.40
2:F:759:ALA:HA	2:F:760:PRO:C	2.41	0.40
1:G:91:VAL:HG12	1:G:92:GLN:N	2.35	0.40
1:G:356:ARG:HH21	1:G:359:GLN:HB3	1.86	0.40
1:A:16:ILE:CD1	1:A:68:PRO:HG3	2.52	0.40
1:A:281:ILE:CG2	1:A:282:GLY:N	2.84	0.40
1:C:124:ASP:OD1	1:C:128:LEU:HD22	2.21	0.40
2:D:696:TYR:C	2:D:697:LYS:HD2	2.41	0.40
2:D:720:GLU:HG2	2:D:724:ARG:HH21	1.86	0.40
1:E:216:LEU:HD23	1:E:216:LEU:HA	1.92	0.40
1:E:228:CYS:O	1:E:230:ASP:N	2.54	0.40
2:F:238:LEU:HD23	2:F:255:MET:HG2	2.03	0.40
2:F:246:ALA:O	2:F:247:ARG:C	2.56	0.40
1:G:345:ALA:O	1:G:346:PRO:C	2.58	0.40
2:H:310:ARG:HD2	2:H:344:PHE:HB3	2.02	0.40
2:H:770:VAL:O	2:H:773:ALA:HB3	2.21	0.40
1:A:308:ARG:HG3	1:A:309:ARG:N	2.37	0.40
1:A:359:GLN:O	1:A:359:GLN:CG	2.59	0.40
1:A:377:ILE:HD11	1:A:406:PHE:HD1	1.87	0.40
2:B:263:MET:HE3	2:B:692:ALA:HA	2.04	0.40
2:B:520:LYS:NZ	2:D:218:ARG:HH12	2.19	0.40
2:B:720:GLU:HA	2:B:724:ARG:HH21	1.85	0.40
1:C:237:THR:OG1	1:C:238:PRO:HD2	2.22	0.40
2:D:92:HIS:CD2	2:D:92:HIS:N	2.89	0.40
2:D:165:CYS:SG	2:D:166:PHE:N	2.92	0.40
2:D:173:HIS:CD2	2:D:341:PHE:CD1	3.09	0.40
1:E:129:LEU:HA	1:E:129:LEU:HD23	1.83	0.40
2:F:179:GLN:O	2:F:180:ALA:HB2	2.21	0.40
2:F:371:LEU:HD12	2:F:371:LEU:HA	1.62	0.40
2:F:407:GLN:CD	2:F:617:ARG:HG2	2.41	0.40
1:G:83:ALA:HA	1:G:84:PRO:HD3	1.96	0.40
1:G:95:MET:CG	1:G:114:MET:HE3	2.51	0.40
1:G:222:VAL:CG1	1:G:223:ALA:N	2.83	0.40
1:G:318:LEU:C	1:G:320:ASP:N	2.75	0.40
1:G:325:TYR:CZ	1:G:326:ARG:HG2	2.56	0.40
1:A:37:GLU:CD	2:B:256:ARG:NH2	2.75	0.40
1:A:318:LEU:O	1:A:319:GLU:C	2.57	0.40
2:B:108:ALA:O	2:B:109:ALA:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:HIS:ND1	2:B:513:ILE:CD1	2.85	0.40
1:C:81:ILE:HD13	1:C:81:ILE:HA	1.94	0.40
7:D:3004:MOS:O2	8:D:4000:141:N8	2.55	0.40
1:E:193:TYR:HE2	1:E:334:GLU:O	2.04	0.40
1:E:266:LEU:HA	1:E:266:LEU:HD12	1.58	0.40
1:E:273:GLU:O	1:E:274:GLN:C	2.57	0.40
1:E:309:ARG:HH11	1:E:309:ARG:HD2	1.73	0.40
2:F:3:VAL:HG21	2:F:723:PHE:CE1	2.56	0.40
2:F:112:ALA:O	2:F:113:ALA:C	2.57	0.40
2:F:342:ARG:NH2	2:F:667:ALA:HB2	2.37	0.40
1:G:56:GLY:HA3	1:G:120:ARG:HH21	1.86	0.40
2:H:360:LEU:HA	2:H:360:LEU:HD12	1.79	0.40
2:H:653:ALA:O	2:H:654:SER:C	2.57	0.40
2:H:672:ALA:C	2:H:674:TRP:N	2.74	0.40
2:H:743:LEU:HA	2:H:743:LEU:HD12	1.13	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:ARG:CD	1:G:152:GLU:OE2[1_655]	2.08	0.12

## 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	446/462 (96%)	385 (86%)	53 (12%)	8 (2%)	8 37
1	C	446/462 (96%)	408 (92%)	31 (7%)	7 (2%)	9 40
1	E	446/462 (96%)	370 (83%)	63 (14%)	13 (3%)	4 24
1	G	446/462 (96%)	375 (84%)	58 (13%)	13 (3%)	4 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	756/777 (97%)	696 (92%)	47 (6%)	13 (2%)	9	39
2	D	756/777 (97%)	697 (92%)	46 (6%)	13 (2%)	9	39
2	F	756/777 (97%)	688 (91%)	57 (8%)	11 (2%)	10	42
2	H	756/777 (97%)	678 (90%)	67 (9%)	11 (2%)	10	42
All	All	4808/4956 (97%)	4297 (89%)	422 (9%)	89 (2%)	8	36

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ALA
2	B	281	ASP
2	B	399	LYS
2	B	458	SER
2	B	561	CYS
1	C	180	ALA
1	C	315	ARG
1	C	374	GLY
2	D	281	ASP
2	D	399	LYS
2	D	458	SER
1	E	374	GLY
2	F	399	LYS
2	F	458	SER
1	G	119	ASP
1	G	180	ALA
1	G	374	GLY
2	H	399	LYS
2	H	458	SER
2	H	560	GLY
2	H	561	CYS
2	H	761	ALA
1	A	163	ALA
1	A	315	ARG
1	A	374	GLY
2	B	187	GLU
2	B	227	GLY
2	B	342	ARG
2	B	560	GLY
2	B	761	ALA
1	C	163	ALA
1	C	375	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	187	GLU
2	D	342	ARG
2	D	560	GLY
1	E	267	LEU
1	E	297	ALA
1	E	395	ALA
1	E	400	ALA
2	F	187	GLU
2	F	227	GLY
2	F	342	ARG
2	F	560	GLY
1	G	163	ALA
1	G	315	ARG
1	G	319	GLU
1	G	400	ALA
2	H	187	GLU
2	H	227	GLY
2	H	342	ARG
2	B	234	GLN
2	D	315	ALA
2	F	561	CYS
1	G	437	ASN
2	H	530	SER
1	A	139	TYR
2	B	692	ALA
2	B	722	ILE
2	D	227	GLY
2	D	234	GLN
2	D	462	THR
2	D	561	CYS
1	E	266	LEU
1	E	315	ARG
1	E	399	ALA
1	E	455	VAL
2	F	611	ARG
1	G	199	ALA
2	H	692	ALA
1	A	221	GLU
1	A	375	SER
1	A	399	ALA
1	C	160	ALA
2	D	72	HIS

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Mol	Chain	Res	Type
2	D	723	PHE
1	E	33	THR
2	F	692	ALA
1	G	375	SER
2	B	731	PRO
1	E	163	ALA
2	F	701	PHE
2	H	141	GLY
1	C	455	VAL
1	G	154	PRO
2	F	722	ILE
1	G	68	PRO
1	G	455	VAL
1	E	68	PRO
1	E	364	VAL

### 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	339/347 (98%)	294 (87%)	45 (13%)	4	17
1	C	339/347 (98%)	295 (87%)	44 (13%)	4	19
1	E	339/347 (98%)	289 (85%)	50 (15%)	3	15
1	G	339/347 (98%)	291 (86%)	48 (14%)	3	16
2	B	571/584 (98%)	499 (87%)	72 (13%)	4	20
2	D	571/584 (98%)	493 (86%)	78 (14%)	3	17
2	F	571/584 (98%)	495 (87%)	76 (13%)	4	17
2	H	571/584 (98%)	500 (88%)	71 (12%)	4	20
All	All	3640/3724 (98%)	3156 (87%)	484 (13%)	4	17

All (484) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	THR
1	A	12	ARG
1	A	15	ARG
1	A	20	THR
1	A	25	GLU
1	A	26	LEU
1	A	33	THR
1	A	40	ASN
1	A	43	ASP
1	A	61	ASN
1	A	68	PRO
1	A	85	ASP
1	A	87	ARG
1	A	96	ILE
1	A	128	LEU
1	A	143	LEU
1	A	156	ASP
1	A	165	THR
1	A	198	GLU
1	A	209	SER
1	A	231	LEU
1	A	237	THR
1	A	257	GLU
1	A	281	ILE
1	A	309	ARG
1	A	316	MET
1	A	326	ARG
1	A	348	LEU
1	A	349	ARG
1	A	359	GLN
1	A	362	SER
1	A	371	THR
1	A	375	SER
1	A	379	THR
1	A	390	VAL
1	A	393	ARG
1	A	401	LEU
1	A	405	ASP
1	A	423	THR
1	A	425	LEU
1	A	428	MET
1	A	435	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	451	SER
1	A	457	VAL
2	B	2	SER
2	B	10	ASP
2	B	16	VAL
2	B	23	LEU
2	B	40	SER
2	B	48	THR
2	B	53	GLU
2	B	66	THR
2	B	77	SER
2	B	90	GLU
2	B	105	SER
2	B	129	LEU
2	B	130	ASP
2	B	133	LEU
2	B	148	ARG
2	B	151	VAL
2	B	161	LEU
2	B	165	CYS
2	B	175	TYR
2	B	190	VAL
2	B	196	SER
2	B	200	SER
2	B	204	HIS
2	B	215	HIS
2	B	221	MET
2	B	222	ARG
2	B	234	GLN
2	B	237	HIS
2	B	247	ARG
2	B	256	ARG
2	B	268	LYS
2	B	296	ARG
2	B	313	LEU
2	B	330	ARG
2	B	341	PHE
2	B	355	ARG
2	B	359	HIS
2	B	364	MET
2	B	381	GLU
2	B	398	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	399	LYS
2	B	423	LYS
2	B	424	SER
2	B	426	ASN
2	B	431	ARG
2	B	442	ARG
2	B	450	LEU
2	B	452	PRO
2	B	458	SER
2	B	461	LEU
2	B	481	LEU
2	B	492	LEU
2	B	512	ARG
2	B	513	ILE
2	B	530	SER
2	B	561	CYS
2	B	574	GLN
2	B	576	SER
2	B	609	TRP
2	B	611	ARG
2	B	617	ARG
2	B	618	PRO
2	B	632	VAL
2	B	641	ARG
2	B	650	ASP
2	B	697	LYS
2	B	704	ARG
2	B	708	PHE
2	B	724	ARG
2	B	741	LEU
2	B	743	LEU
2	B	744	HIS
1	C	11	THR
1	C	12	ARG
1	C	15	ARG
1	C	20	THR
1	C	25	GLU
1	C	26	LEU
1	C	33	THR
1	C	36	LYS
1	C	40	ASN
1	C	41	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	58	ARG
1	C	61	ASN
1	C	65	MET
1	C	87	ARG
1	C	113	SER
1	C	128	LEU
1	C	134	CYS
1	C	143	LEU
1	C	165	THR
1	C	198	GLU
1	C	209	SER
1	C	221	GLU
1	C	231	LEU
1	C	237	THR
1	C	239	ASP
1	C	257	GLU
1	C	291	ILE
1	C	309	ARG
1	C	316	MET
1	C	331	ARG
1	C	344	SER
1	C	349	ARG
1	C	354	SER
1	C	355	LYS
1	C	375	SER
1	C	376	LYS
1	C	379	THR
1	C	381	ARG
1	C	392	LYS
1	C	393	ARG
1	C	425	LEU
1	C	447	VAL
1	C	451	SER
1	C	457	VAL
2	D	2	SER
2	D	10	ASP
2	D	16	VAL
2	D	39	LEU
2	D	48	THR
2	D	66	THR
2	D	129	LEU
2	D	130	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	148	ARG
2	D	151	VAL
2	D	165	CYS
2	D	166	PHE
2	D	175	TYR
2	D	190	VAL
2	D	196	SER
2	D	215	HIS
2	D	221	MET
2	D	222	ARG
2	D	234	GLN
2	D	237	HIS
2	D	247	ARG
2	D	251	ARG
2	D	256	ARG
2	D	268	LYS
2	D	281	ASP
2	D	296	ARG
2	D	313	LEU
2	D	330	ARG
2	D	341	PHE
2	D	355	ARG
2	D	359	HIS
2	D	381	GLU
2	D	398	LYS
2	D	399	LYS
2	D	407	GLN
2	D	416	GLU
2	D	426	ASN
2	D	429	THR
2	D	431	ARG
2	D	441	ASN
2	D	442	ARG
2	D	450	LEU
2	D	451	SER
2	D	452	PRO
2	D	454	LYS
2	D	458	SER
2	D	461	LEU
2	D	465	ASN
2	D	466	GLN
2	D	478	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	496	MET
2	D	498	GLN
2	D	512	ARG
2	D	520	LYS
2	D	541	LYS
2	D	547	LEU
2	D	558	ARG
2	D	574	GLN
2	D	576	SER
2	D	608	SER
2	D	610	ASP
2	D	611	ARG
2	D	617	ARG
2	D	618	PRO
2	D	634	ASP
2	D	641	ARG
2	D	690	THR
2	D	694	SER
2	D	697	LYS
2	D	702	SER
2	D	704	ARG
2	D	706	ARG
2	D	708	PHE
2	D	718	ARG
2	D	724	ARG
2	D	741	LEU
2	D	743	LEU
2	D	744	HIS
1	E	1	MET
1	E	11	THR
1	E	12	ARG
1	E	20	THR
1	E	25	GLU
1	E	26	LEU
1	E	33	THR
1	E	40	ASN
1	E	43	ASP
1	E	58	ARG
1	E	61	ASN
1	E	66	MET
1	E	76	ARG
1	E	79	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	93	GLN
1	E	101	SER
1	E	113	SER
1	E	121	ASP
1	E	128	LEU
1	E	143	LEU
1	E	156	ASP
1	E	159	GLN
1	E	165	THR
1	E	179	PRO
1	E	198	GLU
1	E	209	SER
1	E	221	GLU
1	E	231	LEU
1	E	237	THR
1	E	239	ASP
1	E	257	GLU
1	E	291	ILE
1	E	309	ARG
1	E	313	ARG
1	E	316	MET
1	E	337	GLU
1	E	339	VAL
1	E	341	LEU
1	E	344	SER
1	E	349	ARG
1	E	354	SER
1	E	355	LYS
1	E	359	GLN
1	E	375	SER
1	E	408	GLU
1	E	425	LEU
1	E	435	ARG
1	E	447	VAL
1	E	451	SER
1	E	455	VAL
2	F	2	SER
2	F	10	ASP
2	F	16	VAL
2	F	23	LEU
2	F	39	LEU
2	F	40	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	48	THR
2	F	53	GLU
2	F	66	THR
2	F	105	SER
2	F	129	LEU
2	F	130	ASP
2	F	148	ARG
2	F	151	VAL
2	F	175	TYR
2	F	190	VAL
2	F	196	SER
2	F	215	HIS
2	F	221	MET
2	F	222	ARG
2	F	234	GLN
2	F	237	HIS
2	F	247	ARG
2	F	251	ARG
2	F	256	ARG
2	F	260	ASP
2	F	268	LYS
2	F	296	ARG
2	F	313	LEU
2	F	319	TYR
2	F	330	ARG
2	F	341	PHE
2	F	355	ARG
2	F	359	HIS
2	F	381	GLU
2	F	398	LYS
2	F	399	LYS
2	F	407	GLN
2	F	416	GLU
2	F	426	ASN
2	F	429	THR
2	F	431	ARG
2	F	442	ARG
2	F	450	LEU
2	F	451	SER
2	F	452	PRO
2	F	454	LYS
2	F	461	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	465	ASN
2	F	488	MET
2	F	506	ILE
2	F	512	ARG
2	F	541	LYS
2	F	566	VAL
2	F	574	GLN
2	F	578	LYS
2	F	579	SER
2	F	580	TRP
2	F	609	TRP
2	F	611	ARG
2	F	617	ARG
2	F	618	PRO
2	F	624	TYR
2	F	628	ILE
2	F	632	VAL
2	F	697	LYS
2	F	702	SER
2	F	703	ASP
2	F	704	ARG
2	F	706	ARG
2	F	708	PHE
2	F	718	ARG
2	F	724	ARG
2	F	741	LEU
2	F	743	LEU
2	F	744	HIS
1	G	12	ARG
1	G	20	THR
1	G	25	GLU
1	G	26	LEU
1	G	33	THR
1	G	35	THR
1	G	40	ASN
1	G	58	ARG
1	G	61	ASN
1	G	65	MET
1	G	66	MET
1	G	85	ASP
1	G	87	ARG
1	G	90	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	96	ILE
1	G	128	LEU
1	G	179	PRO
1	G	198	GLU
1	G	209	SER
1	G	221	GLU
1	G	231	LEU
1	G	237	THR
1	G	257	GLU
1	G	281	ILE
1	G	291	ILE
1	G	295	PRO
1	G	309	ARG
1	G	313	ARG
1	G	316	MET
1	G	327	LYS
1	G	331	ARG
1	G	344	SER
1	G	349	ARG
1	G	361	ILE
1	G	362	SER
1	G	371	THR
1	G	375	SER
1	G	376	LYS
1	G	379	THR
1	G	381	ARG
1	G	393	ARG
1	G	408	GLU
1	G	409	ASP
1	G	425	LEU
1	G	428	MET
1	G	435	ARG
1	G	455	VAL
1	G	457	VAL
2	H	2	SER
2	H	10	ASP
2	H	16	VAL
2	H	23	LEU
2	H	39	LEU
2	H	40	SER
2	H	48	THR
2	H	53	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	77	SER
2	H	105	SER
2	H	129	LEU
2	H	130	ASP
2	H	148	ARG
2	H	151	VAL
2	H	165	CYS
2	H	175	TYR
2	H	190	VAL
2	H	196	SER
2	H	215	HIS
2	H	221	MET
2	H	222	ARG
2	H	234	GLN
2	H	237	HIS
2	H	247	ARG
2	H	256	ARG
2	H	260	ASP
2	H	268	LYS
2	H	296	ARG
2	H	313	LEU
2	H	319	TYR
2	H	330	ARG
2	H	341	PHE
2	H	355	ARG
2	H	357	ILE
2	H	359	HIS
2	H	364	MET
2	H	366	ARG
2	H	381	GLU
2	H	398	LYS
2	H	399	LYS
2	H	416	GLU
2	H	423	LYS
2	H	424	SER
2	H	426	ASN
2	H	429	THR
2	H	431	ARG
2	H	442	ARG
2	H	450	LEU
2	H	458	SER
2	H	461	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	465	ASN
2	H	512	ARG
2	H	517	ASP
2	H	530	SER
2	H	561	CYS
2	H	574	GLN
2	H	611	ARG
2	H	617	ARG
2	H	618	PRO
2	H	632	VAL
2	H	661	ILE
2	H	697	LYS
2	H	699	PRO
2	H	704	ARG
2	H	708	PHE
2	H	718	ARG
2	H	724	ARG
2	H	741	LEU
2	H	743	LEU
2	H	744	HIS
2	H	760	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	40	ASN
1	A	61	ASN
1	A	196	HIS
1	A	328	GLN
1	A	359	GLN
2	B	34	HIS
2	B	236	ASN
2	B	293	HIS
2	B	359	HIS
2	B	426	ASN
2	B	744	HIS
1	C	40	ASN
1	C	61	ASN
1	C	196	HIS
2	D	204	HIS
2	D	236	ASN
2	D	359	HIS

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Mol	Chain	Res	Type
2	D	426	ASN
2	D	498	GLN
2	D	691	HIS
2	D	744	HIS
1	E	40	ASN
1	E	61	ASN
1	E	93	GLN
1	E	118	HIS
1	E	196	HIS
1	E	359	GLN
2	F	204	HIS
2	F	236	ASN
2	F	293	HIS
2	F	359	HIS
2	F	426	ASN
2	F	466	GLN
2	F	691	HIS
2	F	744	HIS
1	G	40	ASN
1	G	61	ASN
1	G	196	HIS
1	G	359	GLN
2	H	34	HIS
2	H	236	ASN
2	H	293	HIS
2	H	359	HIS
2	H	426	ASN
2	H	684	HIS
2	H	744	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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MOS	B	3004	6,8	0,2,3	-	-	-		
8	141	H	4000	7	10,12,12	3.20	4 (40%)	10,17,17	2.89	6 (60%)
3	FES	E	3002	1	0,4,4	-	-	-		
8	141	F	4000	7	10,12,12	3.68	5 (50%)	10,17,17	2.60	3 (30%)
6	MTE	H	3003	7	21,26,26	5.76	10 (47%)	21,40,40	5.99	11 (52%)
6	MTE	F	3003	7	21,26,26	5.22	13 (61%)	21,40,40	6.56	11 (52%)
3	FES	C	3001	1	0,4,4	-	-	-		
4	FAD	G	3005	-	53,58,58	1.51	6 (11%)	68,89,89	2.35	28 (41%)
3	FES	A	3001	1	0,4,4	-	-	-		
4	FAD	A	3005	-	53,58,58	1.69	8 (15%)	68,89,89	2.53	29 (42%)
6	MTE	D	3003	7	21,26,26	5.19	11 (52%)	21,40,40	7.33	10 (47%)
3	FES	E	3001	1	0,4,4	-	-	-		
3	FES	G	3001	1	0,4,4	-	-	-		
6	MTE	B	3003	7	21,26,26	4.92	12 (57%)	21,40,40	5.80	11 (52%)
8	141	D	4000	7	10,12,12	3.38	4 (40%)	10,17,17	2.15	2 (20%)
4	FAD	E	3005	-	53,58,58	1.64	10 (18%)	68,89,89	2.62	32 (47%)
3	FES	C	3002	1	0,4,4	-	-	-		
3	FES	A	3002	1	0,4,4	-	-	-		
7	MOS	D	3004	6,8	0,2,3	-	-	-		
7	MOS	H	3004	6,8	0,2,3	-	-	-		
3	FES	G	3002	1	0,4,4	-	-	-		
4	FAD	C	3005	-	53,58,58	1.85	14 (26%)	68,89,89	2.74	32 (47%)
8	141	B	4000	7	10,12,12	3.21	5 (50%)	10,17,17	2.76	3 (30%)
7	MOS	F	3004	6,8	0,2,3	-	-	-		

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
8	141	H	4000	7	-	-	0/2/2/2
3	FES	E	3002	1	-	-	0/1/1/1
8	141	F	4000	7	-	-	0/2/2/2
6	MTE	H	3003	7	-	2/6/34/34	0/3/3/3
6	MTE	F	3003	7	-	0/6/34/34	0/3/3/3
3	FES	C	3001	1	-	-	0/1/1/1
3	FES	A	3001	1	-	-	0/1/1/1
4	FAD	G	3005	-	-	17/30/50/50	0/6/6/6
4	FAD	A	3005	-	-	16/30/50/50	0/6/6/6
6	MTE	D	3003	7	-	5/6/34/34	0/3/3/3
3	FES	E	3001	1	-	-	0/1/1/1
3	FES	G	3001	1	-	-	0/1/1/1
6	MTE	B	3003	7	-	0/6/34/34	0/3/3/3
8	141	D	4000	7	-	-	0/2/2/2
4	FAD	E	3005	-	-	14/30/50/50	0/6/6/6
3	FES	C	3002	1	-	-	0/1/1/1
3	FES	A	3002	1	-	-	0/1/1/1
3	FES	G	3002	1	-	-	0/1/1/1
4	FAD	C	3005	-	-	15/30/50/50	0/6/6/6
8	141	B	4000	7	-	-	0/2/2/2

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	3003	MTE	C7-C6	15.71	1.66	1.53
6	B	3003	MTE	C7-C6	13.70	1.64	1.53
6	F	3003	MTE	C7-C6	12.95	1.63	1.53
6	H	3003	MTE	C6-N5	10.76	1.60	1.45
6	F	3003	MTE	C6-N5	10.69	1.60	1.45
6	H	3003	MTE	C9-C10	10.62	1.61	1.41
6	D	3003	MTE	C9-C10	10.43	1.61	1.41
6	D	3003	MTE	C7-C6	10.25	1.61	1.53
6	D	3003	MTE	C6-N5	9.98	1.59	1.45
8	F	4000	141	O6-C6	9.12	1.40	1.23
6	F	3003	MTE	C9-C10	8.79	1.58	1.41
6	B	3003	MTE	C9-C10	8.44	1.57	1.41
8	H	4000	141	O6-C6	8.20	1.39	1.23
8	D	4000	141	O6-C6	8.12	1.39	1.23
6	B	3003	MTE	C6-N5	7.97	1.56	1.45
8	B	4000	141	O6-C6	7.66	1.38	1.23
6	H	3003	MTE	P-O4'	-7.28	1.36	1.60
6	D	3003	MTE	C4'-C3'	-7.05	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3003	MTE	P-O4'	-6.91	1.38	1.60
6	H	3003	MTE	C4'-C3'	-6.79	1.42	1.52
6	B	3003	MTE	C4'-C3'	-6.66	1.43	1.52
6	D	3003	MTE	C9-N5	6.32	1.51	1.38
6	B	3003	MTE	P-O4'	-6.24	1.40	1.60
6	H	3003	MTE	C9-N5	6.13	1.50	1.38
6	F	3003	MTE	C4'-C3'	-6.11	1.43	1.52
6	F	3003	MTE	P-O4'	-6.06	1.40	1.60
6	D	3003	MTE	P-O3P	-5.82	1.32	1.54
6	F	3003	MTE	C9-N5	5.78	1.49	1.38
6	D	3003	MTE	C9-C4	5.73	1.49	1.41
6	B	3003	MTE	P-O3P	-5.60	1.33	1.54
6	H	3003	MTE	P-O3P	-5.54	1.33	1.54
6	F	3003	MTE	P-O3P	-5.44	1.33	1.54
4	A	3005	FAD	C4X-N5	5.21	1.40	1.30
6	B	3003	MTE	C9-N5	5.11	1.48	1.38
6	F	3003	MTE	C9-C4	5.06	1.48	1.41
6	H	3003	MTE	C9-C4	5.01	1.48	1.41
4	C	3005	FAD	C2B-C1B	-5.00	1.46	1.53
4	A	3005	FAD	C2B-C1B	-4.68	1.46	1.53
4	C	3005	FAD	C2'-C3'	-4.66	1.44	1.53
8	F	4000	141	C7-C5	4.59	1.46	1.38
8	B	4000	141	C5-C4	-4.57	1.37	1.46
4	G	3005	FAD	C4X-N5	4.54	1.39	1.30
8	D	4000	141	C5-C4	-4.52	1.37	1.46
4	C	3005	FAD	C4X-N5	4.12	1.38	1.30
4	C	3005	FAD	C9A-C5X	-4.11	1.34	1.41
4	E	3005	FAD	C2A-N3A	4.10	1.38	1.32
6	D	3003	MTE	O4-C4	3.97	1.34	1.24
4	G	3005	FAD	C2B-C1B	-3.91	1.47	1.53
4	E	3005	FAD	C4X-N5	3.72	1.38	1.30
4	A	3005	FAD	O4B-C4B	-3.70	1.36	1.45
6	F	3003	MTE	O4-C4	3.68	1.33	1.24
6	F	3003	MTE	C4-N3	3.65	1.39	1.33
6	B	3003	MTE	C9-C4	3.60	1.46	1.41
8	D	4000	141	C7-C5	3.52	1.44	1.38
4	A	3005	FAD	C2A-N3A	3.45	1.37	1.32
8	F	4000	141	C4-N3	3.44	1.39	1.32
8	H	4000	141	C5-C4	-3.23	1.39	1.46
4	E	3005	FAD	C2'-C3'	-3.22	1.47	1.53
4	E	3005	FAD	C10-N1	3.14	1.39	1.33
6	D	3003	MTE	C2-N1	3.14	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	3003	MTE	O4-C4	3.13	1.32	1.24
4	C	3005	FAD	O2B-C2B	-3.02	1.35	1.43
4	E	3005	FAD	C2A-N1A	2.99	1.39	1.33
4	E	3005	FAD	C9A-N10	-2.97	1.35	1.41
8	H	4000	141	C4-N3	2.96	1.38	1.32
8	B	4000	141	C4-N3	2.83	1.38	1.32
4	E	3005	FAD	O2B-C2B	-2.81	1.36	1.43
8	H	4000	141	C2-N3	-2.80	1.30	1.36
4	E	3005	FAD	C2B-C1B	-2.79	1.49	1.53
8	F	4000	141	C5-C4	-2.78	1.40	1.46
6	B	3003	MTE	O4-C4	2.74	1.31	1.24
4	C	3005	FAD	C9A-N10	-2.71	1.36	1.41
6	F	3003	MTE	C2-N3	-2.65	1.30	1.35
4	C	3005	FAD	C4-N3	-2.58	1.34	1.38
4	C	3005	FAD	C4X-C10	-2.57	1.36	1.44
8	F	4000	141	C2-N3	-2.55	1.30	1.36
8	B	4000	141	C2-N3	-2.53	1.30	1.36
4	C	3005	FAD	C2A-N3A	2.49	1.36	1.32
6	H	3003	MTE	C4-N3	2.48	1.37	1.33
4	E	3005	FAD	C8-C7	-2.41	1.34	1.40
4	C	3005	FAD	C5X-N5	-2.41	1.34	1.39
4	A	3005	FAD	C9A-N10	-2.39	1.36	1.41
4	A	3005	FAD	C4X-C4	-2.36	1.35	1.44
4	G	3005	FAD	O4B-C4B	-2.33	1.39	1.45
8	D	4000	141	C2-N3	-2.30	1.31	1.36
4	G	3005	FAD	C2A-N3A	2.30	1.35	1.32
4	C	3005	FAD	C6-C5X	-2.30	1.36	1.40
4	E	3005	FAD	C2B-C3B	-2.29	1.47	1.53
4	C	3005	FAD	C4A-N3A	-2.28	1.32	1.35
6	B	3003	MTE	C4-N3	2.28	1.37	1.33
6	F	3003	MTE	P-O2P	-2.25	1.46	1.54
6	B	3003	MTE	C2-N3	-2.21	1.31	1.35
6	F	3003	MTE	P-O1P	2.20	1.57	1.50
8	B	4000	141	C7-C5	2.18	1.42	1.38
4	C	3005	FAD	C8-C7	-2.17	1.35	1.40
6	B	3003	MTE	P-O2P	-2.15	1.46	1.54
4	A	3005	FAD	C2A-N1A	2.14	1.37	1.33
4	G	3005	FAD	O4B-C1B	2.12	1.44	1.41
4	C	3005	FAD	O3B-C3B	-2.11	1.38	1.43
4	A	3005	FAD	C4-N3	-2.06	1.35	1.38
4	G	3005	FAD	O2B-C2B	-2.06	1.38	1.43
6	D	3003	MTE	P-O2P	-2.02	1.47	1.54

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3003	MTE	O3'-C7-C6	-29.62	89.21	108.96
6	F	3003	MTE	O3'-C7-C6	-24.82	92.41	108.96
6	H	3003	MTE	O3'-C7-C6	-23.00	93.63	108.96
6	B	3003	MTE	O3'-C7-C6	-20.63	95.20	108.96
6	D	3003	MTE	C4-C9-N5	9.78	127.33	119.12
6	F	3003	MTE	C4-C9-N5	9.44	127.04	119.12
4	C	3005	FAD	O2'-C2'-C3'	-8.66	88.03	109.10
6	H	3003	MTE	C4-C9-N5	8.43	126.19	119.12
6	B	3003	MTE	C4-C9-N5	7.88	125.73	119.12
6	F	3003	MTE	C2-N1-C10	7.30	130.91	114.54
6	B	3003	MTE	O3'-C7-N8	-7.29	101.08	108.57
4	C	3005	FAD	C1'-C2'-C3'	-7.18	89.73	109.79
4	A	3005	FAD	C5X-C9A-N10	7.12	125.30	117.95
4	G	3005	FAD	N3A-C2A-N1A	-7.04	117.68	128.68
8	B	4000	141	C5-C7-N8	7.04	113.82	107.43
4	C	3005	FAD	O3'-C3'-C4'	7.01	125.75	108.81
4	A	3005	FAD	N3A-C2A-N1A	-6.75	118.12	128.68
8	F	4000	141	C5-C7-N8	6.75	113.56	107.43
6	D	3003	MTE	C2-N3-C4	6.49	126.24	115.93
4	E	3005	FAD	P-O3P-PA	-6.43	110.75	132.83
6	B	3003	MTE	C2-N1-C10	6.42	128.94	114.54
4	E	3005	FAD	N3A-C2A-N1A	-6.33	118.79	128.68
6	H	3003	MTE	O2P-P-O4'	6.01	122.72	106.73
4	A	3005	FAD	P-O3P-PA	-5.96	112.38	132.83
4	E	3005	FAD	O3'-C3'-C4'	5.89	123.04	108.81
8	H	4000	141	C5-C7-N8	5.82	112.71	107.43
8	D	4000	141	C5-C7-N8	5.64	112.56	107.43
6	D	3003	MTE	C2-N1-C10	5.50	126.88	114.54
4	G	3005	FAD	P-O3P-PA	-5.13	115.21	132.83
6	F	3003	MTE	C2-N3-C4	5.06	123.97	115.93
6	H	3003	MTE	C2-N1-C10	5.01	125.77	114.54
4	C	3005	FAD	P-O3P-PA	-4.89	116.04	132.83
4	E	3005	FAD	O3'-C3'-C2'	-4.86	97.07	108.81
6	F	3003	MTE	N2-C2-N3	4.85	124.80	117.25
6	F	3003	MTE	N1-C2-N3	-4.84	117.83	125.42
4	C	3005	FAD	O2'-C2'-C1'	4.83	121.48	109.80
6	B	3003	MTE	O2P-P-O4'	4.82	119.56	106.73
4	E	3005	FAD	O2'-C2'-C1'	4.75	121.29	109.80
6	H	3003	MTE	C9-C10-N8	4.74	122.47	118.13
4	E	3005	FAD	C5'-C4'-C3'	-4.69	103.14	112.20
6	B	3003	MTE	N2-C2-N3	4.69	124.54	117.25
4	G	3005	FAD	O3B-C3B-C4B	-4.66	97.56	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3005	FAD	O4B-C1B-C2B	-4.63	100.17	106.93
4	G	3005	FAD	C7M-C7-C8	-4.61	111.29	120.74
4	A	3005	FAD	C9-C9A-N10	-4.41	115.87	121.84
6	D	3003	MTE	N1-C2-N3	-4.37	118.56	125.42
6	B	3003	MTE	C2-N3-C4	4.35	122.84	115.93
4	E	3005	FAD	C8M-C8-C7	-4.30	111.92	120.74
4	E	3005	FAD	C1'-C2'-C3'	-4.27	97.84	109.79
6	B	3003	MTE	N1-C2-N3	-4.27	118.72	125.42
4	G	3005	FAD	C4X-C10-N10	4.21	122.63	116.48
6	H	3003	MTE	N2-C2-N3	4.16	123.73	117.25
4	E	3005	FAD	C7M-C7-C6	4.14	127.14	119.49
6	F	3003	MTE	C9-C10-N8	4.12	121.90	118.13
4	G	3005	FAD	O5'-C5'-C4'	-4.05	98.56	109.36
6	D	3003	MTE	N2-C2-N3	4.05	123.55	117.25
4	A	3005	FAD	O5'-C5'-C4'	-4.04	98.57	109.36
4	C	3005	FAD	N6A-C6A-N1A	-4.00	110.28	118.57
4	C	3005	FAD	O3'-C3'-C2'	-3.95	99.27	108.81
4	G	3005	FAD	O3B-C3B-C2B	-3.91	99.17	111.82
4	E	3005	FAD	O3B-C3B-C2B	-3.86	99.34	111.82
4	G	3005	FAD	C7M-C7-C6	3.81	126.53	119.49
4	A	3005	FAD	O3B-C3B-C2B	-3.81	99.51	111.82
4	A	3005	FAD	O4-C4-C4X	-3.79	116.54	126.60
4	G	3005	FAD	O2B-C2B-C1B	-3.77	96.91	110.85
6	B	3003	MTE	O3P-P-O4'	3.75	116.70	106.73
4	A	3005	FAD	O4B-C4B-C3B	-3.72	97.74	105.11
6	D	3003	MTE	O3'-C7-N8	-3.72	104.75	108.57
4	C	3005	FAD	C4A-C5A-N7A	-3.71	105.53	109.40
6	B	3003	MTE	C9-C10-N8	3.69	121.51	118.13
6	H	3003	MTE	C2-N3-C4	3.67	121.76	115.93
6	F	3003	MTE	O3P-P-O2P	-3.66	93.66	107.64
4	A	3005	FAD	C9A-N10-C10	-3.65	115.08	120.77
4	G	3005	FAD	O4'-C4'-C5'	-3.61	101.80	109.92
6	H	3003	MTE	P-O4'-C4'	-3.58	108.42	118.30
4	A	3005	FAD	O4'-C4'-C3'	3.57	117.78	109.10
4	A	3005	FAD	C4X-C4-N3	3.57	122.25	113.19
4	C	3005	FAD	O5'-C5'-C4'	-3.56	99.86	109.36
4	A	3005	FAD	O5B-PA-O1A	-3.54	95.24	109.07
4	G	3005	FAD	C8M-C8-C7	-3.53	113.51	120.74
4	E	3005	FAD	C5A-C6A-N6A	-3.51	115.02	120.35
4	E	3005	FAD	C5X-C9A-N10	3.43	121.49	117.95
4	A	3005	FAD	O2'-C2'-C3'	-3.42	100.78	109.10
4	C	3005	FAD	C10-C4X-N5	-3.38	117.69	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3005	FAD	C5A-C6A-N6A	3.37	125.47	120.35
4	C	3005	FAD	C5X-C9A-N10	3.36	121.42	117.95
4	A	3005	FAD	O4B-C4B-C5B	-3.35	98.36	109.37
4	E	3005	FAD	C4'-C3'-C2'	-3.35	106.40	113.36
4	G	3005	FAD	O3'-C3'-C4'	3.34	116.88	108.81
4	E	3005	FAD	N6A-C6A-N1A	3.32	125.46	118.57
4	A	3005	FAD	O2'-C2'-C1'	3.32	117.82	109.80
4	G	3005	FAD	C2B-C3B-C4B	3.28	109.01	102.64
6	F	3003	MTE	P-O4'-C4'	-3.27	109.30	118.30
4	C	3005	FAD	N3A-C2A-N1A	-3.24	123.62	128.68
4	A	3005	FAD	C4X-C10-N10	3.24	121.21	116.48
8	H	4000	141	N1-C2-N3	3.21	125.68	119.38
4	C	3005	FAD	C5'-C4'-C3'	-3.20	106.02	112.20
4	E	3005	FAD	C7M-C7-C8	-3.18	114.21	120.74
6	F	3003	MTE	O2P-P-O4'	3.18	115.19	106.73
4	G	3005	FAD	O4B-C4B-C3B	-3.14	98.89	105.11
4	A	3005	FAD	O2A-PA-O5B	3.14	122.32	107.75
8	H	4000	141	O6-C6-C5	3.13	133.31	125.99
4	A	3005	FAD	C5A-C6A-N6A	-3.09	115.65	120.35
4	E	3005	FAD	C4-N3-C2	-3.07	119.97	125.64
4	C	3005	FAD	C9A-C5X-N5	-3.07	119.10	122.43
4	A	3005	FAD	C4-N3-C2	-3.05	120.00	125.64
6	D	3003	MTE	O3P-P-O1P	-3.05	98.74	110.68
4	G	3005	FAD	C4-N3-C2	-3.05	120.01	125.64
4	C	3005	FAD	C7M-C7-C6	3.01	125.05	119.49
8	B	4000	141	C4-N9-N8	2.99	113.67	110.00
4	E	3005	FAD	O2A-PA-O5B	2.92	121.32	107.75
6	F	3003	MTE	O3P-P-O4'	2.91	114.49	106.73
8	H	4000	141	C4-N3-C2	-2.91	111.10	116.96
4	E	3005	FAD	O4-C4-C4X	-2.91	118.88	126.60
8	H	4000	141	O2-C2-N1	-2.90	113.01	118.65
8	D	4000	141	C4-N9-N8	2.90	113.55	110.00
4	G	3005	FAD	O2-C2-N1	-2.87	117.07	121.83
4	C	3005	FAD	O4B-C4B-C3B	-2.85	99.48	105.11
4	E	3005	FAD	C9-C8-C7	2.84	123.74	119.67
4	E	3005	FAD	C9A-C5X-N5	-2.83	119.35	122.43
6	B	3003	MTE	O3P-P-O2P	-2.80	96.93	107.64
4	C	3005	FAD	O2B-C2B-C1B	-2.77	100.61	110.85
4	C	3005	FAD	C4X-C10-N10	2.77	120.53	116.48
8	F	4000	141	C4-N9-N8	2.76	113.39	110.00
4	G	3005	FAD	C2A-N1A-C6A	2.72	123.41	118.75
4	C	3005	FAD	C4X-C10-N1	-2.69	118.49	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3005	FAD	C8M-C8-C9	-2.68	114.53	119.49
4	E	3005	FAD	O4B-C4B-C3B	-2.68	99.81	105.11
4	A	3005	FAD	O2B-C2B-C3B	-2.67	103.17	111.82
4	A	3005	FAD	C7M-C7-C8	-2.66	115.29	120.74
4	G	3005	FAD	C10-C4X-N5	-2.62	119.29	124.86
4	E	3005	FAD	C8M-C8-C9	2.61	124.31	119.49
4	C	3005	FAD	O4-C4-N3	-2.57	115.18	120.12
4	C	3005	FAD	C4-N3-C2	-2.56	120.92	125.64
4	A	3005	FAD	C7M-C7-C6	2.53	124.16	119.49
4	A	3005	FAD	C9A-C5X-N5	-2.52	119.70	122.43
4	G	3005	FAD	O2'-C2'-C1'	2.50	115.84	109.80
4	E	3005	FAD	O4B-C1B-C2B	-2.47	103.32	106.93
4	G	3005	FAD	C5X-C9A-N10	2.45	120.49	117.95
6	D	3003	MTE	O2P-P-O1P	2.45	120.28	110.68
4	C	3005	FAD	O2B-C2B-C3B	-2.45	103.90	111.82
4	C	3005	FAD	O5B-PA-O1A	-2.43	99.57	109.07
4	C	3005	FAD	O3B-C3B-C4B	-2.42	104.04	111.05
8	B	4000	141	O6-C6-C5	2.42	131.66	125.99
4	E	3005	FAD	C1B-N9A-C4A	2.42	130.89	126.64
4	E	3005	FAD	C4X-C4-N3	2.41	119.31	113.19
8	H	4000	141	O6-C6-N1	-2.39	115.54	120.12
4	E	3005	FAD	C4-C4X-C10	2.37	120.78	116.79
4	A	3005	FAD	C1'-N10-C9A	2.37	124.46	120.51
4	A	3005	FAD	O3'-C3'-C4'	2.34	114.47	108.81
4	C	3005	FAD	O3B-C3B-C2B	-2.34	104.25	111.82
4	G	3005	FAD	C9A-C5X-N5	-2.34	119.89	122.43
4	C	3005	FAD	C4-C4X-C10	2.34	120.72	116.79
4	A	3005	FAD	O2B-C2B-C1B	-2.33	102.25	110.85
4	C	3005	FAD	C5X-N5-C4X	2.32	121.93	118.07
4	C	3005	FAD	C4-C4X-N5	2.32	121.53	118.23
4	G	3005	FAD	C8M-C8-C9	2.31	123.77	119.49
4	G	3005	FAD	C4-C4X-N5	2.29	121.49	118.23
4	E	3005	FAD	O2-C2-N3	-2.26	114.25	118.65
4	E	3005	FAD	O4-C4-N3	-2.25	115.81	120.12
4	E	3005	FAD	C4X-C10-N1	-2.22	119.58	124.73
4	G	3005	FAD	O2B-C2B-C3B	-2.22	104.64	111.82
4	A	3005	FAD	C5X-N5-C4X	-2.22	114.39	118.07
4	G	3005	FAD	O5'-P-O1P	2.18	117.60	109.07
4	A	3005	FAD	C5B-C4B-C3B	-2.18	107.01	115.18
8	F	4000	141	O6-C6-C5	2.14	131.00	125.99
4	G	3005	FAD	P-O5'-C5'	-2.13	109.18	121.68
4	C	3005	FAD	C4X-C4-N3	2.13	118.60	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3005	FAD	O2P-P-O1P	-2.12	101.74	112.24
4	E	3005	FAD	C9-C9A-N10	-2.12	118.97	121.84
4	G	3005	FAD	C4X-C4-N3	2.11	118.56	113.19
6	D	3003	MTE	O2P-P-O4'	2.09	112.30	106.73
6	H	3003	MTE	N2-C2-N1	-2.07	114.03	117.25
4	G	3005	FAD	O2'-C2'-C3'	-2.06	104.09	109.10
6	H	3003	MTE	N1-C2-N3	-2.03	122.24	125.42
4	C	3005	FAD	C6-C5X-C9A	2.02	121.80	118.94
6	H	3003	MTE	C10-N8-C7	-2.01	119.73	123.67
4	E	3005	FAD	O2A-PA-O1A	-2.01	102.31	112.24

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3005	FAD	O4B-C4B-C5B-O5B
4	A	3005	FAD	C2'-C1'-N10-C10
4	A	3005	FAD	N10-C1'-C2'-O2'
4	A	3005	FAD	N10-C1'-C2'-C3'
4	A	3005	FAD	C2'-C3'-C4'-O4'
4	A	3005	FAD	O3'-C3'-C4'-O4'
4	A	3005	FAD	C3'-C4'-C5'-O5'
4	A	3005	FAD	C5'-O5'-P-O3P
4	C	3005	FAD	C5B-O5B-PA-O3P
4	C	3005	FAD	C2'-C1'-N10-C10
4	C	3005	FAD	N10-C1'-C2'-O2'
4	C	3005	FAD	N10-C1'-C2'-C3'
4	C	3005	FAD	C2'-C3'-C4'-O4'
4	C	3005	FAD	C2'-C3'-C4'-C5'
4	C	3005	FAD	O3'-C3'-C4'-O4'
4	C	3005	FAD	O3'-C3'-C4'-C5'
4	C	3005	FAD	C3'-C4'-C5'-O5'
4	C	3005	FAD	O4'-C4'-C5'-O5'
4	E	3005	FAD	C5B-O5B-PA-O3P
4	E	3005	FAD	O4B-C4B-C5B-O5B
4	E	3005	FAD	C2'-C1'-N10-C10
4	E	3005	FAD	N10-C1'-C2'-O2'
4	E	3005	FAD	N10-C1'-C2'-C3'
4	E	3005	FAD	C2'-C3'-C4'-O4'
4	E	3005	FAD	O3'-C3'-C4'-O4'
4	E	3005	FAD	O3'-C3'-C4'-C5'
4	E	3005	FAD	C3'-C4'-C5'-O5'

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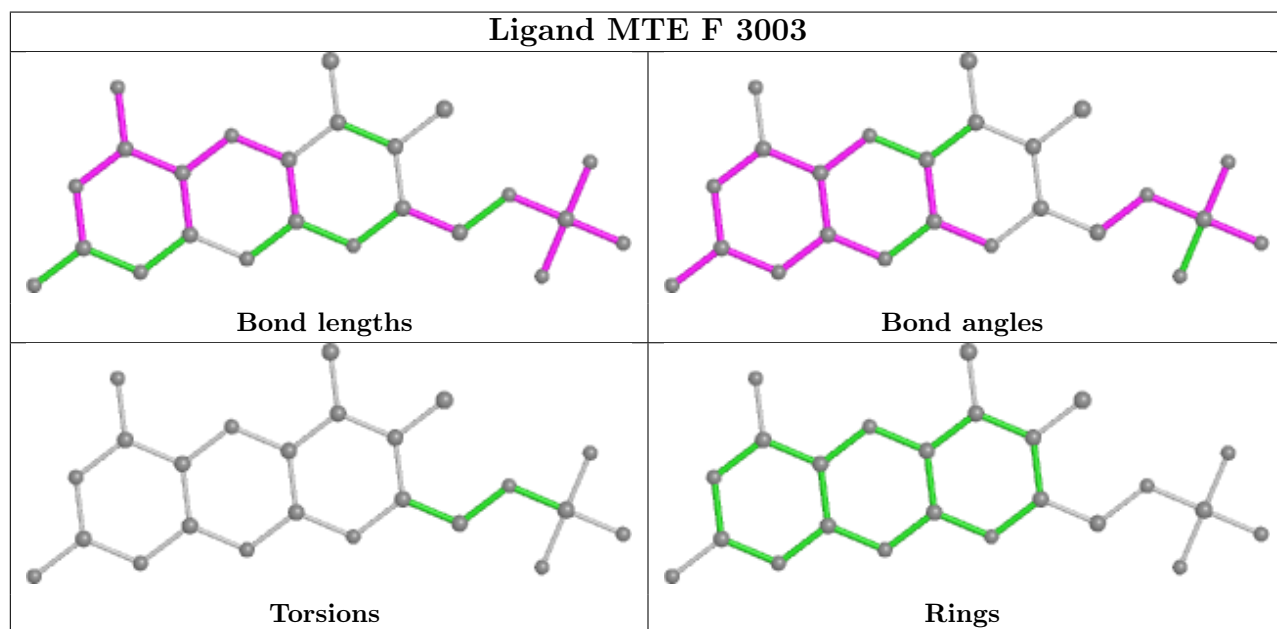
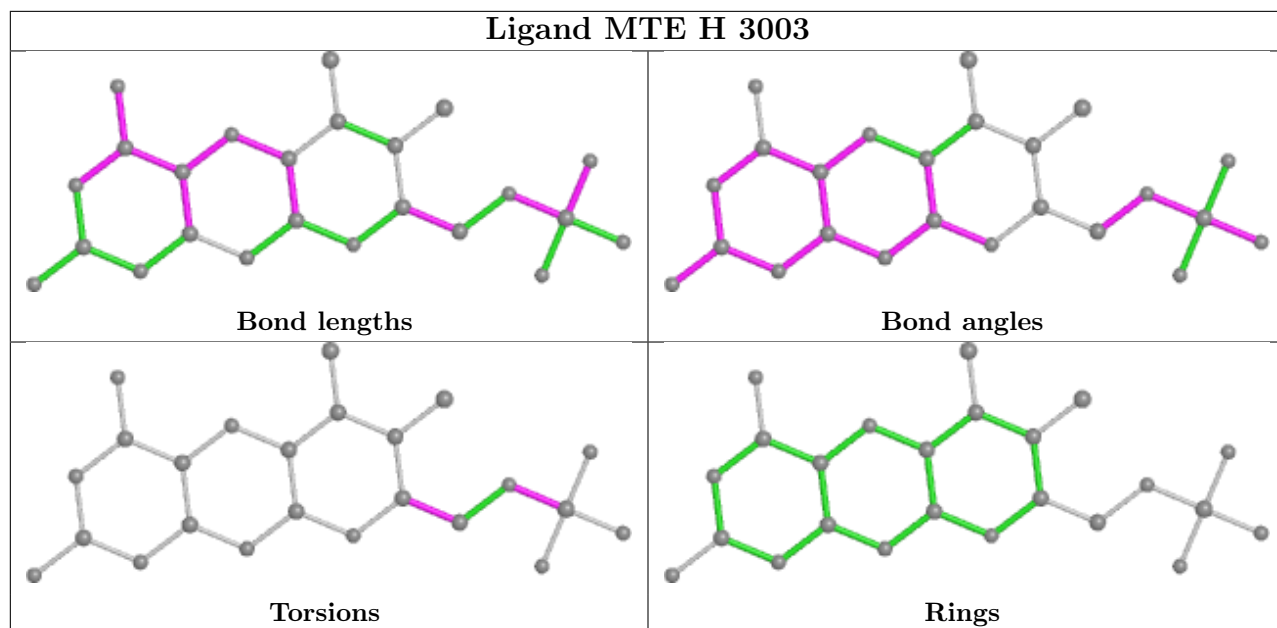
Mol	Chain	Res	Type	Atoms
4	E	3005	FAD	O4'-C4'-C5'-O5'
4	G	3005	FAD	C5B-O5B-PA-O3P
4	G	3005	FAD	N10-C1'-C2'-O2'
4	G	3005	FAD	N10-C1'-C2'-C3'
4	G	3005	FAD	C2'-C3'-C4'-O4'
4	G	3005	FAD	O3'-C3'-C4'-O4'
4	G	3005	FAD	C3'-C4'-C5'-O5'
4	G	3005	FAD	O4'-C4'-C5'-O5'
4	G	3005	FAD	C5'-O5'-P-O3P
6	D	3003	MTE	O3'-C3'-C4'-O4'
6	D	3003	MTE	C4'-O4'-P-O2P
4	C	3005	FAD	C3B-C4B-C5B-O5B
4	A	3005	FAD	O3'-C3'-C4'-C5'
4	G	3005	FAD	O3'-C3'-C4'-C5'
4	A	3005	FAD	C2'-C3'-C4'-C5'
4	E	3005	FAD	C2'-C3'-C4'-C5'
4	G	3005	FAD	C2'-C3'-C4'-C5'
4	E	3005	FAD	C3B-C4B-C5B-O5B
4	G	3005	FAD	O4B-C4B-C5B-O5B
4	G	3005	FAD	C3B-C4B-C5B-O5B
4	A	3005	FAD	O4'-C4'-C5'-O5'
4	C	3005	FAD	O4B-C4B-C5B-O5B
4	G	3005	FAD	C2'-C1'-N10-C10
6	H	3003	MTE	C4'-O4'-P-O2P
4	A	3005	FAD	C5B-O5B-PA-O2A
4	A	3005	FAD	C5'-O5'-P-O1P
4	A	3005	FAD	C5'-O5'-P-O2P
4	C	3005	FAD	C5B-O5B-PA-O1A
4	C	3005	FAD	C5B-O5B-PA-O2A
4	E	3005	FAD	C5B-O5B-PA-O1A
4	E	3005	FAD	C5B-O5B-PA-O2A
4	G	3005	FAD	C5B-O5B-PA-O1A
4	G	3005	FAD	C5B-O5B-PA-O2A
4	G	3005	FAD	C5'-O5'-P-O1P
4	G	3005	FAD	C5'-O5'-P-O2P
6	D	3003	MTE	C2'-C3'-C4'-O4'
6	H	3003	MTE	O3'-C3'-C4'-O4'
6	D	3003	MTE	C4'-O4'-P-O3P
6	D	3003	MTE	C4'-O4'-P-O1P
4	A	3005	FAD	C5B-O5B-PA-O3P
4	C	3005	FAD	C5'-O5'-P-O3P
4	A	3005	FAD	C5B-O5B-PA-O1A

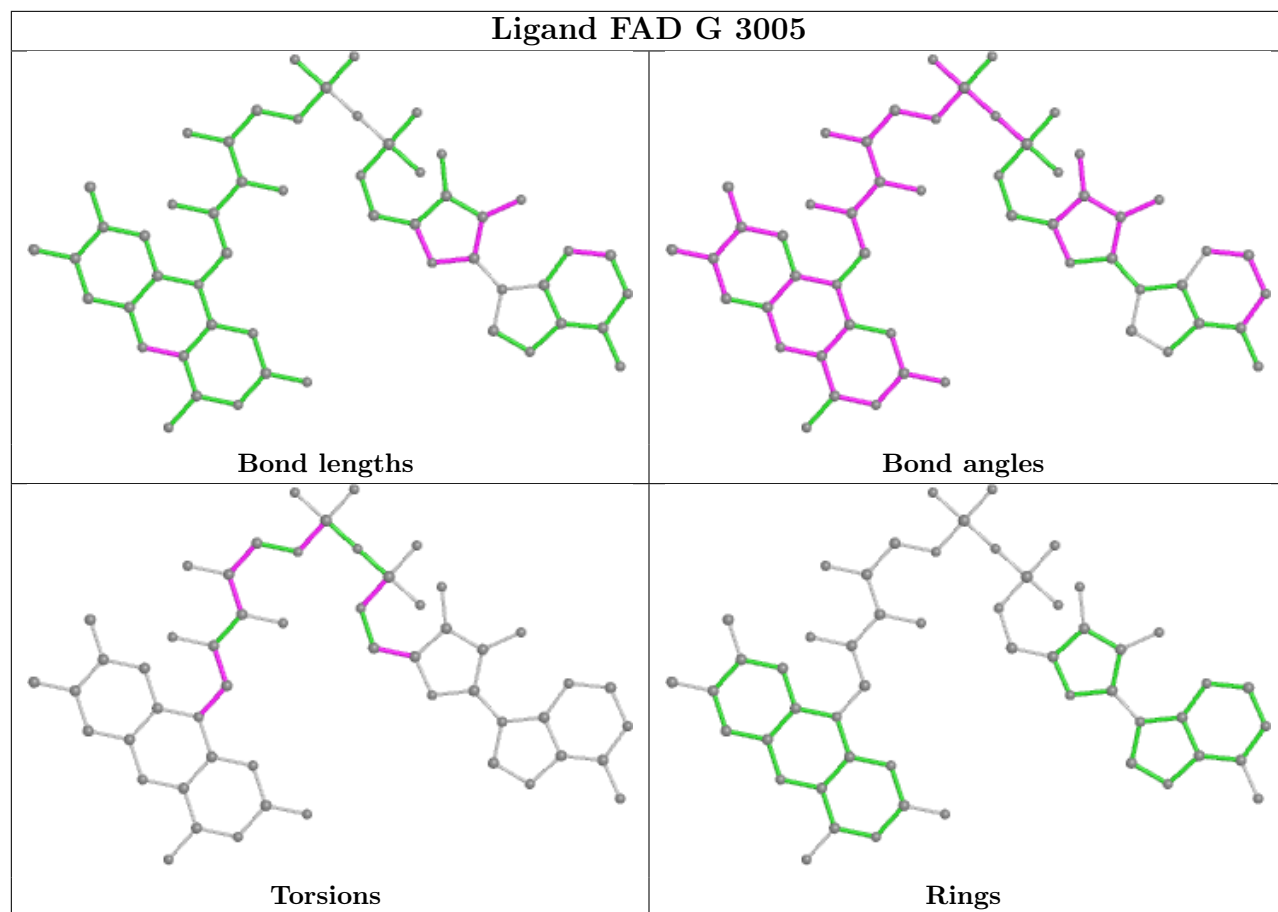
There are no ring outliers.

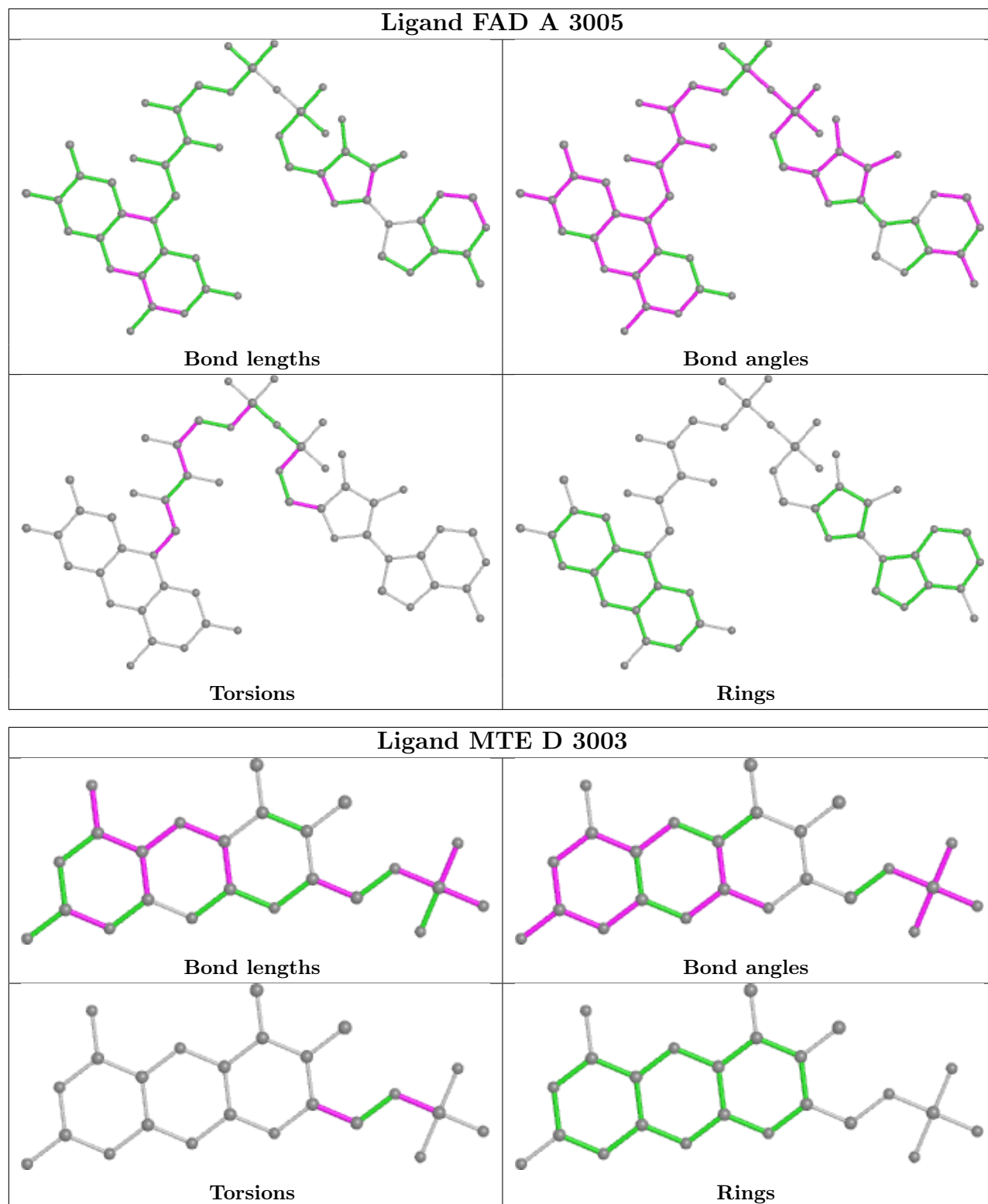
21 monomers are involved in 93 short contacts:

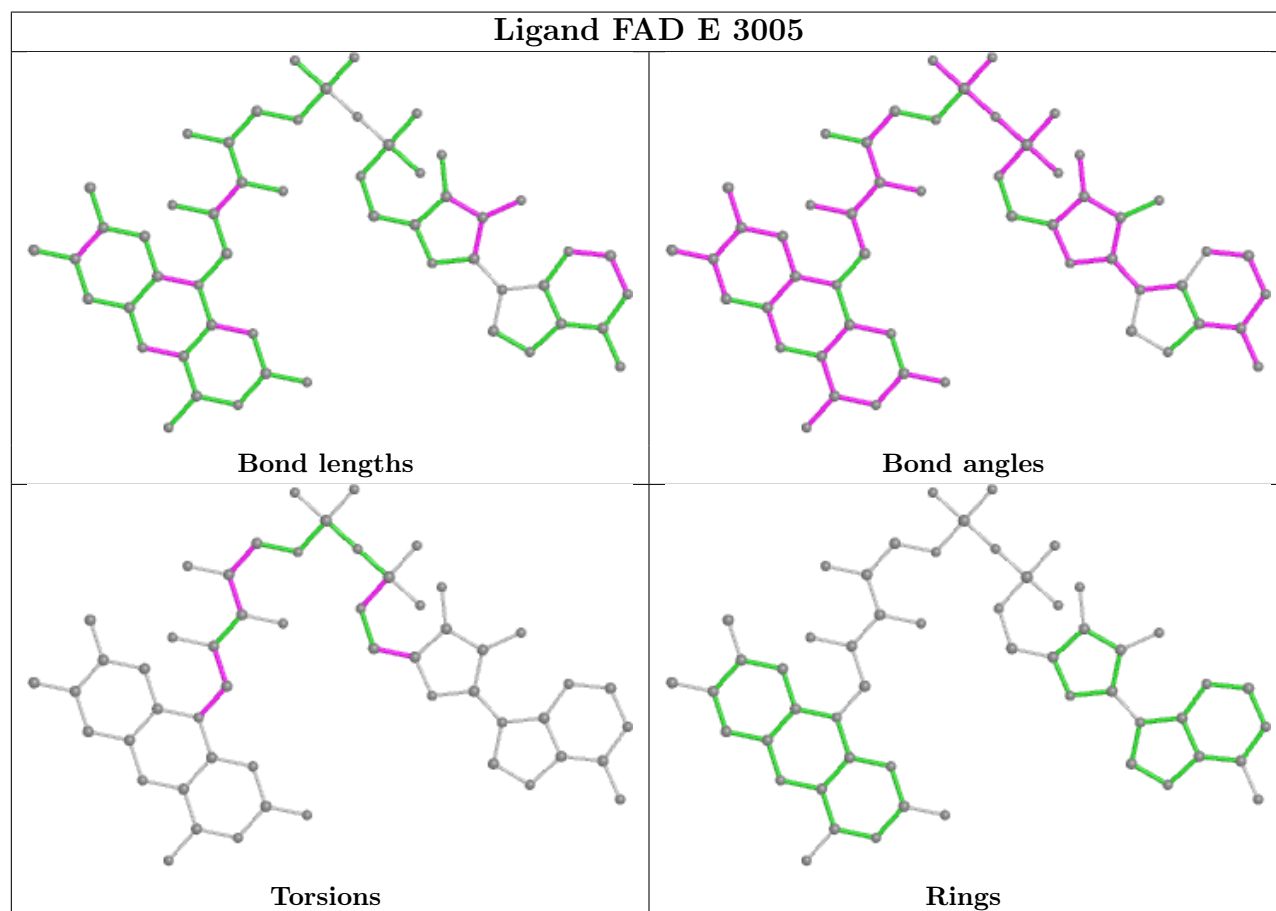
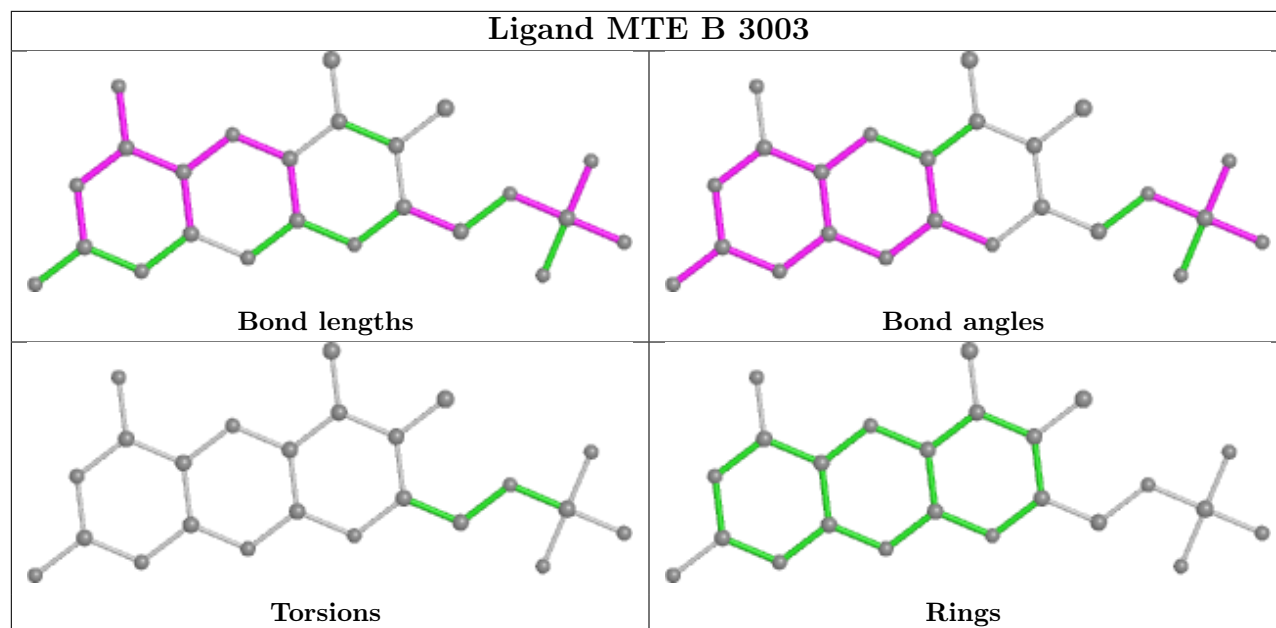
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	3004	MOS	4	0
8	H	4000	141	4	0
3	E	3002	FES	3	0
8	F	4000	141	5	0
6	H	3003	MTE	7	0
6	F	3003	MTE	7	0
4	G	3005	FAD	8	0
4	A	3005	FAD	10	0
6	D	3003	MTE	4	0
3	E	3001	FES	1	0
3	G	3001	FES	2	0
6	B	3003	MTE	4	0
8	D	4000	141	5	0
4	E	3005	FAD	11	0
3	A	3002	FES	1	0
7	D	3004	MOS	7	0
7	H	3004	MOS	5	0
3	G	3002	FES	1	0
4	C	3005	FAD	3	0
8	B	4000	141	9	0
7	F	3004	MOS	8	0

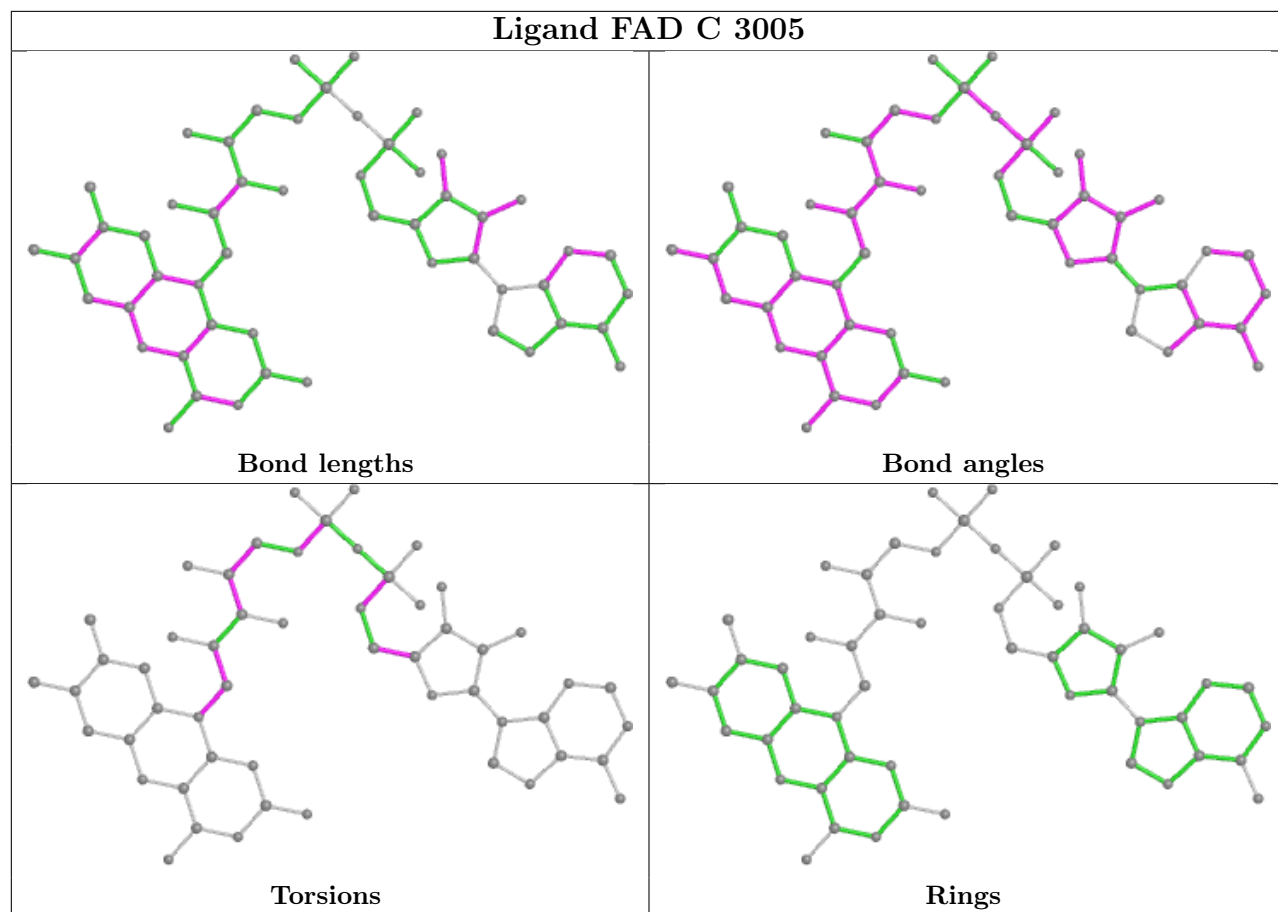
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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