



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 06:33 pm BST

PDB ID : 1JRO  
Title : Crystal Structure of Xanthine Dehydrogenase from Rhodobacter capsulatus  
Authors : Truglio, J.J.; Theis, K.; Leimkuhler, S.; Rappa, R.; Rajagopalan, K.V.; Kisker, C.  
Deposited on : 2001-08-14  
Resolution : 2.70 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.

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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)  
Xtriage (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) : 2.11

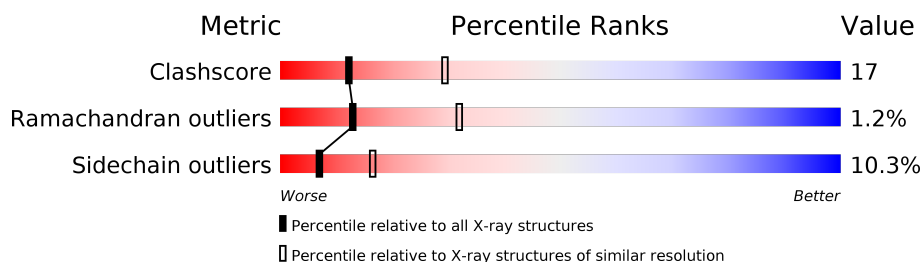
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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 on 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	
1	C	462	
1	E	462	
1	G	462	
2	B	777	
2	D	777	
2	F	777	
2	H	777	

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	G	3001	-	-	X	-
7	MOS	B	3004	-	-	X	-
7	MOS	D	3004	-	-	X	-
7	MOS	F	3004	-	-	X	-
7	MOS	H	3004	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 36831 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
1	A	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	C	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	E	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			
1	G	450	Total	C	N	O	S	0	0	0
			3370	2110	607	628	25			

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

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

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:  $C_{27}H_{33}N_9O_{15}P_2$ ).

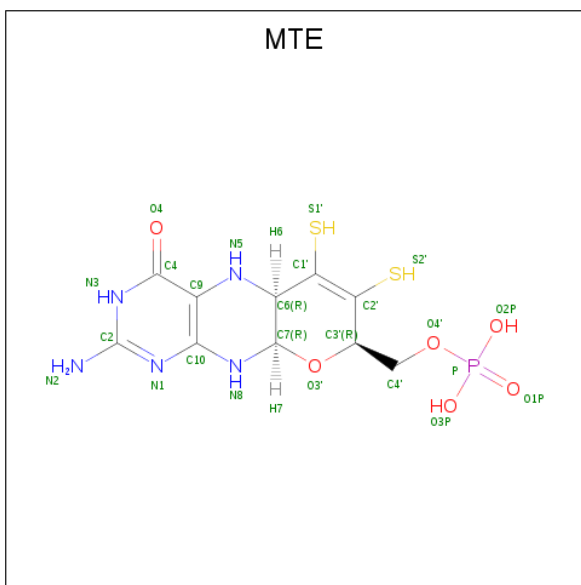


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

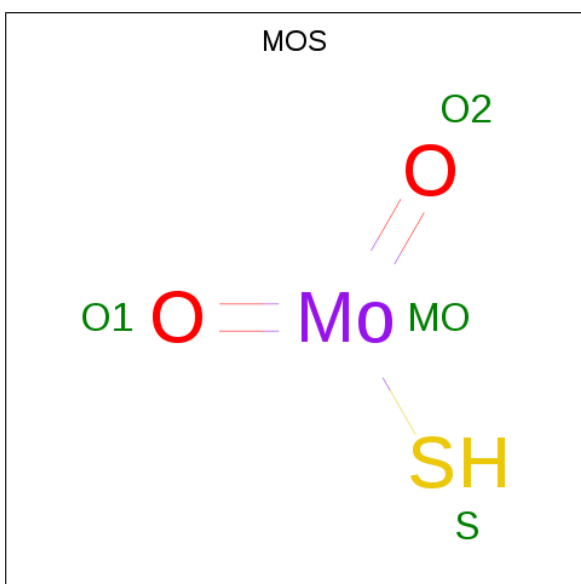
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		

- 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
6	B	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	D	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	F	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
6	H	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total 4	Mo 1	O 2	S 1	0	0
7	D	1	Total 4	Mo 1	O 2	S 1	0	0
7	F	1	Total 4	Mo 1	O 2	S 1	0	0
7	H	1	Total 4	Mo 1	O 2	S 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	11	Total 11	O 11	0	0
8	B	26	Total 26	O 26	0	0
8	C	7	Total 7	O 7	0	0
8	D	25	Total 25	O 25	0	0
8	E	7	Total 7	O 7	0	0
8	F	20	Total 20	O 20	0	0
8	G	6	Total 6	O 6	0	0
8	H	21	Total 21	O 21	0	0

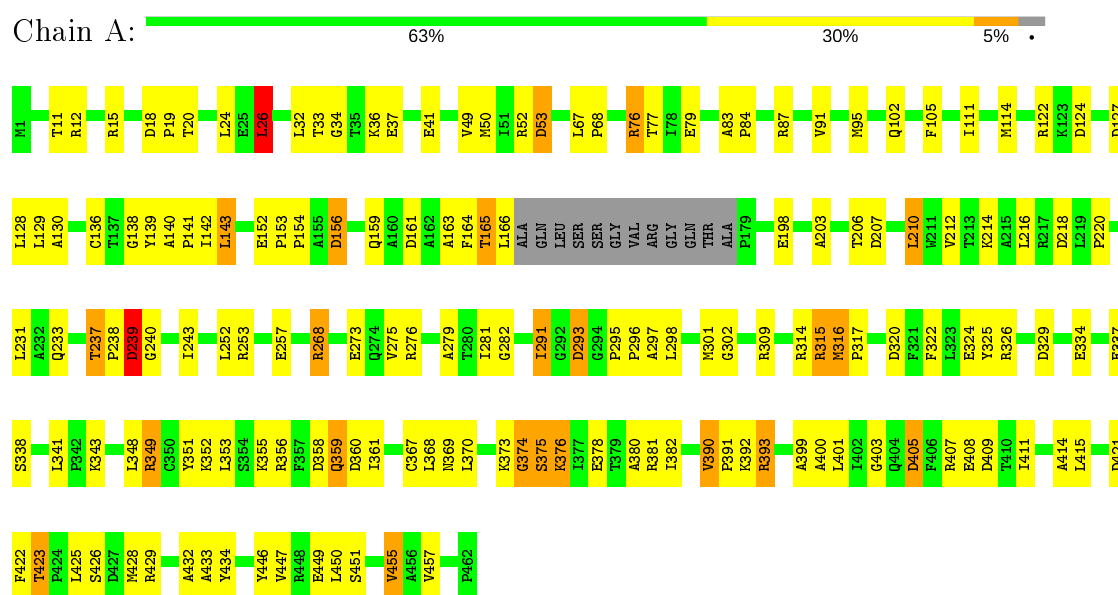


### 3 Residue-property plots

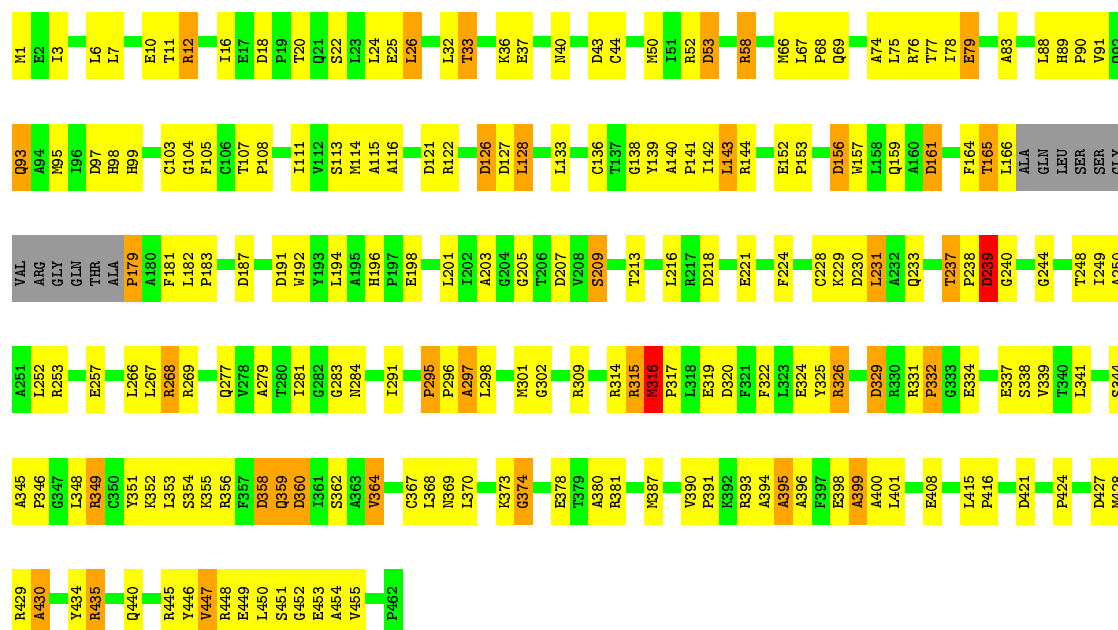
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

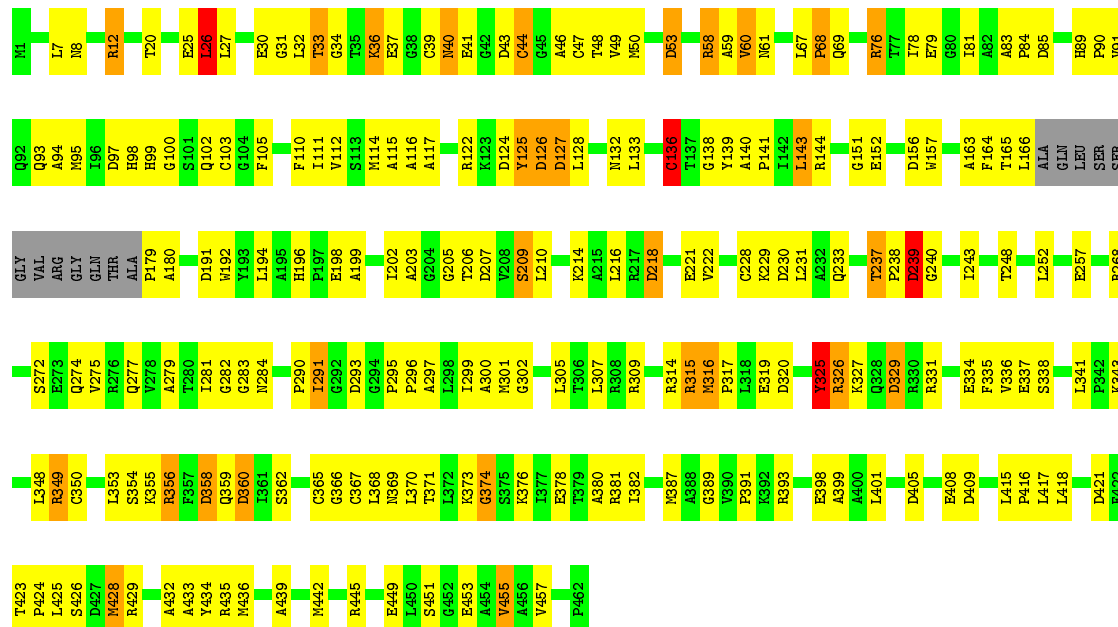


Chain E: 



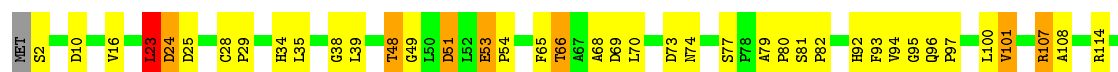
• Molecule 1: xanthine dehydrogenase, chain A

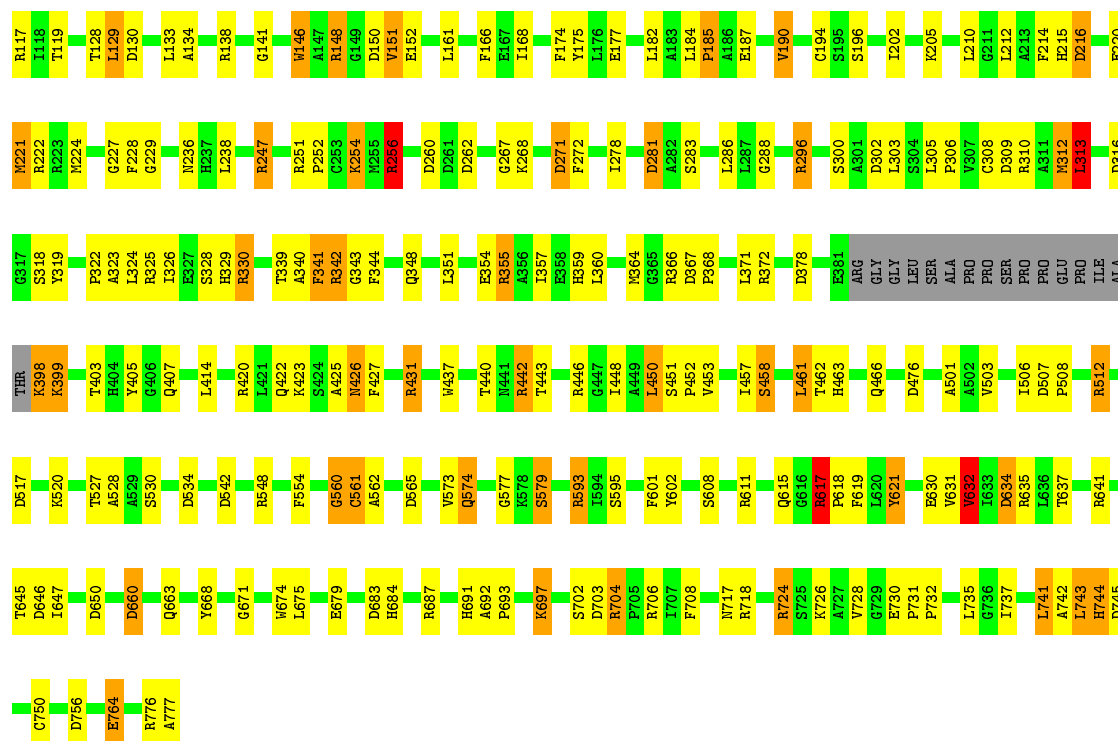
Chain G: 



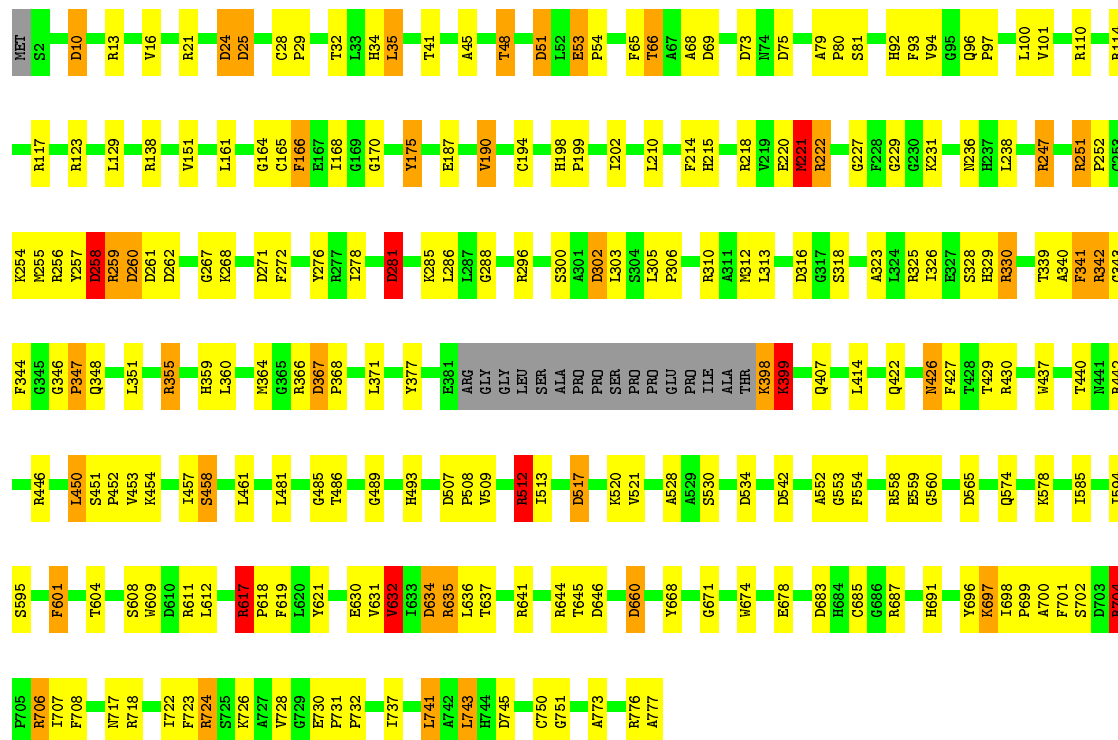
• Molecule 2: xanthine dehydrogenase, chain B

Chain B: 



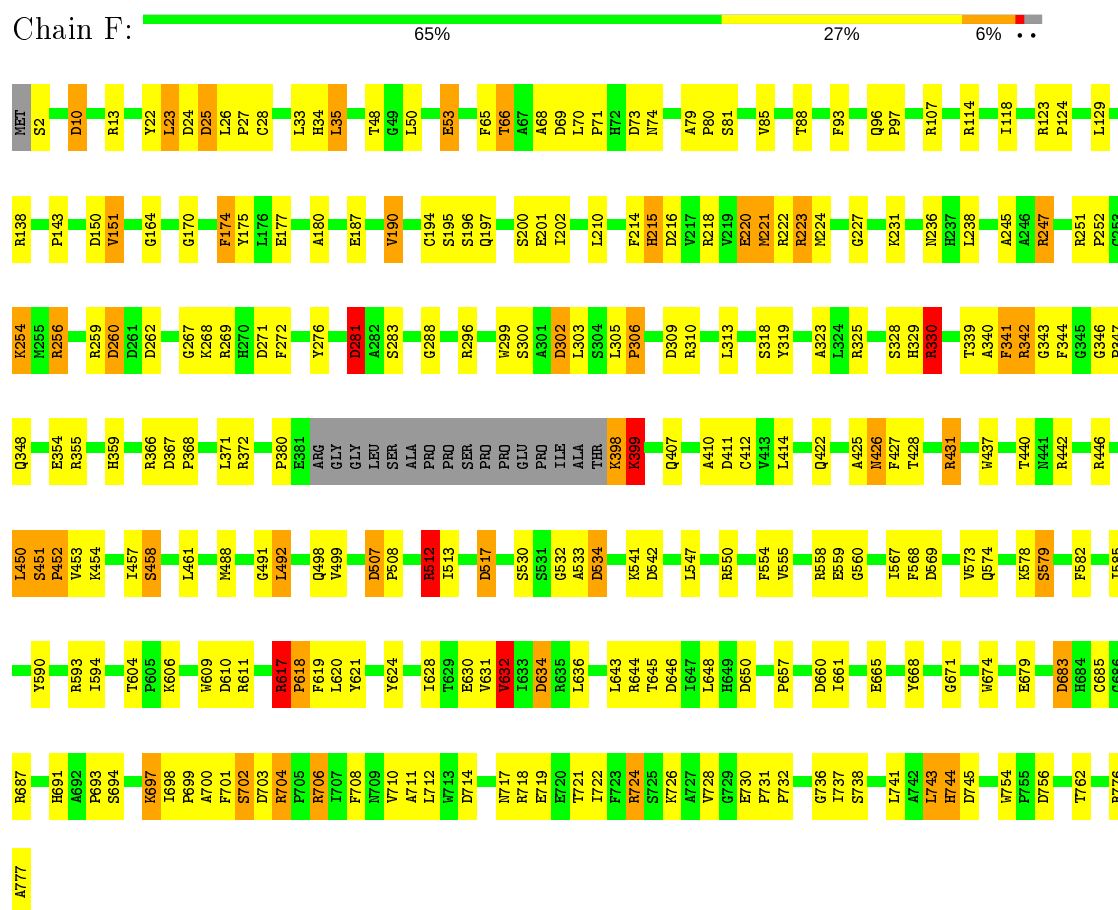


- Molecule 2: xanthine dehydrogenase, chain B



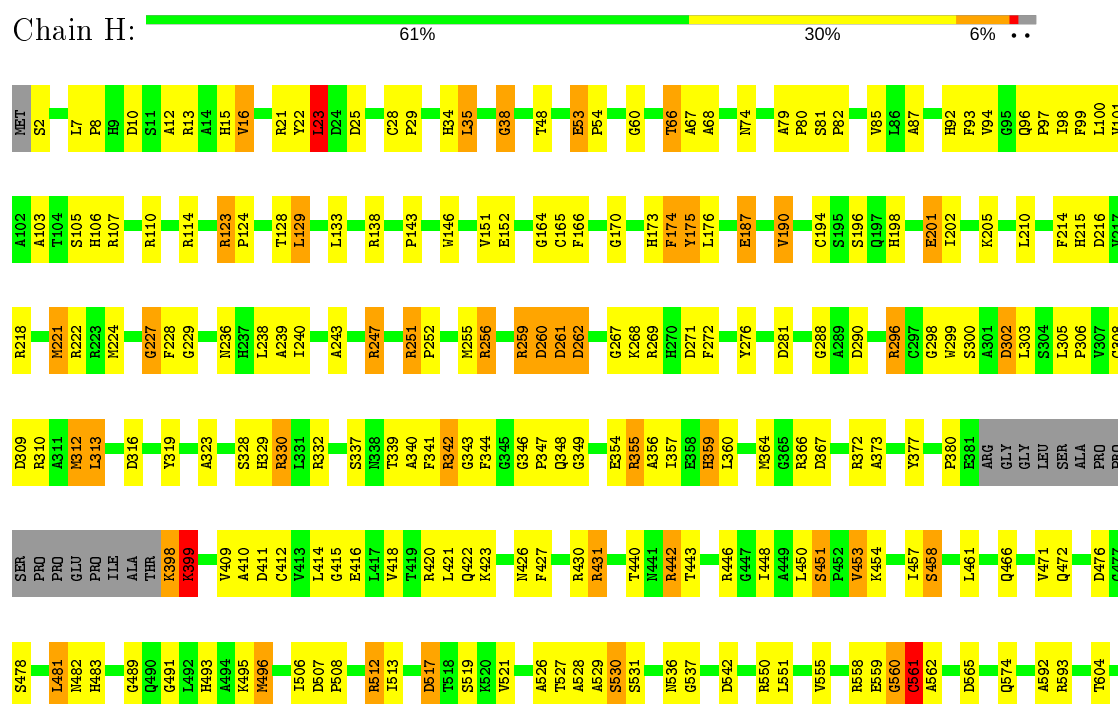
- Molecule 2: xanthine dehydrogenase, chain B

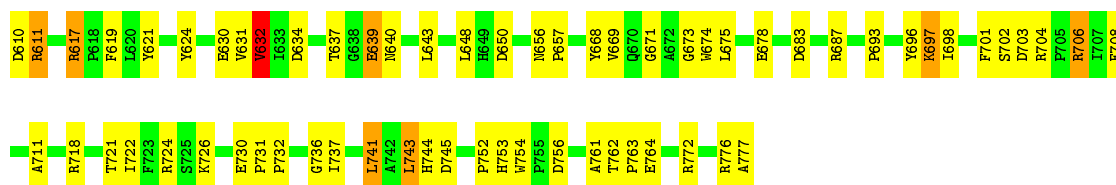
## Chain F:



- Molecule 2: xanthine dehydrogenase, chain B

## Chain H:





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.88Å 141.05Å 158.11Å 109.53° 105.83° 101.33°	Depositor
Resolution (Å)	50.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.2 (50.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.213 , 0.252	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	36831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MOS, CA, FES, FAD, MTE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.94	1/3431 (0.0%)	1.11	17/4647 (0.4%)
1	C	1.17	4/3431 (0.1%)	1.25	23/4647 (0.5%)
1	E	0.99	1/3431 (0.0%)	1.17	20/4647 (0.4%)
1	G	0.98	7/3431 (0.2%)	1.18	26/4647 (0.6%)
2	B	1.16	6/5845 (0.1%)	1.25	49/7942 (0.6%)
2	D	1.26	9/5845 (0.2%)	1.29	47/7942 (0.6%)
2	F	1.17	4/5845 (0.1%)	1.26	43/7942 (0.5%)
2	H	1.14	7/5845 (0.1%)	1.23	38/7942 (0.5%)
All	All	1.13	39/37104 (0.1%)	1.23	263/50356 (0.5%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	258	ASP	CB-CG	-9.22	1.32	1.51
2	H	521	VAL	CA-CB	-8.89	1.36	1.54
1	G	325	TYR	CD1-CE1	-7.39	1.28	1.39
1	G	325	TYR	CB-CG	-7.20	1.40	1.51
1	G	325	TYR	CD2-CE2	-6.99	1.28	1.39
1	C	278	VAL	CB-CG2	-6.82	1.38	1.52
1	C	251	ALA	CA-CB	-6.80	1.38	1.52
2	F	582	PHE	CE1-CZ	6.59	1.49	1.37
2	D	194	CYS	CB-SG	-6.54	1.71	1.82
2	D	312	MET	SD-CE	-6.29	1.42	1.77
2	F	245	ALA	CA-CB	-6.23	1.39	1.52
2	B	621	TYR	CD2-CE2	-6.14	1.30	1.39
2	D	601	PHE	CE2-CZ	6.08	1.48	1.37
2	H	243	ALA	CA-CB	-5.98	1.39	1.52
1	C	276	ARG	CZ-NH1	-5.82	1.25	1.33
2	H	187	GLU	CD-OE2	5.71	1.31	1.25
1	G	60	VAL	CA-CB	-5.65	1.42	1.54
1	G	44	CYS	CB-SG	-5.64	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	200	SER	CB-OG	5.61	1.49	1.42
2	D	231	LYS	CE-NZ	5.57	1.62	1.49
1	A	49	VAL	CB-CG2	-5.54	1.41	1.52
1	G	127	ASP	CB-CG	5.54	1.63	1.51
2	B	146	TRP	CB-CG	-5.51	1.40	1.50
2	H	201	GLU	CD-OE2	5.51	1.31	1.25
2	B	312	MET	SD-CE	-5.42	1.47	1.77
2	D	260	ASP	CB-CG	5.38	1.63	1.51
2	D	257	TYR	CD1-CE1	-5.36	1.31	1.39
2	F	220	GLU	CD-OE2	5.35	1.31	1.25
2	B	220	GLU	CD-OE1	5.32	1.31	1.25
1	E	316	MET	SD-CE	5.26	2.07	1.77
2	H	611	ARG	CB-CG	-5.26	1.38	1.52
2	H	22	TYR	CD1-CE1	5.24	1.47	1.39
2	D	521	VAL	CA-CB	-5.22	1.43	1.54
2	H	16	VAL	CA-CB	-5.16	1.44	1.54
2	D	21	ARG	CG-CD	-5.16	1.39	1.51
1	G	125	TYR	CD2-CE2	-5.10	1.31	1.39
2	B	573	VAL	CB-CG2	-5.08	1.42	1.52
1	C	114	MET	SD-CE	-5.03	1.49	1.77
2	B	228	PHE	CB-CG	-5.01	1.42	1.51

All (263) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	258	ASP	CB-CG-OD1	-13.50	106.15	118.30
1	C	349	ARG	NE-CZ-NH1	13.32	126.96	120.30
2	D	258	ASP	CB-CG-OD2	13.19	130.17	118.30
1	C	429	ARG	NE-CZ-NH2	-12.01	114.30	120.30
2	D	660	ASP	CB-CG-OD2	11.32	128.49	118.30
2	H	481	LEU	CB-CG-CD1	-11.08	92.17	111.00
2	B	512	ARG	NE-CZ-NH2	-10.79	114.90	120.30
2	F	683	ASP	CB-CG-OD2	10.76	127.99	118.30
2	F	617	ARG	NE-CZ-NH1	10.37	125.49	120.30
2	B	190	VAL	CB-CA-C	-10.06	92.29	111.40
2	D	632	VAL	CB-CA-C	-9.98	92.43	111.40
1	C	429	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	C	349	ARG	NE-CZ-NH2	-9.80	115.40	120.30
2	B	660	ASP	CB-CG-OD2	9.56	126.91	118.30
2	D	21	ARG	NE-CZ-NH2	-9.55	115.52	120.30
2	F	617	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	C	76	ARG	NE-CZ-NH1	9.30	124.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	542	ASP	CB-CG-OD2	9.25	126.62	118.30
2	D	24	ASP	CB-CG-OD2	9.11	126.50	118.30
2	D	69	ASP	CB-CG-OD2	9.05	126.44	118.30
2	B	107	ARG	NE-CZ-NH1	-9.04	115.78	120.30
2	B	593	ARG	NE-CZ-NH2	-8.98	115.81	120.30
2	B	309	ASP	CB-CG-OD2	8.95	126.35	118.30
2	B	69	ASP	CB-CG-OD2	8.93	126.34	118.30
2	H	261	ASP	CB-CG-OD2	8.91	126.32	118.30
1	C	320	ASP	CB-CG-OD2	8.88	126.30	118.30
2	D	260	ASP	CB-CG-OD2	8.88	126.29	118.30
2	F	10	ASP	CB-CG-OD2	8.84	126.26	118.30
2	F	632	VAL	CB-CA-C	-8.65	94.97	111.40
1	E	207	ASP	CB-CG-OD2	8.62	126.06	118.30
2	D	704	ARG	NE-CZ-NH1	-8.60	116.00	120.30
1	E	126	ASP	CB-CG-OD2	8.55	126.00	118.30
2	B	262	ASP	CB-CG-OD2	8.46	125.91	118.30
2	F	517	ASP	CB-CG-OD2	8.40	125.86	118.30
2	H	190	VAL	CB-CA-C	-8.39	95.46	111.40
1	G	127	ASP	CB-CG-OD2	8.27	125.74	118.30
2	D	25	ASP	CB-CG-OD2	8.23	125.71	118.30
2	B	632	VAL	CB-CA-C	-8.20	95.83	111.40
2	D	190	VAL	CB-CA-C	-8.02	96.16	111.40
2	H	107	ARG	NE-CZ-NH1	-7.96	116.32	120.30
2	B	542	ASP	CB-CG-OD2	7.89	125.41	118.30
2	F	534	ASP	CB-CG-OD2	7.86	125.38	118.30
1	C	405	ASP	CB-CG-OD2	7.82	125.34	118.30
1	G	207	ASP	CB-CG-OD2	7.81	125.33	118.30
1	C	207	ASP	CB-CG-OD2	7.80	125.32	118.30
1	C	76	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	A	320	ASP	CB-CG-OD2	7.71	125.24	118.30
2	B	271	ASP	CB-CG-OD2	7.60	125.14	118.30
2	B	260	ASP	CB-CG-OD2	7.57	125.11	118.30
1	A	207	ASP	CB-CG-OD2	7.55	125.10	118.30
2	H	21	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	E	18	ASP	CB-CG-OD2	7.45	125.00	118.30
2	B	745	ASP	CB-CG-OD2	7.43	124.99	118.30
2	B	107	ARG	NE-CZ-NH2	7.42	124.01	120.30
1	E	356	ARG	NE-CZ-NH1	-7.41	116.60	120.30
2	B	256	ARG	NE-CZ-NH1	7.40	124.00	120.30
2	D	685	CYS	CB-CA-C	-7.39	95.62	110.40
1	A	127	ASP	CB-CG-OD2	7.20	124.78	118.30
1	E	43	ASP	CB-CG-OD2	7.18	124.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	517	ASP	CB-CG-OD2	7.11	124.70	118.30
1	G	126	ASP	CB-CG-OD2	7.11	124.70	118.30
2	F	634	ASP	CB-CG-OD2	7.10	124.69	118.30
2	F	685	CYS	CB-CA-C	-7.10	96.20	110.40
2	B	565	ASP	CB-CG-OD2	7.08	124.67	118.30
1	C	26	LEU	CB-CG-CD2	7.06	123.01	111.00
2	B	703	ASP	CB-CG-OD2	7.04	124.64	118.30
2	D	302	ASP	CB-CG-OD2	7.04	124.64	118.30
1	A	293	ASP	CB-CG-OD2	7.02	124.61	118.30
2	H	316	ASP	CB-CG-OD2	6.99	124.59	118.30
2	D	73	ASP	CB-CG-OD2	6.96	124.56	118.30
2	H	262	ASP	CB-CG-OD2	6.95	124.55	118.30
2	F	660	ASP	CB-CG-OD2	6.94	124.55	118.30
1	E	127	ASP	CB-CG-OD2	6.90	124.51	118.30
1	E	358	ASP	CB-CG-OD1	6.89	124.51	118.30
1	C	329	ASP	CB-CG-OD2	6.83	124.45	118.30
2	B	23	LEU	CA-CB-CG	-6.83	99.59	115.30
1	C	119	ASP	CB-CG-OD2	6.78	124.41	118.30
2	D	316	ASP	CB-CG-OD2	6.75	124.38	118.30
2	F	646	ASP	CB-CG-OD2	6.74	124.36	118.30
2	B	216	ASP	CB-CG-OD2	6.74	124.36	118.30
1	E	320	ASP	CB-CG-OD2	6.71	124.34	118.30
2	F	569	ASP	CB-CG-OD2	6.71	124.34	118.30
2	F	650	ASP	CB-CG-OD2	6.68	124.31	118.30
1	G	76	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	G	360	ASP	CB-CG-OD2	6.64	124.27	118.30
1	G	230	ASP	CB-CG-OD2	6.63	124.27	118.30
2	H	260	ASP	CB-CG-OD2	6.60	124.24	118.30
2	D	75	ASP	CB-CG-OD2	6.60	124.24	118.30
2	D	745	ASP	CB-CG-OD2	6.59	124.23	118.30
2	F	745	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	156	ASP	CB-CG-OD2	6.57	124.22	118.30
1	E	421	ASP	CB-CG-OD2	6.57	124.21	118.30
2	D	512	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	136	CYS	CA-CB-SG	6.54	125.77	114.00
2	F	190	VAL	CB-CA-C	-6.53	99.00	111.40
2	D	194	CYS	CA-CB-SG	-6.47	102.35	114.00
1	G	26	LEU	CB-CG-CD2	6.45	121.97	111.00
2	F	223	ARG	NE-CZ-NH1	-6.45	117.08	120.30
2	F	411	ASP	CB-CG-OD2	6.42	124.08	118.30
2	B	650	ASP	CB-CG-OD2	6.41	124.07	118.30
2	F	704	ARG	NE-CZ-NH1	-6.40	117.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	703	ASP	CB-CG-OD2	6.40	124.06	118.30
2	B	683	ASP	CB-CG-OD1	6.39	124.05	118.30
1	G	156	ASP	CB-CG-OD2	6.38	124.04	118.30
1	A	76	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	C	156	ASP	CB-CG-OD2	6.33	124.00	118.30
1	C	409	ASP	CB-CG-OD2	6.33	123.99	118.30
2	F	610	ASP	CB-CG-OD2	6.32	123.99	118.30
2	D	481	LEU	CB-CG-CD2	-6.30	100.29	111.00
2	F	512	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	B	73	ASP	CB-CG-OD2	6.26	123.93	118.30
1	E	53	ASP	CB-CG-OD2	6.23	123.90	118.30
2	H	308	CYS	CA-CB-SG	-6.22	102.80	114.00
2	F	756	ASP	CB-CG-OD2	6.21	123.89	118.30
2	H	650	ASP	CB-CG-OD2	6.20	123.88	118.30
2	D	660	ASP	CB-CG-OD1	-6.18	112.73	118.30
2	H	565	ASP	CB-CG-OD2	6.18	123.86	118.30
2	B	316	ASP	CB-CG-OD2	6.17	123.85	118.30
2	H	16	VAL	CG1-CB-CG2	6.17	120.76	110.90
2	D	281	ASP	CB-CG-OD1	-6.16	112.76	118.30
1	A	405	ASP	CB-CG-OD2	6.16	123.84	118.30
1	G	320	ASP	CB-CG-OD2	6.15	123.84	118.30
2	D	367	ASP	CB-CG-OD2	6.15	123.83	118.30
2	H	411	ASP	CB-CG-OD2	6.15	123.83	118.30
2	D	281	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	53	ASP	CB-CG-OD2	6.14	123.82	118.30
1	C	269	ARG	NE-CZ-NH2	-6.11	117.25	120.30
2	F	260	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	50	MET	CG-SD-CE	-6.07	90.48	100.20
2	B	646	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	425	LEU	CA-CB-CG	6.05	129.21	115.30
1	G	365	CYS	CA-CB-SG	-6.05	103.12	114.00
1	E	26	LEU	CB-CG-CD1	6.03	121.25	111.00
2	D	222	ARG	NE-CZ-NH2	6.03	123.31	120.30
2	F	703	ASP	CB-CG-OD2	6.03	123.73	118.30
2	D	646	ASP	CB-CG-OD2	6.02	123.72	118.30
2	H	25	ASP	CB-CG-OD2	6.02	123.72	118.30
2	H	23	LEU	CA-CB-CG	-6.01	101.47	115.30
2	B	150	ASP	CB-CG-OD2	6.01	123.71	118.30
2	F	281	ASP	N-CA-CB	-6.01	99.78	110.60
2	F	107	ARG	NE-CZ-NH1	-6.01	117.30	120.30
2	H	281	ASP	N-CA-CB	-5.98	99.83	110.60
2	B	148	ARG	NE-CZ-NH2	-5.97	117.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	617	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	G	291	ILE	CG1-CB-CG2	-5.94	98.34	111.40
2	D	542	ASP	CB-CG-OD1	-5.93	112.96	118.30
2	D	430	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	26	LEU	CB-CG-CD2	5.91	121.05	111.00
2	F	309	ASP	CB-CG-OD2	5.91	123.62	118.30
2	H	745	ASP	CB-CG-OD2	5.91	123.62	118.30
2	D	565	ASP	CB-CG-OD2	5.91	123.62	118.30
2	B	660	ASP	CB-CG-OD1	-5.91	112.98	118.30
1	E	269	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	H	610	ASP	CB-CG-OD2	5.90	123.61	118.30
2	F	644	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	E	329	ASP	CB-CG-OD2	5.87	123.58	118.30
1	G	293	ASP	CB-CG-OD2	5.86	123.58	118.30
2	B	281	ASP	N-CA-CB	-5.86	100.05	110.60
2	D	281	ASP	N-CA-CB	-5.86	100.05	110.60
2	H	632	VAL	CB-CA-C	-5.84	100.30	111.40
2	F	69	ASP	CB-CG-OD2	5.82	123.54	118.30
1	E	156	ASP	CB-CG-OD2	5.81	123.53	118.30
1	E	360	ASP	CB-CG-OD2	5.81	123.53	118.30
2	F	73	ASP	CB-CG-OD2	5.78	123.50	118.30
2	D	453	VAL	CB-CA-C	-5.76	100.45	111.40
2	F	542	ASP	CB-CG-OD2	5.75	123.48	118.30
2	D	683	ASP	CB-CG-OD2	5.75	123.47	118.30
2	B	24	ASP	CB-CG-OD2	5.74	123.47	118.30
1	E	364	VAL	CB-CA-C	-5.74	100.49	111.40
2	F	254	LYS	CD-CE-NZ	-5.73	98.52	111.70
2	D	10	ASP	CB-CG-OD2	5.73	123.45	118.30
1	G	421	ASP	CB-CG-OD2	5.70	123.43	118.30
2	H	302	ASP	CB-CG-OD2	5.69	123.42	118.30
2	B	378	ASP	CB-CG-OD2	5.68	123.41	118.30
2	B	476	ASP	CB-CG-OD1	5.68	123.41	118.30
2	B	756	ASP	CB-CG-OD2	5.67	123.40	118.30
2	B	313	LEU	CA-CB-CG	5.67	128.33	115.30
2	B	534	ASP	CB-CG-OD2	5.66	123.39	118.30
2	B	617	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	D	347	PRO	N-CD-CG	-5.63	94.75	103.20
1	G	76	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	33	THR	N-CA-CB	-5.60	99.66	110.30
2	B	764	GLU	OE1-CD-OE2	-5.59	116.59	123.30
2	D	512	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	161	ASP	CB-CG-OD2	5.58	123.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	714	ASP	CB-CG-OD2	5.56	123.31	118.30
2	F	330	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	C	127	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	126	ASP	CB-CG-OD2	5.54	123.29	118.30
1	G	356	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	421	ASP	CB-CG-OD2	5.54	123.28	118.30
2	H	517	ASP	CB-CG-OD2	5.53	123.28	118.30
2	D	51	ASP	CB-CG-OD2	5.51	123.26	118.30
1	G	358	ASP	CB-CG-OD1	5.50	123.25	118.30
1	E	230	ASP	CB-CG-OD2	5.49	123.24	118.30
2	H	453	VAL	CB-CA-C	-5.49	100.98	111.40
2	D	634	ASP	CB-CG-OD2	5.47	123.22	118.30
2	H	38	GLY	N-CA-C	-5.46	99.45	113.10
2	H	107	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	H	332	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	G	127	ASP	OD1-CG-OD2	-5.44	112.96	123.30
2	H	355	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	F	25	ASP	CB-CG-OD2	5.41	123.17	118.30
1	G	136	CYS	CA-CB-SG	5.41	123.74	114.00
2	B	182	LEU	CB-CG-CD1	-5.39	101.84	111.00
2	B	101	VAL	CB-CA-C	-5.38	101.17	111.40
2	F	302	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	121	ASP	CB-CG-OD2	5.37	123.13	118.30
2	F	492	LEU	CB-CG-CD1	-5.37	101.87	111.00
2	H	309	ASP	CB-CG-OD2	5.37	123.13	118.30
2	D	221	MET	CG-SD-CE	-5.36	91.63	100.20
1	G	53	ASP	CB-CG-OD2	5.34	123.11	118.30
2	H	290	ASP	CB-CG-OD2	5.33	123.10	118.30
1	E	239	ASP	CB-CG-OD2	5.33	123.10	118.30
2	B	420	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	G	218	ASP	CB-CG-OD2	5.32	123.09	118.30
2	H	312	MET	CG-SD-CE	-5.32	91.69	100.20
2	F	512	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	H	420	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	E	187	ASP	CB-CG-OD2	5.29	123.06	118.30
2	H	110	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	G	329	ASP	CB-CG-OD2	5.27	123.05	118.30
2	F	150	ASP	CB-CG-OD2	5.26	123.04	118.30
1	G	409	ASP	CB-CG-OD2	5.24	123.02	118.30
2	B	453	VAL	CB-CA-C	-5.23	101.46	111.40
1	C	128	LEU	CA-CB-CG	5.23	127.33	115.30
1	C	91	VAL	CG1-CB-CG2	5.23	119.26	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	430	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	D	255	MET	CG-SD-CE	5.22	108.55	100.20
1	G	405	ASP	CB-CG-OD2	5.21	122.99	118.30
2	F	88	THR	OG1-CB-CG2	-5.20	98.03	110.00
1	A	291	ILE	CG1-CB-CG2	-5.20	99.96	111.40
2	B	25	ASP	CB-CG-OD2	5.20	122.98	118.30
2	D	517	ASP	CB-CG-OD1	5.18	122.96	118.30
1	G	417	LEU	CA-CB-CG	-5.18	103.39	115.30
2	D	13	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	447	VAL	CB-CA-C	-5.16	101.59	111.40
1	G	239	ASP	CB-CG-OD2	5.16	122.94	118.30
2	H	476	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	634	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	51	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	254	LYS	CD-CE-NZ	-5.15	99.86	111.70
2	H	35	LEU	CB-CA-C	-5.15	100.42	110.20
2	B	38	GLY	N-CA-C	-5.14	100.24	113.10
2	D	509	VAL	CA-CB-CG1	5.14	118.61	110.90
2	F	262	ASP	CB-CG-OD2	5.14	122.93	118.30
2	D	21	ARG	CB-CA-C	-5.13	100.15	110.40
1	A	218	ASP	CB-CG-OD2	5.11	122.90	118.30
2	H	756	ASP	CB-CG-OD1	5.11	122.90	118.30
2	D	635	ARG	NE-CZ-NH2	-5.11	117.75	120.30
2	H	542	ASP	CB-CG-OD2	5.08	122.88	118.30
2	H	752	PRO	N-CD-CG	-5.08	95.58	103.20
1	A	421	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	239	ASP	CB-CG-OD2	5.07	122.86	118.30
2	B	151	VAL	CB-CA-C	-5.06	101.78	111.40
2	B	462	THR	N-CA-C	5.05	124.65	111.00
1	G	43	ASP	CB-CA-C	-5.05	100.29	110.40
2	F	256	ARG	NE-CZ-NH1	-5.04	117.78	120.30
2	B	185	PRO	CB-CA-C	-5.03	99.42	112.00
1	E	161	ASP	CB-CG-OD2	5.02	122.82	118.30
2	F	507	ASP	CB-CG-OD2	5.02	122.82	118.30
2	D	251	ARG	CA-CB-CG	5.00	124.41	113.40
2	F	259	ARG	NE-CZ-NH1	-5.00	117.80	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	125	0
1	C	3370	0	3368	82	0
1	E	3370	0	3368	177	0
1	G	3370	0	3370	189	0
2	B	5717	0	5630	162	0
2	D	5717	0	5631	153	0
2	F	5717	0	5631	181	0
2	H	5717	0	5630	214	0
3	A	8	0	0	0	0
3	C	8	0	0	0	0
3	E	8	0	0	2	0
3	G	8	0	0	3	0
4	A	53	0	31	6	0
4	C	53	0	30	3	0
4	E	53	0	31	6	0
4	G	53	0	31	11	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	1	0
6	D	24	0	10	2	0
6	F	24	0	10	1	0
6	H	24	0	10	2	0
7	B	4	0	0	5	0
7	D	4	0	0	5	0
7	F	4	0	0	2	0
7	H	4	0	0	5	0
8	A	11	0	0	1	0
8	B	26	0	0	1	0
8	C	7	0	0	0	0
8	D	25	0	0	1	0
8	E	7	0	0	0	0
8	F	20	0	0	0	0
8	G	6	0	0	6	0
8	H	21	0	0	4	0
All	All	36831	0	36159	1239	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (1239) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:MET:SD	1:E:316:MET:CE	2.07	1.42
1:G:325:TYR:CE1	1:G:326:ARG:HG2	1.64	1.33
1:E:325:TYR:O	1:E:326:ARG:HB2	1.41	1.18
2:F:621:TYR:CE1	2:F:726:LYS:HG2	1.84	1.11
1:G:325:TYR:CD1	1:G:326:ARG:HG2	1.85	1.11
1:G:325:TYR:CE1	1:G:326:ARG:CG	2.33	1.10
1:E:381:ARG:HH21	1:E:393:ARG:NH2	1.56	1.04
2:H:66:THR:HG22	2:H:68:ALA:H	1.23	1.03
2:F:446:ARG:NH1	2:F:630:GLU:OE2	1.92	1.02
2:B:247:ARG:HG2	2:B:247:ARG:HH11	1.22	1.00
1:A:358:ASP:OD2	2:B:702:SER:OG	1.80	1.00
1:A:425:LEU:HD12	2:F:579:SER:HB3	1.42	0.99
1:E:381:ARG:HH21	1:E:393:ARG:CZ	1.80	0.95
1:E:445:ARG:NH2	2:F:634:ASP:OD2	2.00	0.94
1:A:348:LEU:HD12	1:A:349:ARG:H	1.27	0.94
2:D:247:ARG:HH11	2:D:247:ARG:HG2	1.30	0.94
1:G:136:CYS:HG	3:G:3001:FES:FE1	0.84	0.92
2:F:559:GLU:OE1	2:F:578:LYS:NZ	2.02	0.90
1:G:325:TYR:O	1:G:326:ARG:HB2	1.69	0.90
2:D:507:ASP:OD1	2:D:508:PRO:HD2	1.69	0.90
4:G:3005:FAD:H8A	4:G:3005:FAD:H51A	1.53	0.90
2:F:621:TYR:HE1	2:F:726:LYS:HG2	1.26	0.88
2:F:216:ASP:OD1	2:H:512:ARG:HD2	1.73	0.88
1:A:348:LEU:HD12	1:A:349:ARG:N	1.89	0.87
2:B:66:THR:HG22	2:B:68:ALA:H	1.38	0.87
2:H:87:ALA:O	8:H:3009:HOH:O	1.92	0.87
1:C:390:VAL:HG22	1:C:391:PRO:HD2	1.55	0.86
4:G:3005:FAD:C8A	4:G:3005:FAD:H51A	2.06	0.86
2:H:671:GLY:O	2:H:674:TRP:HB3	1.75	0.86
2:H:621:TYR:CE1	2:H:726:LYS:HG2	2.12	0.85
2:F:24:ASP:OD2	2:F:254:LYS:NZ	2.09	0.85
1:A:373:LYS:HB2	1:A:378:GLU:HG2	1.58	0.85
2:H:446:ARG:HG2	2:H:632:VAL:HG12	1.57	0.85
1:A:325:TYR:O	1:A:326:ARG:HB2	1.75	0.84
2:H:247:ARG:HH11	2:H:247:ARG:HG2	1.39	0.84
2:D:229:GLY:HA2	7:D:3004:MOS:S	2.18	0.84
1:A:138:GLY:O	1:A:139:TYR:HB2	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ARG:HG2	2:B:247:ARG:NH1	1.90	0.83
1:E:337:GLU:O	1:E:338:SER:HB3	1.79	0.83
2:D:621:TYR:HE1	2:D:726:LYS:HG2	1.42	0.83
1:A:408:GLU:OE1	2:B:442:ARG:NH2	2.11	0.82
2:F:247:ARG:HH11	2:F:247:ARG:HG2	1.42	0.82
2:D:559:GLU:OE1	2:D:578:LYS:NZ	2.11	0.81
4:G:3005:FAD:C5B	4:G:3005:FAD:H8A	2.11	0.81
2:D:621:TYR:CE1	2:D:726:LYS:HG2	2.16	0.81
1:E:352:LYS:HE3	1:E:362:SER:OG	1.80	0.81
1:G:373:LYS:HB2	1:G:378:GLU:HG2	1.63	0.81
2:F:35:LEU:HD23	2:F:35:LEU:N	1.95	0.80
2:H:446:ARG:HG2	2:H:632:VAL:CG1	2.11	0.80
1:G:237:THR:OG1	1:G:238:PRO:HD2	1.82	0.80
1:G:301:MET:CE	1:G:341:LEU:HB3	2.13	0.79
2:D:446:ARG:HG2	2:D:632:VAL:HG13	1.65	0.79
1:E:360:ASP:OD1	2:F:697:LYS:HE3	1.83	0.78
1:E:381:ARG:NH2	1:E:393:ARG:CZ	2.45	0.78
1:E:77:THR:OG1	1:E:79:GLU:HG2	1.83	0.78
2:H:138:ARG:NH2	2:H:329:HIS:ND1	2.30	0.78
2:F:34:HIS:C	2:F:35:LEU:HD23	2.03	0.78
2:B:446:ARG:HG2	2:B:632:VAL:HG13	1.64	0.78
1:A:301:MET:HE1	1:A:341:LEU:HD13	1.66	0.78
1:C:322:PHE:HB3	1:C:390:VAL:CG2	2.14	0.78
2:F:590:TYR:CE1	2:H:466:GLN:NE2	2.51	0.77
2:F:70:LEU:HD12	2:F:74:ASN:HB2	1.65	0.77
1:G:359:GLN:HG3	1:G:359:GLN:O	1.81	0.77
1:G:295:PRO:HB2	1:G:296:PRO:HD3	1.64	0.77
6:H:3003:MTE:S1'	7:H:3004:MOS:S	2.82	0.77
1:C:337:GLU:O	1:C:338:SER:HB3	1.84	0.77
2:H:66:THR:HG22	2:H:68:ALA:N	2.00	0.77
1:E:12:ARG:HH11	1:E:12:ARG:HG3	1.48	0.76
1:A:237:THR:OG1	1:A:238:PRO:HD2	1.85	0.75
1:C:325:TYR:O	1:C:326:ARG:HB2	1.87	0.75
2:H:730:GLU:C	2:H:732:PRO:HD2	2.07	0.75
2:B:138:ARG:NH2	2:B:329:HIS:ND1	2.35	0.74
2:F:138:ARG:NH2	2:F:329:HIS:ND1	2.34	0.74
1:G:252:LEU:CD2	1:G:281:ILE:HD12	2.17	0.74
2:D:267:GLY:C	2:D:268:LYS:HG3	2.07	0.74
1:E:355:LYS:HE2	2:F:679:GLU:OE1	1.87	0.74
1:C:237:THR:OG1	1:C:238:PRO:HD2	1.87	0.74
1:E:302:GLY:HA2	1:E:381:ARG:HH11	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:ASP:OD1	2:D:691:HIS:CD2	2.40	0.74
1:G:237:THR:HG23	1:G:239:ASP:H	1.52	0.74
1:G:393:ARG:HD2	1:G:398:GLU:OE1	1.88	0.74
1:A:359:GLN:O	1:A:359:GLN:HG3	1.87	0.73
2:H:507:ASP:OD1	2:H:508:PRO:HD2	1.88	0.73
2:D:138:ARG:NH2	2:D:329:HIS:ND1	2.35	0.73
4:A:3005:FAD:H51A	4:A:3005:FAD:H8A	1.69	0.73
2:D:631:VAL:HG21	2:D:743:LEU:HD13	1.68	0.73
4:A:3005:FAD:H51A	4:A:3005:FAD:C8A	2.19	0.73
2:B:247:ARG:HH11	2:B:247:ARG:CG	2.02	0.73
2:H:303:LEU:O	2:H:306:PRO:HD2	1.89	0.73
2:B:446:ARG:HG2	2:B:632:VAL:CG1	2.18	0.73
1:E:368:LEU:HD12	1:E:368:LEU:N	2.04	0.73
2:F:507:ASP:OD1	2:F:508:PRO:HD2	1.89	0.72
2:D:305:LEU:HB3	2:D:306:PRO:HD3	1.71	0.72
1:A:24:LEU:HD21	1:A:37:GLU:HB2	1.70	0.72
1:G:368:LEU:HD12	1:G:368:LEU:N	2.03	0.72
1:E:89:HIS:ND1	1:E:90:PRO:HD2	2.05	0.72
1:G:325:TYR:CE1	1:G:326:ARG:HG3	2.24	0.72
7:D:3004:MOS:S	7:D:3004:MOS:MO	2.00	0.72
1:G:138:GLY:O	1:G:139:TYR:HB2	1.89	0.72
1:E:358:ASP:OD2	2:F:702:SER:HB3	1.89	0.72
1:G:50:MET:CE	1:G:116:ALA:HA	2.20	0.72
2:B:776:ARG:O	2:B:777:ALA:HB3	1.89	0.72
2:D:507:ASP:OD1	2:D:508:PRO:CD	2.37	0.72
2:F:451:SER:HB3	2:F:738:SER:HB3	1.69	0.72
1:G:33:THR:O	1:G:36:LYS:NZ	2.16	0.72
2:B:398:LYS:HE3	2:B:398:LYS:N	2.04	0.72
2:H:561:CYS:SG	2:H:562:ALA:N	2.62	0.72
2:D:310:ARG:HD2	2:D:344:PHE:O	1.90	0.71
2:H:247:ARG:NH1	2:H:247:ARG:HG2	2.05	0.71
1:A:423:THR:O	1:A:423:THR:HG22	1.88	0.71
2:D:24:ASP:OD2	2:D:254:LYS:NZ	2.23	0.71
1:E:279:ALA:HB1	4:E:3005:FAD:H4'	1.71	0.71
1:E:301:MET:HE2	1:E:341:LEU:HD13	1.72	0.71
2:H:673:GLY:O	2:H:678:GLU:HB2	1.90	0.71
2:H:66:THR:CG2	2:H:68:ALA:H	2.03	0.71
1:G:325:TYR:O	1:G:326:ARG:CB	2.38	0.71
1:G:367:CYS:C	1:G:368:LEU:HD12	2.10	0.71
2:H:35:LEU:HB2	2:H:255:MET:HG3	1.73	0.71
1:A:455:VAL:HG22	2:B:443:THR:HG21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:305:LEU:HB3	2:F:306:PRO:HD3	1.71	0.71
7:F:3004:MOS:MO	7:F:3004:MOS:S	2.02	0.71
1:G:252:LEU:HD22	1:G:281:ILE:HD12	1.72	0.71
1:E:24:LEU:HD21	1:E:37:GLU:HB2	1.72	0.70
2:F:218:ARG:NE	2:F:220:GLU:OE2	2.24	0.70
2:F:593:ARG:NH1	2:H:604:THR:O	2.20	0.70
2:D:247:ARG:NH1	2:D:247:ARG:HG2	1.98	0.70
1:E:3:ILE:HD13	1:E:16:ILE:HD11	1.73	0.70
1:A:360:ASP:OD1	2:B:697:LYS:HE3	1.91	0.70
1:G:353:LEU:HD21	1:G:434:TYR:OH	1.92	0.70
1:A:390:VAL:HG22	1:A:391:PRO:HD2	1.73	0.70
2:D:398:LYS:HE3	2:D:398:LYS:N	2.07	0.69
2:H:296:ARG:NH1	2:H:296:ARG:HG3	2.06	0.69
1:A:95:MET:HG3	1:A:111:ILE:HD11	1.71	0.69
2:F:425:ALA:O	2:F:426:ASN:HB2	1.92	0.69
1:A:301:MET:CE	1:A:341:LEU:HB3	2.22	0.69
2:H:450:LEU:HG	2:H:451:SER:N	1.99	0.69
1:E:88:LEU:HD21	2:F:13:ARG:NH2	2.08	0.69
2:F:512:ARG:HD2	2:H:216:ASP:OD1	1.93	0.69
1:G:44:CYS:N	3:G:3002:FES:S1	2.63	0.69
2:H:776:ARG:O	2:H:777:ALA:HB3	1.91	0.69
1:E:314:ARG:HD3	1:E:334:GLU:OE1	1.93	0.68
2:H:731:PRO:N	2:H:732:PRO:HD2	2.07	0.68
2:F:247:ARG:NH1	2:F:247:ARG:HG2	2.02	0.68
4:C:3005:FAD:N1	4:C:3005:FAD:H2'	2.08	0.68
2:H:531:SER:OG	8:H:3027:HOH:O	2.11	0.68
2:H:269:ARG:NH2	2:H:341:PHE:CD2	2.62	0.68
1:G:445:ARG:NH2	2:H:634:ASP:OD2	2.27	0.68
1:A:361:ILE:HD12	1:A:429:ARG:NH2	2.08	0.68
1:E:319:GLU:OE2	1:E:319:GLU:N	2.22	0.68
1:E:301:MET:CE	1:E:341:LEU:HB3	2.24	0.68
1:E:322:PHE:HB3	1:E:390:VAL:HG23	1.75	0.68
1:E:415:LEU:HB3	1:E:440:GLN:HG2	1.76	0.68
2:B:34:HIS:C	2:B:35:LEU:HD23	2.14	0.67
1:C:32:LEU:HD22	1:C:79:GLU:HG3	1.75	0.67
2:D:66:THR:HG22	2:D:68:ALA:H	1.59	0.67
1:C:53:ASP:OD2	1:C:58:ARG:NH2	2.27	0.67
2:H:296:ARG:HH11	2:H:296:ARG:HG3	1.57	0.67
2:B:238:LEU:HD12	2:B:238:LEU:H	1.59	0.67
2:H:527:THR:OG1	8:H:3021:HOH:O	2.12	0.67
1:C:359:GLN:HG2	1:C:359:GLN:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:737:ILE:HG22	2:H:741:LEU:CD2	2.24	0.67
2:F:657:PRO:O	2:F:661:ILE:HG12	1.95	0.67
1:E:12:ARG:CG	1:E:12:ARG:HH11	2.08	0.67
1:C:301:MET:HE1	1:C:341:LEU:HD13	1.77	0.67
7:B:3004:MOS:MO	7:B:3004:MOS:S	2.06	0.67
1:E:325:TYR:O	1:E:326:ARG:CB	2.26	0.67
2:B:776:ARG:O	2:B:777:ALA:CB	2.43	0.66
2:F:23:LEU:HD13	2:F:194:CYS:HA	1.77	0.66
1:G:366:GLY:HA3	1:G:442:MET:SD	2.35	0.66
1:E:192:TRP:O	1:E:196:HIS:HD2	1.78	0.66
1:E:237:THR:HG23	1:E:238:PRO:CD	2.24	0.66
1:E:58:ARG:HD3	1:E:277:GLN:OE1	1.96	0.66
1:E:295:PRO:HB2	1:E:296:PRO:HD3	1.77	0.66
2:H:310:ARG:HD2	2:H:344:PHE:O	1.96	0.66
2:B:631:VAL:HG21	2:B:743:LEU:HD13	1.77	0.66
2:D:303:LEU:O	2:D:306:PRO:HD2	1.95	0.66
2:F:260:ASP:OD1	2:F:691:HIS:CD2	2.48	0.66
1:G:111:ILE:HD13	1:G:114:MET:HE3	1.78	0.66
4:G:3005:FAD:C5B	4:G:3005:FAD:C8A	2.71	0.66
2:B:440:THR:HG22	2:B:440:THR:O	1.95	0.66
1:E:252:LEU:HD12	1:E:252:LEU:O	1.96	0.66
2:F:425:ALA:O	2:F:426:ASN:CB	2.44	0.66
7:H:3004:MOS:MO	7:H:3004:MOS:S	2.07	0.66
2:D:377:TYR:CE1	2:D:454:LYS:HE3	2.31	0.66
2:D:660:ASP:OD1	2:D:728:VAL:HG11	1.96	0.66
1:E:322:PHE:HB3	1:E:390:VAL:CG2	2.26	0.66
1:G:37:GLU:CD	2:H:256:ARG:HH21	2.00	0.65
2:D:440:THR:O	2:D:440:THR:HG22	1.97	0.65
2:H:272:PHE:CD2	2:H:348:GLN:HG2	2.31	0.65
1:E:399:ALA:O	1:E:401:LEU:N	2.29	0.65
1:E:7:LEU:HD12	1:E:75:LEU:HD23	1.78	0.65
1:G:95:MET:HG3	1:G:111:ILE:HD11	1.78	0.65
1:A:32:LEU:HD22	1:A:79:GLU:HG3	1.79	0.65
1:E:316:MET:HB2	1:E:317:PRO:HD2	1.79	0.65
1:G:381:ARG:NH1	8:G:3010:HOH:O	2.29	0.65
1:G:408:GLU:OE1	2:H:442:ARG:NH2	2.26	0.65
1:G:37:GLU:CD	2:H:256:ARG:NH2	2.50	0.65
1:A:122:ARG:NH2	1:A:124:ASP:OD2	2.30	0.65
2:B:310:ARG:HD2	2:B:344:PHE:O	1.97	0.65
1:E:138:GLY:O	1:E:139:TYR:HB2	1.97	0.65
1:G:37:GLU:OE2	2:H:256:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:267:GLY:O	2:H:268:LYS:HG3	1.96	0.65
1:E:237:THR:HG23	1:E:239:ASP:H	1.60	0.65
2:D:251:ARG:HB3	2:D:252:PRO:HD2	1.78	0.64
2:D:704:ARG:HG2	2:D:704:ARG:HH11	1.62	0.64
1:C:252:LEU:CD2	1:C:281:ILE:HD12	2.28	0.64
1:A:337:GLU:HG3	1:A:337:GLU:O	1.98	0.64
2:B:251:ARG:HB3	2:B:252:PRO:HD2	1.78	0.64
2:D:704:ARG:HH11	2:D:704:ARG:CG	2.10	0.64
2:B:296:ARG:NH1	2:B:296:ARG:HG3	2.11	0.64
2:F:221:MET:HE1	2:F:224:MET:HG3	1.79	0.64
2:B:367:ASP:OD1	2:B:368:PRO:HD2	1.98	0.64
1:E:233:GLN:OE1	1:E:233:GLN:HA	1.97	0.64
1:G:348:LEU:HD12	1:G:349:ARG:H	1.62	0.64
2:H:440:THR:HG22	2:H:440:THR:O	1.96	0.64
2:D:202:ILE:HD13	2:D:236:ASN:HD22	1.63	0.64
2:F:281:ASP:OD1	2:F:283:SER:OG	2.07	0.64
1:A:237:THR:HG23	1:A:239:ASP:H	1.62	0.64
1:G:58:ARG:HD3	1:G:277:GLN:OE1	1.97	0.64
1:E:115:ALA:O	1:E:116:ALA:C	2.36	0.64
2:B:617:ARG:HD3	2:B:619:PHE:O	1.98	0.64
1:E:373:LYS:HB2	1:E:378:GLU:HG2	1.79	0.64
2:F:532:GLY:N	6:F:3003:MTE:O1P	2.29	0.64
2:F:451:SER:HB3	2:F:738:SER:CB	2.28	0.64
1:G:91:VAL:HG12	1:G:111:ILE:HD12	1.79	0.64
1:A:425:LEU:CD1	2:F:579:SER:HB3	2.24	0.63
1:G:41:GLU:HG3	1:G:214:LYS:HE3	1.79	0.63
1:G:44:CYS:O	8:G:3007:HOH:O	2.15	0.63
2:F:197:GLN:HA	2:F:224:MET:HE1	1.80	0.63
2:H:12:ALA:O	2:H:13:ARG:C	2.35	0.63
7:H:3004:MOS:O2	7:H:3004:MOS:MO	1.70	0.63
2:F:422:GLN:HG2	2:F:427:PHE:CD2	2.33	0.63
2:H:35:LEU:HA	2:H:101:VAL:O	1.98	0.63
2:D:644:ARG:HG3	2:D:707:ILE:HB	1.79	0.63
2:D:728:VAL:HG22	2:D:728:VAL:O	1.97	0.63
7:D:3004:MOS:O2	7:D:3004:MOS:MO	1.70	0.63
1:E:354:SER:HB2	1:E:360:ASP:OD2	1.99	0.63
2:H:372:ARG:O	2:H:373:ALA:C	2.37	0.63
1:A:302:GLY:HA2	8:A:3012:HOH:O	1.98	0.62
4:E:3005:FAD:H2'	4:E:3005:FAD:N1	2.13	0.62
2:F:498:GLN:O	2:F:499:VAL:C	2.33	0.62
2:D:339:THR:OG1	2:D:340:ALA:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1:MET:HE3	1:E:179:PRO:HA	1.81	0.62
2:D:730:GLU:N	2:D:731:PRO:CD	2.62	0.62
2:H:446:ARG:NH1	2:H:630:GLU:OE2	2.28	0.62
2:B:450:LEU:HG	2:B:451:SER:N	2.14	0.62
1:C:360:ASP:OD1	2:D:697:LYS:HE3	2.00	0.62
1:E:302:GLY:HA2	1:E:381:ARG:NH1	2.15	0.62
1:G:34:GLY:HA2	1:G:36:LYS:HZ2	1.65	0.62
1:G:34:GLY:HA2	1:G:36:LYS:NZ	2.15	0.62
2:H:339:THR:OG1	2:H:340:ALA:N	2.28	0.62
2:H:592:ALA:O	2:H:593:ARG:HB2	1.98	0.62
4:A:3005:FAD:N1	4:A:3005:FAD:H2'	2.14	0.62
2:D:776:ARG:O	2:D:777:ALA:HB3	2.00	0.62
2:F:238:LEU:HD12	2:F:238:LEU:H	1.63	0.62
2:F:367:ASP:OD1	2:F:368:PRO:HD2	2.00	0.62
2:F:66:THR:CG2	2:F:68:ALA:H	2.12	0.62
2:B:296:ARG:HH11	2:B:296:ARG:HG3	1.65	0.62
1:C:165:THR:O	1:C:166:LEU:HD23	1.98	0.62
1:E:381:ARG:NH2	1:E:393:ARG:NH2	2.38	0.62
2:F:310:ARG:HD2	2:F:344:PHE:O	2.00	0.62
1:G:50:MET:HE3	1:G:116:ALA:CA	2.29	0.62
2:F:440:THR:O	2:F:440:THR:HG22	2.00	0.62
2:H:305:LEU:HB3	2:H:306:PRO:HD3	1.80	0.62
2:H:559:GLU:O	2:H:560:GLY:O	2.18	0.62
2:D:446:ARG:NH1	2:D:630:GLU:OE2	2.31	0.61
1:G:81:ILE:HG22	1:G:81:ILE:O	2.01	0.61
1:G:127:ASP:OD1	1:G:268:ARG:HD2	2.01	0.61
2:F:512:ARG:NH1	2:H:216:ASP:OD2	2.33	0.61
1:C:301:MET:HE2	1:C:341:LEU:HD22	1.82	0.61
1:E:301:MET:HE3	1:E:341:LEU:HB3	1.82	0.61
2:B:221:MET:O	2:B:221:MET:HG3	2.00	0.61
2:H:457:ILE:O	2:H:458:SER:HB2	1.99	0.61
2:H:621:TYR:HE1	2:H:726:LYS:HG2	1.65	0.61
1:A:337:GLU:O	1:A:338:SER:HB3	2.01	0.61
2:B:24:ASP:OD2	2:B:254:LYS:NZ	2.30	0.60
1:G:44:CYS:C	8:G:3007:HOH:O	2.40	0.60
2:D:110:ARG:NE	2:D:258:ASP:OD2	2.34	0.60
1:G:301:MET:HE1	1:G:341:LEU:HD13	1.82	0.60
1:A:407:ARG:NH1	1:A:409:ASP:OD2	2.34	0.60
2:H:457:ILE:O	2:H:458:SER:CB	2.49	0.60
2:D:422:GLN:HG2	2:D:427:PHE:CD2	2.36	0.60
1:E:33:THR:CG2	2:F:25:ASP:HB3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASN:HB3	1:A:381:ARG:HB2	1.84	0.60
1:C:301:MET:CE	1:C:341:LEU:HB3	2.32	0.60
2:D:731:PRO:N	2:D:732:PRO:HD2	2.17	0.60
1:E:95:MET:SD	1:E:114:MET:CE	2.90	0.60
1:G:297:ALA:HA	1:G:367:CYS:SG	2.42	0.60
2:F:215:HIS:ND1	2:H:478:SER:HB2	2.16	0.60
1:C:322:PHE:HB3	1:C:390:VAL:HG21	1.84	0.60
2:F:339:THR:OG1	2:F:340:ALA:N	2.34	0.60
2:F:507:ASP:OD1	2:F:508:PRO:CD	2.49	0.60
1:G:373:LYS:O	1:G:374:GLY:O	2.20	0.60
1:G:428:MET:N	1:G:428:MET:SD	2.74	0.60
1:E:95:MET:SD	1:E:114:MET:HE3	2.42	0.60
7:B:3004:MOS:MO	7:B:3004:MOS:O2	1.71	0.59
1:E:291:ILE:HG22	1:E:291:ILE:O	2.01	0.59
2:F:218:ARG:NH2	2:F:517:ASP:OD1	2.35	0.59
1:G:50:MET:HE3	1:G:116:ALA:HA	1.84	0.59
1:E:370:LEU:HD22	1:E:380:ALA:HA	1.83	0.59
1:G:281:ILE:HG23	1:G:282:GLY:N	2.17	0.59
1:G:301:MET:HE2	1:G:341:LEU:HB3	1.83	0.59
2:B:328:SER:OG	2:B:330:ARG:NH1	2.34	0.59
2:B:77:SER:O	2:B:205:LYS:NZ	2.29	0.59
2:D:367:ASP:OD1	2:D:368:PRO:HD2	2.02	0.59
1:E:349:ARG:NH1	1:E:450:LEU:HD21	2.16	0.59
2:B:271:ASP:OD2	2:B:296:ARG:NH1	2.35	0.59
1:C:390:VAL:CG2	1:C:391:PRO:HD2	2.30	0.59
1:E:95:MET:HG3	1:E:111:ILE:HD11	1.84	0.59
2:F:305:LEU:HB3	2:F:306:PRO:CD	2.33	0.59
2:H:776:ARG:O	2:H:777:ALA:CB	2.50	0.59
1:A:165:THR:O	1:A:166:LEU:HD23	2.02	0.59
1:E:348:LEU:HD12	1:E:349:ARG:H	1.67	0.59
1:G:359:GLN:O	1:G:359:GLN:CG	2.49	0.59
2:B:704:ARG:HG2	2:B:704:ARG:HH11	1.66	0.59
2:F:66:THR:HG22	2:F:68:ALA:H	1.67	0.59
2:H:221:MET:HE1	2:H:224:MET:HG3	1.84	0.59
2:F:450:LEU:HG	2:F:451:SER:N	2.18	0.59
2:F:617:ARG:HD3	2:F:619:PHE:O	2.02	0.59
1:G:165:THR:O	1:G:165:THR:HG23	2.03	0.59
6:D:3003:MTE:S1'	7:D:3004:MOS:O2	2.61	0.59
1:A:351:TYR:OH	1:A:449:GLU:OE1	2.13	0.59
1:E:205:GLY:O	1:E:209:SER:OG	2.20	0.59
2:H:306:PRO:HB2	2:H:344:PHE:CE2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:507:ASP:OD1	2:H:508:PRO:CD	2.51	0.58
1:E:302:GLY:CA	1:E:381:ARG:HH11	2.16	0.58
2:H:671:GLY:O	2:H:674:TRP:N	2.34	0.58
1:C:3:ILE:HG23	1:C:16:ILE:HD12	1.84	0.58
2:F:632:VAL:HG22	2:F:643:LEU:HD11	1.85	0.58
2:F:196:SER:O	2:F:224:MET:HE2	2.04	0.58
1:C:301:MET:CE	1:C:341:LEU:HD13	2.34	0.58
1:C:192:TRP:O	1:C:196:HIS:HD2	1.87	0.58
1:E:349:ARG:HD3	1:E:449:GLU:OE2	2.03	0.58
2:H:247:ARG:HH11	2:H:247:ARG:CG	2.15	0.58
1:A:122:ARG:HH21	1:A:124:ASP:CG	2.06	0.58
1:E:201:LEU:O	4:E:3005:FAD:O2B	2.11	0.58
1:A:233:GLN:OE1	1:A:233:GLN:HA	2.03	0.58
2:B:229:GLY:HA2	7:B:3004:MOS:S	2.44	0.58
1:C:164:PHE:O	1:C:166:LEU:HG	2.04	0.58
1:A:322:PHE:HB3	1:A:390:VAL:CG2	2.33	0.58
2:B:730:GLU:N	2:B:731:PRO:CD	2.66	0.58
2:D:631:VAL:HG21	2:D:743:LEU:CD1	2.34	0.58
1:E:152:GLU:OE1	1:E:153:PRO:HD2	2.03	0.58
1:E:183:PRO:O	1:E:228:CYS:SG	2.62	0.58
1:E:237:THR:CG2	1:E:239:ASP:H	2.16	0.58
1:E:367:CYS:C	1:E:368:LEU:HD12	2.24	0.58
2:F:730:GLU:OE2	7:F:3004:MOS:O1	2.21	0.58
1:A:143:LEU:HD23	1:A:143:LEU:O	2.03	0.57
1:A:41:GLU:HG3	1:A:214:LYS:HE3	1.85	0.57
2:D:450:LEU:HG	2:D:451:SER:N	2.17	0.57
1:A:105:PHE:CD1	2:B:177:GLU:HB2	2.39	0.57
2:F:776:ARG:O	2:F:777:ALA:HB3	2.04	0.57
2:H:341:PHE:O	2:H:342:ARG:C	2.41	0.57
1:A:390:VAL:HG22	1:A:391:PRO:CD	2.35	0.57
1:A:18:ASP:OD2	1:A:19:PRO:HD2	2.04	0.57
1:C:279:ALA:HB1	4:C:3005:FAD:H4'	1.86	0.57
1:C:252:LEU:HD22	1:C:281:ILE:HD12	1.86	0.57
2:F:661:ILE:HD11	2:F:712:LEU:HG	1.87	0.57
2:F:174:PHE:CZ	2:F:693:PRO:HG3	2.39	0.57
1:G:81:ILE:CG2	1:G:81:ILE:O	2.53	0.57
2:H:205:LYS:HB3	2:H:240:ILE:HD11	1.85	0.57
2:H:94:VAL:HG11	2:H:687:ARG:HG2	1.86	0.57
2:B:134:ALA:HB1	2:F:724:ARG:HH11	1.70	0.57
1:A:95:MET:HG3	1:A:111:ILE:CD1	2.35	0.57
2:B:281:ASP:OD1	2:B:283:SER:N	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:ILE:HD13	1:G:114:MET:CE	2.34	0.57
2:F:457:ILE:O	2:F:458:SER:CB	2.53	0.57
1:G:358:ASP:OD2	2:H:702:SER:OG	2.19	0.57
1:G:455:VAL:HG22	2:H:443:THR:HG21	1.87	0.57
1:A:297:ALA:HA	1:A:367:CYS:SG	2.45	0.57
1:C:314:ARG:O	1:C:315:ARG:HB2	2.05	0.57
1:E:429:ARG:O	1:E:430:ALA:HB2	2.05	0.57
1:G:302:GLY:HA2	8:G:3010:HOH:O	2.05	0.56
2:H:214:PHE:N	2:H:214:PHE:CD1	2.73	0.56
1:A:399:ALA:O	1:A:401:LEU:N	2.38	0.56
2:B:305:LEU:HB3	2:B:306:PRO:HD3	1.86	0.56
1:C:373:LYS:HB2	1:C:378:GLU:HG2	1.87	0.56
2:D:238:LEU:H	2:D:238:LEU:HD12	1.69	0.56
1:E:399:ALA:C	1:E:401:LEU:H	2.08	0.56
1:G:314:ARG:HH22	1:G:329:ASP:CG	2.09	0.56
1:A:111:ILE:HD13	1:A:114:MET:HE3	1.86	0.56
2:H:229:GLY:HA2	7:H:3004:MOS:S	2.46	0.56
2:H:38:GLY:HA3	2:H:99:PHE:CE2	2.40	0.56
2:F:174:PHE:HZ	2:F:693:PRO:HG3	1.70	0.56
2:H:453:VAL:HG12	2:H:454:LYS:N	2.20	0.56
4:E:3005:FAD:H51A	4:E:3005:FAD:H8A	1.88	0.56
1:G:301:MET:HB3	1:G:348:LEU:HD22	1.88	0.56
2:D:214:PHE:N	2:D:214:PHE:CD1	2.74	0.56
1:G:295:PRO:HB2	1:G:296:PRO:CD	2.36	0.56
2:H:412:CYS:HA	2:H:624:TYR:CZ	2.40	0.56
1:C:124:ASP:O	1:C:128:LEU:HD22	2.06	0.56
2:B:216:ASP:OD1	2:D:512:ARG:HD2	2.06	0.56
1:C:237:THR:HG23	1:C:239:ASP:H	1.71	0.56
1:E:314:ARG:HH22	1:E:329:ASP:CG	2.09	0.56
1:E:281:ILE:HD11	1:E:298:LEU:HD11	1.87	0.56
1:A:295:PRO:HB2	1:A:296:PRO:HD3	1.87	0.56
1:E:415:LEU:N	1:E:416:PRO:CD	2.69	0.56
1:E:427:ASP:OD1	1:E:435:ARG:NH2	2.39	0.56
2:F:251:ARG:HB3	2:F:252:PRO:HD2	1.86	0.56
2:H:173:HIS:HA	2:H:341:PHE:CE1	2.39	0.56
2:B:166:PHE:CZ	2:B:355:ARG:HG3	2.40	0.55
2:B:66:THR:HG22	2:B:68:ALA:N	2.15	0.55
1:E:6:LEU:HD12	1:E:10:GLU:C	2.27	0.55
1:E:83:ALA:HB2	1:E:157:TRP:CZ3	2.40	0.55
2:F:328:SER:OG	2:F:330:ARG:NH1	2.36	0.55
1:G:53:ASP:OD1	1:G:53:ASP:C	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PHE:CE1	2:B:177:GLU:HB2	2.41	0.55
1:A:279:ALA:HB1	4:A:3005:FAD:H4'	1.87	0.55
1:C:316:MET:HB2	1:C:317:PRO:HD2	1.89	0.55
1:E:316:MET:HB2	1:E:317:PRO:CD	2.36	0.55
1:E:89:HIS:CE1	1:E:90:PRO:HD2	2.41	0.55
2:F:621:TYR:CE1	2:F:726:LYS:CG	2.76	0.55
2:H:528:ALA:O	2:H:529:ALA:HB3	2.06	0.55
1:A:301:MET:HB3	1:A:348:LEU:HD22	1.88	0.55
2:D:704:ARG:NH1	2:D:704:ARG:CG	2.68	0.55
1:E:237:THR:HG23	1:E:238:PRO:HD2	1.88	0.55
1:G:133:LEU:HD13	2:H:698:ILE:HD11	1.88	0.55
2:D:110:ARG:CZ	2:D:258:ASP:OD2	2.54	0.55
1:G:423:THR:HG22	1:G:423:THR:O	2.05	0.55
1:C:60:VAL:HG21	1:C:65:MET:CE	2.36	0.55
2:H:482:ASN:C	2:H:482:ASN:OD1	2.44	0.55
2:B:660:ASP:OD1	2:B:728:VAL:HG11	2.07	0.55
1:E:297:ALA:HA	1:E:367:CYS:SG	2.47	0.55
1:G:325:TYR:C	1:G:325:TYR:CD1	2.76	0.55
1:G:46:ALA:N	8:G:3007:HOH:O	2.39	0.55
2:H:312:MET:CE	2:H:330:ARG:HH12	2.20	0.55
2:H:736:GLY:O	2:H:737:ILE:C	2.45	0.55
2:B:267:GLY:C	2:B:268:LYS:HG3	2.27	0.55
1:C:390:VAL:HG22	1:C:391:PRO:CD	2.31	0.55
2:B:92:HIS:O	2:B:93:PHE:HB3	2.07	0.55
1:E:390:VAL:HG22	1:E:391:PRO:HD2	1.88	0.55
1:A:325:TYR:O	1:A:326:ARG:CB	2.52	0.54
1:G:348:LEU:HD12	1:G:349:ARG:N	2.23	0.54
2:B:737:ILE:HG22	2:B:741:LEU:HD22	1.89	0.54
2:D:731:PRO:HB2	2:D:732:PRO:HD3	1.88	0.54
2:D:737:ILE:HG22	2:D:741:LEU:HD22	1.89	0.54
1:A:446:TYR:CE2	1:A:450:LEU:HD12	2.42	0.54
1:E:447:VAL:O	1:E:448:ARG:C	2.46	0.54
2:F:573:VAL:HG21	2:F:585:ILE:HG13	1.90	0.54
2:H:448:ILE:O	2:H:448:ILE:HG23	2.07	0.54
2:H:730:GLU:O	2:H:731:PRO:C	2.45	0.54
2:H:668:TYR:O	2:H:669:VAL:C	2.45	0.54
1:A:26:LEU:HD13	1:A:67:LEU:HD11	1.89	0.54
2:D:94:VAL:HG11	2:D:687:ARG:HG2	1.90	0.54
1:E:301:MET:CE	1:E:341:LEU:HD13	2.37	0.54
2:B:407:GLN:OE1	2:B:618:PRO:HD2	2.08	0.54
2:F:704:ARG:O	2:F:704:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:CYS:HG	1:G:136:CYS:HG	1.53	0.54
1:G:237:THR:HG23	1:G:238:PRO:CD	2.38	0.54
1:G:240:GLY:HA2	1:G:343:LYS:HG2	1.88	0.54
2:F:631:VAL:HG21	2:F:743:LEU:HD13	1.89	0.54
1:G:206:THR:HG21	1:G:275:VAL:HG13	1.90	0.54
2:B:730:GLU:H	2:B:731:PRO:CD	2.21	0.54
2:F:604:THR:O	2:H:593:ARG:NH1	2.40	0.54
1:G:136:CYS:SG	3:G:3001:FES:S1	3.05	0.54
2:H:491:GLY:O	2:H:495:LYS:HG3	2.07	0.54
2:D:218:ARG:NE	2:D:220:GLU:OE2	2.40	0.53
2:D:731:PRO:HB2	2:D:732:PRO:CD	2.38	0.53
2:F:491:GLY:O	2:F:492:LEU:C	2.45	0.53
2:D:328:SER:OG	2:D:330:ARG:NH1	2.37	0.53
1:G:356:ARG:NH2	1:G:359:GLN:O	2.40	0.53
2:H:398:LYS:N	2:H:398:LYS:HE3	2.23	0.53
2:H:731:PRO:N	2:H:732:PRO:CD	2.71	0.53
2:H:631:VAL:HG21	2:H:743:LEU:HD13	1.90	0.53
1:A:423:THR:O	1:A:423:THR:CG2	2.56	0.53
2:D:229:GLY:CA	7:D:3004:MOS:S	2.94	0.53
1:E:7:LEU:CD1	1:E:75:LEU:HD23	2.38	0.53
2:F:210:LEU:HD22	2:F:247:ARG:HD3	1.89	0.53
1:E:359:GLN:HG3	1:E:359:GLN:O	2.08	0.53
1:E:445:ARG:HG3	1:E:455:VAL:HG11	1.89	0.53
1:E:68:PRO:HG2	1:E:224:PHE:CE1	2.43	0.53
2:F:164:GLY:HA3	2:F:276:TYR:CZ	2.43	0.53
1:A:165:THR:O	1:A:165:THR:HG23	2.08	0.53
2:H:346:GLY:N	2:H:347:PRO:CD	2.72	0.53
2:B:272:PHE:CD2	2:B:348:GLN:HG2	2.44	0.53
2:B:457:ILE:O	2:B:458:SER:CB	2.56	0.53
2:H:671:GLY:O	2:H:674:TRP:CB	2.51	0.53
2:D:407:GLN:OE1	2:D:618:PRO:HD2	2.07	0.53
4:E:3005:FAD:C8A	4:E:3005:FAD:H51A	2.38	0.53
2:F:728:VAL:HG22	2:F:728:VAL:O	2.09	0.53
2:H:210:LEU:HD22	2:H:247:ARG:HD3	1.89	0.53
2:B:341:PHE:O	2:B:342:ARG:C	2.47	0.53
1:E:133:LEU:HD13	2:F:698:ILE:HD11	1.89	0.53
1:G:237:THR:CB	1:G:238:PRO:HD2	2.39	0.53
2:H:312:MET:HE1	2:H:330:ARG:HH12	1.73	0.53
2:H:306:PRO:HB2	2:H:344:PHE:HE2	1.73	0.53
1:A:273:GLU:OE1	1:A:276:ARG:NH1	2.42	0.53
2:B:601:PHE:CG	2:D:595:SER:HB2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:MET:CE	1:E:341:LEU:HD22	2.39	0.53
2:F:698:ILE:HB	2:F:699:PRO:CD	2.38	0.53
1:G:116:ALA:O	1:G:117:ALA:C	2.46	0.53
2:H:196:SER:O	2:H:224:MET:HE2	2.09	0.53
2:H:701:PHE:O	2:H:704:ARG:HG2	2.09	0.53
1:C:314:ARG:HD3	1:C:334:GLU:OE1	2.09	0.53
1:E:370:LEU:CD2	1:E:380:ALA:HA	2.39	0.53
1:G:369:ASN:HB3	1:G:381:ARG:HB2	1.90	0.53
2:H:683:ASP:C	2:H:683:ASP:OD1	2.48	0.53
1:A:138:GLY:O	1:A:139:TYR:CB	2.52	0.52
1:E:253:ARG:NH2	1:E:268:ARG:HG3	2.23	0.52
2:F:23:LEU:HD22	2:F:180:ALA:HB1	1.91	0.52
2:F:195:SER:O	2:F:231:LYS:HD3	2.09	0.52
2:F:267:GLY:C	2:F:268:LYS:HG3	2.29	0.52
1:G:360:ASP:OD1	2:H:697:LYS:HE3	2.09	0.52
1:G:451:SER:O	1:G:451:SER:OG	2.22	0.52
2:H:453:VAL:CG1	2:H:454:LYS:N	2.70	0.52
2:H:730:GLU:N	2:H:731:PRO:CD	2.71	0.52
1:A:210:LEU:N	1:A:210:LEU:HD23	2.23	0.52
2:B:621:TYR:CE1	2:B:726:LYS:HG2	2.45	0.52
2:D:367:ASP:C	2:D:367:ASP:OD1	2.47	0.52
2:D:723:PHE:O	2:D:724:ARG:HB2	2.09	0.52
1:E:337:GLU:O	1:E:338:SER:CB	2.52	0.52
1:E:33:THR:HG21	2:F:25:ASP:HB3	1.92	0.52
2:F:367:ASP:OD2	2:F:431:ARG:NH1	2.32	0.52
1:G:325:TYR:O	1:G:325:TYR:CG	2.62	0.52
2:D:617:ARG:HD3	2:D:619:PHE:O	2.09	0.52
1:E:12:ARG:CG	1:E:12:ARG:NH1	2.68	0.52
1:E:237:THR:HG23	1:E:238:PRO:N	2.24	0.52
2:F:272:PHE:CD2	2:F:348:GLN:HG2	2.44	0.52
1:G:432:ALA:O	1:G:433:ALA:C	2.45	0.52
2:H:355:ARG:O	2:H:356:ALA:C	2.46	0.52
2:H:730:GLU:H	2:H:731:PRO:CD	2.22	0.52
2:B:174:PHE:HZ	2:B:693:PRO:HG3	1.75	0.52
1:G:359:GLN:NE2	4:G:3005:FAD:H6	2.25	0.52
2:D:306:PRO:HB2	2:D:344:PHE:CE2	2.45	0.52
2:H:79:ALA:HB1	2:H:80:PRO:HD2	1.91	0.52
2:D:210:LEU:HD22	2:D:247:ARG:HD3	1.91	0.52
1:E:395:ALA:O	1:E:396:ALA:C	2.48	0.52
1:E:216:LEU:HD12	2:F:114:ARG:HD2	1.91	0.52
2:H:737:ILE:HG22	2:H:741:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:ALA:O	1:E:253:ARG:N	2.40	0.52
2:H:328:SER:OG	2:H:330:ARG:NH1	2.39	0.52
2:B:210:LEU:HD22	2:B:247:ARG:HD3	1.92	0.52
2:B:634:ASP:OD2	2:B:637:THR:OG1	2.11	0.52
1:C:102:GLN:HB3	2:D:489:GLY:O	2.10	0.52
2:H:238:LEU:HD12	2:H:238:LEU:H	1.74	0.52
2:H:28:CYS:HB2	2:H:29:PRO:HD2	1.92	0.52
2:B:48:THR:HG22	2:B:119:THR:OG1	2.10	0.52
2:B:305:LEU:C	2:B:305:LEU:HD23	2.30	0.51
1:C:165:THR:HG23	1:C:165:THR:O	2.10	0.51
1:G:281:ILE:CG2	1:G:282:GLY:N	2.73	0.51
1:G:337:GLU:HG3	1:G:337:GLU:O	2.08	0.51
2:B:354:GLU:O	2:B:357:ILE:HG22	2.10	0.51
1:G:325:TYR:CZ	1:G:326:ARG:HG3	2.45	0.51
1:G:105:PHE:HD2	2:H:176:LEU:HB3	1.75	0.51
2:H:276:TYR:OH	2:H:359:HIS:HD2	1.94	0.51
4:E:3005:FAD:C2'	4:E:3005:FAD:N1	2.72	0.51
2:D:53:GLU:HA	2:D:53:GLU:OE1	2.09	0.51
2:F:717:ASN:O	2:F:724:ARG:HD3	2.11	0.51
2:F:721:THR:O	2:F:724:ARG:N	2.35	0.51
1:G:102:GLN:HB3	2:H:489:GLY:O	2.11	0.51
2:H:267:GLY:C	2:H:268:LYS:HG3	2.31	0.51
1:A:206:THR:HG21	1:A:275:VAL:HG13	1.92	0.51
2:D:635:ARG:HD3	2:D:750:CYS:SG	2.51	0.51
1:E:349:ARG:NH1	1:E:450:LEU:CD2	2.74	0.51
1:G:164:PHE:O	1:G:166:LEU:HG	2.11	0.51
1:G:387:MET:HE1	1:G:424:PRO:HG3	1.93	0.51
2:H:482:ASN:OD1	2:H:483:HIS:N	2.43	0.51
1:A:353:LEU:HD21	1:A:434:TYR:OH	2.11	0.51
1:C:83:ALA:HB1	1:C:84:PRO:HD2	1.93	0.51
2:D:164:GLY:HA3	2:D:276:TYR:CZ	2.46	0.51
1:E:301:MET:HE2	1:E:341:LEU:HD22	1.93	0.51
2:D:281:ASP:HB2	2:D:285:LYS:O	2.10	0.51
2:D:53:GLU:HB3	2:D:54:PRO:HD3	1.93	0.51
2:D:79:ALA:HB1	2:D:80:PRO:CD	2.41	0.51
1:E:126:ASP:OD1	2:F:704:ARG:NH1	2.33	0.51
1:E:237:THR:OG1	1:E:238:PRO:HD2	2.11	0.51
1:E:314:ARG:O	1:E:315:ARG:HB2	2.11	0.51
2:H:302:ASP:OD1	2:H:303:LEU:N	2.44	0.51
2:H:398:LYS:O	2:H:399:LYS:O	2.28	0.51
1:A:316:MET:HB2	1:A:317:PRO:CD	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:697:LYS:HD2	2:F:697:LYS:N	2.26	0.50
1:G:103:CYS:SG	1:G:136:CYS:SG	3.10	0.50
2:B:574:GLN:HG3	2:B:579:SER:HB2	1.92	0.50
2:F:398:LYS:C	2:F:399:LYS:HD2	2.31	0.50
2:F:730:GLU:N	2:F:731:PRO:CD	2.74	0.50
2:H:23:LEU:HD13	2:H:194:CYS:HA	1.93	0.50
1:A:53:ASP:C	1:A:53:ASP:OD1	2.48	0.50
2:B:214:PHE:N	2:B:214:PHE:CD1	2.77	0.50
1:E:380:ALA:O	1:E:398:GLU:HG2	2.12	0.50
1:E:450:LEU:C	1:E:452:GLY:H	2.14	0.50
1:G:39:CYS:SG	1:G:40:ASN:N	2.84	0.50
2:H:517:ASP:OD2	2:H:519:SER:N	2.33	0.50
2:D:272:PHE:CD2	2:D:348:GLN:HG2	2.46	0.50
1:G:140:ALA:N	1:G:141:PRO:HD2	2.26	0.50
1:G:337:GLU:O	1:G:338:SER:HB3	2.12	0.50
2:H:79:ALA:HB1	2:H:80:PRO:CD	2.41	0.50
2:H:251:ARG:CB	2:H:252:PRO:CD	2.90	0.50
2:H:440:THR:CG2	2:H:440:THR:O	2.60	0.50
1:A:237:THR:CB	1:A:238:PRO:HD2	2.42	0.50
2:F:731:PRO:N	2:F:732:PRO:HD2	2.26	0.50
1:G:295:PRO:CB	1:G:296:PRO:HD3	2.37	0.50
2:H:555:VAL:HG12	2:H:555:VAL:O	2.11	0.50
1:A:399:ALA:C	1:A:401:LEU:H	2.15	0.50
1:G:248:THR:HA	1:G:279:ALA:O	2.12	0.50
2:H:92:HIS:O	2:H:93:PHE:HB3	2.11	0.50
4:G:3005:FAD:H8A	4:G:3005:FAD:H52A	1.93	0.50
2:H:639:GLU:O	2:H:640:ASN:HB3	2.11	0.50
2:B:674:TRP:CE3	2:B:675:LEU:HD21	2.47	0.50
2:F:554:PHE:HB2	2:F:594:ILE:CD1	2.42	0.50
1:G:210:LEU:N	1:G:210:LEU:HD23	2.27	0.50
1:G:314:ARG:HD3	1:G:334:GLU:OE1	2.12	0.50
2:H:74:ASN:OD1	2:H:85:VAL:N	2.37	0.50
1:A:291:ILE:O	1:A:291:ILE:HG22	2.12	0.49
2:B:448:ILE:HG13	2:B:630:GLU:HB2	1.94	0.49
1:A:355:LYS:HE2	2:B:679:GLU:OE1	2.12	0.49
2:B:645:THR:HG21	2:B:668:TYR:CZ	2.47	0.49
1:C:53:ASP:OD1	1:C:53:ASP:C	2.51	0.49
1:E:33:THR:HG23	2:F:25:ASP:HB3	1.94	0.49
1:G:233:GLN:HA	1:G:233:GLN:OE1	2.11	0.49
1:G:299:ILE:O	1:G:300:ALA:C	2.49	0.49
2:H:296:ARG:HH11	2:H:296:ARG:CG	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:ASP:OD1	1:E:218:ASP:C	2.50	0.49
2:F:23:LEU:HD22	2:F:180:ALA:CB	2.42	0.49
1:G:369:ASN:O	1:G:370:LEU:HD23	2.11	0.49
2:B:348:GLN:OE1	2:B:348:GLN:N	2.44	0.49
1:C:337:GLU:O	1:C:337:GLU:HG3	2.11	0.49
2:F:70:LEU:HD12	2:F:74:ASN:CB	2.39	0.49
2:H:166:PHE:CZ	2:H:355:ARG:HG3	2.47	0.49
1:A:368:LEU:N	1:A:368:LEU:HD12	2.27	0.49
2:B:302:ASP:OD1	2:B:303:LEU:N	2.44	0.49
2:B:503:VAL:O	2:B:503:VAL:HG12	2.12	0.49
1:C:138:GLY:O	1:C:139:TYR:HB2	2.13	0.49
2:D:360:LEU:HG	2:D:364:MET:HE3	1.94	0.49
1:E:103:CYS:N	3:E:3001:FES:S1	2.85	0.49
1:G:349:ARG:HD3	1:G:449:GLU:OE2	2.12	0.49
2:F:346:GLY:N	2:F:347:PRO:CD	2.74	0.49
1:G:93:GLN:NE2	1:G:97:ASP:OD1	2.45	0.49
1:G:98:HIS:O	1:G:99:HIS:HB2	2.12	0.49
2:H:634:ASP:OD2	2:H:637:THR:OG1	2.28	0.49
1:E:50:MET:CE	1:E:116:ALA:HA	2.43	0.49
1:E:369:ASN:O	1:E:370:LEU:HD23	2.13	0.49
2:F:256:ARG:O	2:F:256:ARG:HG3	2.12	0.49
1:G:143:LEU:O	1:G:144:ARG:C	2.51	0.49
2:B:731:PRO:N	2:B:732:PRO:CD	2.76	0.49
1:C:237:THR:HG23	1:C:238:PRO:CD	2.43	0.49
1:C:346:PRO:O	1:C:349:ARG:NH2	2.46	0.49
2:D:367:ASP:OD1	2:D:368:PRO:CD	2.60	0.49
1:E:399:ALA:C	1:E:401:LEU:N	2.65	0.49
2:B:174:PHE:CZ	2:B:693:PRO:HG3	2.47	0.49
2:B:577:GLY:O	8:B:3011:HOH:O	2.19	0.49
2:F:440:THR:O	2:F:440:THR:CG2	2.60	0.49
2:F:617:ARG:NH1	2:F:620:LEU:O	2.46	0.49
2:F:74:ASN:OD1	2:F:85:VAL:N	2.42	0.49
1:G:122:ARG:NH2	1:G:124:ASP:OD2	2.46	0.49
1:A:281:ILE:HD11	1:A:298:LEU:HD11	1.94	0.49
2:B:730:GLU:C	2:B:732:PRO:HD2	2.33	0.49
1:E:69:GLN:NE2	1:E:203:ALA:O	2.46	0.49
2:F:33:LEU:HD21	2:F:251:ARG:NH1	2.27	0.49
1:C:359:GLN:O	1:C:359:GLN:CG	2.57	0.48
2:D:776:ARG:O	2:D:777:ALA:CB	2.61	0.48
1:E:249:ILE:O	1:E:250:ALA:C	2.48	0.48
1:G:61:ASN:ND2	1:G:274:GLN:HB3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HD12	2:B:114:ARG:HD2	1.95	0.48
1:C:37:GLU:CD	2:D:256:ARG:HH21	2.17	0.48
2:D:426:ASN:HD22	2:D:429:THR:HB	1.78	0.48
1:E:88:LEU:HD21	2:F:13:ARG:CZ	2.43	0.48
1:G:237:THR:HG23	1:G:238:PRO:N	2.26	0.48
1:A:252:LEU:CD2	1:A:281:ILE:HD12	2.43	0.48
2:B:166:PHE:CE1	2:B:355:ARG:HG3	2.49	0.48
2:B:281:ASP:OD1	2:B:283:SER:OG	2.27	0.48
2:B:635:ARG:HD3	2:B:750:CYS:SG	2.53	0.48
1:C:316:MET:HB2	1:C:317:PRO:CD	2.42	0.48
1:C:33:THR:CG2	2:D:25:ASP:HB3	2.44	0.48
2:F:648:LEU:HA	2:F:711:ALA:O	2.13	0.48
1:G:252:LEU:HD22	1:G:281:ILE:CD1	2.42	0.48
2:B:28:CYS:HB2	2:B:29:PRO:HD2	1.94	0.48
2:D:731:PRO:N	2:D:732:PRO:CD	2.77	0.48
1:E:337:GLU:HG3	1:E:337:GLU:O	2.13	0.48
2:F:398:LYS:N	2:F:398:LYS:HE3	2.27	0.48
1:G:325:TYR:HB2	1:G:389:GLY:CA	2.43	0.48
2:H:471:VAL:HG12	2:H:472:GLN:N	2.27	0.48
1:A:322:PHE:HB3	1:A:390:VAL:HG22	1.96	0.48
2:B:325:ARG:C	2:B:326:ILE:HG13	2.33	0.48
2:F:590:TYR:HE1	2:H:466:GLN:NE2	2.09	0.48
2:F:216:ASP:CG	2:H:512:ARG:HH11	2.16	0.48
2:H:730:GLU:H	2:H:731:PRO:HD2	1.78	0.48
2:B:601:PHE:CD1	2:D:595:SER:HB2	2.49	0.48
2:D:34:HIS:C	2:D:35:LEU:HD23	2.34	0.48
1:E:165:THR:HG23	1:E:165:THR:O	2.13	0.48
1:E:7:LEU:HD21	1:E:32:LEU:HD11	1.94	0.48
2:F:671:GLY:O	2:F:674:TRP:HB3	2.14	0.48
1:G:203:ALA:HB3	4:G:3005:FAD:O1P	2.14	0.48
2:H:34:HIS:C	2:H:35:LEU:HD23	2.34	0.48
1:A:367:CYS:C	1:A:368:LEU:HD12	2.34	0.48
7:B:3004:MOS:S	7:B:3004:MOS:O2	2.71	0.48
2:H:409:VAL:O	2:H:409:VAL:HG12	2.13	0.48
2:B:360:LEU:HG	2:B:364:MET:HE3	1.95	0.48
2:B:595:SER:HB2	2:D:601:PHE:CG	2.49	0.48
1:C:240:GLY:HA2	1:C:343:LYS:HG2	1.96	0.48
1:E:53:ASP:C	1:E:53:ASP:OD1	2.52	0.48
2:F:319:TYR:OH	2:F:372:ARG:HD3	2.12	0.48
2:H:298:GLY:HA3	2:H:337:SER:HA	1.96	0.48
2:B:35:LEU:HA	2:B:101:VAL:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:VAL:HG21	1:C:65:MET:HE1	1.96	0.48
2:D:175:TYR:O	2:D:259:ARG:NH2	2.42	0.48
2:D:218:ARG:NH2	2:D:517:ASP:OD1	2.46	0.48
1:E:387:MET:HE3	1:E:424:PRO:HG3	1.94	0.48
2:D:258:ASP:O	2:D:259:ARG:C	2.51	0.48
2:F:606:LYS:NZ	2:F:719:GLU:OE1	2.36	0.48
1:G:110:PHE:O	1:G:111:ILE:C	2.50	0.48
2:H:60:GLY:O	2:H:103:ALA:HB1	2.14	0.48
2:B:288:GLY:HA2	2:B:323:ALA:O	2.13	0.47
1:G:89:HIS:O	1:G:90:PRO:C	2.53	0.47
1:A:356:ARG:NH2	1:A:359:GLN:O	2.46	0.47
1:G:151:GLY:O	1:G:152:GLU:HG2	2.14	0.47
1:A:67:LEU:HA	1:A:67:LEU:HD23	1.68	0.47
2:B:148:ARG:HD3	2:B:322:PRO:O	2.14	0.47
1:C:237:THR:CB	1:C:238:PRO:HD2	2.44	0.47
1:G:31:GLY:O	1:G:33:THR:N	2.40	0.47
1:G:325:TYR:CZ	1:G:326:ARG:CG	2.93	0.47
2:H:380:PRO:HB3	2:H:410:ALA:O	2.14	0.47
1:A:281:ILE:HG23	1:A:282:GLY:N	2.28	0.47
2:B:560:GLY:O	2:B:561:CYS:HB3	2.15	0.47
1:C:37:GLU:CD	2:D:256:ARG:NH2	2.68	0.47
2:D:29:PRO:O	2:D:32:THR:OG1	2.25	0.47
2:H:448:ILE:O	2:H:448:ILE:CG2	2.62	0.47
2:B:168:ILE:HD13	2:B:351:LEU:HD23	1.97	0.47
1:E:324:GLU:O	1:E:325:TYR:C	2.53	0.47
1:E:322:PHE:CB	1:E:390:VAL:CG2	2.93	0.47
1:A:353:LEU:HD21	1:A:434:TYR:CZ	2.50	0.47
2:B:730:GLU:N	2:B:731:PRO:HD2	2.30	0.47
1:C:25:GLU:HG2	1:C:25:GLU:H	1.57	0.47
2:D:341:PHE:O	2:D:342:ARG:C	2.53	0.47
1:E:373:LYS:O	1:E:374:GLY:O	2.33	0.47
1:E:67:LEU:O	1:E:68:PRO:C	2.52	0.47
1:E:68:PRO:HB2	1:E:224:PHE:CE1	2.49	0.47
2:B:251:ARG:CB	2:B:252:PRO:HD2	2.44	0.47
4:C:3005:FAD:N1	4:C:3005:FAD:C2'	2.72	0.47
2:D:288:GLY:HA2	2:D:323:ALA:O	2.13	0.47
1:E:103:CYS:HB3	1:E:136:CYS:SG	2.55	0.47
1:E:139:TYR:C	1:E:141:PRO:HD2	2.35	0.47
2:H:239:ALA:O	2:H:240:ILE:C	2.53	0.47
2:H:53:GLU:N	2:H:54:PRO:CD	2.77	0.47
2:H:93:PHE:HD1	2:H:94:VAL:O	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:731:PRO:HB2	2:B:732:PRO:HD3	1.97	0.47
2:D:251:ARG:HB3	2:D:252:PRO:CD	2.44	0.47
2:D:621:TYR:CE1	2:D:726:LYS:CG	2.95	0.47
1:G:291:ILE:HG22	1:G:291:ILE:O	2.14	0.47
1:G:50:MET:CE	1:G:116:ALA:CA	2.87	0.47
1:G:67:LEU:HD23	1:G:67:LEU:HA	1.45	0.47
2:H:261:ASP:O	2:H:262:ASP:C	2.51	0.47
2:H:493:HIS:CG	2:H:513:ILE:HG12	2.50	0.47
2:B:28:CYS:HB2	2:B:29:PRO:CD	2.45	0.47
2:D:552:ALA:O	2:D:553:GLY:C	2.53	0.47
2:F:380:PRO:HB3	2:F:410:ALA:O	2.14	0.47
2:F:683:ASP:C	2:F:683:ASP:OD1	2.53	0.47
1:C:427:ASP:OD1	1:C:429:ARG:N	2.31	0.47
1:E:446:TYR:O	1:E:447:VAL:C	2.51	0.47
2:F:371:LEU:HA	2:F:371:LEU:HD12	1.76	0.47
2:F:452:PRO:HG2	2:F:452:PRO:O	2.14	0.47
2:F:721:THR:O	2:F:722:ILE:C	2.51	0.47
1:G:350:CYS:HG	1:G:367:CYS:HG	1.61	0.47
2:H:227:GLY:O	2:H:229:GLY:N	2.48	0.47
2:B:202:ILE:HD13	2:B:236:ASN:HD22	1.80	0.47
2:D:221:MET:HG3	2:D:221:MET:O	2.15	0.47
2:D:310:ARG:HD2	2:D:344:PHE:HB3	1.97	0.47
2:D:346:GLY:N	2:D:347:PRO:CD	2.78	0.47
2:B:422:GLN:HG2	2:B:427:PHE:CD2	2.50	0.46
1:C:373:LYS:O	1:C:374:GLY:O	2.33	0.46
2:D:325:ARG:C	2:D:326:ILE:HG13	2.34	0.46
2:F:568:PHE:CD2	2:F:573:VAL:HG22	2.49	0.46
2:H:536:ASN:O	2:H:537:GLY:C	2.51	0.46
2:H:559:GLU:O	2:H:560:GLY:C	2.53	0.46
1:A:401:LEU:HD11	1:A:411:ILE:HD13	1.97	0.46
1:A:37:GLU:CD	2:B:256:ARG:NH2	2.68	0.46
1:E:453:GLU:HG2	1:E:454:ALA:N	2.31	0.46
1:E:77:THR:O	1:E:78:ILE:C	2.53	0.46
2:F:354:GLU:OE1	2:F:372:ARG:NE	2.42	0.46
1:G:387:MET:HE2	1:G:439:ALA:HB2	1.98	0.46
1:G:83:ALA:HB2	1:G:157:TRP:CD2	2.49	0.46
1:A:153:PRO:HA	1:A:154:PRO:HD3	1.82	0.46
2:B:96:GLN:HA	2:B:97:PRO:HD3	1.86	0.46
1:G:192:TRP:O	1:G:196:HIS:HD2	1.98	0.46
2:H:418:VAL:O	2:H:421:LEU:N	2.47	0.46
2:H:7:LEU:HB3	2:H:8:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:VAL:HG12	1:A:91:VAL:O	2.07	0.46
2:B:671:GLY:O	2:B:674:TRP:HB3	2.16	0.46
1:C:139:TYR:O	1:C:140:ALA:C	2.52	0.46
2:D:221:MET:HE2	2:D:486:THR:HB	1.97	0.46
1:E:68:PRO:CB	1:E:224:PHE:CE1	2.98	0.46
1:E:248:THR:HA	1:E:279:ALA:O	2.15	0.46
2:F:547:LEU:O	2:F:550:ARG:N	2.49	0.46
1:G:348:LEU:HA	1:G:348:LEU:HD12	1.58	0.46
1:G:67:LEU:O	1:G:68:PRO:C	2.52	0.46
1:A:237:THR:HG23	1:A:238:PRO:CD	2.46	0.46
1:A:314:ARG:HD3	1:A:334:GLU:OE1	2.16	0.46
2:B:324:LEU:HD21	2:B:326:ILE:HD11	1.98	0.46
2:D:302:ASP:OD1	2:D:303:LEU:N	2.49	0.46
2:F:247:ARG:CG	2:F:247:ARG:HH11	2.19	0.46
2:H:517:ASP:C	2:H:517:ASP:OD2	2.53	0.46
1:A:141:PRO:HG2	1:A:142:ILE:N	2.31	0.46
2:B:507:ASP:OD1	2:B:508:PRO:HD2	2.16	0.46
1:C:165:THR:C	1:C:166:LEU:HD23	2.35	0.46
1:C:237:THR:HG23	1:C:238:PRO:N	2.31	0.46
1:C:281:ILE:HD11	1:C:298:LEU:HD11	1.96	0.46
1:E:44:CYS:N	3:E:3002:FES:S1	2.88	0.46
2:F:700:ALA:O	2:F:701:PHE:C	2.52	0.46
1:G:370:LEU:CD2	1:G:380:ALA:HA	2.46	0.46
2:H:529:ALA:O	2:H:530:SER:C	2.52	0.46
2:H:66:THR:CG2	2:H:67:ALA:N	2.77	0.46
2:H:701:PHE:HE2	2:H:704:ARG:NH1	2.14	0.46
1:A:376:LYS:HD3	1:A:403:GLY:O	2.14	0.46
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.76	0.46
2:D:51:ASP:HB3	2:D:117:ARG:HB2	1.97	0.46
2:D:645:THR:HG21	2:D:668:TYR:CZ	2.51	0.46
2:F:744:HIS:HE1	2:F:754:TRP:CZ3	2.34	0.46
2:H:133:LEU:HA	2:H:133:LEU:HD12	1.75	0.46
2:H:730:GLU:N	2:H:731:PRO:HD2	2.31	0.46
2:B:308:CYS:O	2:B:312:MET:HG3	2.15	0.46
2:B:51:ASP:HB3	2:B:117:ARG:HB2	1.98	0.46
2:D:278:ILE:HD11	2:D:286:LEU:HD22	1.98	0.46
1:E:89:HIS:ND1	1:E:90:PRO:CD	2.78	0.46
4:G:3005:FAD:N1	4:G:3005:FAD:H2'	2.30	0.46
2:H:128:THR:O	2:H:129:LEU:C	2.52	0.46
2:H:228:PHE:O	2:H:341:PHE:HA	2.16	0.46
2:H:617:ARG:HD3	2:H:619:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ARG:HH22	1:C:329:ASP:CG	2.19	0.46
1:C:67:LEU:HA	1:C:67:LEU:HD23	1.55	0.46
2:D:457:ILE:O	2:D:458:SER:CB	2.64	0.46
1:E:316:MET:CG	1:E:316:MET:CE	2.92	0.46
2:F:450:LEU:HD12	2:F:628:ILE:CG1	2.46	0.46
1:G:216:LEU:HD12	2:H:114:ARG:HD2	1.97	0.46
1:G:202:ILE:HD12	1:G:222:VAL:HG13	1.97	0.46
1:G:382:ILE:O	1:G:393:ARG:HA	2.16	0.46
2:H:632:VAL:HG13	2:H:643:LEU:HD11	1.97	0.46
2:D:79:ALA:HB1	2:D:80:PRO:HD2	1.98	0.46
1:E:390:VAL:HG22	1:E:391:PRO:CD	2.46	0.46
1:A:316:MET:HB2	1:A:317:PRO:HD2	1.98	0.45
1:A:301:MET:HE2	1:A:341:LEU:HB3	1.95	0.45
1:A:91:VAL:CG1	1:A:91:VAL:O	2.55	0.45
2:B:728:VAL:HG22	2:B:728:VAL:O	2.16	0.45
2:F:143:PRO:HB3	2:F:329:HIS:CE1	2.52	0.45
1:A:32:LEU:HD23	1:A:32:LEU:HA	1.67	0.45
1:A:349:ARG:HD3	1:A:449:GLU:OE2	2.15	0.45
1:A:370:LEU:HD23	1:A:380:ALA:HA	1.98	0.45
1:C:3:ILE:HG23	1:C:16:ILE:CD1	2.45	0.45
2:D:48:THR:O	2:D:48:THR:HG23	2.16	0.45
2:D:717:ASN:O	2:D:724:ARG:HD3	2.16	0.45
1:E:164:PHE:CG	1:E:165:THR:N	2.84	0.45
2:F:722:ILE:HA	2:F:722:ILE:HD12	1.78	0.45
1:G:335:PHE:HD1	1:G:336:VAL:O	1.98	0.45
1:A:356:ARG:CZ	2:B:697:LYS:NZ	2.80	0.45
2:B:437:TRP:CZ3	2:B:446:ARG:HG3	2.51	0.45
2:B:466:GLN:HA	2:B:602:TYR:O	2.16	0.45
2:B:704:ARG:CG	2:B:704:ARG:HH11	2.30	0.45
2:F:513:ILE:O	2:F:513:ILE:HG23	2.16	0.45
2:H:35:LEU:HD13	2:H:100:LEU:HD11	1.98	0.45
2:D:634:ASP:OD2	2:D:637:THR:OG1	2.25	0.45
1:E:237:THR:CB	1:E:238:PRO:HD2	2.46	0.45
2:F:450:LEU:HD12	2:F:628:ILE:HG13	1.98	0.45
1:G:418:LEU:HD23	1:G:418:LEU:HA	1.73	0.45
2:F:512:ARG:HH11	2:H:216:ASP:CG	2.19	0.45
6:H:3003:MTE:S1'	7:H:3004:MOS:O2	2.75	0.45
2:B:324:LEU:CD2	2:B:326:ILE:HD11	2.46	0.45
1:E:181:PHE:C	1:E:182:LEU:HD12	2.37	0.45
1:G:83:ALA:HB2	1:G:157:TRP:CE3	2.52	0.45
1:G:237:THR:CG2	1:G:239:ASP:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:ALA:C	1:G:60:VAL:HG13	2.35	0.45
2:H:702:SER:O	2:H:706:ARG:NH2	2.46	0.45
1:A:203:ALA:HB3	4:A:3005:FAD:O1P	2.17	0.45
2:B:697:LYS:N	2:B:697:LYS:HD2	2.31	0.45
1:A:434:TYR:CE1	2:B:764:GLU:HA	2.51	0.45
2:D:702:SER:HB2	2:D:706:ARG:HH22	1.81	0.45
1:E:164:PHE:O	1:E:166:LEU:HG	2.16	0.45
2:F:288:GLY:HA2	2:F:323:ALA:O	2.17	0.45
1:A:314:ARG:O	1:A:315:ARG:HB2	2.16	0.45
1:A:432:ALA:O	1:A:433:ALA:C	2.54	0.45
1:C:324:GLU:O	1:C:325:TYR:C	2.54	0.45
2:D:554:PHE:HB2	2:D:594:ILE:CD1	2.47	0.45
1:G:26:LEU:HG	1:G:26:LEU:O	2.17	0.45
2:H:174:PHE:HZ	2:H:693:PRO:HG3	1.80	0.45
2:H:446:ARG:HG2	2:H:632:VAL:HG13	1.96	0.45
2:H:674:TRP:CE3	2:H:675:LEU:HD21	2.51	0.45
1:E:91:VAL:HG11	1:E:114:MET:HB3	1.99	0.45
1:E:331:ARG:O	1:E:332:PRO:C	2.55	0.45
2:F:446:ARG:HG2	2:F:632:VAL:HG13	1.99	0.45
1:A:392:LYS:HG3	1:A:422:PHE:HE2	1.82	0.45
2:B:730:GLU:HB2	2:B:731:PRO:HD3	1.98	0.45
2:D:367:ASP:OD1	2:D:368:PRO:N	2.50	0.45
1:E:358:ASP:OD2	2:F:702:SER:CB	2.63	0.45
1:E:369:ASN:C	1:E:370:LEU:HD23	2.37	0.45
1:G:354:SER:HB2	1:G:360:ASP:OD2	2.17	0.45
1:E:316:MET:CB	1:E:317:PRO:CD	2.95	0.45
2:F:214:PHE:N	2:F:214:PHE:CD1	2.84	0.45
2:F:407:GLN:CD	2:F:617:ARG:HG2	2.36	0.45
2:F:776:ARG:O	2:F:777:ALA:CB	2.65	0.45
2:F:93:PHE:CE2	2:F:299:TRP:NE1	2.85	0.45
1:G:353:LEU:HD21	1:G:434:TYR:CZ	2.51	0.45
2:H:551:LEU:HD23	2:H:551:LEU:HA	1.65	0.45
2:B:561:CYS:SG	2:B:562:ALA:N	2.90	0.44
2:D:247:ARG:HH11	2:D:247:ARG:CG	2.14	0.44
2:D:698:ILE:HB	2:D:699:PRO:CD	2.47	0.44
1:E:83:ALA:HB2	1:E:157:TRP:CH2	2.52	0.44
2:F:645:THR:HG21	2:F:668:TYR:CZ	2.52	0.44
1:G:434:TYR:CE1	2:H:764:GLU:HA	2.52	0.44
2:H:555:VAL:O	2:H:555:VAL:CG1	2.64	0.44
1:A:414:ALA:O	1:A:415:LEU:C	2.53	0.44
2:B:128:THR:O	2:B:129:LEU:C	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:717:ASN:O	2:B:724:ARG:HD3	2.17	0.44
1:E:143:LEU:O	1:E:144:ARG:C	2.55	0.44
1:A:399:ALA:C	1:A:401:LEU:N	2.71	0.44
1:C:407:ARG:NH1	1:C:409:ASP:OD2	2.50	0.44
2:B:595:SER:HB2	2:D:601:PHE:CD1	2.52	0.44
1:E:32:LEU:HA	1:E:32:LEU:HD23	1.83	0.44
2:F:306:PRO:HB2	2:F:344:PHE:CE2	2.52	0.44
1:G:301:MET:HE1	1:G:341:LEU:HD22	1.99	0.44
2:H:743:LEU:HD12	2:H:743:LEU:HA	1.65	0.44
2:B:405:TYR:O	2:B:615:GLN:HA	2.18	0.44
1:C:281:ILE:HG23	1:C:282:GLY:N	2.31	0.44
2:D:214:PHE:N	2:D:214:PHE:HD1	2.13	0.44
1:C:33:THR:HG23	2:D:25:ASP:HB3	1.99	0.44
2:D:700:ALA:O	2:D:701:PHE:C	2.56	0.44
1:G:61:ASN:H	1:G:61:ASN:ND2	2.15	0.44
2:H:288:GLY:HA2	2:H:323:ALA:O	2.17	0.44
2:H:143:PRO:HB3	2:H:329:HIS:CE1	2.53	0.44
1:A:324:GLU:O	1:A:325:TYR:C	2.55	0.44
1:C:427:ASP:C	1:C:427:ASP:OD1	2.56	0.44
1:C:446:TYR:CZ	1:C:450:LEU:HD11	2.53	0.44
2:F:454:LYS:CG	2:F:454:LYS:O	2.63	0.44
1:G:316:MET:HB2	1:G:317:PRO:HD2	1.99	0.44
1:G:27:LEU:HD22	1:G:32:LEU:HD12	1.99	0.44
2:H:146:TRP:CZ3	2:H:313:LEU:HD13	2.53	0.44
1:E:67:LEU:O	1:E:69:GLN:N	2.50	0.44
2:F:66:THR:HG22	2:F:68:ALA:N	2.30	0.44
1:A:83:ALA:HB1	1:A:84:PRO:HD2	2.00	0.44
2:B:440:THR:O	2:B:440:THR:CG2	2.63	0.44
2:B:730:GLU:O	2:B:731:PRO:C	2.54	0.44
1:E:368:LEU:CD1	1:E:368:LEU:N	2.78	0.44
2:F:453:VAL:HG12	2:F:454:LYS:N	2.32	0.44
2:F:736:GLY:O	2:F:737:ILE:C	2.56	0.44
2:F:79:ALA:HB1	2:F:80:PRO:HD2	2.00	0.44
1:G:49:VAL:HA	1:G:112:VAL:HG11	1.98	0.44
1:G:78:ILE:HG23	1:G:79:GLU:N	2.33	0.44
1:A:348:LEU:CD1	1:A:349:ARG:N	2.74	0.44
1:A:382:ILE:O	1:A:393:ARG:HA	2.16	0.44
2:B:501:ALA:HB1	2:B:506:ILE:O	2.17	0.44
2:B:647:ILE:HD13	2:B:735:LEU:HD13	1.99	0.44
2:D:251:ARG:CB	2:D:252:PRO:CD	2.96	0.44
2:D:343:GLY:O	2:D:344:PHE:C	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:730:GLU:N	2:D:731:PRO:HD2	2.31	0.44
1:G:399:ALA:C	1:G:401:LEU:H	2.21	0.44
2:H:319:TYR:OH	2:H:372:ARG:HD3	2.17	0.44
2:B:319:TYR:OH	2:B:372:ARG:HD3	2.18	0.44
1:E:140:ALA:N	1:E:141:PRO:CD	2.81	0.44
1:E:266:LEU:O	1:E:268:ARG:N	2.51	0.44
1:G:453:GLU:OE1	2:H:442:ARG:NH1	2.51	0.44
2:H:218:ARG:NH2	2:H:517:ASP:OD1	2.51	0.44
2:H:354:GLU:O	2:H:357:ILE:HG22	2.18	0.44
2:B:414:LEU:HA	2:B:414:LEU:HD23	1.83	0.43
2:D:528:ALA:HA	6:D:3003:MTE:S2'	2.57	0.43
2:D:485:GLY:HA2	8:D:3021:HOH:O	2.18	0.43
2:D:66:THR:HG22	2:D:68:ALA:N	2.31	0.43
2:D:671:GLY:O	2:D:674:TRP:HB3	2.19	0.43
2:F:618:PRO:HG2	2:F:619:PHE:CD1	2.52	0.43
2:F:96:GLN:HA	2:F:97:PRO:HD3	1.84	0.43
1:G:67:LEU:O	1:G:69:GLN:N	2.52	0.43
2:H:348:GLN:O	2:H:349:GLY:C	2.54	0.43
1:C:22:SER:OG	1:C:25:GLU:HG2	2.17	0.43
1:C:445:ARG:NH2	2:D:634:ASP:OD2	2.52	0.43
1:G:325:TYR:HA	1:G:389:GLY:O	2.17	0.43
1:G:59:ALA:C	1:G:60:VAL:CG1	2.84	0.43
2:B:35:LEU:HD23	2:B:35:LEU:N	2.32	0.43
2:B:691:HIS:O	2:B:692:ALA:HB2	2.18	0.43
1:E:95:MET:SD	1:E:114:MET:HE1	2.58	0.43
2:H:201:GLU:O	2:H:202:ILE:C	2.57	0.43
1:A:77:THR:OG1	1:A:79:GLU:HG2	2.19	0.43
2:B:461:LEU:HD12	2:B:463:HIS:CE1	2.54	0.43
2:B:79:ALA:HB1	2:B:80:PRO:CD	2.48	0.43
1:C:216:LEU:HD12	2:D:114:ARG:NH1	2.33	0.43
1:E:209:SER:O	1:E:213:THR:HG23	2.18	0.43
2:F:26:LEU:HA	2:F:27:PRO:HD3	1.90	0.43
2:F:706:ARG:HA	2:F:706:ARG:HD3	1.78	0.43
1:G:115:ALA:O	1:G:116:ALA:C	2.57	0.43
1:G:12:ARG:HH11	1:G:12:ARG:CG	2.31	0.43
1:G:279:ALA:HB1	4:G:3005:FAD:H4'	1.99	0.43
2:H:105:SER:O	2:H:106:HIS:C	2.53	0.43
4:G:3005:FAD:H1'2	4:G:3005:FAD:H9	1.71	0.43
2:H:214:PHE:HD1	2:H:214:PHE:N	2.14	0.43
2:B:70:LEU:HD12	2:B:74:ASN:HB2	2.01	0.43
2:D:371:LEU:HA	2:D:371:LEU:HD12	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:TYR:O	1:E:142:ILE:N	2.51	0.43
1:E:394:ALA:O	1:E:395:ALA:C	2.56	0.43
2:F:170:GLY:N	2:F:271:ASP:HB3	2.33	0.43
2:F:310:ARG:HD2	2:F:344:PHE:HB3	2.01	0.43
2:F:683:ASP:OD2	2:F:687:ARG:NE	2.47	0.43
1:G:415:LEU:HB2	1:G:416:PRO:HD3	2.00	0.43
1:A:152:GLU:OE1	1:A:153:PRO:HD2	2.19	0.43
1:A:291:ILE:HD13	1:A:291:ILE:HG21	1.71	0.43
1:A:450:LEU:HD23	1:A:450:LEU:HA	1.38	0.43
1:C:129:LEU:O	1:C:130:ALA:C	2.56	0.43
2:D:198:HIS:N	2:D:199:PRO:HD3	2.33	0.43
2:D:507:ASP:HA	2:D:508:PRO:HD3	1.87	0.43
1:E:122:ARG:HB3	1:E:128:LEU:HD21	2.00	0.43
1:E:283:GLY:O	1:E:284:ASN:C	2.55	0.43
2:F:53:GLU:OE1	2:F:53:GLU:HA	2.19	0.43
1:G:205:GLY:O	1:G:209:SER:OG	2.35	0.43
1:G:319:GLU:OE2	1:G:319:GLU:N	2.48	0.43
1:G:428:MET:SD	1:G:429:ARG:N	2.92	0.43
2:H:174:PHE:CD2	2:H:698:ILE:HD13	2.53	0.43
2:H:360:LEU:HG	2:H:364:MET:CE	2.48	0.43
1:A:102:GLN:OE1	2:B:663:GLN:NE2	2.52	0.43
1:A:253:ARG:NH2	1:A:268:ARG:HG3	2.34	0.43
1:A:314:ARG:HH22	1:A:329:ASP:CG	2.22	0.43
2:B:367:ASP:OD1	2:B:368:PRO:CD	2.67	0.43
2:B:403:THR:HG23	2:B:407:GLN:O	2.18	0.43
1:E:348:LEU:HA	1:E:348:LEU:HD12	1.59	0.43
2:F:201:GLU:O	2:F:202:ILE:C	2.58	0.43
2:F:367:ASP:OD1	2:F:368:PRO:CD	2.66	0.43
1:G:305:LEU:HD21	1:G:307:LEU:HD21	2.01	0.43
1:G:7:LEU:O	1:G:8:ASN:C	2.57	0.43
2:H:414:LEU:O	2:H:415:GLY:C	2.58	0.43
1:A:374:GLY:O	1:A:375:SER:HB3	2.19	0.43
2:B:107:ARG:O	2:B:108:ALA:C	2.56	0.43
2:B:196:SER:O	2:B:224:MET:HE2	2.19	0.43
2:B:343:GLY:O	2:B:344:PHE:C	2.56	0.43
1:C:432:ALA:O	1:C:433:ALA:C	2.56	0.43
2:D:414:LEU:HD23	2:D:414:LEU:HA	1.86	0.43
2:D:743:LEU:HD12	2:D:743:LEU:HA	1.80	0.43
1:E:98:HIS:O	1:E:99:HIS:HB2	2.19	0.43
1:G:122:ARG:NH2	1:G:124:ASP:OD1	2.52	0.43
1:G:355:LYS:N	1:G:360:ASP:OD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ALA:HB3	1:A:141:PRO:CD	2.48	0.42
1:A:67:LEU:N	1:A:68:PRO:HD2	2.34	0.42
1:E:364:VAL:CG2	1:E:435:ARG:HG2	2.49	0.42
4:G:3005:FAD:H51A	4:G:3005:FAD:H2B	1.39	0.42
2:H:367:ASP:OD2	2:H:431:ARG:NH1	2.33	0.42
2:D:45:ALA:HA	2:D:123:ARG:HG3	1.99	0.42
2:D:260:ASP:OD1	2:D:691:HIS:HD2	1.96	0.42
2:D:440:THR:O	2:D:440:THR:CG2	2.66	0.42
2:F:70:LEU:HA	2:F:71:PRO:HD3	1.94	0.42
2:F:79:ALA:HB1	2:F:80:PRO:CD	2.49	0.42
1:G:89:HIS:CE1	1:G:91:VAL:HG23	2.54	0.42
2:H:123:ARG:HB3	2:H:124:PRO:HD2	2.00	0.42
1:G:102:GLN:O	2:H:15:HIS:CE1	2.71	0.42
2:H:93:PHE:CE2	2:H:299:TRP:NE1	2.87	0.42
1:A:129:LEU:O	1:A:130:ALA:C	2.55	0.42
2:B:367:ASP:OD2	2:B:431:ARG:NH1	2.43	0.42
1:C:444:LEU:HD23	1:C:444:LEU:HA	1.87	0.42
1:C:95:MET:HG3	1:C:111:ILE:HD11	2.01	0.42
2:B:425:ALA:O	2:B:426:ASN:CB	2.68	0.42
2:D:96:GLN:HA	2:D:97:PRO:HD3	1.89	0.42
2:F:151:VAL:HG21	2:F:325:ARG:HB2	2.01	0.42
1:G:83:ALA:HB1	1:G:84:PRO:HD2	2.00	0.42
2:B:184:LEU:HA	2:B:185:PRO:HD2	1.81	0.42
2:B:39:LEU:HD22	2:B:95:GLY:O	2.20	0.42
1:C:319:GLU:N	1:C:319:GLU:OE2	2.42	0.42
2:D:697:LYS:N	2:D:697:LYS:CD	2.82	0.42
1:E:353:LEU:HD21	1:E:434:TYR:OH	2.19	0.42
1:E:401:LEU:HA	1:E:401:LEU:HD12	1.57	0.42
2:F:341:PHE:HD2	2:F:342:ARG:N	2.17	0.42
2:F:50:LEU:CD1	2:F:118:ILE:HG12	2.50	0.42
2:H:550:ARG:O	2:H:551:LEU:C	2.51	0.42
2:B:23:LEU:O	2:B:23:LEU:HG	2.17	0.42
2:D:585:ILE:HA	2:D:585:ILE:HD13	1.81	0.42
2:D:730:GLU:H	2:D:731:PRO:CD	2.33	0.42
1:E:133:LEU:HD22	2:F:698:ILE:HD11	2.02	0.42
2:F:269:ARG:NH2	2:F:341:PHE:CD2	2.87	0.42
2:H:348:GLN:N	2:H:348:GLN:OE1	2.37	0.42
2:B:34:HIS:O	2:B:35:LEU:HD23	2.20	0.42
1:C:237:THR:HG23	1:C:238:PRO:HD2	2.00	0.42
2:D:65:PHE:HB2	2:D:100:LEU:HB3	2.01	0.42
2:D:678:GLU:OE1	2:D:696:TYR:OH	2.29	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:437:TRP:CZ3	2:F:446:ARG:HG3	2.54	0.42
2:F:555:VAL:CG1	2:F:555:VAL:O	2.63	0.42
2:H:170:GLY:N	2:H:271:ASP:HB3	2.34	0.42
2:H:343:GLY:O	2:H:344:PHE:C	2.58	0.42
2:B:305:LEU:HB3	2:B:306:PRO:CD	2.48	0.42
1:C:228:CYS:HB2	1:C:231:LEU:HB2	2.01	0.42
2:D:493:HIS:CG	2:D:513:ILE:HG12	2.55	0.42
1:E:22:SER:OG	1:E:25:GLU:HG2	2.19	0.42
1:E:301:MET:HB3	1:E:348:LEU:HD22	2.01	0.42
2:F:302:ASP:OD1	2:F:303:LEU:N	2.51	0.42
1:G:218:ASP:C	1:G:218:ASP:OD1	2.58	0.42
1:G:325:TYR:HB2	1:G:389:GLY:HA3	2.01	0.42
1:G:418:LEU:HB3	1:G:436:MET:CE	2.49	0.42
2:H:360:LEU:HG	2:H:364:MET:HE3	2.02	0.42
2:H:744:HIS:HE1	2:H:754:TRP:CZ3	2.38	0.42
1:A:140:ALA:N	1:A:141:PRO:HD2	2.35	0.42
1:A:237:THR:HG23	1:A:238:PRO:N	2.34	0.42
1:C:382:ILE:O	1:C:393:ARG:HA	2.18	0.42
2:D:318:SER:HB3	2:D:414:LEU:CD1	2.49	0.42
2:D:92:HIS:O	2:D:93:PHE:HB3	2.19	0.42
1:E:105:PHE:CD1	2:F:177:GLU:HB2	2.55	0.42
2:F:341:PHE:O	2:F:342:ARG:C	2.57	0.42
2:H:496:MET:HE2	2:H:496:MET:HA	2.00	0.42
1:A:281:ILE:CG2	1:A:282:GLY:N	2.82	0.42
1:A:243:ILE:HD12	1:A:341:LEU:HG	2.02	0.42
2:B:65:PHE:N	2:B:100:LEU:O	2.47	0.42
2:B:744:HIS:C	2:B:744:HIS:CD2	2.91	0.42
1:E:237:THR:HG22	1:E:240:GLY:O	2.20	0.42
2:F:457:ILE:O	2:F:458:SER:OG	2.30	0.42
2:F:636:LEU:HD23	2:F:636:LEU:HA	1.82	0.42
1:G:44:CYS:O	1:G:132:ASN:HA	2.20	0.42
2:H:81:SER:HA	2:H:82:PRO:HD3	1.81	0.42
1:A:41:GLU:HG2	1:A:210:LEU:HD13	2.02	0.41
1:C:268:ARG:HH11	1:C:268:ARG:HD2	1.61	0.41
1:C:295:PRO:HB2	1:C:296:PRO:HD3	2.02	0.41
2:D:202:ILE:HD13	2:D:236:ASN:ND2	2.31	0.41
1:E:191:ASP:O	1:E:194:LEU:HB3	2.19	0.41
1:E:349:ARG:HG2	1:E:351:TYR:OH	2.20	0.41
2:F:251:ARG:HB3	2:F:252:PRO:CD	2.50	0.41
2:F:343:GLY:O	2:F:344:PHE:C	2.58	0.41
2:F:412:CYS:HA	2:F:624:TYR:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:65:PHE:CD1	2:F:65:PHE:N	2.88	0.41
2:F:701:PHE:O	2:F:704:ARG:HG2	2.19	0.41
1:G:191:ASP:O	1:G:194:LEU:HB3	2.20	0.41
2:H:643:LEU:HA	2:H:643:LEU:HD23	1.89	0.41
2:H:696:TYR:HA	8:H:3020:HOH:O	2.19	0.41
1:A:52:ARG:HG2	1:A:53:ASP:N	2.34	0.41
2:D:166:PHE:CZ	2:D:355:ARG:HG3	2.55	0.41
2:F:66:THR:HG23	2:F:68:ALA:H	1.84	0.41
1:G:125:TYR:O	1:G:126:ASP:C	2.58	0.41
1:G:290:PRO:HA	1:G:391:PRO:HD3	2.01	0.41
1:G:48:THR:C	1:G:49:VAL:HG13	2.38	0.41
2:H:730:GLU:C	2:H:732:PRO:CD	2.85	0.41
2:B:81:SER:HA	2:B:82:PRO:HD3	1.79	0.41
2:D:35:LEU:HA	2:D:101:VAL:O	2.20	0.41
2:D:517:ASP:C	2:D:517:ASP:OD2	2.58	0.41
2:D:698:ILE:HG21	2:D:698:ILE:HD13	1.70	0.41
1:E:237:THR:CG2	1:E:238:PRO:N	2.84	0.41
1:G:299:ILE:HA	8:G:3010:HOH:O	2.20	0.41
1:G:314:ARG:O	1:G:315:ARG:HB2	2.20	0.41
2:H:310:ARG:HB3	2:H:344:PHE:O	2.19	0.41
2:H:656:ASN:OD1	2:H:656:ASN:C	2.57	0.41
1:A:293:ASP:OD2	1:A:352:LYS:NZ	2.46	0.41
2:B:503:VAL:O	2:B:503:VAL:CG1	2.66	0.41
1:C:450:LEU:HA	1:C:450:LEU:HD23	1.74	0.41
2:B:593:ARG:NH1	2:D:604:THR:O	2.44	0.41
1:E:140:ALA:N	1:E:141:PRO:HD2	2.35	0.41
1:G:27:LEU:O	1:G:30:GLU:HB2	2.20	0.41
1:G:382:ILE:HG22	1:G:382:ILE:O	2.19	0.41
1:A:356:ARG:NH2	2:B:697:LYS:NZ	2.67	0.41
1:C:361:ILE:HD12	1:C:429:ARG:NH2	2.36	0.41
2:D:731:PRO:CB	2:D:732:PRO:CD	2.96	0.41
1:E:231:LEU:O	1:E:244:GLY:HA3	2.20	0.41
2:H:276:TYR:OH	2:H:359:HIS:CD2	2.71	0.41
2:B:53:GLU:N	2:B:54:PRO:CD	2.83	0.41
2:D:398:LYS:O	2:D:399:LYS:HD2	2.21	0.41
1:E:267:LEU:HA	1:E:267:LEU:HD23	1.83	0.41
1:E:104:GLY:HA3	2:F:22:TYR:OH	2.21	0.41
2:H:202:ILE:HD13	2:H:236:ASN:HD22	1.85	0.41
2:H:367:ASP:CG	2:H:431:ARG:HH12	2.19	0.41
2:H:96:GLN:HA	2:H:97:PRO:HD3	1.88	0.41
2:B:527:THR:O	2:B:528:ALA:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:706:ARG:HD3	2:B:706:ARG:HA	1.63	0.41
1:E:381:ARG:NH2	1:E:393:ARG:NE	2.68	0.41
2:F:123:ARG:HB3	2:F:124:PRO:HD2	2.03	0.41
1:G:283:GLY:O	1:G:284:ASN:C	2.56	0.41
1:A:252:LEU:HD22	1:A:281:ILE:HD12	2.02	0.41
4:A:3005:FAD:HM82	4:A:3005:FAD:HM71	1.90	0.41
1:A:37:GLU:CD	2:B:256:ARG:HH22	2.24	0.41
2:B:743:LEU:HD12	2:B:743:LEU:HA	1.71	0.41
1:E:52:ARG:N	1:E:74:ALA:O	2.52	0.41
2:F:238:LEU:HD12	2:F:238:LEU:N	2.32	0.41
2:F:665:GLU:HG2	2:F:710:VAL:HG21	2.03	0.41
1:G:39:CYS:O	1:G:40:ASN:CB	2.68	0.41
1:G:89:HIS:C	1:G:91:VAL:N	2.74	0.41
1:G:94:ALA:O	1:G:98:HIS:HB2	2.20	0.41
2:H:164:GLY:HA3	2:H:276:TYR:CZ	2.56	0.41
2:H:721:THR:O	2:H:722:ILE:C	2.57	0.41
1:A:32:LEU:HD22	1:A:79:GLU:CG	2.48	0.41
1:A:353:LEU:HD21	1:A:434:TYR:CE2	2.55	0.41
2:B:278:ILE:HD11	2:B:286:LEU:HD22	2.03	0.41
2:B:704:ARG:CG	2:B:704:ARG:NH1	2.83	0.41
1:C:158:LEU:HA	1:C:158:LEU:HD23	1.81	0.41
1:C:233:GLN:OE1	1:C:233:GLN:HA	2.21	0.41
2:D:636:LEU:HA	2:D:636:LEU:HD23	1.86	0.41
2:D:751:GLY:HA3	2:D:773:ALA:O	2.21	0.41
2:F:202:ILE:HD13	2:F:236:ASN:HD22	1.86	0.41
2:F:762:THR:H	2:F:762:THR:HG23	1.68	0.41
1:G:151:GLY:C	1:G:152:GLU:HG2	2.40	0.41
2:H:560:GLY:O	2:H:561:CYS:HB3	2.21	0.41
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.91	0.41
2:B:210:LEU:CD1	2:B:212:LEU:HD12	2.51	0.41
1:C:429:ARG:O	1:C:430:ALA:HB2	2.20	0.41
2:F:318:SER:HB3	2:F:414:LEU:HD13	2.03	0.41
1:G:126:ASP:OD1	2:H:704:ARG:NH1	2.44	0.41
1:G:272:SER:O	1:G:275:VAL:N	2.53	0.41
2:H:98:ILE:HG21	2:H:98:ILE:HD13	1.77	0.41
2:B:318:SER:HB3	2:B:414:LEU:CD1	2.51	0.41
2:B:684:HIS:CE1	2:F:567:ILE:HD11	2.55	0.41
2:B:742:ALA:O	2:B:743:LEU:C	2.59	0.41
2:D:170:GLY:N	2:D:271:ASP:HB3	2.36	0.41
1:E:345:ALA:N	1:E:346:PRO:HD3	2.36	0.41
2:F:23:LEU:HD13	2:F:194:CYS:CA	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:243:ILE:CD1	1:G:341:LEU:HD11	2.51	0.41
1:G:326:ARG:HA	1:G:326:ARG:HD3	1.89	0.41
2:H:422:GLN:HG2	2:H:427:PHE:CD2	2.56	0.41
2:H:656:ASN:HA	2:H:657:PRO:HD3	1.90	0.41
2:H:674:TRP:CD2	2:H:675:LEU:HD21	2.56	0.41
2:B:146:TRP:CZ3	2:B:313:LEU:HD13	2.56	0.40
2:B:451:SER:HA	2:B:452:PRO:HD3	1.97	0.40
2:D:168:ILE:HD13	2:D:351:LEU:HD23	2.03	0.40
2:D:612:LEU:HD23	2:D:612:LEU:HA	1.80	0.40
1:E:93:GLN:NE2	1:E:97:ASP:OD1	2.55	0.40
1:G:216:LEU:HD23	1:G:216:LEU:HA	1.92	0.40
1:G:237:THR:HG23	1:G:238:PRO:HD2	2.03	0.40
1:G:237:THR:HG1	1:G:238:PRO:HD2	1.82	0.40
1:G:302:GLY:HA2	1:G:381:ARG:NH1	2.36	0.40
2:H:701:PHE:CE2	2:H:704:ARG:NH1	2.89	0.40
1:A:164:PHE:O	1:A:166:LEU:HG	2.22	0.40
1:C:32:LEU:HD22	1:C:79:GLU:CG	2.47	0.40
1:E:76:ARG:HH11	1:E:161:ASP:CG	2.19	0.40
2:F:22:TYR:CE2	2:F:223:ARG:HD3	2.56	0.40
1:G:12:ARG:NH1	1:G:12:ARG:CG	2.82	0.40
2:H:753:HIS:HB2	2:H:772:ARG:O	2.21	0.40
2:B:214:PHE:N	2:B:214:PHE:HD1	2.17	0.40
6:B:3003:MTE:S1'	7:B:3004:MOS:S	3.19	0.40
2:B:371:LEU:HA	2:B:371:LEU:HD12	1.91	0.40
2:B:94:VAL:HG11	2:B:687:ARG:HG2	2.03	0.40
2:D:261:ASP:O	2:D:262:ASP:C	2.59	0.40
2:D:437:TRP:CZ3	2:D:446:ARG:HG3	2.57	0.40
1:E:228:CYS:O	1:E:229:LYS:C	2.59	0.40
2:F:533:ALA:O	2:F:534:ASP:C	2.56	0.40
2:H:175:TYR:O	2:H:259:ARG:NH2	2.47	0.40
2:H:377:TYR:CE1	2:H:454:LYS:HE3	2.57	0.40
2:H:481:LEU:HD12	2:H:482:ASN:N	2.36	0.40
2:H:198:HIS:ND1	2:H:526:ALA:HB2	2.35	0.40
2:H:704:ARG:O	2:H:704:ARG:HG3	2.20	0.40
1:A:240:GLY:HA2	1:A:343:LYS:HG2	2.02	0.40
2:B:724:ARG:HD2	2:B:724:ARG:HH11	1.74	0.40
2:D:165:CYS:O	2:D:166:PHE:HB3	2.20	0.40
2:D:507:ASP:OD1	2:D:508:PRO:N	2.54	0.40
1:E:348:LEU:HD12	1:E:349:ARG:N	2.33	0.40
1:G:47:CYS:O	1:G:49:VAL:HG13	2.21	0.40
2:H:507:ASP:OD1	2:H:508:PRO:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:648:LEU:HD12	2:H:711:ALA:O	2.21	0.40
1:A:34:GLY:O	1:A:36:LYS:HE2	2.21	0.40
2:B:23:LEU:HD13	2:B:194:CYS:HA	2.03	0.40
2:B:339:THR:OG1	2:B:340:ALA:N	2.53	0.40
2:B:48:THR:HG22	2:B:49:GLY:N	2.36	0.40
2:D:706:ARG:HA	2:D:706:ARG:HD3	1.82	0.40
1:E:107:THR:HB	1:E:108:PRO:HD3	2.03	0.40
2:F:452:PRO:O	2:F:452:PRO:CG	2.69	0.40
2:F:717:ASN:ND2	2:F:726:LYS:HG3	2.36	0.40
1:G:228:CYS:O	1:G:229:LYS:C	2.60	0.40
1:G:34:GLY:CA	1:G:36:LYS:NZ	2.84	0.40
2:H:722:ILE:HD12	2:H:722:ILE:HA	1.89	0.40
2:H:762:THR:HB	2:H:763:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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%)	401 (90%)	41 (9%)	4 (1%)	17	40
1	C	446/462 (96%)	415 (93%)	27 (6%)	4 (1%)	17	40
1	E	446/462 (96%)	383 (86%)	53 (12%)	10 (2%)	6	17
1	G	446/462 (96%)	395 (89%)	44 (10%)	7 (2%)	9	24
2	B	756/777 (97%)	708 (94%)	40 (5%)	8 (1%)	14	34
2	D	756/777 (97%)	718 (95%)	31 (4%)	7 (1%)	17	40
2	F	756/777 (97%)	709 (94%)	39 (5%)	8 (1%)	14	34
2	H	756/777 (97%)	700 (93%)	47 (6%)	9 (1%)	13	32
All	All	4808/4956 (97%)	4429 (92%)	322 (7%)	57 (1%)	13	32

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	399	LYS
2	B	458	SER
1	C	180	ALA
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	374	GLY
2	H	399	LYS
2	H	458	SER
1	A	315	ARG
1	A	374	GLY
1	A	400	ALA
2	B	187	GLU
2	B	342	ARG
2	B	560	GLY
2	B	608	SER
2	D	187	GLU
2	D	342	ARG
1	E	395	ALA
1	E	400	ALA
2	F	342	ARG
2	H	187	GLU
2	H	342	ARG
2	H	560	GLY
2	H	761	ALA
1	A	163	ALA
1	E	315	ARG
1	E	326	ARG
1	E	399	ALA
2	F	187	GLU
2	F	426	ASN
1	G	180	ALA
1	G	315	ARG
1	G	326	ARG
2	H	227	GLY
2	H	561	CYS
2	H	639	GLU
1	C	315	ARG

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Mol	Chain	Res	Type
1	E	297	ALA
1	E	447	VAL
1	G	199	ALA
1	C	163	ALA
2	D	227	GLY
2	F	281	ASP
2	F	560	GLY
1	G	163	ALA
2	B	227	GLY
1	E	430	ALA
2	D	560	GLY
2	F	227	GLY
2	B	141	GLY
1	G	100	GLY
1	E	332	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/347 (98%)	302 (89%)	37 (11%)	6	14
1	C	339/347 (98%)	302 (89%)	37 (11%)	6	14
1	E	339/347 (98%)	301 (89%)	38 (11%)	6	13
1	G	339/347 (98%)	302 (89%)	37 (11%)	6	14
2	B	571/584 (98%)	515 (90%)	56 (10%)	8	18
2	D	571/584 (98%)	514 (90%)	57 (10%)	7	18
2	F	571/584 (98%)	513 (90%)	58 (10%)	7	17
2	H	571/584 (98%)	516 (90%)	55 (10%)	8	19
All	All	3640/3724 (98%)	3265 (90%)	375 (10%)	7	16

All (375) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	11	THR
1	A	12	ARG
1	A	15	ARG
1	A	20	THR
1	A	26	LEU
1	A	33	THR
1	A	76	ARG
1	A	87	ARG
1	A	128	LEU
1	A	143	LEU
1	A	156	ASP
1	A	159	GLN
1	A	165	THR
1	A	198	GLU
1	A	210	LEU
1	A	212	VAL
1	A	220	PRO
1	A	231	LEU
1	A	237	THR
1	A	239	ASP
1	A	257	GLU
1	A	268	ARG
1	A	309	ARG
1	A	316	MET
1	A	349	ARG
1	A	359	GLN
1	A	375	SER
1	A	376	LYS
1	A	390	VAL
1	A	393	ARG
1	A	405	ASP
1	A	423	THR
1	A	426	SER
1	A	428	MET
1	A	451	SER
1	A	455	VAL
1	A	457	VAL
2	B	2	SER
2	B	10	ASP
2	B	16	VAL
2	B	23	LEU
2	B	48	THR
2	B	53	GLU

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Mol	Chain	Res	Type
2	B	66	THR
2	B	129	LEU
2	B	130	ASP
2	B	133	LEU
2	B	151	VAL
2	B	152	GLU
2	B	161	LEU
2	B	175	TYR
2	B	190	VAL
2	B	215	HIS
2	B	221	MET
2	B	222	ARG
2	B	247	ARG
2	B	256	ARG
2	B	296	ARG
2	B	300	SER
2	B	313	LEU
2	B	330	ARG
2	B	341	PHE
2	B	355	ARG
2	B	359	HIS
2	B	366	ARG
2	B	398	LYS
2	B	399	LYS
2	B	423	LYS
2	B	426	ASN
2	B	431	ARG
2	B	442	ARG
2	B	450	LEU
2	B	461	LEU
2	B	512	ARG
2	B	520	LYS
2	B	530	SER
2	B	548	ARG
2	B	554	PHE
2	B	561	CYS
2	B	574	GLN
2	B	579	SER
2	B	611	ARG
2	B	617	ARG
2	B	632	VAL
2	B	641	ARG

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Mol	Chain	Res	Type
2	B	697	LYS
2	B	704	ARG
2	B	708	PHE
2	B	718	ARG
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	19	PRO
1	C	20	THR
1	C	25	GLU
1	C	26	LEU
1	C	33	THR
1	C	40	ASN
1	C	76	ARG
1	C	87	ARG
1	C	91	VAL
1	C	128	LEU
1	C	143	LEU
1	C	165	THR
1	C	198	GLU
1	C	209	SER
1	C	221	GLU
1	C	226	SER
1	C	231	LEU
1	C	237	THR
1	C	239	ASP
1	C	257	GLU
1	C	268	ARG
1	C	309	ARG
1	C	316	MET
1	C	326	ARG
1	C	331	ARG
1	C	349	ARG
1	C	354	SER
1	C	376	LYS
1	C	379	THR
1	C	393	ARG
1	C	428	MET

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Mol	Chain	Res	Type
1	C	447	VAL
1	C	451	SER
1	C	455	VAL
2	D	10	ASP
2	D	16	VAL
2	D	28	CYS
2	D	35	LEU
2	D	41	THR
2	D	48	THR
2	D	53	GLU
2	D	66	THR
2	D	81	SER
2	D	129	LEU
2	D	151	VAL
2	D	161	LEU
2	D	166	PHE
2	D	175	TYR
2	D	190	VAL
2	D	215	HIS
2	D	221	MET
2	D	222	ARG
2	D	247	ARG
2	D	258	ASP
2	D	259	ARG
2	D	296	ARG
2	D	300	SER
2	D	313	LEU
2	D	330	ARG
2	D	341	PHE
2	D	355	ARG
2	D	359	HIS
2	D	366	ARG
2	D	398	LYS
2	D	399	LYS
2	D	426	ASN
2	D	442	ARG
2	D	450	LEU
2	D	452	PRO
2	D	461	LEU
2	D	512	ARG
2	D	520	LYS
2	D	530	SER

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Mol	Chain	Res	Type
2	D	534	ASP
2	D	558	ARG
2	D	574	GLN
2	D	608	SER
2	D	609	TRP
2	D	611	ARG
2	D	617	ARG
2	D	632	VAL
2	D	641	ARG
2	D	697	LYS
2	D	704	ARG
2	D	706	ARG
2	D	708	PHE
2	D	718	ARG
2	D	722	ILE
2	D	724	ARG
2	D	741	LEU
2	D	743	LEU
1	E	11	THR
1	E	12	ARG
1	E	20	THR
1	E	26	LEU
1	E	33	THR
1	E	36	LYS
1	E	40	ASN
1	E	58	ARG
1	E	66	MET
1	E	79	GLU
1	E	93	GLN
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

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Mol	Chain	Res	Type
1	E	239	ASP
1	E	257	GLU
1	E	268	ARG
1	E	295	PRO
1	E	309	ARG
1	E	316	MET
1	E	339	VAL
1	E	344	SER
1	E	349	ARG
1	E	359	GLN
1	E	408	GLU
1	E	428	MET
1	E	435	ARG
1	E	451	SER
2	F	2	SER
2	F	10	ASP
2	F	23	LEU
2	F	28	CYS
2	F	35	LEU
2	F	48	THR
2	F	53	GLU
2	F	66	THR
2	F	81	SER
2	F	129	LEU
2	F	151	VAL
2	F	174	PHE
2	F	175	TYR
2	F	190	VAL
2	F	215	HIS
2	F	221	MET
2	F	222	ARG
2	F	247	ARG
2	F	296	ARG
2	F	300	SER
2	F	306	PRO
2	F	313	LEU
2	F	330	ARG
2	F	341	PHE
2	F	355	ARG
2	F	359	HIS
2	F	366	ARG
2	F	398	LYS

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Mol	Chain	Res	Type
2	F	399	LYS
2	F	428	THR
2	F	431	ARG
2	F	442	ARG
2	F	450	LEU
2	F	451	SER
2	F	452	PRO
2	F	461	LEU
2	F	488	MET
2	F	512	ARG
2	F	530	SER
2	F	541	LYS
2	F	558	ARG
2	F	574	GLN
2	F	579	SER
2	F	609	TRP
2	F	611	ARG
2	F	617	ARG
2	F	618	PRO
2	F	632	VAL
2	F	694	SER
2	F	697	LYS
2	F	702	SER
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	36	LYS
1	G	40	ASN
1	G	58	ARG
1	G	68	PRO
1	G	76	ARG
1	G	85	ASP
1	G	128	LEU

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Mol	Chain	Res	Type
1	G	136	CYS
1	G	143	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	239	ASP
1	G	257	GLU
1	G	309	ARG
1	G	316	MET
1	G	325	TYR
1	G	327	LYS
1	G	331	ARG
1	G	349	ARG
1	G	362	SER
1	G	371	THR
1	G	376	LYS
1	G	425	LEU
1	G	426	SER
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	48	THR
2	H	53	GLU
2	H	66	THR
2	H	123	ARG
2	H	129	LEU
2	H	151	VAL
2	H	152	GLU
2	H	165	CYS
2	H	174	PHE
2	H	175	TYR
2	H	190	VAL
2	H	215	HIS
2	H	221	MET

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Mol	Chain	Res	Type
2	H	222	ARG
2	H	247	ARG
2	H	251	ARG
2	H	256	ARG
2	H	259	ARG
2	H	260	ASP
2	H	296	ARG
2	H	300	SER
2	H	313	LEU
2	H	330	ARG
2	H	359	HIS
2	H	366	ARG
2	H	398	LYS
2	H	399	LYS
2	H	416	GLU
2	H	423	LYS
2	H	426	ASN
2	H	431	ARG
2	H	442	ARG
2	H	451	SER
2	H	461	LEU
2	H	496	MET
2	H	506	ILE
2	H	512	ARG
2	H	530	SER
2	H	558	ARG
2	H	561	CYS
2	H	574	GLN
2	H	611	ARG
2	H	617	ARG
2	H	632	VAL
2	H	697	LYS
2	H	706	ARG
2	H	708	PHE
2	H	718	ARG
2	H	724	ARG
2	H	741	LEU
2	H	743	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	118	HIS
1	A	196	HIS
1	A	328	GLN
2	B	204	HIS
2	B	208	HIS
2	B	236	ASN
2	B	359	HIS
2	B	426	ASN
2	B	463	HIS
2	B	574	GLN
2	B	744	HIS
1	C	40	ASN
1	C	61	ASN
1	C	196	HIS
1	C	359	GLN
2	D	106	HIS
2	D	236	ASN
2	D	359	HIS
2	D	426	ASN
2	D	691	HIS
2	D	744	HIS
1	E	40	ASN
1	E	93	GLN
1	E	196	HIS
1	E	284	ASN
1	E	328	GLN
2	F	208	HIS
2	F	236	ASN
2	F	359	HIS
2	F	691	HIS
2	F	744	HIS
1	G	40	ASN
1	G	61	ASN
1	G	196	HIS
1	G	328	GLN
1	G	359	GLN
2	H	204	HIS
2	H	208	HIS
2	H	236	ASN
2	H	359	HIS
2	H	426	ASN
2	H	744	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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
4	FAD	C	3005	-	51,58,58	2.03	14 (27%)	60,89,89	3.10	30 (50%)
3	FES	A	3001	1	0,4,4	0.00	-	-		
4	FAD	A	3005	-	51,58,58	1.59	10 (19%)	60,89,89	2.93	20 (33%)
3	FES	E	3001	1	0,4,4	0.00	-	-		
3	FES	C	3002	1	0,4,4	0.00	-	-		
6	MTE	B	3003	7	21,26,26	5.38	10 (47%)	21,40,40	3.09	7 (33%)
6	MTE	F	3003	7	21,26,26	5.35	10 (47%)	21,40,40	4.71	9 (42%)
6	MTE	D	3003	7	21,26,26	4.61	12 (57%)	21,40,40	5.62	10 (47%)
3	FES	C	3001	1	0,4,4	0.00	-	-		
3	FES	E	3002	1	0,4,4	0.00	-	-		
7	MOS	F	3004	6	0,3,3	0.00	-	-		
7	MOS	H	3004	6	0,3,3	0.00	-	-		
3	FES	A	3002	1	0,4,4	0.00	-	-		
7	MOS	D	3004	6	0,3,3	0.00	-	-		
6	MTE	H	3003	7	21,26,26	5.27	11 (52%)	21,40,40	5.05	9 (42%)
7	MOS	B	3004	6	0,3,3	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FAD	G	3005	-	51,58,58	1.58	14 (27%)	60,89,89	2.49	24 (40%)
3	FES	G	3002	1	0,4,4	0.00	-	-	-	-
4	FAD	E	3005	-	51,58,58	1.52	9 (17%)	60,89,89	2.57	26 (43%)
3	FES	G	3001	1	0,4,4	0.00	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	C	3005	-	-	14/30/50/50	0/6/6/6
3	FES	A	3001	1	-	-	0/1/1/1
4	FAD	A	3005	-	-	16/30/50/50	0/6/6/6
3	FES	E	3001	1	-	-	0/1/1/1
3	FES	C	3002	1	-	-	0/1/1/1
6	MTE	B	3003	7	-	0/6/34/34	0/3/3/3
3	FES	E	3002	1	-	-	0/1/1/1
6	MTE	D	3003	7	-	2/6/34/34	0/3/3/3
3	FES	C	3001	1	-	-	0/1/1/1
6	MTE	F	3003	7	-	4/6/34/34	0/3/3/3
6	MTE	H	3003	7	-	1/6/34/34	0/3/3/3
3	FES	A	3002	1	-	-	0/1/1/1
4	FAD	G	3005	-	-	11/30/50/50	0/6/6/6
3	FES	G	3002	1	-	-	0/1/1/1
4	FAD	E	3005	-	-	12/30/50/50	0/6/6/6
3	FES	G	3001	1	-	-	0/1/1/1

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	3003	MTE	C7-C6	14.92	1.65	1.53
6	B	3003	MTE	C7-C6	14.34	1.65	1.53
6	H	3003	MTE	C7-C6	12.73	1.63	1.53
6	D	3003	MTE	C7-C6	10.22	1.61	1.53
6	F	3003	MTE	C9-C10	9.79	1.59	1.41
6	H	3003	MTE	C9-C10	9.75	1.59	1.41
6	B	3003	MTE	C9-C10	9.74	1.59	1.41
6	F	3003	MTE	C4'-C3'	-9.38	1.39	1.52
6	H	3003	MTE	C6-N5	9.09	1.58	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	3003	MTE	C4'-C3'	-9.00	1.39	1.52
6	D	3003	MTE	C9-C10	8.91	1.58	1.41
6	B	3003	MTE	P-O4'	-8.09	1.34	1.60
6	B	3003	MTE	C4'-C3'	-8.06	1.41	1.52
6	D	3003	MTE	C4'-C3'	-7.31	1.42	1.52
6	F	3003	MTE	C6-N5	7.25	1.55	1.45
6	B	3003	MTE	C6-N5	7.09	1.55	1.45
6	H	3003	MTE	P-O4'	-6.97	1.37	1.60
6	D	3003	MTE	C6-N5	6.71	1.54	1.45
6	D	3003	MTE	P-O4'	-6.47	1.39	1.60
6	F	3003	MTE	P-O4'	-6.26	1.40	1.60
6	B	3003	MTE	C9-N5	6.10	1.50	1.38
6	H	3003	MTE	C9-N5	5.85	1.50	1.38
4	C	3005	FAD	C2B-C1B	-5.52	1.45	1.53
6	D	3003	MTE	C4-C9	5.29	1.48	1.41
6	H	3003	MTE	P-O3P	-5.24	1.34	1.54
6	B	3003	MTE	C4-C9	5.23	1.48	1.41
6	B	3003	MTE	P-O3P	-5.14	1.35	1.54
6	D	3003	MTE	P-O3P	-5.11	1.35	1.54
6	F	3003	MTE	C9-N5	5.00	1.48	1.38
4	C	3005	FAD	C2'-C3'	-4.81	1.44	1.53
6	D	3003	MTE	C9-N5	4.71	1.47	1.38
6	F	3003	MTE	P-O3P	-4.56	1.37	1.54
4	C	3005	FAD	C4X-N5	4.50	1.39	1.33
4	A	3005	FAD	C4X-N5	4.40	1.39	1.33
4	E	3005	FAD	C2A-N3A	4.38	1.39	1.32
6	H	3003	MTE	C4-C9	4.15	1.47	1.41
6	F	3003	MTE	C4-N3	4.10	1.40	1.33
6	B	3003	MTE	C4-N3	4.06	1.40	1.33
4	C	3005	FAD	C10-N1	4.02	1.38	1.33
4	G	3005	FAD	C4X-N5	3.92	1.38	1.33
4	A	3005	FAD	C1'-N10	3.78	1.52	1.48
4	C	3005	FAD	C9A-N10	3.78	1.43	1.38
6	F	3003	MTE	C4-C9	3.73	1.46	1.41
4	A	3005	FAD	C10-N1	3.68	1.38	1.33
6	F	3003	MTE	O4-C4	3.55	1.33	1.24
4	E	3005	FAD	C10-N1	3.50	1.37	1.33
4	G	3005	FAD	C4-N3	3.48	1.39	1.33
4	E	3005	FAD	C4X-N5	3.40	1.38	1.33
6	H	3003	MTE	O4-C4	3.38	1.33	1.24
6	D	3003	MTE	C4-N3	3.36	1.38	1.33
4	C	3005	FAD	O2B-C2B	-3.25	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3005	FAD	C2'-C3'	-3.25	1.47	1.53
4	A	3005	FAD	C9A-N10	3.22	1.42	1.38
6	D	3003	MTE	C2-N1	3.21	1.41	1.35
4	E	3005	FAD	C2A-N1A	3.20	1.39	1.33
4	G	3005	FAD	C10-N1	3.18	1.37	1.33
4	C	3005	FAD	C1'-N10	3.16	1.51	1.48
6	H	3003	MTE	C4-N3	3.11	1.38	1.33
4	C	3005	FAD	C9A-C5X	-3.09	1.36	1.42
4	C	3005	FAD	C6-C5X	-3.01	1.37	1.41
6	D	3003	MTE	O4-C4	2.93	1.31	1.24
4	G	3005	FAD	C1'-N10	2.85	1.51	1.48
6	D	3003	MTE	C2-N3	-2.85	1.30	1.35
4	E	3005	FAD	C9A-C5X	-2.84	1.36	1.42
4	A	3005	FAD	C2A-N3A	2.82	1.36	1.32
4	C	3005	FAD	O4B-C4B	-2.69	1.39	1.45
4	G	3005	FAD	O4'-C4'	-2.67	1.37	1.43
6	B	3003	MTE	C2-N1	2.66	1.40	1.35
4	C	3005	FAD	C2A-N3A	2.66	1.36	1.32
4	C	3005	FAD	O4B-C1B	2.64	1.44	1.41
4	A	3005	FAD	C4X-C10	2.62	1.41	1.38
4	A	3005	FAD	O4B-C4B	-2.55	1.39	1.45
4	A	3005	FAD	C4'-C3'	2.53	1.58	1.53
4	G	3005	FAD	C2A-N3A	2.38	1.35	1.32
4	G	3005	FAD	C5X-N5	2.37	1.39	1.35
4	G	3005	FAD	O4B-C1B	2.29	1.44	1.41
4	G	3005	FAD	C5'-C4'	-2.28	1.48	1.51
4	G	3005	FAD	O4B-C4B	-2.27	1.39	1.45
4	C	3005	FAD	C8-C7	-2.19	1.35	1.40
6	H	3003	MTE	C2-N3	-2.17	1.31	1.35
4	E	3005	FAD	C4-N3	2.17	1.36	1.33
4	G	3005	FAD	C2A-N1A	2.15	1.37	1.33
4	E	3005	FAD	C2B-C1B	-2.14	1.50	1.53
4	G	3005	FAD	O5B-C5B	-2.12	1.36	1.44
4	A	3005	FAD	C2B-C1B	-2.12	1.50	1.53
4	C	3005	FAD	C4-C4X	-2.07	1.37	1.41
4	G	3005	FAD	C9A-C5X	-2.06	1.38	1.42
4	A	3005	FAD	C2A-N1A	2.06	1.37	1.33
4	E	3005	FAD	O4B-C1B	2.06	1.43	1.41
4	G	3005	FAD	C4-C4X	-2.02	1.37	1.41

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3003	MTE	O3'-C7-C6	-19.89	95.70	108.96
6	F	3003	MTE	O3'-C7-C6	-16.03	98.27	108.96
6	H	3003	MTE	O3'-C7-C6	-15.63	98.54	108.96
6	D	3003	MTE	C4-C9-N5	9.89	127.42	119.12
4	A	3005	FAD	C1'-N10-C9A	9.36	125.66	118.29
4	A	3005	FAD	C4-N3-C2	9.23	122.94	115.14
6	H	3003	MTE	C4-C9-N5	9.23	126.86	119.12
6	B	3003	MTE	C4-C9-N5	8.89	126.58	119.12
4	C	3005	FAD	C1'-N10-C9A	7.85	124.47	118.29
4	C	3005	FAD	O2'-C2'-C3'	-7.83	90.07	109.10
4	E	3005	FAD	C4-N3-C2	7.45	121.43	115.14
4	A	3005	FAD	C5X-C9A-N10	7.31	123.01	117.72
4	G	3005	FAD	C5X-C9A-N10	6.98	122.77	117.72
6	H	3003	MTE	O3'-C7-N8	-6.68	101.70	108.57
4	C	3005	FAD	C1'-C2'-C3'	-6.59	91.36	109.79
6	F	3003	MTE	C2-N1-C10	6.34	128.76	114.54
4	C	3005	FAD	C4-N3-C2	6.30	120.46	115.14
4	C	3005	FAD	O3'-C3'-C4'	6.20	123.79	108.81
6	D	3003	MTE	C2-N1-C10	6.19	128.42	114.54
4	E	3005	FAD	C1'-N10-C9A	6.09	123.08	118.29
4	C	3005	FAD	O2'-C2'-C1'	6.03	124.11	109.59
4	G	3005	FAD	N3A-C2A-N1A	-5.98	119.33	128.68
4	G	3005	FAD	P-O3P-PA	-5.97	112.33	132.83
4	E	3005	FAD	N3A-C2A-N1A	-5.90	119.46	128.68
6	F	3003	MTE	N2-C2-N3	5.90	126.42	117.25
6	B	3003	MTE	C2-N1-C10	5.87	127.69	114.54
6	H	3003	MTE	N2-C2-N3	5.82	126.31	117.25
6	D	3003	MTE	C4-N3-C2	5.81	125.15	115.93
6	H	3003	MTE	C2-N1-C10	5.72	127.36	114.54
4	A	3005	FAD	P-O3P-PA	-5.55	113.78	132.83
4	C	3005	FAD	O5'-C5'-C4'	-5.50	94.68	109.36
6	H	3003	MTE	C4-N3-C2	5.50	124.66	115.93
6	F	3003	MTE	O3'-C7-N8	-5.45	102.96	108.57
4	E	3005	FAD	C5X-C9A-N10	5.34	121.58	117.72
6	D	3003	MTE	O3'-C7-N8	-5.30	103.12	108.57
4	G	3005	FAD	C4-N3-C2	5.24	119.57	115.14
4	A	3005	FAD	O2'-C2'-C3'	-5.24	96.36	109.10
4	C	3005	FAD	N3A-C2A-N1A	-5.16	120.62	128.68
6	F	3003	MTE	C4-C9-N5	5.06	123.37	119.12
4	A	3005	FAD	N3A-C2A-N1A	-4.89	121.03	128.68
6	F	3003	MTE	C4-N3-C2	4.89	123.69	115.93
6	D	3003	MTE	N3-C2-N1	-4.82	117.85	125.42
6	B	3003	MTE	O3'-C7-N8	-4.80	103.63	108.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3005	FAD	O5'-C5'-C4'	-4.75	96.67	109.36
4	C	3005	FAD	C5X-C9A-N10	4.75	121.16	117.72
4	E	3005	FAD	O2'-C2'-C1'	4.68	120.87	109.59
4	A	3005	FAD	O2'-C2'-C1'	4.67	120.85	109.59
4	C	3005	FAD	C4X-N5-C5X	4.60	121.37	116.77
4	C	3005	FAD	O3'-C3'-C2'	-4.57	97.77	108.81
4	G	3005	FAD	O4'-C4'-C5'	-4.49	99.82	109.92
6	H	3003	MTE	C9-C10-N8	4.47	122.22	118.13
6	B	3003	MTE	N2-C2-N3	4.39	124.09	117.25
4	A	3005	FAD	C4X-C4-N3	-4.35	117.49	123.43
4	E	3005	FAD	P-O3P-PA	-4.34	117.92	132.83
4	A	3005	FAD	C9A-N10-C10	-4.30	116.27	121.91
6	H	3003	MTE	O2P-P-O4'	4.29	118.14	106.73
6	F	3003	MTE	N3-C2-N1	-4.18	118.86	125.42
4	G	3005	FAD	O5'-C5'-C4'	-4.08	98.48	109.36
4	E	3005	FAD	C4X-C4-N3	-3.90	118.09	123.43
6	H	3003	MTE	N3-C2-N1	-3.82	119.43	125.42
4	G	3005	FAD	O4B-C4B-C3B	-3.78	97.64	105.11
4	E	3005	FAD	C5'-C4'-C3'	-3.74	104.98	112.20
4	C	3005	FAD	O4B-C1B-C2B	-3.73	101.47	106.93
6	D	3003	MTE	O3P-P-O4'	3.71	116.61	106.73
4	G	3005	FAD	C4X-C4-N3	-3.63	118.47	123.43
6	F	3003	MTE	O3P-P-O4'	3.63	116.38	106.73
4	E	3005	FAD	O3B-C3B-C2B	-3.58	100.24	111.82
4	G	3005	FAD	C5B-C4B-C3B	-3.54	101.92	115.18
4	G	3005	FAD	O3'-C3'-C4'	3.42	117.08	108.81
4	E	3005	FAD	C5A-C6A-N6A	-3.39	115.20	120.35
4	E	3005	FAD	O3'-C3'-C2'	-3.35	100.71	108.81
4	C	3005	FAD	O4'-C4'-C3'	3.32	117.18	109.10
4	C	3005	FAD	P-O3P-PA	-3.31	121.45	132.83
4	C	3005	FAD	C8M-C8-C7	-3.27	114.04	120.74
4	A	3005	FAD	C4A-C5A-N7A	-3.26	106.00	109.40
4	E	3005	FAD	C1'-C2'-C3'	-3.18	100.90	109.79
4	C	3005	FAD	C6-C5X-C9A	3.18	123.22	119.05
4	E	3005	FAD	O2A-PA-O5B	3.17	122.48	107.75
4	E	3005	FAD	N6A-C6A-N1A	3.17	125.15	118.57
4	A	3005	FAD	O4'-C4'-C3'	3.15	116.77	109.10
4	C	3005	FAD	C9-C9A-C5X	-3.12	114.54	119.88
4	G	3005	FAD	C1'-N10-C9A	3.11	120.74	118.29
4	A	3005	FAD	O3'-C3'-C4'	3.09	116.27	108.81
6	B	3003	MTE	O3'-C7-C6	-3.05	106.93	108.96
4	E	3005	FAD	C4X-N5-C5X	3.02	119.78	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3005	FAD	O4B-C4B-C3B	-2.99	99.20	105.11
6	D	3003	MTE	N2-C2-N3	2.95	121.84	117.25
4	G	3005	FAD	O4B-C4B-C5B	-2.94	99.69	109.37
4	E	3005	FAD	O3'-C3'-C4'	2.94	115.92	108.81
6	B	3003	MTE	N3-C2-N1	-2.91	120.85	125.42
4	C	3005	FAD	C4X-C4-N3	-2.86	119.52	123.43
6	B	3003	MTE	C4-N3-C2	2.83	120.43	115.93
4	C	3005	FAD	O3B-C3B-C2B	-2.81	102.72	111.82
4	G	3005	FAD	C5A-C6A-N6A	-2.79	116.11	120.35
4	G	3005	FAD	C9A-C5X-N5	-2.78	118.01	122.36
4	A	3005	FAD	O4B-C4B-C5B	-2.75	100.32	109.37
4	G	3005	FAD	C2A-N1A-C6A	2.74	123.45	118.75
4	E	3005	FAD	C2B-C3B-C4B	-2.73	97.34	102.64
4	A	3005	FAD	C9-C9A-C5X	-2.69	115.28	119.88
4	G	3005	FAD	O5B-PA-O1A	-2.67	98.62	109.07
4	E	3005	FAD	O2A-PA-O1A	-2.67	99.05	112.24
4	G	3005	FAD	C5'-C4'-C3'	2.62	117.28	112.20
4	C	3005	FAD	C7M-C7-C8	-2.62	115.37	120.74
4	C	3005	FAD	C8M-C8-C9	2.59	126.55	120.34
4	A	3005	FAD	O4B-C1B-C2B	-2.57	103.17	106.93
4	G	3005	FAD	O3B-C3B-C4B	-2.55	103.67	111.05
4	C	3005	FAD	C1'-N10-C10	-2.52	116.15	118.41
4	E	3005	FAD	O2'-C2'-C3'	-2.50	103.02	109.10
4	A	3005	FAD	O3'-C3'-C2'	-2.43	102.94	108.81
4	C	3005	FAD	C2A-N1A-C6A	2.43	122.91	118.75
4	G	3005	FAD	C9A-N10-C10	-2.42	118.73	121.91
4	G	3005	FAD	C4X-N5-C5X	2.41	119.18	116.77
6	F	3003	MTE	C4-C9-C10	2.36	116.67	114.57
4	E	3005	FAD	C6-C7-C8	-2.34	115.97	119.91
4	C	3005	FAD	O4'-C4'-C5'	-2.30	104.74	109.92
4	G	3005	FAD	O5'-P-O1P	2.29	118.00	109.07
4	A	3005	FAD	C5'-C4'-C3'	2.28	116.60	112.20
4	C	3005	FAD	C4A-C5A-N7A	-2.25	107.05	109.40
6	D	3003	MTE	O3P-P-O2P	-2.25	99.05	107.64
4	E	3005	FAD	O2P-P-O5'	2.21	118.02	107.75
4	C	3005	FAD	C7M-C7-C6	2.21	125.62	120.34
4	G	3005	FAD	C7M-C7-C8	-2.18	116.28	120.74
4	C	3005	FAD	O2B-C2B-C1B	-2.17	102.84	110.85
4	C	3005	FAD	C9A-N10-C10	-2.14	119.10	121.91
4	G	3005	FAD	O4B-C1B-C2B	-2.14	103.80	106.93
4	C	3005	FAD	C9A-C5X-N5	-2.13	119.03	122.36
6	D	3003	MTE	O2P-P-O1P	2.12	118.99	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3005	FAD	C9A-N10-C10	-2.10	119.16	121.91
4	A	3005	FAD	C6-C5X-C9A	2.10	121.80	119.05
4	E	3005	FAD	C10-C4X-N5	-2.10	119.81	121.26
4	E	3005	FAD	C4'-C3'-C2'	-2.07	109.05	113.36
4	G	3005	FAD	C4-C4X-C10	2.07	121.32	119.95
4	E	3005	FAD	C9-C9A-C5X	-2.07	116.35	119.88
4	C	3005	FAD	C4'-C3'-C2'	-2.04	109.12	113.36
4	E	3005	FAD	C6-C5X-C9A	2.03	121.71	119.05

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3005	FAD	C5B-O5B-PA-O1A
4	C	3005	FAD	C2'-C1'-N10-C9A
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	O3'-C3'-C4'-O4'
4	C	3005	FAD	O3'-C3'-C4'-C5'
6	F	3003	MTE	C2'-C3'-C4'-O4'
4	A	3005	FAD	C5B-O5B-PA-O2A
4	A	3005	FAD	C5B-O5B-PA-O3P
4	A	3005	FAD	C2'-C1'-N10-C9A
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'-C5'
4	A	3005	FAD	C3'-C4'-C5'-O5'
4	A	3005	FAD	C5'-O5'-P-O3P
4	G	3005	FAD	C2'-C1'-N10-C9A
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	C2'-C3'-C4'-C5'
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
4	E	3005	FAD	C5B-O5B-PA-O3P
4	E	3005	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
4	E	3005	FAD	C2'-C1'-N10-C9A
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	A	3005	FAD	O4B-C4B-C5B-O5B
4	A	3005	FAD	C2'-C3'-C4'-O4'
4	A	3005	FAD	O3'-C3'-C4'-C5'
4	G	3005	FAD	O3'-C3'-C4'-C5'
4	C	3005	FAD	C2'-C3'-C4'-C5'
4	E	3005	FAD	C2'-C3'-C4'-C5'
4	A	3005	FAD	O3'-C3'-C4'-O4'
4	C	3005	FAD	O4'-C4'-C5'-O5'
4	A	3005	FAD	O4'-C4'-C5'-O5'
4	C	3005	FAD	C3'-C4'-C5'-O5'
6	F	3003	MTE	C4'-O4'-P-O1P
6	D	3003	MTE	C4'-O4'-P-O2P
4	C	3005	FAD	C5B-O5B-PA-O3P
4	C	3005	FAD	C5'-O5'-P-O3P
4	A	3005	FAD	C5B-O5B-PA-O1A
4	E	3005	FAD	C5B-O5B-PA-O2A
4	E	3005	FAD	C3'-C4'-C5'-O5'
6	D	3003	MTE	O3'-C3'-C4'-O4'
6	F	3003	MTE	O3'-C3'-C4'-O4'
6	H	3003	MTE	O3'-C3'-C4'-O4'
6	F	3003	MTE	C4'-O4'-P-O2P
4	G	3005	FAD	O4B-C4B-C5B-O5B
4	C	3005	FAD	C5'-O5'-P-O2P
4	A	3005	FAD	C5'-O5'-P-O1P

There are no ring outliers.

16 monomers are involved in 50 short contacts:

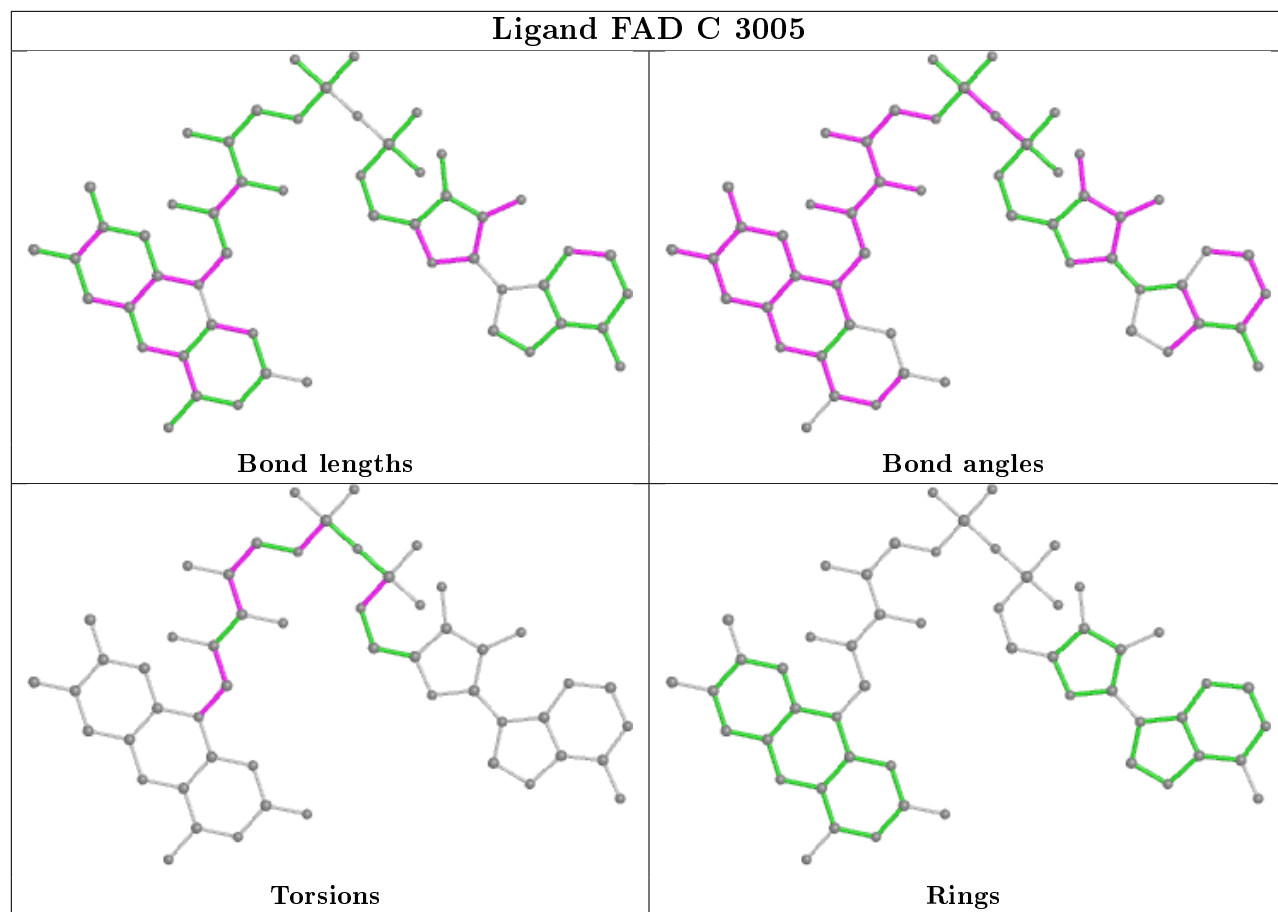
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3005	FAD	3	0
4	A	3005	FAD	6	0
3	E	3001	FES	1	0
6	B	3003	MTE	1	0
6	F	3003	MTE	1	0
6	D	3003	MTE	2	0

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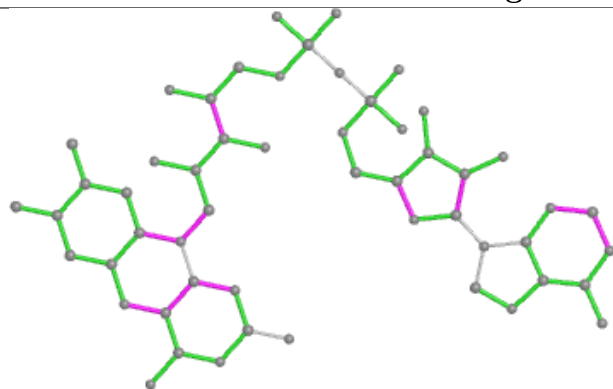
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	3002	FES	1	0
7	F	3004	MOS	2	0
7	H	3004	MOS	5	0
7	D	3004	MOS	5	0
6	H	3003	MTE	2	0
7	B	3004	MOS	5	0
4	G	3005	FAD	11	0
3	G	3002	FES	1	0
4	E	3005	FAD	6	0
3	G	3001	FES	2	0

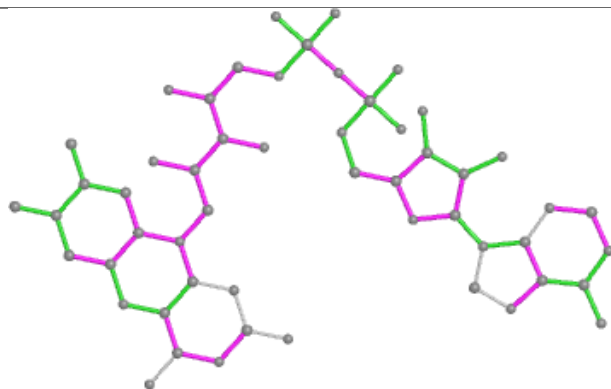
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



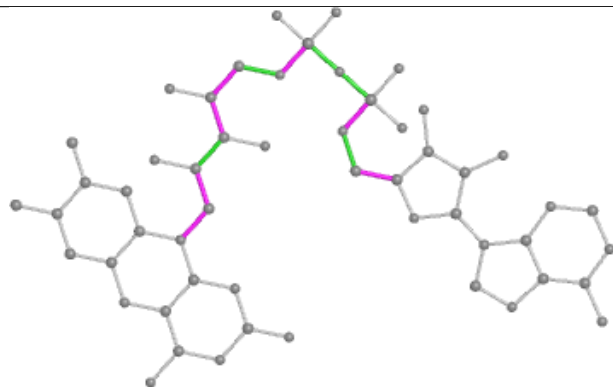
## Ligand FAD A 3005



Bond lengths



Bond angles

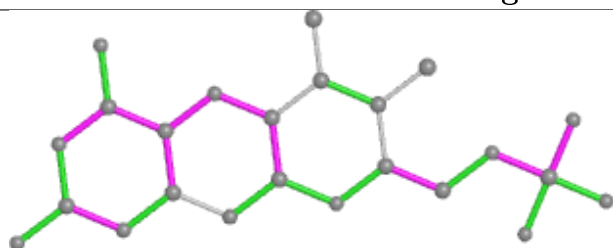


Torsions

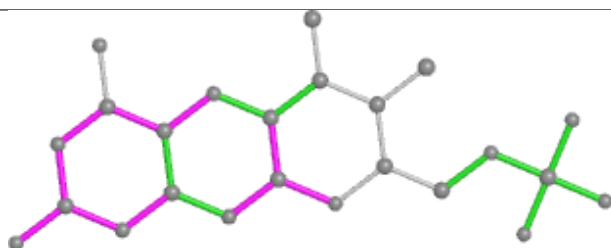


Rings

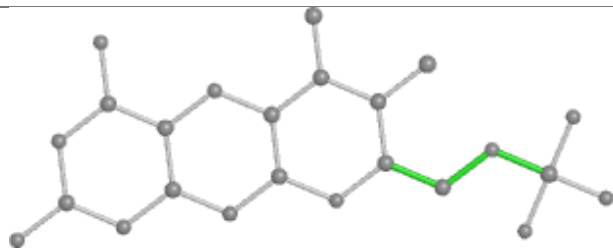
## Ligand MTE B 3003



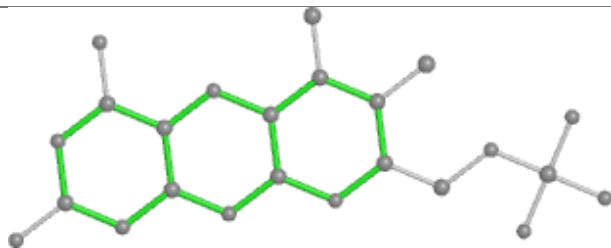
Bond lengths



Bond angles

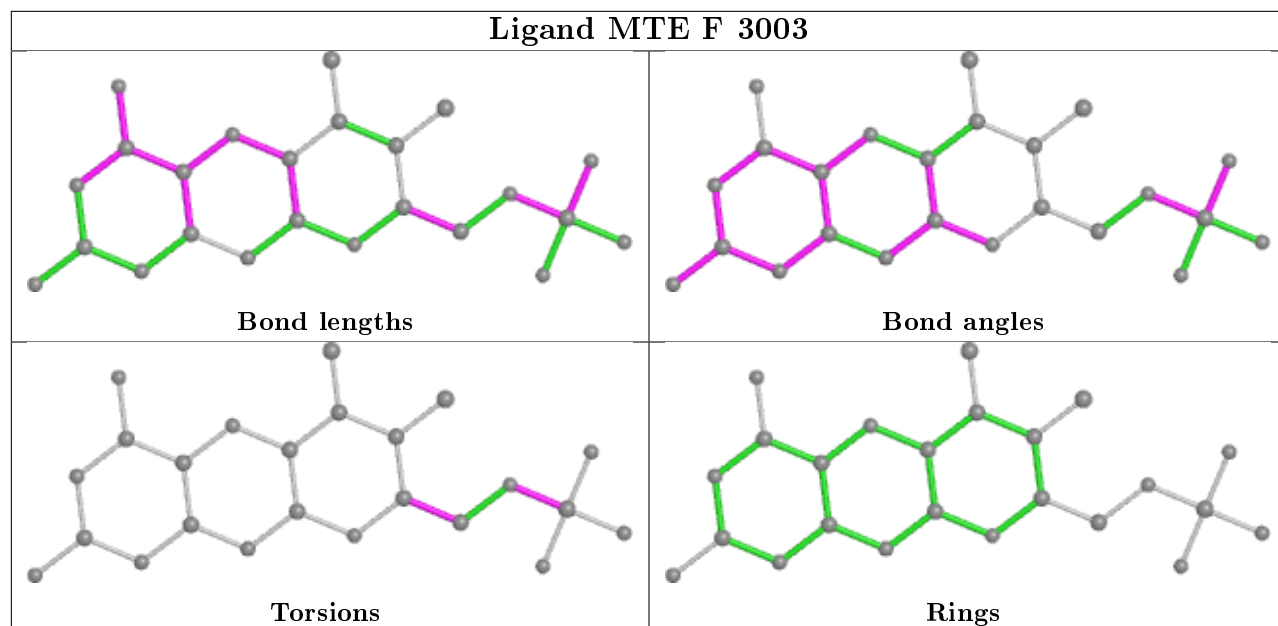


Torsions

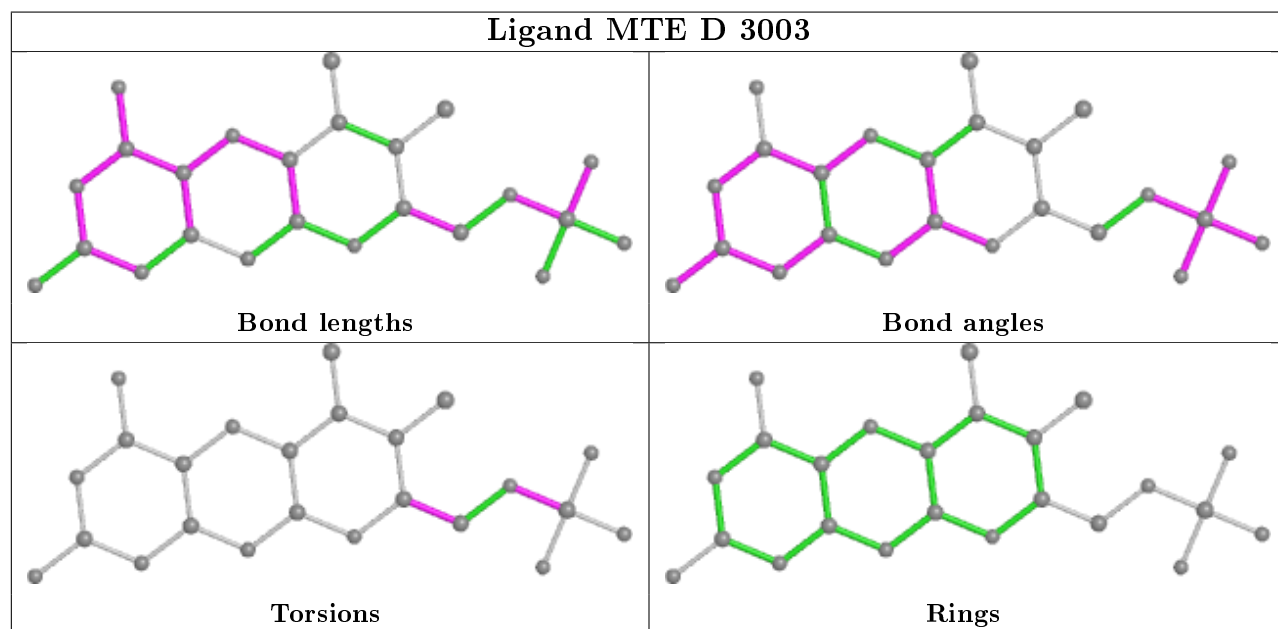


Rings

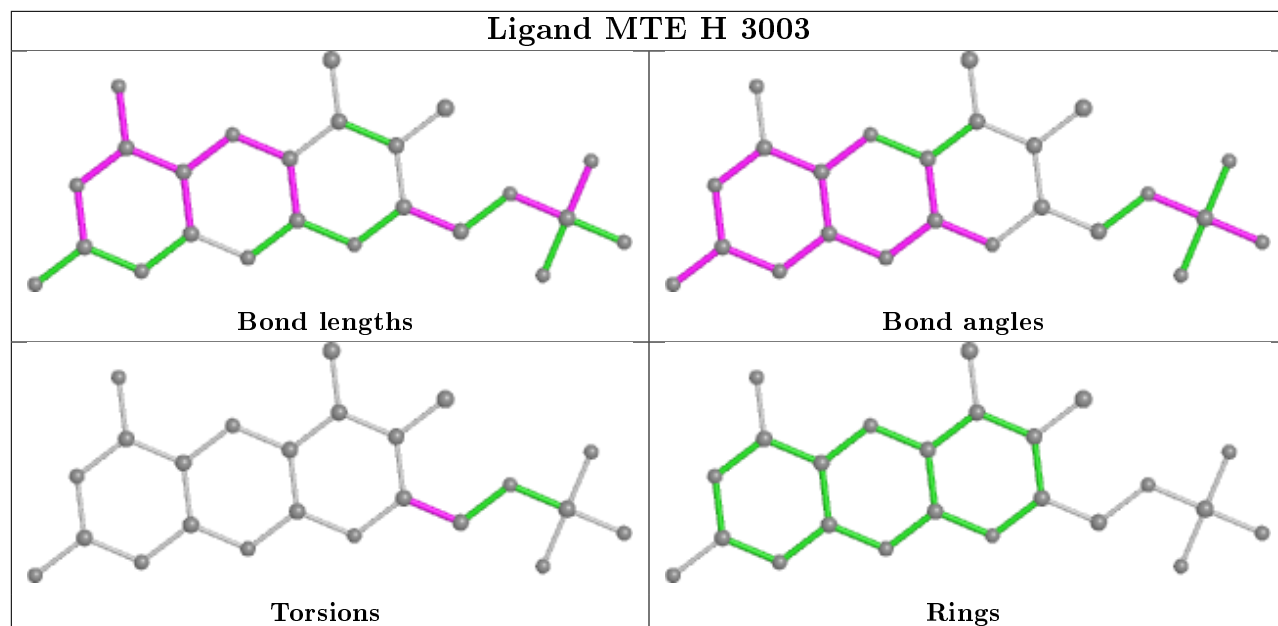
## Ligand MTE F 3003



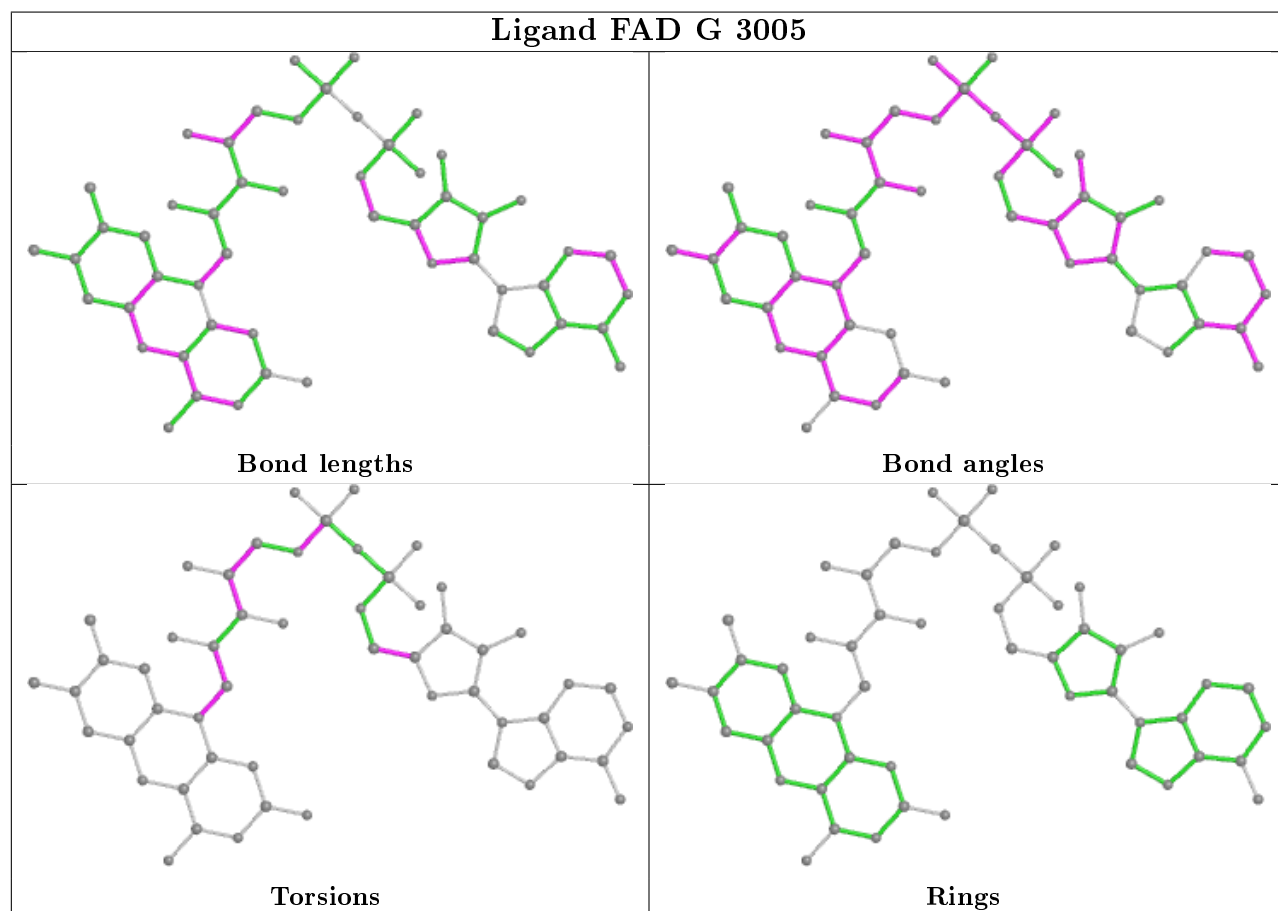
## Ligand MTE D 3003



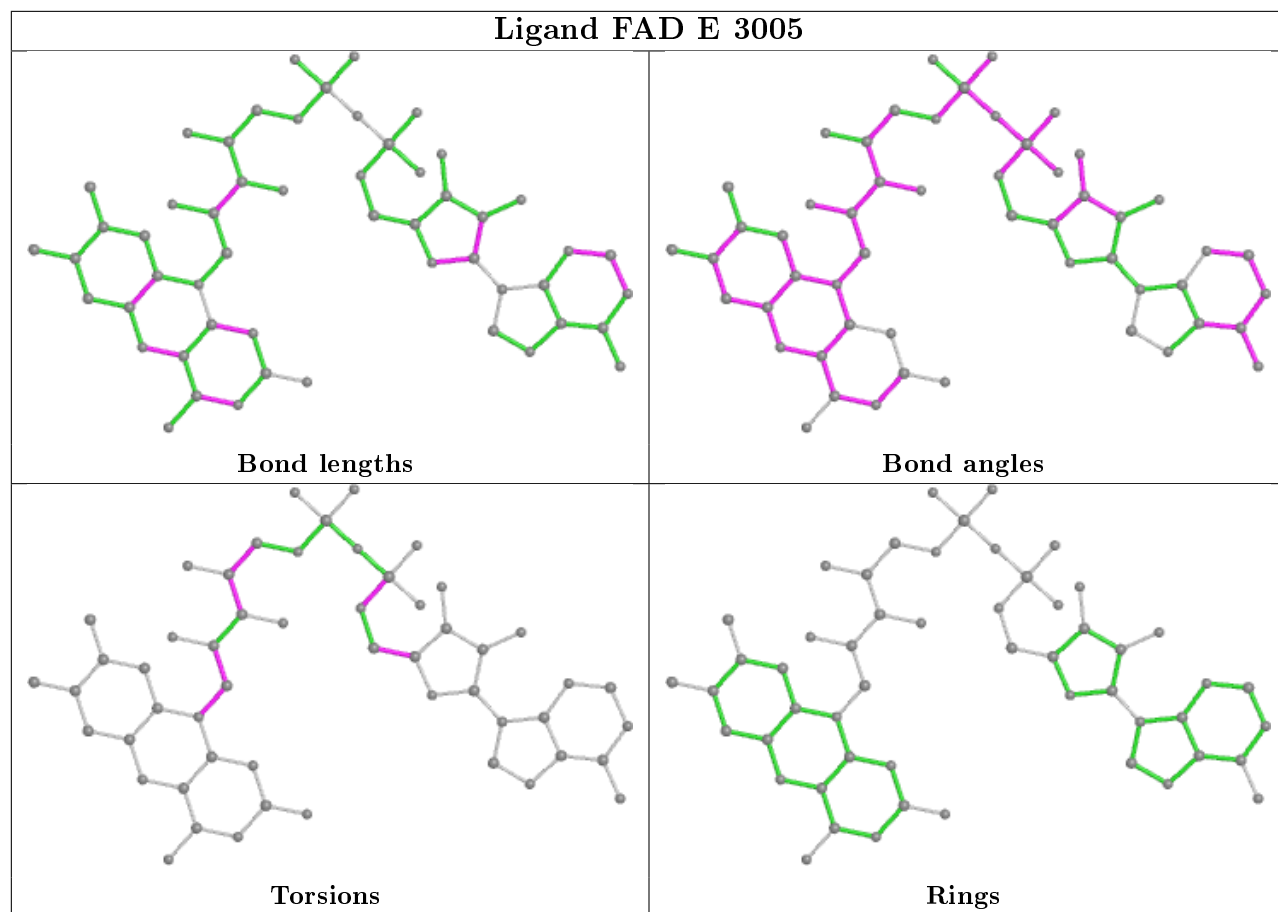
## Ligand MTE H 3003



## Ligand FAD G 3005







## 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.