



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2021 – 03:43 PM EDT

PDB ID : 2B76
Title : E. coli Quinol fumarate reductase FrdA E49Q mutation
Authors : Maklashina, E.; Iverson, T.M.; Sher, Y.; Kotlyar, V.; Mirza, O.; Andrell, J.; Hudson, J.M.; Armstrong, F.A.; Cecchini, G.
Deposited on : 2005-10-03
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

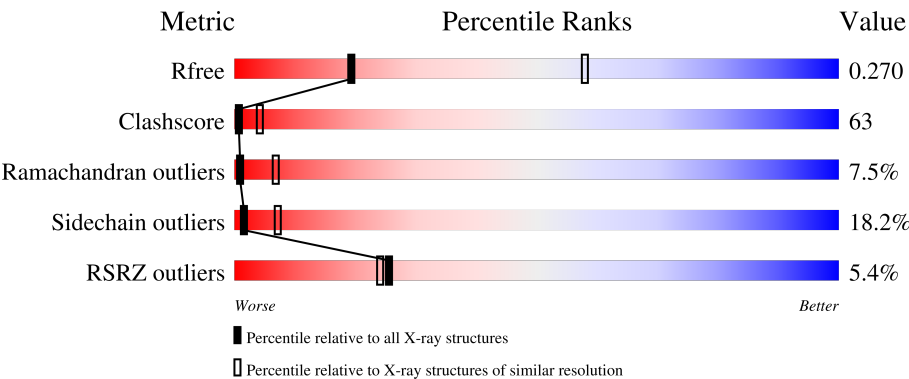
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	602	<div><div></div><div><div>28%</div><div>41%</div><div>21%</div><div>5%</div><div></div></div></div>
1	M	602	<div><div>16%</div><div><div>24%</div><div>56%</div><div>13%</div><div>5%</div><div></div></div></div>
2	B	243	<div><div></div><div><div>35%</div><div>54%</div><div>9%</div><div></div></div></div>
2	N	243	<div><div>5%</div><div><div>21%</div><div>59%</div><div>19%</div><div></div></div></div>
3	C	130	<div><div></div><div><div>31%</div><div>54%</div><div>15%</div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
3	O	130	
4	D	119	
4	P	119	

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
10	MQ7	D	700	-	-	-	X
10	MQ7	P	800	-	-	-	X
5	FLC	A	702	-	-	X	-
5	FLC	M	802	-	-	-	X
9	SF4	N	246	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16840 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 Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4448	2775	803	839	31			
1	M	572	Total	C	N	O	S	0	0	0
			4414	2752	798	833	31			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	49	GLN	GLU	engineered mutation	GB P00363
M	49	GLN	GLU	engineered mutation	GB P00363

- Molecule 2 is a protein called Fumarate reductase iron-sulfur protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			
2	N	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			

- Molecule 3 is a protein called Fumarate reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			
3	O	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

- Molecule 4 is a protein called Fumarate reductase subunit D.

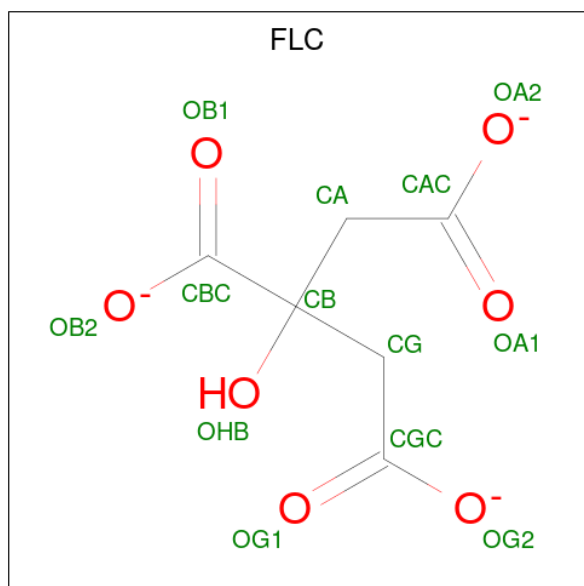
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

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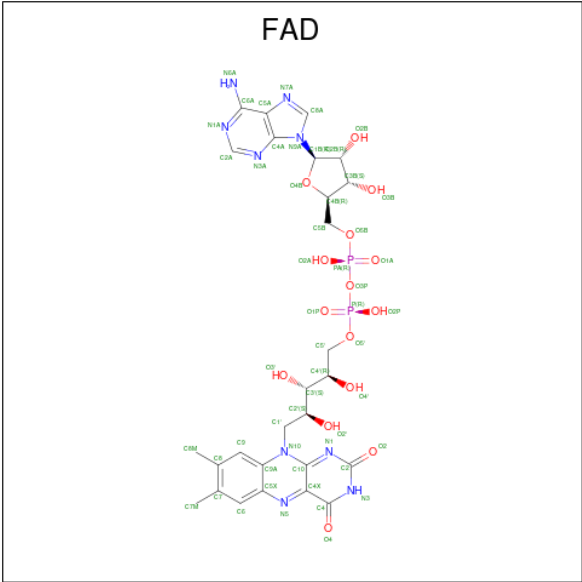
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7^-$).



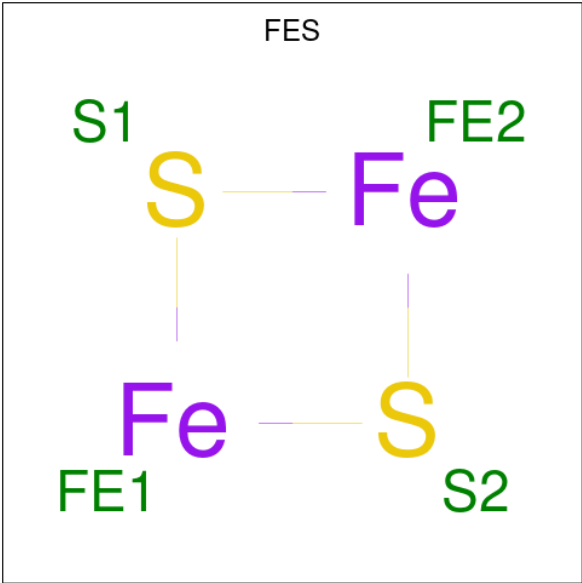
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		
5	M	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



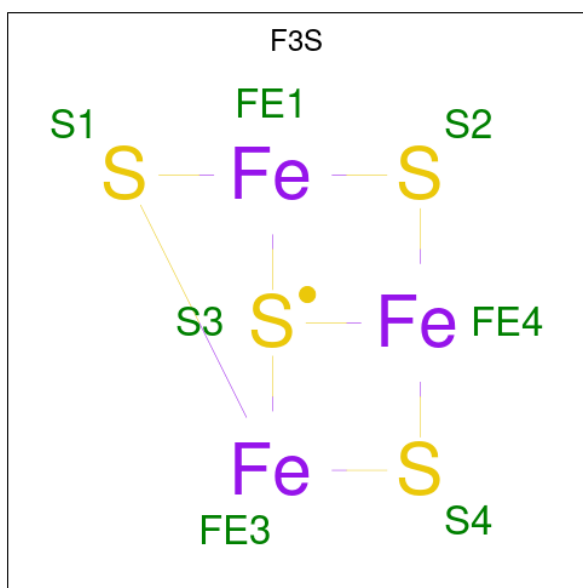
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 52	C 27	N 9	O 14	P 2	0	0
6	M	1	Total 52	C 27	N 9	O 14	P 2	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



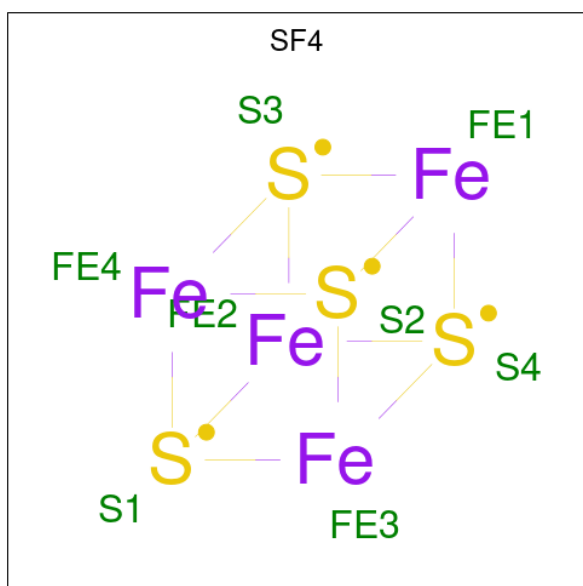
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		
8	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



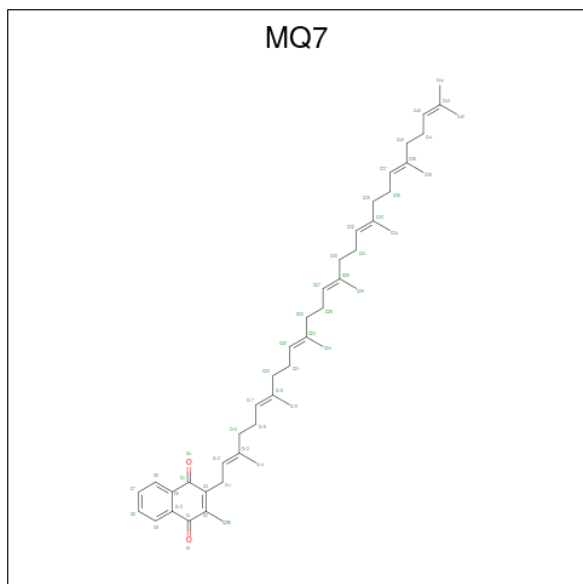
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	N	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 10 is MENAQUINONE-7 (three-letter code: MQ7) (formula: $C_{46}H_{64}O_2$).

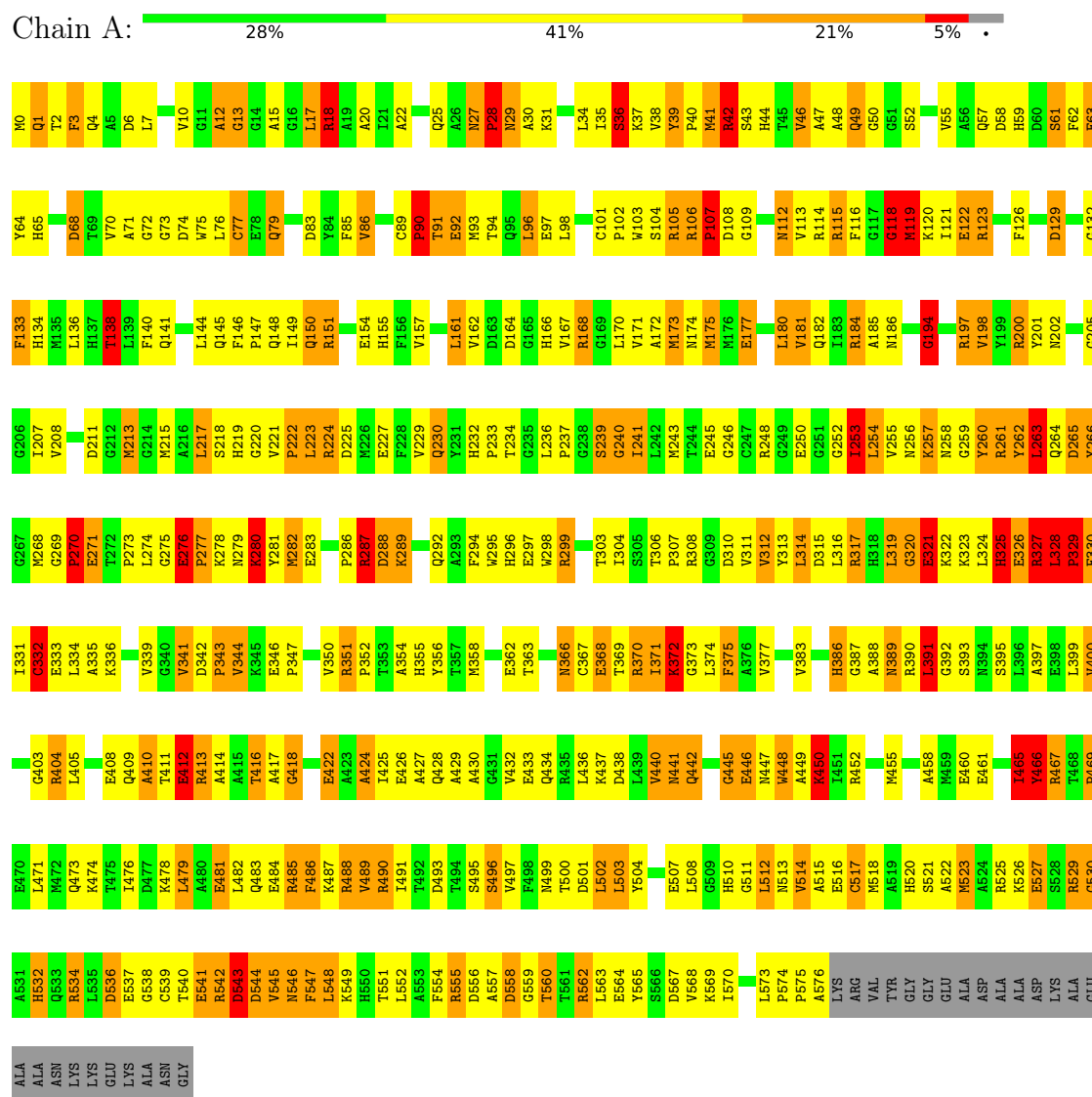


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			33	31	2		
10	P	1	Total	C	O	0	0
			33	31	2		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

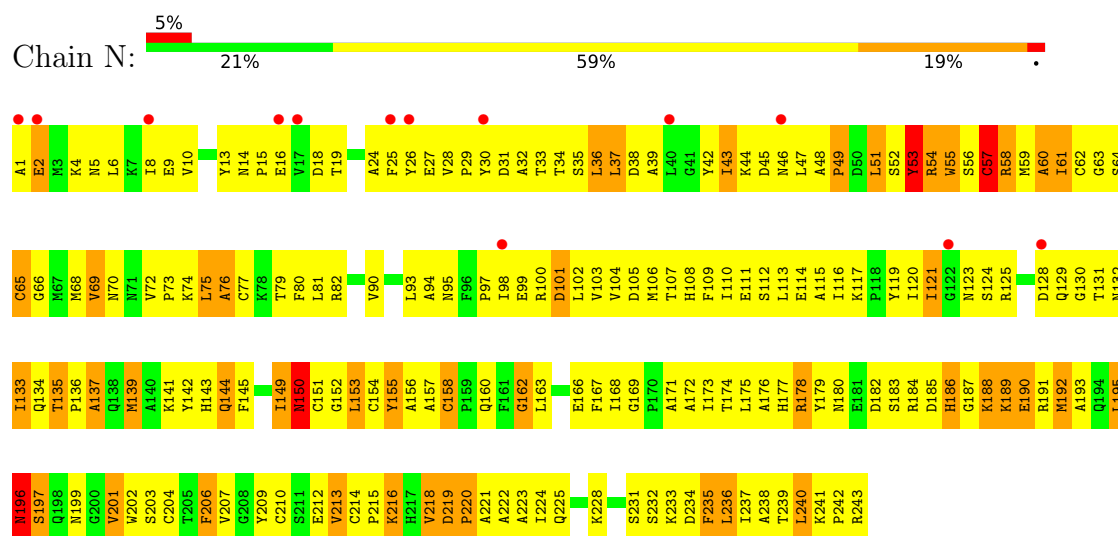
• Molecule 1: Fumarate reductase flavoprotein subunit



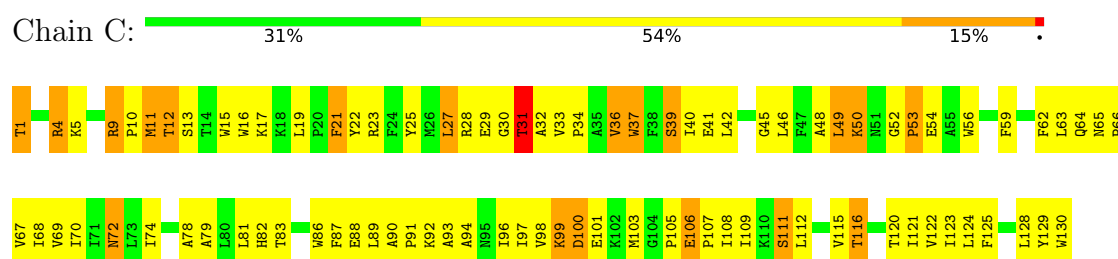
• Molecule 1: Fumarate reductase flavoprotein subunit



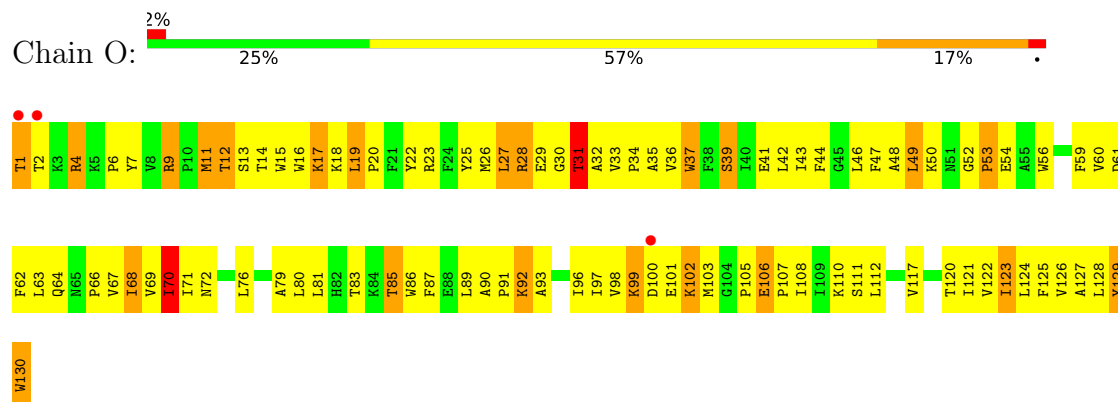
- Molecule 2: Fumarate reductase iron-sulfur protein



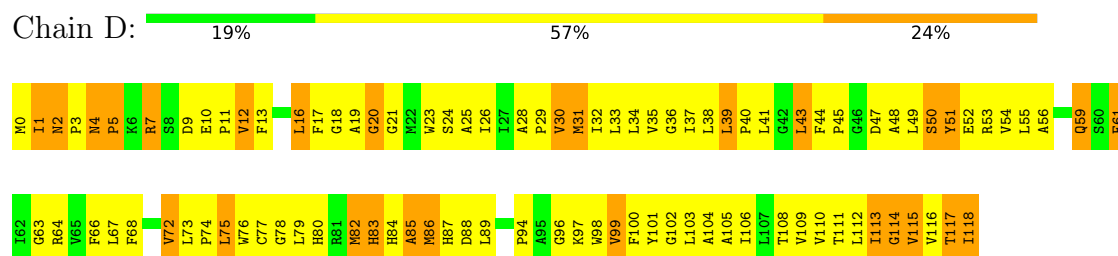
- Molecule 3: Fumarate reductase subunit C



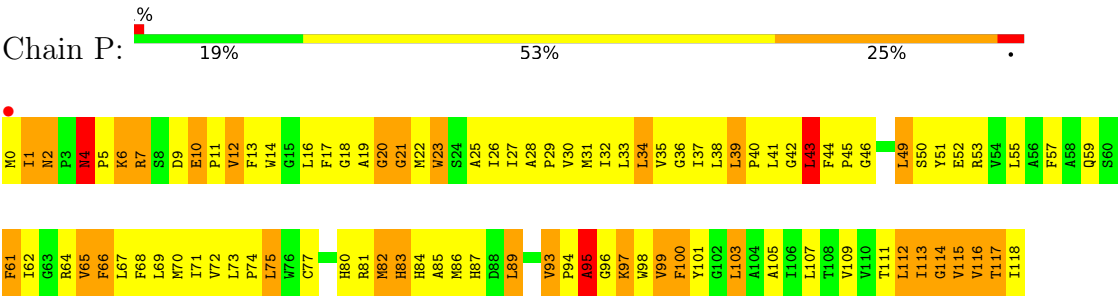
- Molecule 3: Fumarate reductase subunit C



- Molecule 4: Fumarate reductase subunit D



● Molecule 4: Fumarate reductase subunit D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.80Å 139.53Å 273.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.30 39.53 – 3.30	Depositor EDS
% Data completeness (in resolution range)	83.5 (20.00-3.30) 83.4 (39.53-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.12 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.284 0.237 , 0.270	Depositor DCC
R_{free} test set	1096 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16840	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, FES, SF4, FAD, F3S, MQ7

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.71	79/4540 (1.7%)	1.81	109/6139 (1.8%)
1	M	0.36	0/4504	0.71	0/6087
2	B	1.01	2/1931 (0.1%)	1.15	8/2617 (0.3%)
2	N	0.41	0/1931	0.71	0/2617
3	C	0.98	0/1094	1.12	6/1496 (0.4%)
3	O	0.92	1/1094 (0.1%)	1.11	5/1496 (0.3%)
4	D	0.77	0/956	1.03	1/1303 (0.1%)
4	P	0.70	1/956 (0.1%)	1.06	3/1303 (0.2%)
All	All	1.06	83/17006 (0.5%)	1.22	132/23058 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	3
3	O	0	1
All	All	0	8

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	450	LYS	CD-CE	10.77	1.78	1.51
1	A	372	LYS	CB-CG	9.71	1.78	1.52
1	A	277	PRO	CA-C	9.18	1.71	1.52
1	A	484	GLU	CG-CD	8.83	1.65	1.51
1	A	240	GLY	C-O	-8.45	1.10	1.23
1	A	129	ASP	CB-CG	8.43	1.69	1.51
1	A	576	ALA	CA-CB	8.32	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	517	CYS	CB-SG	-8.04	1.68	1.82
1	A	352	PRO	CA-C	8.02	1.68	1.52
1	A	269	GLY	N-CA	-7.89	1.34	1.46
1	A	270	PRO	CA-C	7.79	1.68	1.52
1	A	63	GLU	C-O	-7.52	1.09	1.23
1	A	220	GLY	C-O	-7.09	1.12	1.23
1	A	543	ASP	CA-CB	6.98	1.69	1.53
1	A	90	PRO	CA-CB	-6.80	1.40	1.53
1	A	333	GLU	CG-CD	6.76	1.62	1.51
1	A	22	ALA	CA-CB	-6.76	1.38	1.52
1	A	77	CYS	CB-SG	-6.73	1.70	1.82
1	A	85	PHE	CE2-CZ	-6.66	1.24	1.37
3	O	1	THR	C-O	6.66	1.35	1.23
1	A	221	VAL	CA-CB	-6.64	1.40	1.54
1	A	424	ALA	CA-CB	6.58	1.66	1.52
1	A	287	ARG	C-O	-6.57	1.10	1.23
1	A	36	SER	CA-CB	-6.57	1.43	1.52
1	A	469	PRO	CA-C	-6.56	1.39	1.52
1	A	113	VAL	CB-CG1	-6.51	1.39	1.52
1	A	465	ILE	CA-CB	-6.51	1.39	1.54
1	A	276	GLU	N-CA	-6.35	1.33	1.46
1	A	64	TYR	CD2-CE2	6.32	1.48	1.39
1	A	145	GLN	C-O	-6.31	1.11	1.23
1	A	172	ALA	CA-CB	-6.25	1.39	1.52
1	A	372	LYS	CG-CD	6.24	1.73	1.52
1	A	177	GLU	CD-OE2	6.21	1.32	1.25
1	A	229	VAL	C-O	-6.21	1.11	1.23
1	A	276	GLU	CA-CB	6.19	1.67	1.53
1	A	372	LYS	CD-CE	6.19	1.66	1.51
2	B	56	SER	C-O	-6.15	1.11	1.23
1	A	327	ARG	CG-CD	6.07	1.67	1.51
1	A	330	PHE	CB-CG	6.01	1.61	1.51
1	A	90	PRO	N-CD	-6.00	1.39	1.47
1	A	119	MET	CA-C	5.96	1.68	1.52
1	A	386	HIS	C-O	-5.89	1.12	1.23
2	B	207	VAL	CA-CB	-5.89	1.42	1.54
1	A	574	PRO	CA-CB	-5.88	1.41	1.53
1	A	138	THR	CA-CB	5.85	1.68	1.53
1	A	90	PRO	CA-C	-5.81	1.41	1.52
1	A	312	VAL	CA-CB	-5.77	1.42	1.54
1	A	28	PRO	CA-C	-5.75	1.41	1.52
1	A	460	GLU	CD-OE2	5.75	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	522	ALA	CA-CB	5.73	1.64	1.52
1	A	61	SER	CA-CB	-5.72	1.44	1.52
1	A	371	ILE	CA-CB	5.63	1.67	1.54
1	A	410	ALA	C-O	-5.63	1.12	1.23
1	A	481	GLU	CD-OE1	5.58	1.31	1.25
1	A	198	VAL	CB-CG2	-5.50	1.41	1.52
1	A	328	LEU	N-CA	5.48	1.57	1.46
1	A	486	PHE	CE2-CZ	5.47	1.47	1.37
4	P	95	ALA	CA-CB	-5.43	1.41	1.52
1	A	157	VAL	CB-CG1	-5.38	1.41	1.52
1	A	514	VAL	CA-CB	-5.38	1.43	1.54
1	A	375	PHE	CE1-CZ	5.34	1.47	1.37
1	A	450	LYS	CE-NZ	5.33	1.62	1.49
1	A	549	LYS	CG-CD	5.32	1.70	1.52
1	A	46	VAL	CB-CG1	-5.31	1.41	1.52
1	A	28	PRO	N-CA	-5.26	1.38	1.47
1	A	400	VAL	CA-CB	-5.26	1.43	1.54
1	A	473	GLN	CB-CG	-5.23	1.38	1.52
1	A	253	ILE	CA-CB	5.20	1.66	1.54
1	A	368	GLU	CA-CB	-5.16	1.42	1.53
1	A	270	PRO	N-CD	5.13	1.55	1.47
1	A	146	PHE	CE1-CZ	5.13	1.47	1.37
1	A	461	GLU	CA-CB	5.12	1.65	1.53
1	A	547	PHE	CE2-CZ	-5.12	1.27	1.37
1	A	173	MET	SD-CE	5.10	2.06	1.77
1	A	35	ILE	C-O	-5.09	1.13	1.23
1	A	460	GLU	CD-OE1	5.07	1.31	1.25
1	A	10	VAL	CB-CG1	-5.07	1.42	1.52
1	A	474	LYS	CD-CE	5.06	1.64	1.51
1	A	136	LEU	C-O	-5.05	1.13	1.23
1	A	391	LEU	CA-CB	-5.03	1.42	1.53
1	A	64	TYR	CZ-OH	5.03	1.46	1.37
1	A	3	PHE	CD2-CE2	5.01	1.49	1.39
1	A	213	MET	CG-SD	5.01	1.94	1.81

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	GLY	C-N-CD	-13.40	91.12	120.60
1	A	370	ARG	NE-CZ-NH1	-13.35	113.63	120.30
1	A	68	ASP	CB-CG-OD1	-10.64	108.72	118.30
1	A	68	ASP	CB-CG-OD2	10.35	127.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	501	ASP	CB-CG-OD2	10.22	127.50	118.30
1	A	164	ASP	CB-CG-OD2	9.37	126.73	118.30
1	A	161	LEU	CA-CB-CG	-8.92	94.78	115.30
1	A	269	GLY	CA-C-N	-8.85	92.31	117.10
1	A	501	ASP	CB-CG-OD1	-8.76	110.42	118.30
1	A	200	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	A	467	ARG	NE-CZ-NH1	-8.56	116.02	120.30
1	A	269	GLY	O-C-N	8.51	137.26	121.10
2	B	13	TYR	CB-CG-CD1	-8.50	115.90	121.00
1	A	325	HIS	C-N-CA	-8.45	100.58	121.70
1	A	269	GLY	N-CA-C	8.29	133.82	113.10
1	A	266	TYR	N-CA-CB	-8.14	95.94	110.60
1	A	18	ARG	CG-CD-NE	-8.10	94.79	111.80
1	A	42	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	151	ARG	NE-CZ-NH1	-7.91	116.35	120.30
1	A	120	LYS	CA-CB-CG	7.80	130.57	113.40
1	A	351	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	A	563	LEU	CB-CG-CD1	-7.63	98.04	111.00
1	A	164	ASP	CB-CG-OD1	-7.47	111.57	118.30
1	A	391	LEU	CB-CG-CD1	-7.47	98.31	111.00
1	A	391	LEU	CB-CA-C	-7.42	96.11	110.20
1	A	277	PRO	N-CA-C	-7.39	92.88	112.10
1	A	248	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	42	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	545	VAL	CB-CA-C	-7.28	97.57	111.40
3	C	99	LYS	N-CA-C	-7.20	91.55	111.00
1	A	225	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	A	488	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	106	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	321	GLU	N-CA-C	6.66	128.98	111.00
1	A	276	GLU	CB-CA-C	-6.64	97.12	110.40
1	A	544	ASP	N-CA-CB	6.62	122.52	110.60
1	A	372	LYS	CB-CG-CD	6.61	128.79	111.60
1	A	460	GLU	OE1-CD-OE2	6.59	131.21	123.30
1	A	106	ARG	CB-CA-C	-6.58	97.24	110.40
1	A	544	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	479	LEU	CB-CG-CD2	-6.54	99.88	111.00
1	A	270	PRO	N-CA-C	-6.53	95.12	112.10
1	A	466	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	A	270	PRO	CB-CA-C	6.51	128.27	112.00
1	A	194	GLY	N-CA-C	6.50	129.35	113.10
1	A	485	ARG	NE-CZ-NH1	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	39	LEU	CA-CB-CG	-6.45	100.46	115.30
1	A	418	GLY	N-CA-C	-6.44	97.00	113.10
1	A	270	PRO	CA-C-N	6.34	131.15	117.20
1	A	136	LEU	CA-CB-CG	-6.31	100.80	115.30
1	A	229	VAL	O-C-N	-6.28	112.65	122.70
1	A	327	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	543	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	517	CYS	CB-CA-C	6.22	122.84	110.40
1	A	118	GLY	O-C-N	-6.15	112.86	122.70
1	A	448	TRP	CB-CA-C	-6.10	98.21	110.40
2	B	13	TYR	CB-CA-C	-6.07	98.27	110.40
1	A	64	TYR	CB-CG-CD2	6.04	124.62	121.00
1	A	223	LEU	N-CA-C	-5.97	94.87	111.00
1	A	549	LYS	CD-CE-NZ	5.96	125.40	111.70
1	A	517	CYS	N-CA-CB	-5.95	99.89	110.60
1	A	446	GLU	C-N-CA	-5.94	106.85	121.70
1	A	445	GLY	N-CA-C	5.89	127.83	113.10
1	A	556	ASP	O-C-N	-5.89	113.27	122.70
1	A	61	SER	CB-CA-C	-5.88	98.92	110.10
3	C	100	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	556	ASP	CA-C-N	5.87	130.11	117.20
1	A	28	PRO	C-N-CA	-5.86	107.05	121.70
3	O	70	ILE	N-CA-C	-5.86	95.18	111.00
3	C	27	LEU	CA-CB-CG	-5.78	102.00	115.30
1	A	412	GLU	CG-CD-OE2	-5.75	106.80	118.30
1	A	13	GLY	N-CA-C	-5.75	98.73	113.10
1	A	263	LEU	CB-CG-CD1	-5.74	101.24	111.00
1	A	366	ASN	CB-CA-C	-5.74	98.92	110.40
2	B	13	TYR	CB-CG-CD2	5.73	124.44	121.00
1	A	105	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	332	CYS	CA-CB-SG	5.68	124.22	114.00
1	A	502	LEU	CB-CG-CD2	-5.64	101.40	111.00
3	C	1	THR	C-N-CA	-5.64	107.60	121.70
2	B	93	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	262	TYR	N-CA-C	5.61	126.14	111.00
1	A	254	LEU	CA-CB-CG	5.60	128.18	115.30
2	B	13	TYR	CA-CB-CG	-5.59	102.78	113.40
1	A	265	ASP	CB-CA-C	-5.58	99.24	110.40
1	A	479	LEU	CA-CB-CG	-5.56	102.52	115.30
1	A	248	ARG	CG-CD-NE	-5.55	100.15	111.80
1	A	326	GLU	CA-C-N	-5.54	105.00	117.20
1	A	312	VAL	N-CA-C	-5.52	96.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	39	TYR	CB-CG-CD1	-5.47	117.72	121.00
1	A	412	GLU	OE1-CD-OE2	5.46	129.85	123.30
1	A	269	GLY	CA-C-O	5.45	130.41	120.60
1	A	448	TRP	N-CA-CB	5.45	120.41	110.60
1	A	466	TYR	CB-CG-CD1	5.45	124.27	121.00
1	A	185	ALA	N-CA-CB	5.43	117.70	110.10
1	A	503	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	A	277	PRO	CA-N-CD	-5.41	103.93	111.50
3	O	63	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	330	PHE	CB-CA-C	5.37	121.15	110.40
1	A	465	ILE	CB-CA-C	-5.37	100.85	111.60
1	A	233	PRO	N-CD-CG	-5.37	95.15	103.20
1	A	1	GLN	N-CA-C	-5.35	96.55	111.00
1	A	177	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	A	486	PHE	N-CA-CB	-5.33	101.00	110.60
3	C	130	TRP	N-CA-C	5.30	125.32	111.00
2	B	16	GLU	CA-CB-CG	5.29	125.05	113.40
3	C	4	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	123	ARG	NE-CZ-NH1	-5.29	117.66	120.30
2	B	15	PRO	C-N-CA	-5.29	108.49	121.70
1	A	68	ASP	CB-CA-C	-5.27	99.86	110.40
1	A	488	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	O	99	LYS	N-CA-C	-5.24	96.84	111.00
1	A	311	VAL	CB-CA-C	-5.22	101.48	111.40
1	A	538	GLY	C-N-CA	-5.22	108.66	121.70
2	B	13	TYR	C-N-CA	-5.21	108.66	121.70
3	O	28	ARG	NE-CZ-NH2	-5.20	117.70	120.30
4	P	49	LEU	CA-CB-CG	5.19	127.24	115.30
4	P	4	ASN	N-CA-C	-5.19	97.00	111.00
1	A	329	PRO	N-CA-C	5.17	125.55	112.10
1	A	106	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	274	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	548	LEU	CB-CG-CD2	-5.12	102.30	111.00
1	A	239	SER	CB-CA-C	-5.11	100.38	110.10
4	D	39	LEU	C-N-CD	5.11	139.13	128.40
3	O	27	LEU	CA-CB-CG	-5.10	103.57	115.30
1	A	12	ALA	N-CA-C	5.06	124.66	111.00
1	A	496	SER	N-CA-CB	-5.06	102.92	110.50
1	A	180	LEU	CB-CA-C	-5.05	100.60	110.20
1	A	112	ASN	CB-CA-C	-5.05	100.31	110.40
1	A	280	LYS	CD-CE-NZ	5.04	123.28	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	GLN	N-CA-CB	-5.03	101.54	110.60
1	A	555	ARG	C-N-CA	-5.02	109.14	121.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	GLY	Mainchain
1	A	276	GLU	Mainchain
1	A	341	VAL	Mainchain
1	A	422	GLU	Mainchain
2	B	15	PRO	Mainchain
2	B	16	GLU	Mainchain
2	B	185	ASP	Mainchain
3	O	129	TYR	Sidechain

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	4448	0	4337	457	0
1	M	4414	0	4300	755	0
2	B	1888	0	1837	172	0
2	N	1888	0	1837	315	0
3	C	1058	0	1108	122	0
3	O	1058	0	1108	133	0
4	D	926	0	971	140	0
4	P	926	0	971	130	0
5	A	13	0	5	14	0
5	M	13	0	5	3	0
6	A	52	0	29	17	0
6	M	52	0	29	14	0
7	B	4	0	0	0	0
7	N	4	0	0	0	0
8	B	7	0	0	0	0
8	N	7	0	0	1	0
9	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	N	8	0	0	3	0
10	D	33	0	37	7	0
10	P	33	0	37	12	0
All	All	16840	0	16611	2099	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 63.

All (2099) 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:A:207:ILE:CG1	1:A:207:ILE:CD1	1.79	1.57
1:A:450:LYS:CE	1:A:450:LYS:CD	1.78	1.57
1:A:372:LYS:CB	1:A:372:LYS:CG	1.78	1.56
1:A:173:MET:CE	1:A:173:MET:SD	2.06	1.43
1:M:44:HIS:NE2	6:M:803:FAD:HM82	1.13	1.42
1:M:44:HIS:NE2	6:M:803:FAD:C8M	1.81	1.42
1:A:44:HIS:NE2	6:A:703:FAD:HM82	1.27	1.42
1:A:44:HIS:NE2	6:A:703:FAD:C8M	1.86	1.36
1:A:253:ILE:HG22	1:A:315:ASP:CB	1.72	1.18
1:A:27:ASN:C	1:A:27:ASN:HD22	1.35	1.16
1:A:253:ILE:CG2	1:A:315:ASP:HB3	1.74	1.16
1:A:275:GLY:O	1:A:277:PRO:HD2	1.45	1.16
1:A:261:ARG:NH1	1:A:282:MET:HE3	1.58	1.16
1:M:48:ALA:HB3	1:M:132:GLY:HA3	1.18	1.12
5:A:702:FLC:OG2	5:A:702:FLC:HA1	1.33	1.12
3:C:50:LYS:NZ	4:D:118:ILE:HD12	1.65	1.12
2:N:162:GLY:O	3:O:11:MET:HG3	1.50	1.12
1:M:74:ASP:HB3	1:M:388:ALA:HB3	1.27	1.11
1:A:543:ASP:OD2	1:A:546:ASN:ND2	1.85	1.10
1:M:38:VAL:HB	2:N:54:ARG:HH22	1.15	1.10
1:M:391:LEU:HG	1:M:392:GLY:H	1.14	1.10
2:N:65:CYS:HB2	2:N:76:ALA:HB3	1.30	1.09
1:A:253:ILE:HG22	1:A:315:ASP:HB3	1.30	1.09
1:M:227:GLU:HG2	1:M:518:MET:HB3	1.34	1.09
4:D:55:LEU:HG	4:D:59:GLN:NE2	1.69	1.08
2:B:225:GLN:HG2	3:C:93:ALA:HB2	1.36	1.08
3:O:87:PHE:HD2	3:O:112:LEU:HD13	1.08	1.07
1:M:72:GLY:HA3	1:M:391:LEU:HD22	1.33	1.06
1:M:227:GLU:HG3	1:M:463:CYS:SG	1.95	1.06
1:A:18:ARG:NH1	1:A:92:GLU:OE1	1.88	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LEU:O	1:A:268:MET:HB2	1.55	1.05
1:M:225:ASP:H	1:M:550:HIS:HB3	1.18	1.05
1:A:287:ARG:HG3	1:A:287:ARG:NH1	1.56	1.04
1:A:263:LEU:HB3	1:A:268:MET:CE	1.88	1.04
1:A:287:ARG:HH11	1:A:287:ARG:CG	1.70	1.04
4:D:55:LEU:HG	4:D:59:GLN:HE22	1.18	1.04
2:B:180:ASN:ND2	2:B:188:LYS:HG3	1.72	1.03
3:O:2:THR:HG22	3:O:4:ARG:H	1.19	1.03
1:M:360:GLY:H	1:M:382:SER:HB2	1.24	1.02
1:M:527:GLU:HA	1:M:539:CYS:SG	1.97	1.02
1:A:101:CYS:HB2	1:A:138:THR:HG21	1.40	1.02
1:M:467:ARG:NH2	1:M:532:HIS:HA	1.73	1.02
2:N:98:ILE:HG12	3:O:9:ARG:HH21	1.23	1.02
1:M:15:ALA:HB2	1:M:399:LEU:HD22	1.40	1.02
1:A:261:ARG:HH11	1:A:282:MET:HE3	1.23	1.01
4:P:10:GLU:HG3	4:P:10:GLU:O	1.56	1.01
2:N:69:VAL:HG11	2:N:79:THR:HG21	1.43	1.01
2:B:110:ILE:HA	2:B:113:LEU:HD12	1.42	1.00
2:B:210:CYS:SG	2:B:220:PRO:HG2	2.02	1.00
1:M:476:ILE:HG12	1:M:519:ALA:HB1	1.42	0.99
1:A:253:ILE:HG12	1:A:261:ARG:HD3	1.41	0.99
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.19	0.99
3:O:87:PHE:CD2	3:O:112:LEU:HD13	1.97	0.99
1:M:360:GLY:N	1:M:382:SER:HB2	1.77	0.99
2:B:238:ALA:HA	2:B:241:LYS:HB3	1.43	0.98
3:O:50:LYS:HE2	4:P:118:ILE:HG22	1.42	0.98
1:A:527:GLU:HG2	1:A:547:PHE:CB	1.94	0.97
1:M:74:ASP:HB3	1:M:388:ALA:CB	1.95	0.97
1:M:548:LEU:HD21	1:M:570:ILE:HD11	1.46	0.97
1:A:234:THR:HG22	1:A:350:VAL:HG21	1.46	0.97
1:A:236:LEU:HD21	1:A:243:MET:CE	1.95	0.96
1:A:115:ARG:HH11	1:A:115:ARG:HG3	1.24	0.96
1:A:253:ILE:CG2	1:A:315:ASP:CB	2.39	0.96
1:M:55:VAL:HB	1:M:90:PRO:HG3	1.48	0.96
1:M:106:ARG:HB3	1:M:112:ASN:HB2	1.48	0.96
1:M:232:HIS:O	1:M:352:PRO:HA	1.64	0.95
3:O:4:ARG:HE	3:O:6:PRO:HG3	1.31	0.95
2:N:149:ILE:HG13	2:N:151:CYS:HB3	1.45	0.95
1:A:427:ALA:O	1:A:430:ALA:HB3	1.67	0.95
1:M:178:GLY:HA3	1:M:496:SER:HB2	1.48	0.95
1:A:295:TRP:CZ3	1:A:299:ARG:HD2	2.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:NE2	6:A:703:FAD:HM81	1.80	0.94
1:M:227:GLU:HB2	1:M:518:MET:O	1.67	0.94
1:A:542:ARG:NE	1:A:544:ASP:OD2	2.00	0.94
1:A:27:ASN:C	1:A:27:ASN:ND2	2.09	0.94
1:M:53:ALA:H	1:M:394:ASN:HD22	1.16	0.94
1:M:82:VAL:HG22	1:M:385:LEU:HA	1.46	0.94
1:M:113:VAL:HB	1:M:124:THR:O	1.69	0.93
1:A:562:ARG:HH11	1:A:562:ARG:HG3	1.32	0.93
1:M:223:LEU:HG	1:M:360:GLY:HA2	1.49	0.93
1:M:448:TRP:O	1:M:452:ARG:HD3	1.67	0.93
3:C:50:LYS:HD3	4:D:118:ILE:HB	1.48	0.93
2:N:214:CYS:SG	2:N:218:VAL:HG23	2.09	0.93
1:M:93:MET:HB3	1:M:125:TRP:CZ3	2.03	0.92
1:M:474:LYS:HD2	1:M:478:LYS:HE2	1.52	0.92
1:A:261:ARG:NH1	1:A:282:MET:CE	2.33	0.92
1:A:288:ASP:OD2	1:A:288:ASP:N	1.98	0.92
1:M:361:ILE:H	1:M:382:SER:H	0.94	0.92
1:M:217:LEU:HD11	1:M:555:ARG:HD2	1.50	0.92
1:M:151:ARG:HH11	1:M:151:ARG:HB2	1.35	0.92
2:N:75:LEU:HD21	2:N:215:PRO:HB3	1.51	0.92
1:A:44:HIS:CE1	6:A:703:FAD:HM82	2.04	0.92
1:M:273:PRO:HG2	1:M:276:GLU:HB2	1.49	0.92
3:O:4:ARG:NE	3:O:6:PRO:HG3	1.86	0.91
1:M:44:HIS:NE2	6:M:803:FAD:HM81	1.84	0.91
1:M:44:HIS:HE1	1:M:204:ASN:HA	1.33	0.91
4:P:43:LEU:HD23	4:P:43:LEU:N	1.84	0.91
2:B:44:LYS:HA	2:B:48:ALA:O	1.71	0.90
1:A:275:GLY:O	1:A:277:PRO:CD	2.19	0.90
2:N:30:TYR:HB3	2:N:81:LEU:HD13	1.54	0.90
1:A:493:ASP:HB3	1:A:499:ASN:HD21	1.36	0.90
1:M:391:LEU:HG	1:M:392:GLY:N	1.86	0.90
2:B:7:LYS:HE2	2:B:27:GLU:HG3	1.53	0.90
3:C:63:LEU:HB3	4:D:40:PRO:HG3	1.53	0.89
1:M:361:ILE:H	1:M:382:SER:N	1.70	0.89
2:B:14:ASN:N	2:B:18:ASP:OD2	2.06	0.89
2:N:144:GLN:HG3	3:O:102:LYS:NZ	1.88	0.89
1:M:242:LEU:CD2	1:M:244:THR:H	1.85	0.89
3:C:50:LYS:HZ3	4:D:118:ILE:HD12	1.22	0.89
3:O:53:PRO:HB3	4:P:51:TYR:CD2	2.08	0.88
2:N:44:LYS:HA	2:N:48:ALA:O	1.73	0.88
1:A:13:GLY:O	1:A:17:LEU:HB2	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:28:ARG:O	3:C:31:THR:HB	1.73	0.88
2:N:169:GLY:O	2:N:173:ILE:HG13	1.73	0.88
1:A:416:THR:CG2	1:A:416:THR:O	2.22	0.88
1:A:287:ARG:HG3	1:A:287:ARG:HH11	0.77	0.87
1:M:403:GLY:HA2	1:M:406:ALA:HB3	1.55	0.87
3:O:87:PHE:HD2	3:O:112:LEU:CD1	1.88	0.87
3:O:123:ILE:HD11	10:P:800:MQ7:H162	1.54	0.87
1:M:433:GLU:HG3	1:M:434:GLN:N	1.89	0.87
1:M:224:ARG:HE	1:M:550:HIS:CD2	1.91	0.87
1:M:38:VAL:HB	2:N:54:ARG:NH2	1.89	0.87
5:A:702:FLC:OG2	5:A:702:FLC:CA	2.22	0.86
1:A:184:ARG:HH11	1:A:184:ARG:CG	1.88	0.86
3:C:111:SER:O	3:C:115:VAL:HG23	1.73	0.86
2:N:196:ASN:HD22	2:N:196:ASN:N	1.74	0.86
1:M:471:LEU:HD12	1:M:472:MET:N	1.90	0.86
1:M:167:VAL:HG21	1:M:374:LEU:HD13	1.56	0.86
1:M:490:ARG:H	1:M:490:ARG:HD3	1.41	0.86
3:O:123:ILE:CD1	10:P:800:MQ7:H162	2.06	0.86
1:M:224:ARG:HE	1:M:550:HIS:HD2	1.21	0.86
1:A:263:LEU:HB3	1:A:268:MET:HE3	1.58	0.85
1:M:279:ASN:HD22	1:M:280:LYS:N	1.74	0.85
1:A:540:THR:O	1:A:541:GLU:OE2	1.94	0.85
2:N:14:ASN:O	2:N:18:ASP:HB3	1.76	0.85
1:A:27:ASN:ND2	1:A:27:ASN:O	2.06	0.85
2:B:12:ARG:NH2	2:B:101:ASP:OD1	2.10	0.85
1:M:53:ALA:CB	1:M:394:ASN:HD22	1.89	0.85
1:M:230:GLN:HE21	1:M:287:ARG:NH1	1.73	0.85
1:M:42:ARG:HH22	2:N:54:ARG:HB3	1.42	0.85
3:O:4:ARG:HE	3:O:6:PRO:CG	1.90	0.85
3:C:50:LYS:CE	3:C:50:LYS:HA	2.07	0.85
1:M:44:HIS:CE1	6:M:803:FAD:HM82	2.12	0.84
1:A:261:ARG:HH11	1:A:282:MET:CE	1.88	0.84
2:N:144:GLN:HG3	3:O:102:LYS:HZ2	1.42	0.84
4:D:0:MET:HG3	4:D:1:ILE:H	1.41	0.84
4:D:99:VAL:HG12	4:D:100:PHE:N	1.91	0.84
2:N:54:ARG:HG2	2:N:54:ARG:HH11	1.41	0.84
1:M:92:GLU:HA	1:M:95:GLN:HB3	1.60	0.83
2:B:241:LYS:O	2:B:243:ARG:N	2.11	0.83
2:N:196:ASN:HD22	2:N:196:ASN:H	1.24	0.83
1:A:65:HIS:ND1	1:A:86:VAL:HG22	1.92	0.83
1:M:44:HIS:CE1	1:M:204:ASN:HA	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:60:VAL:HG12	3:O:64:GLN:HE21	1.41	0.83
1:A:446:GLU:HG2	1:A:488:ARG:O	1.77	0.83
1:M:225:ASP:N	1:M:550:HIS:HB3	1.94	0.83
3:O:87:PHE:CD2	3:O:112:LEU:HB3	2.13	0.83
3:C:87:PHE:CD1	3:C:112:LEU:HB3	2.14	0.83
4:D:1:ILE:O	4:D:1:ILE:HG22	1.79	0.83
1:A:57:GLN:NE2	1:A:122:GLU:HG2	1.94	0.82
1:M:49:GLN:HE21	1:M:49:GLN:H	1.22	0.82
3:C:49:LEU:O	3:C:49:LEU:HD23	1.80	0.82
1:A:314:LEU:HD11	1:A:316:LEU:HD21	1.59	0.82
2:N:145:PHE:HA	2:N:218:VAL:HG13	1.60	0.82
4:P:26:ILE:HG22	4:P:27:ILE:HG13	1.61	0.82
2:N:168:ILE:HD11	2:N:173:ILE:HG12	1.61	0.82
3:C:45:GLY:HA3	10:D:700:MQ7:H8	1.61	0.82
1:M:49:GLN:H	1:M:49:GLN:NE2	1.76	0.82
1:M:24:ALA:O	1:M:26:ALA:N	2.13	0.82
1:A:200:ARG:HD3	1:A:201:TYR:CE1	2.15	0.82
2:B:26:TYR:HD2	2:B:47:LEU:HD13	1.42	0.82
1:M:256:ASN:HD21	1:M:260:TYR:HB3	1.44	0.82
1:M:526:LYS:HD2	1:M:526:LYS:O	1.80	0.81
1:M:551:THR:O	1:M:552:LEU:HD23	1.81	0.81
1:M:52:SER:HB2	1:M:396:LEU:CB	2.10	0.81
1:A:263:LEU:CB	1:A:268:MET:HE3	2.10	0.81
2:N:69:VAL:HG21	2:N:74:LYS:HB2	1.61	0.81
1:A:548:LEU:HD23	1:A:548:LEU:O	1.81	0.81
1:A:306:THR:HB	1:A:307:PRO:CD	2.10	0.81
1:M:53:ALA:H	1:M:394:ASN:ND2	1.78	0.81
1:M:77:CYS:SG	1:M:387:GLY:HA2	2.20	0.81
3:O:17:LYS:HG3	3:O:23:ARG:HH21	1.47	0.81
3:O:128:LEU:HD13	4:P:45:PRO:HD2	1.63	0.80
1:A:306:THR:HB	1:A:307:PRO:HD2	1.60	0.80
1:A:253:ILE:O	1:A:314:LEU:HA	1.82	0.80
1:A:388:ALA:O	1:A:389:ASN:HB2	1.80	0.80
3:O:90:ALA:N	3:O:91:PRO:HD2	1.97	0.80
1:M:180:LEU:HD13	1:M:433:GLU:HB2	1.62	0.80
1:M:356:TYR:HE2	1:M:379:GLU:HG3	1.46	0.80
1:A:90:PRO:HG2	1:A:91:THR:N	1.95	0.80
1:M:116:PHE:HB2	1:M:124:THR:HG21	1.64	0.80
2:B:50:ASP:C	2:B:50:ASP:OD1	2.19	0.80
1:M:65:HIS:HB2	1:M:123:ARG:NH1	1.96	0.80
1:M:377:VAL:HG22	1:M:402:PHE:HE2	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:HIS:CD2	1:A:174:ASN:HA	2.17	0.80
1:M:130:LYS:NZ	2:N:216:LYS:HD3	1.97	0.79
2:B:211:SER:OG	2:B:220:PRO:HD2	1.82	0.79
1:M:439:LEU:HD23	1:M:442:GLN:NE2	1.98	0.79
1:M:230:GLN:HE21	1:M:287:ARG:HH11	1.26	0.79
4:P:41:LEU:O	4:P:43:LEU:HD23	1.81	0.79
3:C:124:LEU:HD23	4:D:34:LEU:HD21	1.62	0.79
1:M:60:ASP:HB2	1:M:123:ARG:CZ	2.12	0.79
1:M:361:ILE:HG12	1:M:376:ALA:HB3	1.64	0.79
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.18	0.79
2:B:180:ASN:HD22	2:B:188:LYS:HG3	1.42	0.79
1:M:133:PHE:HZ	2:N:149:ILE:HA	1.46	0.79
1:M:242:LEU:C	1:M:242:LEU:HD23	2.03	0.79
1:M:38:VAL:CG1	2:N:54:ARG:HH12	1.96	0.79
2:N:6:LEU:HD13	2:N:81:LEU:HD21	1.65	0.79
1:M:53:ALA:N	1:M:394:ASN:HD22	1.80	0.78
1:M:113:VAL:HG21	1:M:123:ARG:HA	1.65	0.78
1:M:226:MET:HG2	1:M:517:CYS:HB2	1.65	0.78
3:C:90:ALA:N	3:C:91:PRO:HD2	1.97	0.78
1:M:479:LEU:HD13	1:M:516:GLU:OE1	1.83	0.78
2:B:238:ALA:HA	2:B:241:LYS:CB	2.13	0.78
1:A:198:VAL:HG23	1:A:455:MET:CE	2.14	0.78
2:N:113:LEU:O	2:N:116:ILE:HG12	1.84	0.78
1:A:497:VAL:O	1:A:497:VAL:HG12	1.82	0.78
3:C:31:THR:HG21	3:C:82:HIS:HB2	1.64	0.78
1:M:361:ILE:N	1:M:382:SER:H	1.78	0.78
1:M:467:ARG:HH22	1:M:532:HIS:HA	1.46	0.78
2:B:211:SER:HA	2:B:220:PRO:HD2	1.64	0.77
1:M:159:ASP:HB3	1:M:432:VAL:HG13	1.66	0.77
1:M:514:VAL:O	1:M:518:MET:HG3	1.83	0.77
1:M:549:LYS:HG3	1:M:565:TYR:HB3	1.67	0.77
1:A:493:ASP:HB3	1:A:499:ASN:ND2	1.99	0.77
1:A:253:ILE:HG21	1:A:315:ASP:HB3	1.67	0.77
1:M:222:PRO:HB3	1:M:552:LEU:HD22	1.66	0.77
3:C:36:VAL:HG22	4:D:75:LEU:HD22	1.66	0.77
1:M:52:SER:HB2	1:M:396:LEU:HB3	1.66	0.77
1:M:229:VAL:HG12	1:M:531:ALA:HB1	1.66	0.77
1:A:416:THR:O	1:A:416:THR:HG23	1.85	0.77
1:M:227:GLU:HG2	1:M:518:MET:CB	2.14	0.77
1:A:262:TYR:CD1	1:A:297:GLU:HG3	2.19	0.77
1:A:545:VAL:HG12	1:A:546:ASN:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:PRO:C	2:B:104:VAL:HG23	2.05	0.77
1:M:433:GLU:HG3	1:M:434:GLN:H	1.48	0.77
2:N:28:VAL:HG22	2:N:43:ILE:HG13	1.65	0.77
3:O:49:LEU:HG	3:O:49:LEU:O	1.85	0.77
1:A:147:PRO:HD2	1:A:148:GLN:OE1	1.85	0.77
1:A:491:ILE:O	1:A:491:ILE:HG22	1.85	0.77
1:A:213:MET:O	1:A:217:LEU:HD12	1.85	0.77
1:M:46:VAL:HG13	1:M:136:LEU:HD23	1.65	0.77
3:C:50:LYS:HA	3:C:50:LYS:HE3	1.67	0.76
1:M:242:LEU:HD21	1:M:244:THR:H	1.51	0.76
2:N:69:VAL:N	2:N:72:VAL:O	2.14	0.76
4:P:80:HIS:CD2	4:P:84:HIS:CD2	2.72	0.76
1:M:226:MET:HG3	1:M:518:MET:HG2	1.68	0.76
1:A:253:ILE:CG1	1:A:261:ARG:HD3	2.14	0.76
4:D:44:PHE:CE1	4:D:49:LEU:HB2	2.20	0.76
1:M:48:ALA:HB3	1:M:132:GLY:CA	2.09	0.76
1:M:230:GLN:HG2	1:M:390:ARG:HH21	1.51	0.76
3:O:53:PRO:HD3	4:P:51:TYR:CZ	2.19	0.76
4:D:83:HIS:O	4:D:86:MET:HB2	1.86	0.76
4:P:43:LEU:HD23	4:P:43:LEU:H	1.46	0.76
1:A:114:ARG:HD3	1:A:126:PHE:CD2	2.20	0.76
3:C:94:ALA:HB1	3:C:96:ILE:HD11	1.68	0.76
1:M:220:GLY:N	1:M:371:ILE:HD11	2.00	0.76
1:M:368:GLU:HG2	1:M:409:GLN:OE1	1.85	0.76
4:P:67:LEU:O	4:P:71:ILE:HD12	1.86	0.76
1:M:42:ARG:NH2	2:N:64:SER:OG	2.18	0.76
1:M:346:GLU:HG3	1:M:347:PRO:HD2	1.66	0.76
1:A:46:VAL:HG23	1:A:47:ALA:N	2.00	0.76
1:A:527:GLU:HG2	1:A:547:PHE:HB3	1.65	0.76
2:B:32:ALA:O	2:B:82:ARG:NH1	2.18	0.76
1:A:328:LEU:CD1	1:A:331:ILE:HG13	2.16	0.76
4:D:0:MET:HG3	4:D:1:ILE:N	2.00	0.76
1:M:223:LEU:HA	1:M:360:GLY:O	1.86	0.76
1:M:227:GLU:CG	1:M:518:MET:HB3	2.15	0.76
1:A:44:HIS:CD2	6:A:703:FAD:C8M	2.69	0.75
2:N:81:LEU:HD23	2:N:81:LEU:O	1.86	0.75
2:B:43:ILE:HG23	2:B:47:LEU:HD12	1.68	0.75
2:N:168:ILE:HG23	2:N:199:ASN:O	1.86	0.75
4:P:10:GLU:O	4:P:10:GLU:CG	2.34	0.75
1:A:390:ARG:HH12	5:A:702:FLC:CAC	1.99	0.75
2:B:13:TYR:CD2	2:B:13:TYR:O	2.40	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:TYR:HE1	2:B:171:ALA:HB3	1.52	0.75
4:D:12:VAL:HG12	4:D:13:PHE:N	2.02	0.75
2:B:43:ILE:HG23	2:B:47:LEU:CD1	2.17	0.75
1:M:226:MET:HG3	1:M:518:MET:CA	2.16	0.75
1:M:296:HIS:O	1:M:300:LYS:HB2	1.85	0.75
2:N:97:PRO:HA	3:O:7:TYR:O	1.87	0.75
2:N:233:LYS:O	2:N:237:ILE:HD13	1.86	0.75
4:P:117:THR:O	4:P:118:ILE:HB	1.85	0.75
1:M:467:ARG:CZ	1:M:532:HIS:HA	2.15	0.75
1:A:27:ASN:ND2	1:A:29:ASN:N	2.34	0.75
1:M:551:THR:HG22	1:M:552:LEU:N	2.00	0.75
4:D:41:LEU:O	4:D:43:LEU:HD23	1.86	0.74
1:M:256:ASN:HB3	1:M:262:TYR:HD2	1.51	0.74
2:N:75:LEU:O	2:N:77:CYS:N	2.21	0.74
1:A:73:GLY:O	1:A:74:ASP:HB2	1.87	0.74
3:O:60:VAL:CG1	3:O:64:GLN:HE21	1.99	0.74
2:B:99:GLU:OE2	3:C:4:ARG:NH1	2.19	0.74
4:D:48:ALA:HA	4:D:53:ARG:HD3	1.68	0.74
1:M:242:LEU:HD23	1:M:244:THR:H	1.52	0.74
1:A:115:ARG:H	1:A:115:ARG:HD2	1.52	0.74
3:O:50:LYS:HE2	4:P:118:ILE:CG2	2.16	0.74
1:A:324:LEU:O	1:A:328:LEU:N	2.19	0.74
1:M:9:ILE:HD13	1:M:19:ALA:HB3	1.68	0.74
1:M:447:ASN:HB3	1:M:450:LYS:HG2	1.70	0.74
2:B:97:PRO:O	2:B:104:VAL:HG23	1.87	0.73
1:M:42:ARG:NH2	2:N:54:ARG:NE	2.36	0.73
2:B:182:ASP:OD1	2:B:184:ARG:NH1	2.20	0.73
1:M:57:GLN:O	1:M:58:ASP:HB2	1.88	0.73
1:M:133:PHE:CZ	2:N:149:ILE:HG22	2.23	0.73
1:M:356:TYR:CE2	1:M:379:GLU:HG3	2.22	0.73
2:N:8:ILE:HG22	2:N:9:GLU:N	2.04	0.73
1:A:255:VAL:HG12	1:A:261:ARG:HG2	1.70	0.73
1:A:493:ASP:CB	1:A:499:ASN:HD21	2.00	0.73
1:M:42:ARG:NH2	2:N:54:ARG:CZ	2.52	0.73
1:A:44:HIS:CD2	6:A:703:FAD:HM81	2.23	0.73
2:N:8:ILE:HG22	2:N:9:GLU:H	1.52	0.73
2:N:206:PHE:CE1	2:N:225:GLN:HG2	2.24	0.73
2:N:210:CYS:SG	2:N:221:ALA:HB2	2.27	0.73
4:D:73:LEU:HB2	4:D:74:PRO:HD3	1.70	0.73
1:M:187:ALA:HB1	1:M:410:ALA:HB1	1.70	0.73
1:M:256:ASN:HB3	1:M:262:TYR:CD2	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:55:LEU:CG	4:D:59:GLN:HE22	2.01	0.73
1:M:93:MET:HB3	1:M:125:TRP:CH2	2.23	0.72
2:N:36:LEU:HB2	2:N:76:ALA:O	1.89	0.72
2:B:13:TYR:O	2:B:13:TYR:CG	2.38	0.72
1:M:113:VAL:CG2	1:M:123:ARG:HA	2.18	0.72
2:B:155:TYR:CE2	2:B:169:GLY:HA3	2.23	0.72
1:M:248:ARG:HG2	1:M:248:ARG:HH11	1.52	0.72
2:N:155:TYR:CE1	2:N:171:ALA:HB3	2.24	0.72
1:A:523:MET:O	1:A:526:LYS:NZ	2.22	0.72
1:A:103:TRP:O	2:B:139:MET:HE1	1.90	0.72
2:B:72:VAL:HG12	2:B:73:PRO:HD2	1.71	0.72
1:M:377:VAL:HG13	1:M:402:PHE:CD2	2.25	0.72
2:N:215:PRO:HD2	9:N:246:SF4:S3	2.29	0.72
1:A:40:PRO:HG2	1:A:140:PHE:CE1	2.25	0.72
3:C:53:PRO:HD3	4:D:51:TYR:CZ	2.25	0.72
4:P:113:ILE:HG22	4:P:117:THR:HG21	1.71	0.72
2:B:60:ALA:N	2:B:77:CYS:SG	2.62	0.72
1:M:391:LEU:CG	1:M:392:GLY:H	1.97	0.72
1:M:399:LEU:HD21	6:M:803:FAD:H5'2	1.71	0.71
1:M:552:LEU:HB2	1:M:564:GLU:HB2	1.71	0.71
1:A:79:GLN:HG3	1:A:570:ILE:HA	1.72	0.71
1:A:118:GLY:O	1:A:280:LYS:NZ	2.14	0.71
4:P:14:TRP:O	4:P:17:PHE:HB3	1.89	0.71
2:B:212:GLU:HG3	3:C:21:PHE:HE1	1.56	0.71
1:M:228:PHE:CE2	1:M:388:ALA:HA	2.24	0.71
2:N:145:PHE:HD1	2:N:218:VAL:HG12	1.55	0.71
1:A:527:GLU:HG2	1:A:547:PHE:CG	2.26	0.71
1:M:200:ARG:HD2	1:M:457:LEU:HB2	1.71	0.71
4:P:6:LYS:HG3	4:P:6:LYS:O	1.91	0.71
1:M:60:ASP:HB3	1:M:121:ILE:HG21	1.71	0.71
1:M:187:ALA:O	1:M:188:VAL:HG23	1.91	0.71
1:M:227:GLU:OE1	1:M:227:GLU:HA	1.91	0.71
1:M:385:LEU:HD12	1:M:386:HIS:N	2.05	0.71
2:N:177:HIS:HA	2:N:180:ASN:HB2	1.70	0.71
3:O:70:ILE:HG22	3:O:71:ILE:N	2.04	0.71
4:P:2:ASN:ND2	4:P:4:ASN:O	2.24	0.71
1:M:92:GLU:O	1:M:96:LEU:HG	1.90	0.71
1:M:341:VAL:HG13	1:M:346:GLU:HB3	1.73	0.71
4:P:80:HIS:CD2	4:P:84:HIS:HD2	2.08	0.71
1:A:182:GLN:NE2	1:A:184:ARG:HH12	1.88	0.71
2:B:143:HIS:O	2:B:146:SER:OG	2.07	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:166:HIS:HD2	1:M:413:ARG:HH21	1.39	0.71
1:M:383:VAL:HG21	1:M:398:GLU:HG2	1.73	0.70
3:O:83:THR:CG2	3:O:87:PHE:CE1	2.74	0.70
1:A:236:LEU:HD21	1:A:243:MET:HE1	1.72	0.70
2:B:238:ALA:CA	2:B:241:LYS:HB3	2.20	0.70
1:M:377:VAL:HG22	1:M:402:PHE:CE2	2.26	0.70
2:N:218:VAL:O	2:N:219:ASP:HB2	1.89	0.70
1:A:253:ILE:HG22	1:A:315:ASP:HB2	1.68	0.70
1:M:255:VAL:HG23	1:M:313:TYR:HB2	1.73	0.70
4:P:31:MET:HG3	4:P:70:MET:SD	2.31	0.70
2:B:67:MET:HE3	2:B:76:ALA:HB2	1.74	0.70
1:M:455:MET:SD	1:M:508:LEU:HD11	2.31	0.70
1:M:94:THR:HB	2:N:130:GLY:O	1.92	0.70
1:M:229:VAL:HB	1:M:467:ARG:HH22	1.56	0.70
1:M:242:LEU:HD21	1:M:244:THR:N	2.06	0.70
1:M:53:ALA:CB	1:M:394:ASN:ND2	2.54	0.70
1:A:211:ASP:HB3	6:A:703:FAD:H61A	1.56	0.70
2:B:68:MET:HE3	2:B:72:VAL:O	1.92	0.70
2:N:241:LYS:C	2:N:243:ARG:H	1.94	0.70
3:O:97:ILE:HG23	3:O:101:GLU:O	1.92	0.70
1:A:177:GLU:HA	1:A:177:GLU:OE2	1.92	0.70
4:D:105:ALA:O	4:D:109:VAL:HG23	1.92	0.70
1:M:194:GLY:H	1:M:208:VAL:HG13	1.55	0.70
1:M:255:VAL:O	1:M:312:VAL:HG13	1.92	0.69
2:N:240:LEU:N	2:N:240:LEU:HD23	2.06	0.69
1:M:358:MET:SD	1:M:386:HIS:HB2	2.32	0.69
1:M:550:HIS:O	1:M:565:TYR:HA	1.92	0.69
2:N:149:ILE:HG23	2:N:216:LYS:HG3	1.73	0.69
2:B:9:GLU:OE2	2:B:23:SER:HB3	1.92	0.69
2:N:26:TYR:HE2	2:N:48:ALA:HB3	1.56	0.69
1:M:76:LEU:HD21	1:M:525:ARG:HH12	1.57	0.69
1:M:106:ARG:HG2	1:M:110:SER:O	1.93	0.69
1:M:130:LYS:HZ1	2:N:216:LYS:HD3	1.55	0.69
2:N:6:LEU:HD21	2:N:81:LEU:HD11	1.75	0.69
2:N:241:LYS:HB3	2:N:242:PRO:HD3	1.74	0.69
1:A:184:ARG:HG2	1:A:184:ARG:NH1	2.01	0.69
1:A:294:PHE:O	1:A:298:TRP:N	2.23	0.69
1:M:555:ARG:NE	1:M:560:THR:H	1.91	0.69
2:N:37:LEU:HD11	2:N:58:ARG:HA	1.74	0.69
3:O:125:PHE:CZ	3:O:130:TRP:CZ3	2.81	0.69
1:A:62:PHE:HD2	1:A:86:VAL:HG13	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:73:PRO:HG2	2:N:213:VAL:HG11	1.75	0.69
1:A:314:LEU:HD11	1:A:316:LEU:CD2	2.23	0.69
1:A:341:VAL:HG13	1:A:346:GLU:HG3	1.75	0.69
1:M:227:GLU:H	1:M:518:MET:HA	1.58	0.69
1:M:467:ARG:NH2	1:M:532:HIS:CA	2.53	0.69
3:C:59:PHE:CE1	3:C:63:LEU:HD11	2.27	0.68
4:D:34:LEU:HD23	4:D:38:LEU:HD12	1.75	0.68
4:D:44:PHE:CD1	4:D:49:LEU:HB2	2.28	0.68
1:M:177:GLU:OE2	3:O:2:THR:HG23	1.91	0.68
1:M:554:PHE:HB3	1:M:562:ARG:H	1.58	0.68
2:N:155:TYR:HE1	2:N:171:ALA:HB3	1.59	0.68
1:M:53:ALA:HA	1:M:125:TRP:CD1	2.28	0.68
1:M:194:GLY:H	1:M:208:VAL:CG1	2.05	0.68
2:N:151:CYS:SG	2:N:153:LEU:HB2	2.34	0.68
1:A:446:GLU:HB2	1:A:489:VAL:HB	1.74	0.68
3:C:87:PHE:CE1	3:C:112:LEU:HB3	2.28	0.68
1:M:22:ALA:HB2	1:M:404:ARG:HA	1.74	0.68
1:A:27:ASN:ND2	1:A:30:ALA:H	1.91	0.68
1:A:321:GLU:O	1:A:324:LEU:N	2.27	0.68
1:A:328:LEU:HD13	1:A:331:ILE:HG13	1.74	0.68
4:P:73:LEU:N	4:P:73:LEU:HD23	2.08	0.68
4:P:113:ILE:HG22	4:P:117:THR:CG2	2.24	0.68
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.75	0.68
1:M:52:SER:O	1:M:125:TRP:HB2	1.94	0.68
1:M:433:GLU:CG	1:M:434:GLN:H	2.07	0.68
2:N:220:PRO:O	2:N:223:ALA:N	2.27	0.68
4:P:72:VAL:O	4:P:75:LEU:HB2	1.94	0.68
4:D:111:THR:O	4:D:115:VAL:HG22	1.93	0.68
4:D:113:ILE:HG22	4:D:114:GLY:N	2.09	0.68
1:M:151:ARG:HH11	1:M:151:ARG:CB	2.06	0.68
1:M:329:PRO:HA	1:M:332:CYS:SG	2.34	0.68
1:M:455:MET:HE2	1:M:482:LEU:HD13	1.75	0.68
1:A:27:ASN:ND2	1:A:30:ALA:N	2.42	0.67
1:A:198:VAL:HG23	1:A:455:MET:HE1	1.75	0.67
1:M:46:VAL:HA	1:M:132:GLY:O	1.93	0.67
1:M:192:THR:HG21	1:M:212:GLY:H	1.58	0.67
4:P:57:PHE:CZ	10:P:800:MQ7:H151	2.29	0.67
1:M:72:GLY:CA	1:M:391:LEU:HD22	2.18	0.67
1:M:46:VAL:HA	1:M:133:PHE:HA	1.75	0.67
1:M:390:ARG:HD3	1:M:395:SER:OG	1.93	0.67
1:A:168:ARG:HG2	1:A:425:ILE:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LEU:HD23	1:A:436:LEU:C	2.14	0.67
3:O:87:PHE:CE2	3:O:112:LEU:HB3	2.29	0.67
4:P:68:PHE:O	4:P:72:VAL:HG22	1.94	0.67
1:M:220:GLY:H	1:M:371:ILE:HD11	1.60	0.67
1:M:555:ARG:HE	1:M:560:THR:H	1.43	0.67
2:N:36:LEU:HD13	2:N:79:THR:HB	1.76	0.67
1:M:76:LEU:HD21	1:M:525:ARG:NH1	2.10	0.67
1:M:226:MET:HG3	1:M:518:MET:HA	1.76	0.67
1:A:262:TYR:CE1	1:A:263:LEU:HD23	2.30	0.67
2:B:105:ASP:C	2:B:105:ASP:OD1	2.32	0.67
3:C:37:TRP:CZ2	3:C:41:GLU:OE2	2.47	0.67
3:O:83:THR:CG2	3:O:87:PHE:HE1	2.06	0.67
1:M:251:GLY:HA2	1:M:277:PRO:HG2	1.76	0.67
2:N:10:VAL:HG13	2:N:90:VAL:HB	1.77	0.67
2:N:235:PHE:C	2:N:237:ILE:H	1.98	0.67
1:A:254:LEU:HD12	1:A:283:GLU:HG3	1.77	0.66
1:M:225:ASP:O	1:M:226:MET:O	2.13	0.66
2:N:75:LEU:HD21	2:N:215:PRO:CB	2.23	0.66
4:D:50:SER:O	4:D:51:TYR:C	2.34	0.66
1:M:242:LEU:CD2	1:M:244:THR:N	2.56	0.66
4:P:13:PHE:HE2	4:P:97:LYS:HG2	1.59	0.66
1:M:144:LEU:HD21	2:N:114:GLU:O	1.95	0.66
1:M:230:GLN:NE2	1:M:287:ARG:HH11	1.92	0.66
1:M:551:THR:HG22	1:M:552:LEU:H	1.59	0.66
4:P:105:ALA:O	4:P:109:VAL:HG23	1.94	0.66
1:A:182:GLN:NE2	1:A:184:ARG:NH1	2.43	0.66
1:A:263:LEU:HB3	1:A:268:MET:HE2	1.76	0.66
2:B:26:TYR:HD2	2:B:47:LEU:CD1	2.07	0.66
1:M:233:PRO:HG2	1:M:234:THR:H	1.59	0.66
1:M:346:GLU:HG3	1:M:347:PRO:CD	2.25	0.66
1:M:192:THR:HG21	1:M:212:GLY:N	2.10	0.66
2:N:167:PHE:HA	2:N:199:ASN:HA	1.78	0.66
1:A:181:VAL:HG23	1:A:182:GLN:N	2.11	0.66
1:A:529:ARG:O	1:A:530:GLY:C	2.34	0.66
2:N:6:LEU:CD2	2:N:81:LEU:HD11	2.26	0.66
2:N:75:LEU:CD2	2:N:215:PRO:HB3	2.23	0.66
1:A:234:THR:HG22	1:A:350:VAL:CG2	2.24	0.66
2:B:116:ILE:HD13	2:B:176:ALA:HB2	1.77	0.66
1:M:46:VAL:HB	1:M:133:PHE:HD1	1.60	0.66
1:M:53:ALA:HB2	1:M:124:THR:HG23	1.77	0.66
1:A:166:HIS:HB3	1:A:168:ARG:NH2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:78:GLU:H	1:M:224:ARG:HH22	1.44	0.66
2:N:97:PRO:O	2:N:104:VAL:HA	1.96	0.66
2:N:120:ILE:O	2:N:121:ILE:HG23	1.94	0.66
1:A:437:LYS:HA	1:A:440:VAL:HG23	1.77	0.66
3:C:9:ARG:HG2	3:C:9:ARG:HH11	1.61	0.66
2:N:145:PHE:HE1	2:N:219:ASP:HB3	1.61	0.66
3:O:130:TRP:HA	3:O:130:TRP:CE3	2.29	0.66
3:C:30:GLY:O	3:C:32:ALA:N	2.29	0.65
1:M:195:ALA:O	1:M:198:VAL:HG22	1.96	0.65
1:M:433:GLU:CG	1:M:434:GLN:N	2.59	0.65
2:N:54:ARG:HG2	2:N:54:ARG:NH1	2.07	0.65
3:O:50:LYS:CE	4:P:118:ILE:HG22	2.22	0.65
1:M:78:GLU:N	1:M:224:ARG:HH22	1.94	0.65
2:N:98:ILE:HD12	2:N:98:ILE:N	2.11	0.65
2:N:149:ILE:CG1	2:N:151:CYS:HB3	2.25	0.65
1:M:217:LEU:HD11	1:M:555:ARG:CD	2.26	0.65
3:C:53:PRO:HD3	4:D:51:TYR:OH	1.97	0.65
2:B:14:ASN:OD1	2:B:16:GLU:N	2.17	0.65
4:D:72:VAL:HG12	4:D:73:LEU:HD23	1.78	0.65
1:M:452:ARG:CD	1:M:508:LEU:HD22	2.26	0.65
4:D:67:LEU:CD1	10:D:700:MQ7:H6	2.26	0.65
1:M:38:VAL:HG12	2:N:54:ARG:HH12	1.60	0.65
1:M:103:TRP:CZ3	1:M:131:THR:HG23	2.32	0.65
1:M:188:VAL:HG12	1:M:188:VAL:O	1.96	0.65
1:M:194:GLY:O	1:M:357:THR:HG21	1.97	0.65
1:M:467:ARG:O	1:M:534:ARG:HA	1.97	0.65
3:C:48:ALA:C	3:C:50:LYS:H	1.99	0.65
1:M:121:ILE:HD12	1:M:123:ARG:NH2	2.12	0.65
1:M:247:CYS:HB3	1:M:331:ILE:HD13	1.79	0.65
3:C:50:LYS:HZ2	4:D:118:ILE:HD12	1.57	0.64
2:N:106:MET:O	2:N:110:ILE:HG12	1.96	0.64
1:A:253:ILE:CG2	1:A:315:ASP:HB2	2.26	0.64
2:B:65:CYS:O	2:B:67:MET:HE3	1.97	0.64
4:D:72:VAL:O	4:D:75:LEU:HB2	1.97	0.64
4:D:87:HIS:O	4:D:89:LEU:N	2.30	0.64
1:A:562:ARG:HG3	1:A:562:ARG:NH1	2.09	0.64
1:M:51:GLY:HA3	1:M:125:TRP:O	1.96	0.64
1:A:65:HIS:ND1	1:A:86:VAL:CG2	2.60	0.64
2:N:155:TYR:HE1	2:N:171:ALA:CB	2.10	0.64
1:A:455:MET:SD	1:A:512:LEU:HD23	2.37	0.64
1:M:226:MET:SD	1:M:518:MET:HG2	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:HH22	1:A:404:ARG:HD2	1.62	0.64
1:M:232:HIS:O	1:M:352:PRO:CA	2.44	0.64
2:N:192:MET:O	2:N:195:LEU:N	2.29	0.64
4:D:36:GLY:C	4:D:37:ILE:HD12	2.18	0.64
2:N:44:LYS:HB2	2:N:49:PRO:HA	1.80	0.64
2:B:206:PHE:CD2	2:B:206:PHE:O	2.51	0.64
1:M:230:GLN:NE2	1:M:287:ARG:NH1	2.46	0.64
2:N:30:TYR:CB	2:N:81:LEU:HD13	2.27	0.64
2:N:73:PRO:O	2:N:74:LYS:HG3	1.98	0.64
4:P:30:VAL:O	4:P:33:LEU:HB3	1.98	0.64
1:A:38:VAL:O	1:A:38:VAL:CG2	2.44	0.63
1:A:542:ARG:NH2	1:A:544:ASP:OD1	2.31	0.63
1:M:53:ALA:N	1:M:394:ASN:HB2	2.14	0.63
1:M:15:ALA:HB2	1:M:399:LEU:CD2	2.25	0.63
1:A:253:ILE:HG22	1:A:315:ASP:CA	2.29	0.63
1:A:388:ALA:O	1:A:389:ASN:CB	2.41	0.63
1:A:527:GLU:OE2	1:A:529:ARG:NH1	2.30	0.63
2:B:132:ASN:ND2	2:B:184:ARG:HD3	2.13	0.63
3:C:65:ASN:O	3:C:69:VAL:HG23	1.98	0.63
1:M:32:ILE:HG23	1:M:149:ILE:HA	1.79	0.63
1:M:214:GLY:HA3	1:M:510:HIS:HB3	1.81	0.63
1:A:41:MET:CE	2:B:150:ASN:HD22	2.11	0.63
1:A:279:ASN:O	1:A:280:LYS:HB2	1.99	0.63
1:M:466:TYR:O	1:M:467:ARG:HG3	1.97	0.63
1:M:527:GLU:HB3	1:M:543:ASP:OD2	1.98	0.63
2:N:206:PHE:CD1	2:N:225:GLN:HG2	2.34	0.63
1:A:455:MET:O	1:A:458:ALA:HB3	1.98	0.63
1:A:479:LEU:HB3	1:A:516:GLU:HG2	1.81	0.63
1:A:279:ASN:HD21	1:A:280:LYS:HD3	1.63	0.63
1:A:529:ARG:NH2	1:A:544:ASP:OD2	2.32	0.63
2:B:4:LYS:HB2	2:B:4:LYS:HZ2	1.62	0.63
1:M:403:GLY:HA2	1:M:406:ALA:CB	2.27	0.63
1:A:90:PRO:HG2	1:A:91:THR:H	1.62	0.63
2:N:99:GLU:HB2	2:N:103:VAL:HB	1.80	0.63
1:M:161:LEU:HD21	1:M:429:ALA:HA	1.79	0.62
1:M:9:ILE:HG12	1:M:189:VAL:HB	1.81	0.62
2:B:67:MET:CE	2:B:76:ALA:HB2	2.29	0.62
1:M:83:ASP:O	1:M:87:HIS:ND1	2.33	0.62
1:M:182:GLN:NE2	1:M:429:ALA:HB1	2.15	0.62
1:M:311:VAL:HB	1:M:350:VAL:O	1.99	0.62
2:N:160:GLN:HA	2:N:160:GLN:NE2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:GLU:HG3	1:A:413:ARG:N	2.06	0.62
1:M:105:ARG:HH12	1:M:109:GLY:HA2	1.64	0.62
1:M:228:PHE:HE2	1:M:387:GLY:O	1.82	0.62
2:N:152:GLY:N	9:N:246:SF4:S4	2.72	0.62
1:A:44:HIS:CE1	1:A:205:GLY:H	2.16	0.62
1:M:18:ARG:O	1:M:18:ARG:HD3	1.99	0.62
2:N:4:LYS:C	2:N:5:ASN:HD22	2.02	0.62
2:N:37:LEU:HD23	2:N:38:ASP:H	1.64	0.62
2:N:109:PHE:CE1	2:N:113:LEU:HD11	2.34	0.62
2:N:192:MET:O	2:N:193:ALA:C	2.38	0.62
1:A:27:ASN:HD21	1:A:30:ALA:N	1.98	0.62
2:B:118:PRO:O	2:B:179:TYR:CE2	2.53	0.62
2:B:211:SER:CA	2:B:220:PRO:HD2	2.29	0.62
1:M:53:ALA:H	1:M:394:ASN:HB2	1.64	0.62
1:M:73:GLY:CA	1:M:387:GLY:HA3	2.30	0.62
2:N:75:LEU:HD23	2:N:75:LEU:H	1.64	0.62
2:N:196:ASN:O	2:N:197:SER:HB3	2.00	0.62
2:B:189:LYS:HE3	2:B:190:GLU:OE1	2.00	0.62
1:M:328:LEU:HD12	1:M:331:ILE:HD11	1.82	0.62
3:O:48:ALA:C	3:O:50:LYS:H	2.03	0.62
1:A:447:ASN:O	1:A:448:TRP:C	2.36	0.62
1:A:467:ARG:O	1:A:534:ARG:HA	1.99	0.62
1:A:536:ASP:OD1	1:A:536:ASP:N	2.32	0.62
2:B:157:ALA:HB1	2:B:209:TYR:CD2	2.34	0.62
2:B:206:PHE:O	2:B:206:PHE:HD2	1.83	0.62
1:M:5:ALA:O	1:M:185:ALA:HA	2.00	0.62
1:A:115:ARG:HG3	1:A:115:ARG:NH1	2.02	0.62
1:A:408:GLU:O	1:A:411:THR:N	2.33	0.62
1:M:182:GLN:HG3	1:M:182:GLN:O	2.00	0.62
3:O:60:VAL:HG12	3:O:64:GLN:NE2	2.13	0.62
1:M:43:SER:HB3	1:M:136:LEU:HD21	1.82	0.61
1:M:103:TRP:HZ3	1:M:131:THR:HG23	1.65	0.61
1:M:229:VAL:HB	1:M:467:ARG:NH2	2.14	0.61
1:A:335:ALA:O	1:A:339:VAL:CG2	2.49	0.61
1:A:335:ALA:O	1:A:339:VAL:HG23	2.00	0.61
4:D:35:VAL:HG13	10:D:700:MQ7:O1	2.00	0.61
1:M:549:LYS:HB2	1:M:566:SER:H	1.65	0.61
1:M:525:ARG:HA	1:M:547:PHE:CE2	2.35	0.61
1:A:155:HIS:CD2	1:A:174:ASN:CA	2.84	0.61
4:D:12:VAL:CG1	4:D:13:PHE:N	2.63	0.61
1:M:46:VAL:HG23	1:M:47:ALA:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:78:GLU:O	1:M:80:ASP:N	2.33	0.61
1:M:223:LEU:HD22	1:M:517:CYS:SG	2.39	0.61
1:M:434:GLN:O	1:M:437:LYS:N	2.30	0.61
2:N:149:ILE:O	2:N:151:CYS:N	2.33	0.61
3:O:76:LEU:HD12	3:O:76:LEU:O	2.01	0.61
1:A:41:MET:HE2	2:B:150:ASN:HD22	1.65	0.61
1:A:166:HIS:HB3	1:A:168:ARG:HH21	1.66	0.61
3:O:49:LEU:HD21	4:P:55:LEU:HA	1.81	0.61
1:A:562:ARG:HH11	1:A:562:ARG:CG	2.09	0.61
1:M:439:LEU:HD23	1:M:442:GLN:HE22	1.64	0.61
1:A:27:ASN:HD21	1:A:29:ASN:N	1.97	0.61
1:A:236:LEU:HD21	1:A:243:MET:SD	2.39	0.61
1:M:236:LEU:HG	1:M:237:PRO:HD2	1.81	0.61
1:A:287:ARG:NH2	5:A:702:FLC:OB1	2.33	0.61
2:B:173:ILE:HG23	2:B:195:LEU:CD2	2.31	0.61
2:N:189:LYS:O	2:N:191:ARG:N	2.31	0.61
3:O:39:SER:OG	4:P:71:ILE:O	2.18	0.61
4:P:23:TRP:C	4:P:23:TRP:CD1	2.74	0.61
1:A:390:ARG:NH1	5:A:702:FLC:CAC	2.64	0.61
1:M:356:TYR:HB2	1:M:390:ARG:NH2	2.15	0.61
1:M:405:LEU:HA	1:M:408:GLU:HB2	1.82	0.61
1:M:430:ALA:O	1:M:433:GLU:HG2	2.01	0.61
1:M:455:MET:HG2	1:M:456:GLY:N	2.15	0.61
1:A:263:LEU:CB	1:A:268:MET:CE	2.68	0.61
1:M:226:MET:HG3	1:M:518:MET:N	2.14	0.61
1:M:356:TYR:HD1	1:M:390:ARG:CZ	2.14	0.61
1:A:441:ASN:O	1:A:442:GLN:C	2.37	0.60
2:B:26:TYR:CD2	2:B:47:LEU:CD1	2.85	0.60
1:M:12:ALA:HB2	1:M:36:SER:HB2	1.83	0.60
1:M:208:VAL:O	1:M:208:VAL:HG12	2.01	0.60
1:M:264:GLN:HB3	1:M:282:MET:HE1	1.82	0.60
1:M:446:GLU:HB3	1:M:488:ARG:O	2.01	0.60
1:A:239:SER:CB	1:A:241:ILE:HD12	2.30	0.60
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.82	0.60
1:M:55:VAL:CB	1:M:90:PRO:HG3	2.29	0.60
2:N:75:LEU:CD2	2:N:75:LEU:N	2.63	0.60
4:P:43:LEU:N	4:P:43:LEU:CD2	2.60	0.60
1:A:211:ASP:CB	6:A:703:FAD:H61A	2.12	0.60
1:A:545:VAL:HG12	1:A:546:ASN:CG	2.20	0.60
4:D:99:VAL:CG1	4:D:100:PHE:N	2.64	0.60
1:M:72:GLY:HA3	1:M:391:LEU:CD2	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:236:LEU:HD22	1:M:241:ILE:HD12	1.84	0.60
3:O:53:PRO:HB3	4:P:51:TYR:CE2	2.35	0.60
3:O:83:THR:HG23	3:O:87:PHE:CE1	2.35	0.60
1:M:226:MET:CG	1:M:518:MET:HG2	2.31	0.60
1:M:395:SER:O	1:M:398:GLU:HB3	2.00	0.60
2:N:204:CYS:O	2:N:228:LYS:NZ	2.34	0.60
5:A:702:FLC:OA2	6:A:703:FAD:C2	2.50	0.60
1:M:553:ALA:O	1:M:562:ARG:HG2	2.01	0.60
1:M:55:VAL:HG22	1:M:65:HIS:HD2	1.65	0.60
1:M:56:ALA:C	1:M:57:GLN:HG2	2.21	0.60
1:M:462:GLY:HA2	1:M:471:LEU:HD13	1.84	0.60
2:N:120:ILE:HD13	2:N:185:ASP:HB2	1.81	0.60
3:O:27:LEU:HD23	3:O:81:LEU:CD2	2.31	0.60
1:A:447:ASN:ND2	1:A:449:ALA:HB3	2.16	0.60
1:M:551:THR:CG2	1:M:552:LEU:H	2.14	0.60
1:M:554:PHE:O	1:M:555:ARG:HG3	2.02	0.60
1:A:1:GLN:NE2	1:A:3:PHE:CZ	2.69	0.60
1:M:243:MET:HE2	1:M:348:ILE:HG21	1.84	0.60
3:C:36:VAL:HG22	4:D:75:LEU:CD2	2.32	0.60
1:M:35:ILE:HG22	1:M:36:SER:N	2.16	0.60
1:M:57:GLN:O	1:M:58:ASP:CB	2.50	0.60
1:M:228:PHE:CZ	1:M:388:ALA:HA	2.36	0.60
1:M:42:ARG:CZ	2:N:54:ARG:NE	2.64	0.60
1:M:175:MET:HG2	1:M:503:LEU:HD11	1.83	0.60
1:M:315:ASP:OD1	1:M:317:ARG:HG2	2.02	0.60
4:P:32:ILE:O	4:P:33:LEU:C	2.38	0.60
1:A:256:ASN:OD1	1:A:260:TYR:N	2.34	0.59
1:M:552:LEU:HD12	1:M:564:GLU:HB3	1.84	0.59
2:N:239:THR:C	2:N:240:LEU:HD23	2.22	0.59
4:D:79:LEU:HD12	4:D:104:ALA:HB2	1.83	0.59
1:M:89:CYS:HB3	1:M:90:PRO:HD3	1.83	0.59
1:M:180:LEU:CD1	1:M:433:GLU:HB2	2.29	0.59
2:N:236:LEU:HD12	2:N:240:LEU:HD21	1.84	0.59
3:O:4:ARG:HH21	3:O:6:PRO:HG2	1.66	0.59
2:B:225:GLN:HG2	3:C:93:ALA:CB	2.23	0.59
1:M:55:VAL:HG22	1:M:65:HIS:CD2	2.36	0.59
1:M:551:THR:HA	1:M:564:GLU:O	2.02	0.59
4:D:67:LEU:HD13	10:D:700:MQ7:H6	1.83	0.59
1:M:82:VAL:O	1:M:86:VAL:HG22	2.01	0.59
2:N:173:ILE:HG23	2:N:195:LEU:CD2	2.33	0.59
2:N:193:ALA:HB1	4:P:5:PRO:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:18:ARG:NH1	1:M:22:ALA:HB2	2.17	0.59
2:N:13:TYR:O	2:N:100:ARG:HG3	2.02	0.59
1:M:44:HIS:CE1	6:M:803:FAD:C8M	2.76	0.59
1:M:161:LEU:HD13	1:M:425:ILE:HG22	1.84	0.59
2:B:173:ILE:HG23	2:B:195:LEU:HD22	1.84	0.59
1:M:43:SER:HB3	1:M:136:LEU:CD2	2.33	0.59
1:M:171:VAL:HA	1:M:181:VAL:O	2.03	0.59
1:M:281:TYR:O	1:M:282:MET:HB3	2.02	0.59
1:M:295:TRP:CZ3	1:M:466:TYR:HB3	2.38	0.59
1:M:304:ILE:HD12	1:M:304:ILE:N	2.18	0.59
4:P:41:LEU:O	4:P:43:LEU:CD2	2.50	0.59
1:A:279:ASN:ND2	1:A:280:LYS:HD3	2.17	0.59
1:A:282:MET:HE3	1:A:283:GLU:OE1	2.03	0.59
1:A:324:LEU:O	1:A:326:GLU:N	2.36	0.59
1:A:493:ASP:CB	1:A:499:ASN:ND2	2.63	0.59
1:M:39:TYR:HB3	1:M:40:PRO:HD2	1.84	0.59
1:M:451:ILE:O	1:M:455:MET:HB3	2.03	0.59
2:N:241:LYS:C	2:N:243:ARG:N	2.56	0.59
3:O:30:GLY:O	3:O:32:ALA:N	2.35	0.59
3:O:105:PRO:HD2	3:O:106:GLU:HG3	1.84	0.59
3:C:128:LEU:HD22	4:D:45:PRO:HD2	1.85	0.58
1:A:2:THR:CG2	1:A:3:PHE:N	2.65	0.58
1:A:68:ASP:OD2	1:A:119:MET:HB3	2.03	0.58
1:M:42:ARG:NH2	2:N:54:ARG:HB3	2.15	0.58
1:M:356:TYR:HD1	1:M:390:ARG:NE	2.01	0.58
2:N:108:HIS:O	2:N:112:SER:N	2.30	0.58
4:P:35:VAL:HG22	10:P:800:MQ7:O1	2.03	0.58
4:P:113:ILE:O	4:P:114:GLY:C	2.42	0.58
1:A:329:PRO:HD2	1:A:330:PHE:H	1.68	0.58
1:M:539:CYS:SG	1:M:541:GLU:O	2.60	0.58
2:N:6:LEU:HD21	2:N:8:ILE:HD11	1.85	0.58
2:N:196:ASN:N	2:N:196:ASN:ND2	2.47	0.58
1:A:91:THR:HG22	1:A:92:GLU:N	2.17	0.58
4:D:23:TRP:C	4:D:25:ALA:H	2.06	0.58
1:M:263:LEU:CD1	1:M:283:GLU:H	2.16	0.58
2:N:36:LEU:HB3	2:N:76:ALA:HB1	1.85	0.58
2:N:98:ILE:HD11	3:O:9:ARG:HE	1.69	0.58
2:B:72:VAL:CG1	2:B:73:PRO:HD2	2.33	0.58
3:C:50:LYS:HD3	4:D:118:ILE:CB	2.26	0.58
1:M:226:MET:HG3	1:M:518:MET:CG	2.32	0.58
2:N:8:ILE:CG2	2:N:9:GLU:H	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:15:ALA:HB1	1:M:377:VAL:HG12	1.86	0.58
1:M:214:GLY:HA3	1:M:510:HIS:CG	2.39	0.58
1:M:485:ARG:O	1:M:485:ARG:HG2	2.03	0.58
2:N:9:GLU:HG3	2:N:24:ALA:O	2.03	0.58
2:N:68:MET:CE	2:N:73:PRO:HB3	2.33	0.58
2:B:75:LEU:CD2	2:B:153:LEU:HD11	2.33	0.58
1:M:53:ALA:HB2	1:M:394:ASN:ND2	2.18	0.58
2:N:193:ALA:HB1	4:P:5:PRO:CG	2.34	0.58
1:A:18:ARG:NH2	1:A:404:ARG:HD2	2.18	0.58
1:M:54:ALA:N	1:M:125:TRP:CD1	2.71	0.58
1:M:84:TYR:CE2	1:M:405:LEU:HD11	2.39	0.58
1:M:115:ARG:HD3	1:M:122:GLU:HA	1.86	0.58
1:M:225:ASP:OD2	1:M:550:HIS:CE1	2.57	0.58
1:M:263:LEU:HD12	1:M:283:GLU:N	2.19	0.58
2:N:196:ASN:HA	2:N:201:VAL:CG1	2.34	0.58
2:B:121:ILE:HB	2:B:187:GLY:HA3	1.86	0.58
2:B:180:ASN:ND2	2:B:188:LYS:CG	2.60	0.58
4:D:82:MET:HA	4:D:85:ALA:HB3	1.86	0.58
1:M:147:PRO:C	1:M:149:ILE:H	2.07	0.58
1:A:306:THR:CB	1:A:307:PRO:CD	2.73	0.58
1:M:554:PHE:HD2	1:M:560:THR:HB	1.69	0.58
4:P:72:VAL:O	4:P:75:LEU:N	2.36	0.58
1:M:9:ILE:HB	1:M:34:LEU:HD12	1.84	0.57
1:M:78:GLU:H	1:M:224:ARG:NH2	2.02	0.57
2:N:37:LEU:HD22	2:N:77:CYS:HA	1.85	0.57
3:O:32:ALA:O	3:O:35:ALA:HB3	2.04	0.57
4:P:117:THR:O	4:P:118:ILE:CB	2.51	0.57
1:A:42:ARG:HD3	2:B:62:CYS:O	2.03	0.57
2:B:135:THR:O	2:B:137:ALA:N	2.37	0.57
1:M:332:CYS:O	1:M:336:LYS:HG3	2.04	0.57
1:M:551:THR:CG2	1:M:552:LEU:N	2.65	0.57
2:N:167:PHE:HA	2:N:199:ASN:CA	2.34	0.57
3:O:17:LYS:HG3	3:O:23:ARG:NH2	2.17	0.57
4:P:75:LEU:HD11	4:P:107:LEU:HD13	1.86	0.57
1:A:262:TYR:CE1	1:A:263:LEU:CD2	2.87	0.57
1:M:92:GLU:CD	1:M:400:VAL:HG12	2.25	0.57
1:A:273:PRO:HG2	1:A:276:GLU:HB2	1.85	0.57
1:A:417:ALA:C	1:A:418:GLY:O	2.40	0.57
2:B:211:SER:HA	2:B:220:PRO:CD	2.35	0.57
4:D:2:ASN:OD1	4:D:4:ASN:O	2.23	0.57
1:M:78:GLU:HB3	1:M:81:VAL:HG23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:95:GLN:O	1:M:98:LEU:HB3	2.04	0.57
1:M:207:ILE:HG23	1:M:208:VAL:HG23	1.86	0.57
2:N:149:ILE:O	2:N:150:ASN:C	2.42	0.57
1:A:224:ARG:HB2	1:A:552:LEU:HD23	1.87	0.57
1:A:256:ASN:HD21	1:A:260:TYR:HB3	1.69	0.57
5:A:702:FLC:OA1	6:A:703:FAD:C10	2.52	0.57
2:B:109:PHE:CD1	2:B:113:LEU:HD11	2.39	0.57
4:D:9:ASP:C	4:D:11:PRO:HD2	2.24	0.57
1:M:77:CYS:O	1:M:568:VAL:HG13	2.04	0.57
2:N:196:ASN:H	2:N:196:ASN:ND2	2.00	0.57
3:O:130:TRP:HA	3:O:130:TRP:HE3	1.70	0.57
4:P:112:LEU:O	4:P:116:VAL:HG22	2.05	0.57
1:A:465:ILE:HG22	1:A:465:ILE:O	2.02	0.57
3:C:9:ARG:H	3:C:9:ARG:HD3	1.70	0.57
1:M:103:TRP:O	1:M:105:ARG:HD2	2.05	0.57
2:N:133:ILE:HG23	2:N:133:ILE:O	2.04	0.57
2:N:51:LEU:HA	2:N:101:ASP:OD2	2.04	0.57
1:A:12:ALA:HB2	1:A:34:LEU:HD21	1.87	0.57
1:A:253:ILE:HG12	1:A:261:ARG:CD	2.24	0.57
4:D:55:LEU:O	4:D:59:GLN:HB2	2.05	0.57
1:M:33:ALA:HA	1:M:150:GLN:O	2.05	0.57
1:M:194:GLY:N	1:M:208:VAL:CG1	2.67	0.57
2:B:31:ASP:C	2:B:31:ASP:OD2	2.43	0.57
3:C:21:PHE:HD2	3:C:21:PHE:O	1.88	0.57
1:M:103:TRP:HE3	1:M:126:PHE:O	1.88	0.57
1:M:256:ASN:HD22	1:M:262:TYR:HB3	1.69	0.57
1:M:537:GLU:H	1:M:537:GLU:CD	2.06	0.57
2:N:68:MET:HE3	2:N:93:LEU:HD12	1.87	0.57
2:N:125:ARG:NH2	2:N:131:THR:O	2.38	0.57
2:N:149:ILE:HG13	2:N:149:ILE:O	2.05	0.57
1:A:70:VAL:HG11	1:A:573:LEU:HD23	1.87	0.57
1:M:372:LYS:O	1:M:413:ARG:NE	2.38	0.57
1:A:40:PRO:CG	1:A:140:PHE:CE1	2.87	0.56
1:A:424:ALA:O	1:A:427:ALA:HB3	2.05	0.56
1:A:523:MET:O	1:A:523:MET:HG3	2.04	0.56
4:D:23:TRP:O	4:D:25:ALA:N	2.37	0.56
1:M:129:ASP:HB2	1:M:328:LEU:HB3	1.87	0.56
1:M:194:GLY:HA3	1:M:379:GLU:HG2	1.87	0.56
1:M:276:GLU:N	1:M:277:PRO:CD	2.66	0.56
1:M:568:VAL:HG12	1:M:570:ILE:HG13	1.86	0.56
3:C:45:GLY:CA	3:C:59:PHE:CE2	2.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:40:PRO:HG3	1:M:140:PHE:CE1	2.40	0.56
2:N:112:SER:O	2:N:116:ILE:HG23	2.05	0.56
1:A:230:GLN:NE2	1:A:287:ARG:HE	2.03	0.56
1:A:324:LEU:C	1:A:326:GLU:N	2.56	0.56
3:C:17:LYS:HG2	3:C:23:ARG:HH22	1.70	0.56
1:M:102:PRO:HD2	1:M:134:HIS:HB3	1.86	0.56
1:M:151:ARG:HH12	1:M:153:ASP:CG	2.07	0.56
1:M:452:ARG:HG3	1:M:508:LEU:HD22	1.86	0.56
1:M:483:GLN:HG3	1:M:512:LEU:HD13	1.88	0.56
4:P:42:GLY:O	4:P:44:PHE:N	2.35	0.56
1:M:32:ILE:HG22	1:M:148:GLN:O	2.05	0.56
1:M:114:ARG:O	1:M:115:ARG:HG2	2.04	0.56
1:A:282:MET:CE	1:A:283:GLU:OE1	2.54	0.56
4:D:78:GLY:O	4:D:82:MET:HG2	2.05	0.56
1:A:2:THR:HG22	1:A:3:PHE:N	2.20	0.56
3:C:17:LYS:HG3	3:C:23:ARG:HH12	1.70	0.56
3:C:45:GLY:HA2	3:C:59:PHE:CE2	2.40	0.56
3:C:83:THR:HG23	3:C:87:PHE:CE2	2.40	0.56
4:D:87:HIS:C	4:D:89:LEU:H	2.07	0.56
1:M:162:VAL:HG12	1:M:163:ASP:N	2.20	0.56
3:O:28:ARG:O	3:O:31:THR:HB	2.06	0.56
2:B:180:ASN:HD21	2:B:188:LYS:HG3	1.68	0.56
1:A:416:THR:O	1:A:416:THR:HG22	2.01	0.56
2:B:68:MET:HE3	2:B:72:VAL:C	2.25	0.56
3:C:123:ILE:HG23	10:D:700:MQ7:H161	1.88	0.56
4:D:87:HIS:C	4:D:89:LEU:N	2.59	0.56
1:M:295:TRP:CH2	1:M:535:LEU:HD11	2.41	0.56
3:O:15:TRP:CD2	3:O:16:TRP:N	2.74	0.56
1:M:53:ALA:HB2	1:M:394:ASN:HD22	1.71	0.56
2:N:166:GLU:HB2	2:N:199:ASN:OD1	2.06	0.56
2:N:175:LEU:O	2:N:178:ARG:HB3	2.05	0.56
4:P:7:ARG:HH11	4:P:7:ARG:HB2	1.71	0.56
2:N:162:GLY:O	3:O:11:MET:CG	2.41	0.56
3:C:36:VAL:HG12	3:C:37:TRP:N	2.21	0.55
1:M:93:MET:CB	1:M:125:TRP:CH2	2.89	0.55
1:M:222:PRO:CB	1:M:552:LEU:HD22	2.35	0.55
4:P:28:ALA:N	4:P:29:PRO:HD2	2.21	0.55
1:A:46:VAL:CG2	1:A:47:ALA:N	2.69	0.55
3:C:45:GLY:N	3:C:59:PHE:CE2	2.74	0.55
1:M:76:LEU:HB2	1:M:529:ARG:HD3	1.88	0.55
1:M:144:LEU:HD13	2:N:114:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:252:GLY:O	1:M:283:GLU:HG2	2.06	0.55
4:P:19:ALA:O	4:P:20:GLY:O	2.24	0.55
1:A:37:LYS:HG3	1:A:38:VAL:HG13	1.86	0.55
2:B:63:GLY:CA	2:B:149:ILE:HD12	2.36	0.55
2:B:68:MET:CE	2:B:72:VAL:C	2.74	0.55
1:M:263:LEU:HD12	1:M:283:GLU:CA	2.36	0.55
1:M:499:ASN:O	1:M:503:LEU:HG	2.07	0.55
1:M:555:ARG:CG	1:M:560:THR:H	2.19	0.55
2:N:221:ALA:O	2:N:225:GLN:NE2	2.39	0.55
1:A:37:LYS:HG3	1:A:38:VAL:CG1	2.36	0.55
1:A:106:ARG:O	1:A:108:ASP:N	2.40	0.55
1:A:168:ARG:HG2	1:A:425:ILE:HD11	1.88	0.55
1:A:286:PRO:O	1:A:289:LYS:HB2	2.06	0.55
2:B:167:PHE:HA	2:B:199:ASN:HB3	1.87	0.55
1:M:53:ALA:HB2	1:M:124:THR:CG2	2.37	0.55
1:M:57:GLN:C	1:M:60:ASP:OD1	2.45	0.55
1:M:115:ARG:HA	1:M:124:THR:OG1	2.07	0.55
1:M:268:MET:HB3	1:M:282:MET:HB3	1.88	0.55
1:A:446:GLU:HB2	1:A:489:VAL:HA	1.88	0.55
3:C:98:VAL:O	3:C:99:LYS:HB2	2.07	0.55
1:M:264:GLN:HB3	1:M:282:MET:CE	2.36	0.55
1:A:254:LEU:HA	1:A:313:TYR:O	2.07	0.55
1:M:276:GLU:O	1:M:277:PRO:C	2.44	0.55
1:M:527:GLU:OE1	1:M:543:ASP:HB2	2.07	0.55
1:A:298:TRP:HA	1:A:303:THR:HG23	1.89	0.55
3:C:49:LEU:HD11	4:D:54:VAL:HG12	1.89	0.55
1:M:35:ILE:HA	1:M:152:PHE:O	2.06	0.55
1:M:228:PHE:CE1	1:M:532:HIS:HB2	2.42	0.55
4:P:112:LEU:O	4:P:112:LEU:HG	2.07	0.55
1:A:93:MET:HE1	1:A:397:ALA:HA	1.88	0.55
1:A:236:LEU:HD21	1:A:243:MET:HE2	1.87	0.55
1:M:279:ASN:HD22	1:M:280:LYS:H	1.55	0.55
1:M:386:HIS:O	1:M:387:GLY:O	2.25	0.55
2:N:54:ARG:C	2:N:55:TRP:CD1	2.81	0.55
2:N:121:ILE:N	2:N:185:ASP:OD1	2.39	0.55
2:N:210:CYS:SG	2:N:221:ALA:N	2.80	0.55
4:P:101:TYR:CD1	4:P:101:TYR:N	2.75	0.55
1:A:411:THR:O	1:A:414:ALA:HB3	2.07	0.55
2:B:75:LEU:C	2:B:77:CYS:N	2.52	0.55
1:M:52:SER:C	1:M:125:TRP:HB2	2.27	0.55
2:N:6:LEU:CD1	2:N:81:LEU:HD21	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ALA:O	1:A:430:ALA:C	2.45	0.54
2:B:75:LEU:C	2:B:77:CYS:H	2.06	0.54
4:D:73:LEU:HD23	4:D:73:LEU:N	2.22	0.54
1:M:114:ARG:NH1	1:M:114:ARG:HB2	2.21	0.54
1:M:447:ASN:HB3	1:M:450:LYS:CG	2.38	0.54
1:M:455:MET:CE	1:M:508:LEU:HD21	2.37	0.54
2:N:98:ILE:HG12	3:O:9:ARG:NH2	2.07	0.54
2:N:116:ILE:HG21	2:N:172:ALA:HB1	1.88	0.54
1:A:446:GLU:OE1	1:A:485:ARG:HD3	2.06	0.54
3:C:65:ASN:OD1	3:C:66:PRO:HD2	2.06	0.54
4:D:113:ILE:O	4:D:114:GLY:C	2.45	0.54
1:M:78:GLU:N	1:M:224:ARG:NH2	2.55	0.54
1:M:225:ASP:O	1:M:225:ASP:CG	2.44	0.54
1:M:467:ARG:HH22	1:M:532:HIS:CA	2.18	0.54
3:O:50:LYS:HG2	4:P:118:ILE:HG23	1.89	0.54
1:A:324:LEU:HB2	1:A:325:HIS:ND1	2.22	0.54
2:B:135:THR:C	2:B:137:ALA:N	2.58	0.54
4:D:7:ARG:HG2	4:D:7:ARG:O	2.06	0.54
1:M:426:GLU:HA	1:M:429:ALA:HB3	1.90	0.54
1:A:38:VAL:HG23	1:A:39:TYR:O	2.08	0.54
1:M:75:TRP:HB2	1:M:529:ARG:NH2	2.23	0.54
1:M:96:LEU:HB2	1:M:103:TRP:HE1	1.72	0.54
2:B:128:ASP:OD1	2:B:128:ASP:N	2.40	0.54
3:O:83:THR:HG22	3:O:87:PHE:CE1	2.41	0.54
1:A:89:CYS:N	1:A:90:PRO:HD2	2.22	0.54
1:M:9:ILE:HB	1:M:34:LEU:CD1	2.37	0.54
1:M:60:ASP:HB3	1:M:121:ILE:CG2	2.36	0.54
1:M:82:VAL:CG2	1:M:385:LEU:HA	2.30	0.54
2:N:154:CYS:C	2:N:156:ALA:H	2.10	0.54
2:N:192:MET:O	2:N:196:ASN:ND2	2.41	0.54
1:A:541:GLU:OE2	1:A:541:GLU:HA	2.08	0.54
1:M:99:TRP:CE3	1:M:142:THR:HG21	2.42	0.54
1:M:166:HIS:HB2	1:M:373:GLY:HA3	1.90	0.54
1:M:516:GLU:OE1	1:M:516:GLU:HA	2.08	0.54
2:N:109:PHE:O	2:N:113:LEU:HG	2.08	0.54
2:N:175:LEU:O	2:N:176:ALA:C	2.44	0.54
2:B:241:LYS:O	2:B:242:PRO:C	2.46	0.54
1:M:13:GLY:N	6:M:803:FAD:H4B	2.23	0.54
1:M:361:ILE:CG1	1:M:376:ALA:HB3	2.36	0.54
2:N:28:VAL:HG12	2:N:29:PRO:HD2	1.90	0.54
2:N:120:ILE:CD1	2:N:185:ASP:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:64:ARG:NH2	4:P:118:ILE:HA	2.22	0.54
1:A:71:ALA:HA	1:A:75:TRP:CZ3	2.42	0.54
1:A:448:TRP:CG	1:A:449:ALA:N	2.75	0.54
2:B:216:LYS:HE2	2:B:216:LYS:HA	1.88	0.54
1:M:28:PRO:O	1:M:30:ALA:N	2.41	0.54
2:N:69:VAL:HG11	2:N:79:THR:CG2	2.29	0.54
2:N:75:LEU:CD2	2:N:75:LEU:H	2.19	0.54
1:A:109:GLY:O	2:B:133:ILE:HG23	2.08	0.54
4:D:20:GLY:HA3	4:D:77:CYS:HB2	1.90	0.54
4:D:37:ILE:HD12	4:D:37:ILE:N	2.22	0.54
1:M:130:LYS:HZ3	2:N:216:LYS:HD3	1.72	0.54
1:M:525:ARG:HA	1:M:547:PHE:CD2	2.42	0.54
2:N:125:ARG:HA	2:N:129:GLN:OE1	2.08	0.54
3:O:50:LYS:C	3:O:52:GLY:H	2.11	0.54
1:A:263:LEU:HB2	1:A:268:MET:HE3	1.87	0.53
2:B:26:TYR:CD2	2:B:47:LEU:HD13	2.33	0.53
1:M:103:TRP:CE3	1:M:126:PHE:O	2.61	0.53
1:M:467:ARG:HB2	1:M:533:GLN:O	2.08	0.53
1:M:549:LYS:CB	1:M:566:SER:O	2.56	0.53
2:N:206:PHE:O	2:N:206:PHE:CD2	2.62	0.53
3:O:12:THR:OG1	3:O:13:SER:N	2.40	0.53
1:A:106:ARG:O	1:A:107:PRO:C	2.45	0.53
1:M:204:ASN:O	2:N:58:ARG:CZ	2.56	0.53
1:M:363:THR:HA	1:M:368:GLU:O	2.08	0.53
1:M:474:LYS:O	1:M:478:LYS:HG2	2.08	0.53
2:N:166:GLU:O	2:N:199:ASN:HB3	2.08	0.53
3:O:28:ARG:HG3	3:O:85:THR:HG21	1.90	0.53
1:A:319:LEU:HD12	1:A:323:LYS:CE	2.37	0.53
2:B:126:THR:H	2:B:129:GLN:HG3	1.73	0.53
1:M:53:ALA:CA	1:M:394:ASN:HD22	2.21	0.53
1:M:216:ALA:O	1:M:217:LEU:C	2.47	0.53
1:A:115:ARG:HH11	1:A:115:ARG:CG	2.09	0.53
1:A:366:ASN:HB3	1:A:409:GLN:HG3	1.89	0.53
2:B:212:GLU:HG3	3:C:21:PHE:CE1	2.41	0.53
1:M:49:GLN:HE21	1:M:49:GLN:N	2.00	0.53
1:M:162:VAL:HG12	1:M:163:ASP:H	1.74	0.53
1:M:228:PHE:HE1	1:M:532:HIS:HB2	1.73	0.53
1:M:320:GLY:O	1:M:324:LEU:HB2	2.09	0.53
2:N:154:CYS:O	2:N:156:ALA:N	2.39	0.53
3:C:36:VAL:CG2	4:D:75:LEU:HD22	2.38	0.53
2:N:8:ILE:CG2	2:N:9:GLU:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:73:PRO:HB2	2:N:153:LEU:CD2	2.39	0.53
1:M:46:VAL:O	1:M:48:ALA:N	2.40	0.53
1:M:157:VAL:HA	1:M:172:ALA:HA	1.91	0.53
2:N:44:LYS:C	2:N:46:ASN:H	2.10	0.53
2:N:70:ASN:C	2:N:72:VAL:H	2.11	0.53
4:P:59:GLN:O	4:P:64:ARG:NH1	2.41	0.53
4:D:103:LEU:HA	4:D:106:ILE:HD12	1.89	0.53
1:M:194:GLY:N	1:M:208:VAL:HG12	2.24	0.53
1:M:256:ASN:ND2	1:M:260:TYR:HB3	2.19	0.53
1:M:552:LEU:HD12	1:M:564:GLU:CB	2.38	0.53
2:N:144:GLN:HG3	3:O:102:LYS:HZ1	1.68	0.53
2:N:192:MET:HE3	2:N:195:LEU:HB2	1.89	0.53
4:P:13:PHE:CE2	4:P:97:LYS:HG2	2.43	0.53
1:A:57:GLN:HE21	1:A:122:GLU:HG2	1.72	0.53
1:M:363:THR:OG1	1:M:367:CYS:HA	2.09	0.53
2:N:219:ASP:CG	2:N:222:ALA:HB3	2.29	0.53
1:A:500:THR:OG1	2:B:52:SER:HB3	2.09	0.53
2:B:53:TYR:HA	2:B:103:VAL:HG22	1.91	0.53
4:D:110:VAL:O	4:D:113:ILE:HB	2.09	0.53
1:M:8:ALA:HB1	1:M:170:LEU:CD1	2.39	0.53
1:M:281:TYR:O	1:M:282:MET:CB	2.57	0.53
1:M:554:PHE:O	1:M:560:THR:O	2.26	0.53
2:N:168:ILE:CD1	2:N:173:ILE:HG12	2.36	0.53
4:P:20:GLY:HA3	4:P:77:CYS:HB2	1.91	0.53
4:P:80:HIS:HD2	4:P:84:HIS:HD2	1.54	0.53
1:A:496:SER:OG	2:B:16:GLU:OE1	2.19	0.52
1:M:74:ASP:O	1:M:74:ASP:OD1	2.26	0.52
1:M:263:LEU:CD1	1:M:283:GLU:HA	2.39	0.52
2:N:51:LEU:C	2:N:51:LEU:HD12	2.28	0.52
2:N:155:TYR:CZ	2:N:169:GLY:HA3	2.45	0.52
2:N:157:ALA:HB2	2:N:213:VAL:HG21	1.91	0.52
2:N:236:LEU:O	2:N:240:LEU:HD21	2.09	0.52
3:O:126:VAL:CG1	10:P:800:MQ7:H141	2.38	0.52
2:N:94:ALA:O	2:N:95:ASN:HB2	2.09	0.52
3:O:120:THR:HG23	4:P:30:VAL:HB	1.91	0.52
2:B:110:ILE:CA	2:B:113:LEU:HD12	2.27	0.52
1:M:78:GLU:C	1:M:80:ASP:H	2.11	0.52
2:N:101:ASP:O	2:N:102:LEU:HD23	2.09	0.52
1:A:390:ARG:NH2	5:A:702:FLC:OA1	2.42	0.52
2:B:15:PRO:HB3	3:C:5:LYS:H	1.75	0.52
2:B:219:ASP:OD2	2:B:222:ALA:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:78:GLU:HB2	1:M:224:ARG:HH22	1.74	0.52
1:M:110:SER:O	1:M:111:VAL:C	2.47	0.52
1:M:549:LYS:HB3	1:M:566:SER:O	2.10	0.52
2:N:134:GLN:O	2:N:135:THR:O	2.27	0.52
2:N:173:ILE:HG23	2:N:195:LEU:HD22	1.90	0.52
1:A:48:ALA:HB3	1:A:132:GLY:HA3	1.92	0.52
1:M:242:LEU:HD21	1:M:244:THR:HA	1.92	0.52
1:A:377:VAL:HG21	1:A:403:GLY:HA2	1.92	0.52
4:D:48:ALA:CA	4:D:53:ARG:HD3	2.38	0.52
1:M:96:LEU:HD12	1:M:103:TRP:HZ2	1.74	0.52
1:M:174:ASN:ND2	1:M:177:GLU:CG	2.73	0.52
1:M:363:THR:HB	1:M:367:CYS:C	2.30	0.52
1:A:253:ILE:O	1:A:314:LEU:CA	2.55	0.52
1:A:446:GLU:CG	1:A:488:ARG:O	2.53	0.52
4:D:103:LEU:O	4:D:103:LEU:HD23	2.10	0.52
4:D:112:LEU:HA	4:D:115:VAL:CG2	2.40	0.52
1:M:219:HIS:HB3	1:M:371:ILE:HD11	1.92	0.52
1:M:242:LEU:HD21	1:M:244:THR:CA	2.40	0.52
1:M:329:PRO:O	1:M:333:GLU:HG3	2.09	0.52
3:C:22:TYR:O	3:C:25:TYR:HB3	2.10	0.52
1:M:79:GLN:CD	1:M:570:ILE:HG23	2.30	0.52
2:N:108:HIS:HA	2:N:111:GLU:HB2	1.91	0.52
4:P:35:VAL:HG22	10:P:800:MQ7:C1	2.40	0.52
4:P:50:SER:O	4:P:51:TYR:C	2.48	0.52
1:A:102:PRO:O	1:A:103:TRP:C	2.48	0.52
1:A:253:ILE:HG21	1:A:315:ASP:CB	2.29	0.52
2:B:95:ASN:HD21	2:B:162:GLY:HA3	1.74	0.52
4:D:30:VAL:O	4:D:33:LEU:HB3	2.09	0.52
1:M:211:ASP:CG	1:M:507:GLU:HA	2.30	0.52
1:M:555:ARG:HG2	1:M:558:ASP:O	2.09	0.52
1:A:96:LEU:HD11	1:A:400:VAL:HG21	1.91	0.52
3:C:15:TRP:CD2	3:C:16:TRP:N	2.78	0.52
4:D:41:LEU:O	4:D:43:LEU:CD2	2.57	0.52
1:M:41:MET:CE	1:M:42:ARG:HG3	2.39	0.51
1:M:60:ASP:OD2	1:M:123:ARG:HD3	2.10	0.51
1:M:106:ARG:HD2	1:M:110:SER:OG	2.10	0.51
1:M:158:LEU:HB3	1:M:436:LEU:CD1	2.41	0.51
1:M:229:VAL:CG2	1:M:467:ARG:CZ	2.87	0.51
1:M:242:LEU:HD23	1:M:242:LEU:O	2.10	0.51
1:M:388:ALA:HB1	1:M:529:ARG:HB3	1.92	0.51
2:B:209:TYR:O	2:B:213:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:73:GLY:HA2	1:M:387:GLY:HA3	1.90	0.51
1:M:106:ARG:HG3	1:M:108:ASP:OD1	2.09	0.51
1:M:211:ASP:HB3	6:M:803:FAD:H61A	1.75	0.51
2:N:73:PRO:HB2	2:N:153:LEU:HD22	1.93	0.51
2:B:162:GLY:O	3:C:11:MET:SD	2.68	0.51
1:M:92:GLU:OE2	1:M:401:VAL:HA	2.10	0.51
1:M:97:GLU:OE1	2:N:132:ASN:HB2	2.10	0.51
1:M:495:SER:HB3	2:N:16:GLU:OE2	2.11	0.51
1:A:184:ARG:CG	1:A:184:ARG:NH1	2.57	0.51
1:A:292:GLN:HG2	1:A:466:TYR:CZ	2.45	0.51
1:A:410:ALA:O	1:A:411:THR:C	2.47	0.51
2:B:65:CYS:O	2:B:67:MET:CE	2.59	0.51
3:C:97:ILE:HG23	3:C:101:GLU:O	2.10	0.51
4:D:72:VAL:HG12	4:D:73:LEU:N	2.24	0.51
1:M:42:ARG:HH22	2:N:54:ARG:CB	2.20	0.51
2:N:149:ILE:CG2	2:N:216:LYS:HG3	2.41	0.51
4:P:66:PHE:C	4:P:66:PHE:CD2	2.84	0.51
1:A:493:ASP:CG	1:A:499:ASN:ND2	2.64	0.51
2:B:70:ASN:O	2:B:71:ASN:HB2	2.09	0.51
1:M:58:ASP:C	1:M:60:ASP:H	2.13	0.51
1:M:84:TYR:HE2	1:M:405:LEU:HD11	1.76	0.51
1:M:467:ARG:NH2	1:M:533:GLN:H	2.07	0.51
2:N:31:ASP:CG	2:N:32:ALA:H	2.13	0.51
1:A:12:ALA:HB1	1:A:40:PRO:HB3	1.92	0.51
1:A:198:VAL:CG2	1:A:455:MET:CE	2.88	0.51
1:A:245:GLU:O	1:A:246:GLY:C	2.47	0.51
1:A:256:ASN:OD1	1:A:259:GLY:N	2.42	0.51
1:A:328:LEU:HD11	1:A:331:ILE:HG13	1.93	0.51
4:D:68:PHE:CE1	4:D:72:VAL:HG21	2.45	0.51
1:M:295:TRP:CD1	1:M:295:TRP:C	2.83	0.51
1:M:468:THR:O	1:M:472:MET:HG3	2.11	0.51
2:N:214:CYS:HA	9:N:246:SF4:S3	2.50	0.51
3:C:50:LYS:C	3:C:52:GLY:H	2.14	0.51
3:C:121:ILE:O	3:C:123:ILE:N	2.44	0.51
3:C:123:ILE:HG13	10:D:700:MQ7:H192	1.92	0.51
1:M:382:SER:HG	1:M:386:HIS:CE1	2.25	0.51
1:M:434:GLN:HA	1:M:437:LYS:HB2	1.93	0.51
3:O:87:PHE:CD2	3:O:112:LEU:CD1	2.75	0.51
3:O:90:ALA:N	3:O:91:PRO:CD	2.73	0.51
1:A:114:ARG:HD3	1:A:126:PHE:CE2	2.44	0.51
1:M:3:PHE:HB3	1:M:183:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:191:ALA:HB2	1:M:377:VAL:O	2.10	0.51
3:C:87:PHE:HD1	3:C:112:LEU:HD13	1.75	0.51
1:M:42:ARG:NE	2:N:54:ARG:NH2	2.59	0.51
1:M:106:ARG:HB3	1:M:112:ASN:CB	2.29	0.51
1:M:194:GLY:HA3	1:M:379:GLU:CG	2.41	0.51
1:M:328:LEU:HD23	1:M:328:LEU:H	1.75	0.51
1:M:467:ARG:NH2	1:M:533:GLN:N	2.59	0.51
2:N:204:CYS:CB	2:N:224:ILE:HG21	2.41	0.51
4:P:83:HIS:O	4:P:86:MET:HB2	2.11	0.51
1:A:65:HIS:CG	1:A:86:VAL:CG2	2.94	0.51
1:A:399:LEU:N	1:A:399:LEU:HD23	2.25	0.51
3:C:12:THR:HG22	3:C:13:SER:H	1.75	0.51
3:C:88:GLU:HA	3:C:109:ILE:HD13	1.93	0.51
1:M:53:ALA:HB3	1:M:394:ASN:ND2	2.26	0.51
1:M:66:PHE:O	1:M:70:VAL:HG23	2.10	0.51
1:M:221:VAL:HG23	1:M:371:ILE:HG13	1.92	0.51
1:M:223:LEU:CD2	1:M:517:CYS:SG	2.99	0.51
1:M:266:TYR:CE2	1:M:296:HIS:HB3	2.45	0.51
2:N:37:LEU:CD2	2:N:77:CYS:HA	2.41	0.51
4:P:103:LEU:HD21	4:P:107:LEU:HD11	1.93	0.51
1:A:557:ALA:C	1:A:559:GLY:H	2.15	0.50
4:D:28:ALA:O	4:D:32:ILE:HG13	2.11	0.50
1:M:104:SER:OG	1:M:128:ALA:N	2.43	0.50
1:M:214:GLY:HA3	1:M:510:HIS:CB	2.41	0.50
1:M:461:GLU:HA	1:M:466:TYR:OH	2.11	0.50
2:N:108:HIS:O	2:N:109:PHE:C	2.49	0.50
3:O:22:TYR:O	3:O:25:TYR:HB3	2.11	0.50
3:O:37:TRP:CZ2	3:O:41:GLU:OE1	2.64	0.50
3:O:59:PHE:O	3:O:62:PHE:HB3	2.10	0.50
1:A:239:SER:OG	1:A:240:GLY:N	2.42	0.50
1:A:268:MET:O	1:A:282:MET:HG2	2.11	0.50
1:A:280:LYS:C	1:A:281:TYR:HD1	2.15	0.50
1:M:167:VAL:CG2	1:M:374:LEU:HD13	2.36	0.50
2:N:28:VAL:HG11	2:N:39:ALA:O	2.11	0.50
1:A:224:ARG:HB2	1:A:552:LEU:CD2	2.41	0.50
3:C:17:LYS:CG	3:C:23:ARG:HH12	2.24	0.50
1:M:105:ARG:NH1	1:M:109:GLY:HA2	2.25	0.50
1:M:213:MET:SD	1:M:216:ALA:HB3	2.51	0.50
1:M:548:LEU:HG	1:M:568:VAL:HB	1.93	0.50
2:N:163:LEU:HG	3:O:11:MET:HE3	1.94	0.50
2:N:207:VAL:HG22	3:O:25:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:241:LYS:O	2:N:243:ARG:N	2.44	0.50
4:P:30:VAL:O	4:P:33:LEU:N	2.44	0.50
1:A:215:MET:O	1:A:219:HIS:HD2	1.93	0.50
1:A:250:GLU:HG3	1:A:328:LEU:HD23	1.93	0.50
1:A:255:VAL:HB	1:A:259:GLY:HA2	1.92	0.50
1:A:270:PRO:O	1:A:271:GLU:C	2.50	0.50
1:A:527:GLU:HG2	1:A:547:PHE:HB2	1.90	0.50
1:M:266:TYR:HE2	1:M:296:HIS:HB3	1.77	0.50
2:N:31:ASP:CG	2:N:32:ALA:N	2.64	0.50
2:N:134:GLN:OE1	2:N:184:ARG:HG3	2.12	0.50
4:P:94:PRO:O	4:P:95:ALA:C	2.50	0.50
1:A:413:ARG:CZ	1:A:413:ARG:HB2	2.41	0.50
1:M:39:TYR:HD1	1:M:39:TYR:H	1.58	0.50
1:M:79:GLN:NE2	1:M:570:ILE:HG23	2.26	0.50
2:N:120:ILE:C	2:N:121:ILE:HG13	2.32	0.50
2:N:196:ASN:HB3	2:N:231:SER:OG	2.12	0.50
1:M:92:GLU:CA	1:M:95:GLN:HB3	2.38	0.50
1:M:358:MET:SD	1:M:386:HIS:CB	3.00	0.50
2:N:135:THR:O	2:N:137:ALA:N	2.41	0.50
4:P:39:LEU:HD13	4:P:49:LEU:CD1	2.42	0.50
1:A:525:ARG:O	1:A:527:GLU:N	2.42	0.50
3:O:70:ILE:CG2	3:O:71:ILE:N	2.74	0.50
3:O:106:GLU:HB2	3:O:107:PRO:HD3	1.94	0.50
4:P:80:HIS:NE2	4:P:84:HIS:NE2	2.60	0.50
1:M:166:HIS:HD2	1:M:413:ARG:NH2	2.09	0.50
2:N:219:ASP:H	2:N:220:PRO:CD	2.25	0.50
1:A:59:HIS:CD2	1:A:121:ILE:HD12	2.47	0.50
1:A:253:ILE:HG22	1:A:315:ASP:H	1.77	0.50
1:A:266:TYR:CE2	1:A:296:HIS:HB3	2.46	0.50
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.94	0.50
2:B:176:ALA:O	2:B:177:HIS:C	2.48	0.50
4:D:23:TRP:C	4:D:25:ALA:N	2.64	0.50
1:M:74:ASP:CB	1:M:388:ALA:HB3	2.19	0.50
1:M:115:ARG:CD	1:M:122:GLU:HA	2.42	0.50
1:M:151:ARG:NH1	1:M:153:ASP:OD1	2.39	0.50
1:M:396:LEU:O	1:M:399:LEU:HB2	2.11	0.50
2:N:52:SER:C	2:N:53:TYR:HD1	2.15	0.50
1:A:0:MET:HG3	1:A:182:GLN:HG2	1.94	0.49
1:A:232:HIS:HD2	1:A:234:THR:H	1.60	0.49
1:A:237:PRO:HB2	1:A:308:ARG:HB3	1.94	0.49
1:A:567:ASP:OD1	1:A:568:VAL:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:67:LEU:HD11	10:D:700:MQ7:H6	1.92	0.49
1:M:527:GLU:CA	1:M:539:CYS:SG	2.87	0.49
1:A:141:GLN:NE2	2:B:175:LEU:HD21	2.27	0.49
1:A:155:HIS:NE2	1:A:174:ASN:HB2	2.27	0.49
1:A:166:HIS:ND1	1:A:167:VAL:N	2.60	0.49
1:A:239:SER:HB2	1:A:241:ILE:HD12	1.94	0.49
1:A:252:GLY:HA2	1:A:316:LEU:HD23	1.93	0.49
1:A:328:LEU:HD13	1:A:331:ILE:CG1	2.41	0.49
3:C:36:VAL:CG1	3:C:37:TRP:N	2.75	0.49
1:M:203:THR:HA	1:M:240:GLY:O	2.12	0.49
2:B:142:TYR:CD1	2:B:142:TYR:C	2.86	0.49
2:B:184:ARG:HH11	2:B:184:ARG:HG3	1.77	0.49
1:M:21:ILE:CD1	1:M:139:LEU:HD22	2.41	0.49
1:M:72:GLY:C	1:M:74:ASP:H	2.14	0.49
1:M:112:ASN:O	1:M:126:PHE:HE2	1.94	0.49
1:M:127:ALA:HB3	1:M:131:THR:OG1	2.13	0.49
1:M:162:VAL:HG13	1:M:219:HIS:CE1	2.48	0.49
1:M:227:GLU:HB2	1:M:518:MET:C	2.30	0.49
3:O:15:TRP:CE3	3:O:16:TRP:N	2.80	0.49
1:A:133:PHE:C	1:A:133:PHE:CD2	2.86	0.49
1:A:317:ARG:HB2	1:A:344:VAL:O	2.12	0.49
1:A:390:ARG:NH1	5:A:702:FLC:OA2	2.44	0.49
2:B:50:ASP:OD1	2:B:51:LEU:N	2.44	0.49
2:B:75:LEU:HD21	2:B:153:LEU:HD11	1.94	0.49
1:M:257:LYS:HB2	1:M:302:ASN:C	2.32	0.49
1:M:356:TYR:CD1	1:M:390:ARG:CZ	2.95	0.49
1:M:491:ILE:HD13	1:M:502:LEU:HD13	1.94	0.49
2:N:201:VAL:HG13	2:N:202:TRP:CD1	2.48	0.49
2:N:235:PHE:C	2:N:237:ILE:N	2.62	0.49
4:P:19:ALA:O	4:P:20:GLY:C	2.50	0.49
1:A:307:PRO:HD2	1:A:308:ARG:HG3	1.93	0.49
1:A:489:VAL:O	1:A:489:VAL:HG22	2.12	0.49
4:D:12:VAL:HG12	4:D:13:PHE:H	1.78	0.49
1:M:45:THR:HB	1:M:136:LEU:HD22	1.95	0.49
1:M:448:TRP:O	1:M:452:ARG:NH1	2.42	0.49
3:O:125:PHE:HZ	3:O:130:TRP:CZ3	2.29	0.49
4:P:23:TRP:C	4:P:25:ALA:H	2.15	0.49
4:P:37:ILE:HG22	4:P:38:LEU:N	2.26	0.49
3:C:121:ILE:O	3:C:122:VAL:C	2.47	0.49
1:M:52:SER:HB2	1:M:396:LEU:HB2	1.91	0.49
1:M:53:ALA:H	1:M:394:ASN:CB	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:165:GLY:O	1:M:166:HIS:HB3	2.11	0.49
1:M:244:THR:O	1:M:247:CYS:SG	2.52	0.49
1:M:263:LEU:HD13	1:M:283:GLU:H	1.76	0.49
1:M:468:THR:OG1	1:M:471:LEU:HG	2.13	0.49
1:M:554:PHE:O	1:M:555:ARG:CB	2.61	0.49
1:A:437:LYS:HG3	1:A:441:ASN:HD21	1.77	0.49
1:A:446:GLU:HB2	1:A:489:VAL:CB	2.41	0.49
1:M:32:ILE:HG12	1:M:33:ALA:N	2.27	0.49
1:M:39:TYR:CD1	1:M:39:TYR:N	2.80	0.49
1:M:426:GLU:O	1:M:430:ALA:N	2.45	0.49
1:M:461:GLU:CD	1:M:461:GLU:H	2.16	0.49
2:N:209:TYR:HD1	2:N:212:GLU:HB3	1.76	0.49
3:O:33:VAL:HB	3:O:34:PRO:CD	2.43	0.49
2:B:95:ASN:ND2	2:B:162:GLY:HA3	2.27	0.49
2:B:153:LEU:HD12	2:B:215:PRO:HD3	1.95	0.49
4:D:13:PHE:CE1	4:D:101:TYR:CD1	3.00	0.49
4:D:72:VAL:HG22	4:D:108:THR:HG23	1.94	0.49
1:M:226:MET:HG2	1:M:517:CYS:CB	2.40	0.49
1:M:328:LEU:HB2	1:M:331:ILE:CD1	2.43	0.49
2:N:37:LEU:HD23	2:N:37:LEU:N	2.27	0.49
2:N:192:MET:O	2:N:195:LEU:HB2	2.13	0.49
4:P:30:VAL:HG13	4:P:31:MET:N	2.28	0.49
4:P:62:ILE:HD13	10:P:800:MQ7:H212	1.94	0.49
1:A:436:LEU:HD23	1:A:437:LYS:N	2.27	0.49
2:B:36:LEU:O	2:B:40:LEU:HG	2.12	0.49
2:B:57:CYS:O	2:B:58:ARG:HB2	2.12	0.49
4:D:51:TYR:O	4:D:52:GLU:C	2.49	0.49
4:D:98:TRP:O	4:D:99:VAL:C	2.51	0.49
3:O:53:PRO:HB3	4:P:51:TYR:CG	2.47	0.49
1:A:103:TRP:O	2:B:139:MET:CE	2.60	0.49
1:A:350:VAL:CG2	1:A:350:VAL:O	2.61	0.49
1:M:53:ALA:HA	1:M:125:TRP:HB2	1.94	0.49
1:M:443:ASP:HA	1:M:490:ARG:HA	1.95	0.49
1:M:469:PRO:HD3	1:M:536:ASP:OD2	2.13	0.49
2:N:80:PHE:HB2	2:N:82:ARG:HG2	1.95	0.49
2:N:116:ILE:O	2:N:191:ARG:HG3	2.13	0.49
1:A:134:HIS:O	1:A:138:THR:HB	2.13	0.48
1:A:363:THR:OG1	1:A:383:VAL:HA	2.13	0.48
2:B:54:ARG:NE	2:B:103:VAL:CG1	2.76	0.48
2:B:111:GLU:OE1	4:D:0:MET:HB2	2.13	0.48
1:M:35:ILE:CG2	1:M:36:SER:N	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:106:ARG:HB2	1:M:112:ASN:HD22	1.78	0.48
1:M:355:HIS:NE2	5:M:802:FLC:OB1	2.46	0.48
1:M:361:ILE:HG22	1:M:363:THR:HG23	1.96	0.48
1:A:261:ARG:O	1:A:264:GLN:NE2	2.31	0.48
2:B:26:TYR:CB	2:B:43:ILE:HD13	2.43	0.48
2:B:182:ASP:C	2:B:182:ASP:OD2	2.51	0.48
3:C:48:ALA:C	3:C:50:LYS:N	2.66	0.48
1:M:60:ASP:HB2	1:M:123:ARG:NH1	2.28	0.48
1:M:158:LEU:HD13	1:M:436:LEU:HD12	1.94	0.48
1:M:338:TYR:O	2:N:33:THR:HG22	2.13	0.48
1:M:377:VAL:HG13	1:M:402:PHE:HD2	1.75	0.48
2:N:31:ASP:H	2:N:34:THR:HG21	1.78	0.48
4:P:23:TRP:HE1	4:P:70:MET:CE	2.26	0.48
4:P:64:ARG:HH22	4:P:118:ILE:HA	1.78	0.48
1:A:294:PHE:CZ	1:A:351:ARG:HG3	2.49	0.48
1:A:366:ASN:O	1:A:367:CYS:CB	2.60	0.48
1:A:490:ARG:HG2	1:A:491:ILE:N	2.28	0.48
3:C:37:TRP:CE2	3:C:41:GLU:OE2	2.67	0.48
4:D:0:MET:CG	4:D:1:ILE:H	2.21	0.48
4:D:4:ASN:C	4:D:4:ASN:ND2	2.67	0.48
1:M:8:ALA:HB1	1:M:170:LEU:HD12	1.95	0.48
1:M:34:LEU:O	1:M:152:PHE:N	2.44	0.48
1:M:65:HIS:HB2	1:M:123:ARG:CZ	2.42	0.48
1:M:159:ASP:OD2	1:M:432:VAL:HG22	2.14	0.48
1:A:232:HIS:CD2	1:A:234:THR:H	2.32	0.48
1:M:455:MET:HB2	1:M:482:LEU:HD21	1.95	0.48
1:M:476:ILE:HG12	1:M:519:ALA:CB	2.29	0.48
1:M:517:CYS:O	1:M:521:SER:HB2	2.12	0.48
4:P:0:MET:O	4:P:1:ILE:HG12	2.12	0.48
2:N:235:PHE:O	2:N:237:ILE:N	2.45	0.48
3:O:15:TRP:CE3	3:O:16:TRP:HA	2.49	0.48
3:O:27:LEU:HD23	3:O:81:LEU:HD21	1.95	0.48
1:M:42:ARG:CZ	2:N:54:ARG:CZ	2.92	0.48
1:M:174:ASN:HD22	1:M:177:GLU:HB2	1.79	0.48
1:M:371:ILE:HD12	1:M:374:LEU:HD23	1.96	0.48
1:M:529:ARG:O	1:M:530:GLY:C	2.52	0.48
2:N:53:TYR:O	2:N:54:ARG:HG3	2.13	0.48
3:O:62:PHE:CE1	3:O:68:ILE:HG12	2.48	0.48
1:A:448:TRP:CZ2	1:A:504:TYR:HD1	2.32	0.48
2:B:13:TYR:OH	3:C:5:LYS:HE3	2.14	0.48
2:B:121:ILE:O	2:B:186:HIS:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:LEU:CB	4:D:40:PRO:HG3	2.36	0.48
1:M:104:SER:H	1:M:127:ALA:HA	1.78	0.48
1:M:192:THR:CG2	1:M:212:GLY:H	2.25	0.48
1:M:227:GLU:HG3	1:M:463:CYS:HG	1.74	0.48
1:M:452:ARG:CG	1:M:508:LEU:HD22	2.42	0.48
1:M:490:ARG:H	1:M:490:ARG:CD	2.21	0.48
3:O:56:TRP:O	3:O:59:PHE:HB3	2.13	0.48
1:A:540:THR:C	1:A:541:GLU:OE2	2.49	0.48
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.94	0.48
1:M:78:GLU:C	1:M:80:ASP:N	2.66	0.48
1:M:225:ASP:O	1:M:225:ASP:OD1	2.32	0.48
1:M:263:LEU:HD12	1:M:283:GLU:HA	1.94	0.48
3:O:79:ALA:O	3:O:80:LEU:C	2.50	0.48
3:C:124:LEU:O	3:C:128:LEU:HB2	2.14	0.48
4:D:66:PHE:C	4:D:66:PHE:CD2	2.87	0.48
1:M:46:VAL:C	1:M:48:ALA:H	2.16	0.48
4:P:32:ILE:O	4:P:36:GLY:N	2.45	0.48
1:M:92:GLU:OE1	1:M:400:VAL:HG12	2.13	0.48
1:M:440:VAL:HA	1:M:491:ILE:HD12	1.96	0.48
1:A:17:LEU:HD11	1:A:140:PHE:HA	1.95	0.47
1:A:109:GLY:C	2:B:133:ILE:HG23	2.34	0.47
1:A:253:ILE:HG22	1:A:315:ASP:N	2.29	0.47
3:C:98:VAL:HG23	3:C:99:LYS:HE3	1.96	0.47
1:M:555:ARG:CD	1:M:559:GLY:HA2	2.44	0.47
2:N:104:VAL:HG23	2:N:106:MET:SD	2.53	0.47
2:N:216:LYS:HA	2:N:216:LYS:NZ	2.29	0.47
3:O:67:VAL:C	3:O:69:VAL:N	2.66	0.47
1:A:427:ALA:HA	1:A:430:ALA:HB2	1.97	0.47
3:C:27:LEU:O	3:C:28:ARG:C	2.49	0.47
4:D:10:GLU:N	4:D:11:PRO:HD2	2.29	0.47
2:N:31:ASP:H	2:N:34:THR:CG2	2.27	0.47
1:A:43:SER:O	1:A:46:VAL:HG13	2.14	0.47
4:D:32:ILE:O	4:D:36:GLY:N	2.42	0.47
1:M:157:VAL:HG12	1:M:215:MET:SD	2.54	0.47
1:M:228:PHE:CE2	1:M:387:GLY:O	2.65	0.47
1:M:255:VAL:CG2	1:M:313:TYR:HB2	2.42	0.47
2:N:4:LYS:C	2:N:5:ASN:ND2	2.67	0.47
2:N:10:VAL:HG22	2:N:90:VAL:CG2	2.44	0.47
2:N:64:SER:O	2:N:66:GLY:N	2.47	0.47
2:N:157:ALA:CB	2:N:213:VAL:HG21	2.43	0.47
1:A:479:LEU:HD23	1:A:479:LEU:HA	1.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ASP:OD2	1:A:560:THR:OG1	2.32	0.47
1:M:448:TRP:CG	1:M:449:ALA:N	2.82	0.47
1:M:483:GLN:CG	1:M:512:LEU:HD13	2.45	0.47
2:N:145:PHE:CE1	2:N:219:ASP:HB3	2.45	0.47
2:N:201:VAL:O	2:N:201:VAL:HG22	2.14	0.47
1:A:287:ARG:NH1	1:A:287:ARG:CG	2.42	0.47
1:A:551:THR:O	1:A:552:LEU:HD23	2.15	0.47
3:C:27:LEU:C	3:C:29:GLU:N	2.65	0.47
4:D:30:VAL:CG1	4:D:31:MET:N	2.78	0.47
1:M:46:VAL:CG2	1:M:47:ALA:N	2.78	0.47
1:M:53:ALA:HB3	1:M:392:GLY:O	2.14	0.47
1:M:268:MET:HG2	1:M:282:MET:HA	1.97	0.47
1:M:470:GLU:O	1:M:470:GLU:CD	2.53	0.47
1:M:555:ARG:HG3	1:M:560:THR:H	1.78	0.47
2:N:107:THR:O	2:N:111:GLU:HG3	2.14	0.47
2:N:174:THR:HG21	2:N:218:VAL:HG11	1.96	0.47
1:A:182:GLN:O	1:A:182:GLN:HG3	2.14	0.47
1:A:261:ARG:HD2	1:A:282:MET:HE1	1.95	0.47
5:A:702:FLC:OA1	6:A:703:FAD:N1	2.47	0.47
2:B:73:PRO:O	2:B:74:LYS:HG3	2.15	0.47
1:M:131:THR:O	1:M:135:MET:HB2	2.15	0.47
4:P:39:LEU:HG	4:P:40:PRO:N	2.29	0.47
1:A:2:THR:OG1	1:A:182:GLN:NE2	2.47	0.47
1:A:109:GLY:HA3	2:B:133:ILE:CG2	2.45	0.47
1:A:154:GLU:OE2	2:B:54:ARG:NH2	2.48	0.47
1:A:277:PRO:O	1:A:277:PRO:HG2	2.15	0.47
1:A:511:GLY:O	1:A:512:LEU:C	2.50	0.47
2:B:180:ASN:OD1	2:B:191:ARG:HD2	2.14	0.47
2:B:242:PRO:O	2:B:243:ARG:C	2.51	0.47
3:C:50:LYS:NZ	4:D:118:ILE:CD1	2.57	0.47
3:C:82:HIS:HE2	4:D:25:ALA:HB2	1.79	0.47
1:M:22:ALA:CB	1:M:404:ARG:HA	2.45	0.47
1:M:224:ARG:HG3	1:M:550:HIS:HB2	1.97	0.47
1:M:452:ARG:N	1:M:452:ARG:HD2	2.29	0.47
2:N:30:TYR:CG	2:N:81:LEU:HD22	2.50	0.47
2:N:44:LYS:C	2:N:46:ASN:N	2.68	0.47
2:N:70:ASN:O	2:N:72:VAL:N	2.47	0.47
3:O:102:LYS:HG3	3:O:102:LYS:O	2.13	0.47
4:P:34:LEU:HA	4:P:38:LEU:HB2	1.96	0.47
1:A:91:THR:O	1:A:94:THR:HB	2.15	0.47
1:A:298:TRP:HA	1:A:303:THR:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:LEU:HB3	2:B:77:CYS:HB3	1.97	0.47
1:M:388:ALA:HB1	1:M:529:ARG:CB	2.45	0.47
1:M:526:LYS:O	1:M:526:LYS:CD	2.58	0.47
2:N:4:LYS:O	2:N:5:ASN:ND2	2.41	0.47
2:N:175:LEU:O	2:N:178:ARG:N	2.48	0.47
4:P:13:PHE:HE2	4:P:97:LYS:CG	2.27	0.47
1:A:386:HIS:O	1:A:387:GLY:C	2.49	0.47
2:B:119:TYR:O	2:B:121:ILE:HG13	2.15	0.47
4:D:64:ARG:HH21	4:D:118:ILE:HA	1.80	0.47
1:M:244:THR:O	1:M:244:THR:HG23	2.14	0.47
1:M:518:MET:O	1:M:521:SER:HB3	2.15	0.47
3:O:123:ILE:HD12	10:P:800:MQ7:H162	1.93	0.47
1:A:230:GLN:CD	1:A:287:ARG:HE	2.17	0.47
4:D:61:PHE:HA	4:D:64:ARG:HB2	1.97	0.47
4:D:105:ALA:O	4:D:106:ILE:C	2.53	0.47
1:M:230:GLN:HG2	1:M:390:ARG:NH2	2.25	0.47
1:M:279:ASN:HD22	1:M:279:ASN:C	2.15	0.47
3:C:88:GLU:HA	3:C:109:ILE:CD1	2.45	0.46
1:M:194:GLY:HA3	1:M:379:GLU:CD	2.35	0.46
1:M:228:PHE:HE1	1:M:532:HIS:CB	2.28	0.46
2:N:56:SER:O	2:N:57:CYS:HB3	2.15	0.46
3:O:43:ILE:O	3:O:44:PHE:C	2.53	0.46
4:P:65:VAL:O	4:P:69:LEU:HG	2.16	0.46
1:A:324:LEU:C	1:A:326:GLU:H	2.18	0.46
1:M:49:GLN:O	1:M:50:GLY:C	2.54	0.46
1:M:236:LEU:CB	1:M:241:ILE:H	2.28	0.46
1:M:263:LEU:CD1	1:M:283:GLU:N	2.77	0.46
1:M:279:ASN:O	1:M:280:LYS:HG2	2.15	0.46
1:M:418:GLY:O	1:M:419:ASN:CG	2.53	0.46
2:N:35:SER:HB3	2:N:77:CYS:HA	1.97	0.46
1:A:2:THR:O	1:A:3:PHE:CD1	2.68	0.46
1:A:197:ARG:HB2	1:A:208:VAL:O	2.16	0.46
1:A:427:ALA:C	1:A:430:ALA:HB3	2.35	0.46
4:D:1:ILE:O	4:D:1:ILE:CG2	2.56	0.46
4:D:10:GLU:C	4:D:12:VAL:H	2.18	0.46
4:D:100:PHE:C	4:D:102:GLY:N	2.68	0.46
1:M:193:GLY:HA3	1:M:208:VAL:HA	1.96	0.46
1:M:297:GLU:HA	1:M:297:GLU:OE1	2.14	0.46
1:M:521:SER:O	1:M:525:ARG:HG3	2.16	0.46
2:N:220:PRO:HG2	2:N:221:ALA:H	1.80	0.46
3:O:14:THR:O	3:O:17:LYS:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:49:LEU:HD11	4:P:55:LEU:HB2	1.98	0.46
1:A:181:VAL:CG2	1:A:182:GLN:N	2.78	0.46
1:A:504:TYR:HA	1:A:507:GLU:OE1	2.16	0.46
1:M:103:TRP:CE3	1:M:127:ALA:HB2	2.51	0.46
1:M:147:PRO:C	1:M:149:ILE:N	2.69	0.46
1:M:237:PRO:O	1:M:239:SER:N	2.37	0.46
2:N:108:HIS:CE1	2:N:112:SER:OG	2.68	0.46
2:N:209:TYR:CD1	2:N:212:GLU:HB3	2.50	0.46
4:P:10:GLU:N	4:P:11:PRO:HD3	2.31	0.46
4:D:53:ARG:O	4:D:56:ALA:HB3	2.15	0.46
1:M:56:ALA:O	1:M:57:GLN:HG2	2.16	0.46
1:M:80:ASP:O	1:M:83:ASP:HB3	2.16	0.46
1:M:187:ALA:CB	1:M:410:ALA:HB1	2.43	0.46
1:M:503:LEU:C	1:M:505:THR:H	2.18	0.46
2:N:189:LYS:C	2:N:191:ARG:H	2.15	0.46
3:O:48:ALA:C	3:O:50:LYS:N	2.68	0.46
4:P:98:TRP:O	4:P:99:VAL:C	2.52	0.46
1:A:255:VAL:CG1	1:A:261:ARG:HG2	2.43	0.46
1:A:328:LEU:CD1	1:A:331:ILE:CG1	2.91	0.46
1:A:391:LEU:O	1:A:392:GLY:C	2.51	0.46
2:B:97:PRO:O	2:B:104:VAL:CG2	2.62	0.46
2:B:127:ALA:C	2:B:129:GLN:N	2.68	0.46
3:C:27:LEU:O	3:C:29:GLU:N	2.48	0.46
4:D:84:HIS:O	4:D:86:MET:N	2.48	0.46
1:M:10:VAL:CG1	1:M:157:VAL:HG21	2.46	0.46
1:M:42:ARG:NE	2:N:54:ARG:HH21	2.14	0.46
1:M:130:LYS:HB2	1:M:134:HIS:CE1	2.51	0.46
1:M:383:VAL:HG13	1:M:402:PHE:CD1	2.50	0.46
4:P:103:LEU:CD2	4:P:107:LEU:HD11	2.46	0.46
1:A:168:ARG:HD3	1:A:168:ARG:HA	1.67	0.46
2:B:43:ILE:HG22	2:B:48:ALA:HB3	1.97	0.46
3:C:17:LYS:HG2	3:C:23:ARG:NH2	2.30	0.46
1:M:52:SER:HB2	1:M:396:LEU:CD2	2.45	0.46
1:M:61:SER:O	1:M:62:PHE:C	2.54	0.46
1:M:360:GLY:C	1:M:361:ILE:HD12	2.36	0.46
4:P:29:PRO:HG2	4:P:30:VAL:H	1.81	0.46
1:A:49:GLN:CG	1:A:129:ASP:O	2.63	0.46
1:A:161:LEU:HA	1:A:161:LEU:HD23	1.70	0.46
1:A:280:LYS:O	1:A:281:TYR:CD1	2.68	0.46
1:A:342:ASP:O	1:A:344:VAL:N	2.49	0.46
1:A:541:GLU:OE2	1:A:541:GLU:CA	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:LEU:HD21	4:D:55:LEU:HD12	1.98	0.46
4:D:75:LEU:O	4:D:76:TRP:C	2.54	0.46
1:M:143:SER:O	1:M:149:ILE:HD12	2.15	0.46
2:N:54:ARG:C	2:N:55:TRP:HD1	2.18	0.46
4:P:18:GLY:O	4:P:19:ALA:C	2.53	0.46
4:P:72:VAL:O	4:P:75:LEU:CB	2.64	0.46
1:A:133:PHE:CD2	1:A:134:HIS:N	2.84	0.46
2:B:121:ILE:O	2:B:186:HIS:HB2	2.15	0.46
1:M:142:THR:O	1:M:145:GLN:HB3	2.16	0.46
1:M:151:ARG:HB2	1:M:151:ARG:NH1	2.16	0.46
1:M:229:VAL:CB	1:M:467:ARG:NH2	2.78	0.46
1:M:363:THR:HB	1:M:368:GLU:N	2.31	0.46
1:M:399:LEU:HD11	6:M:803:FAD:C4'	2.45	0.46
1:M:449:ALA:O	1:M:452:ARG:HB2	2.15	0.46
2:N:37:LEU:HD23	2:N:38:ASP:N	2.29	0.46
3:O:27:LEU:O	3:O:28:ARG:C	2.52	0.46
4:P:49:LEU:HD22	10:P:800:MQ7:H2M3	1.98	0.46
1:A:38:VAL:O	1:A:38:VAL:HG22	2.14	0.46
1:A:425:ILE:O	1:A:426:GLU:C	2.53	0.46
4:D:84:HIS:C	4:D:86:MET:N	2.69	0.46
1:M:42:ARG:CZ	2:N:54:ARG:HE	2.28	0.46
1:M:133:PHE:CZ	2:N:149:ILE:HA	2.38	0.46
1:M:203:THR:OG1	6:M:803:FAD:HM83	2.16	0.46
2:N:37:LEU:CD2	2:N:37:LEU:N	2.79	0.46
1:A:399:LEU:HD13	6:A:703:FAD:O1P	2.15	0.45
2:B:9:GLU:OE2	2:B:23:SER:CB	2.62	0.45
2:B:50:ASP:O	2:B:100:ARG:NH2	2.49	0.45
3:C:21:PHE:O	3:C:21:PHE:CD2	2.67	0.45
3:C:86:TRP:CH2	4:D:21:GLY:HA3	2.51	0.45
1:M:11:GLY:HA3	1:M:191:ALA:O	2.16	0.45
1:M:11:GLY:HA2	6:M:803:FAD:H1B	1.98	0.45
1:M:106:ARG:HB2	1:M:107:PRO:HD2	1.98	0.45
1:M:330:PHE:HA	1:M:333:GLU:HB2	1.97	0.45
1:M:490:ARG:O	1:M:490:ARG:HG2	2.16	0.45
1:M:555:ARG:NE	1:M:560:THR:N	2.61	0.45
1:M:555:ARG:HE	1:M:560:THR:N	2.10	0.45
1:M:570:ILE:H	1:M:570:ILE:HD12	1.81	0.45
1:A:332:CYS:HA	1:A:343:PRO:HG2	1.97	0.45
1:A:515:ALA:O	1:A:516:GLU:C	2.55	0.45
3:C:15:TRP:CE3	3:C:16:TRP:HA	2.51	0.45
4:D:55:LEU:CG	4:D:59:GLN:NE2	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:13:GLY:C	1:M:15:ALA:N	2.67	0.45
1:M:170:LEU:O	1:M:182:GLN:HA	2.16	0.45
1:M:269:GLY:O	1:M:282:MET:HE3	2.15	0.45
1:M:428:GLN:O	1:M:432:VAL:HG23	2.16	0.45
1:M:476:ILE:HG21	1:M:520:HIS:CE1	2.51	0.45
2:N:75:LEU:N	2:N:75:LEU:HD22	2.30	0.45
3:O:49:LEU:O	3:O:49:LEU:CG	2.59	0.45
3:O:125:PHE:HZ	3:O:130:TRP:HZ3	1.63	0.45
4:P:30:VAL:CG1	4:P:31:MET:N	2.78	0.45
1:A:237:PRO:CB	1:A:308:ARG:HB3	2.46	0.45
1:A:326:GLU:HB3	1:A:327:ARG:HG3	1.99	0.45
4:D:28:ALA:N	4:D:29:PRO:CD	2.80	0.45
1:M:53:ALA:HA	1:M:125:TRP:HD1	1.78	0.45
1:M:113:VAL:CB	1:M:124:THR:O	2.53	0.45
1:M:174:ASN:HD22	1:M:177:GLU:CG	2.30	0.45
2:N:73:PRO:CG	2:N:213:VAL:HG11	2.43	0.45
2:N:206:PHE:O	2:N:206:PHE:HD2	1.98	0.45
4:P:94:PRO:O	4:P:96:GLY:N	2.49	0.45
1:A:97:GLU:OE2	1:A:98:LEU:HD23	2.17	0.45
1:A:520:HIS:O	1:A:521:SER:C	2.53	0.45
2:B:43:ILE:HG23	2:B:47:LEU:HD11	1.93	0.45
2:B:95:ASN:ND2	2:B:162:GLY:CA	2.79	0.45
3:C:30:GLY:C	3:C:32:ALA:H	2.19	0.45
3:C:112:LEU:HA	3:C:112:LEU:HD23	1.68	0.45
3:C:120:THR:CG2	4:D:30:VAL:HG23	2.45	0.45
4:D:34:LEU:HA	4:D:38:LEU:HB2	1.98	0.45
1:M:38:VAL:HG12	2:N:54:ARG:NH1	2.29	0.45
1:M:42:ARG:CZ	2:N:64:SER:CB	2.94	0.45
1:M:60:ASP:O	1:M:123:ARG:NH1	2.49	0.45
1:M:158:LEU:HB3	1:M:436:LEU:HD12	1.99	0.45
1:M:371:ILE:O	1:M:372:LYS:HB2	2.16	0.45
2:N:162:GLY:O	3:O:11:MET:CE	2.64	0.45
2:N:188:LYS:O	2:N:192:MET:HB2	2.15	0.45
2:N:231:SER:O	2:N:234:ASP:HB3	2.17	0.45
1:A:167:VAL:HG11	1:A:373:GLY:C	2.37	0.45
1:A:289:LYS:HD3	1:A:289:LYS:HA	1.62	0.45
2:B:135:THR:O	2:B:138:GLN:N	2.49	0.45
2:B:211:SER:CB	2:B:220:PRO:HD2	2.47	0.45
4:D:84:HIS:C	4:D:86:MET:H	2.18	0.45
1:M:44:HIS:CE1	1:M:204:ASN:ND2	2.85	0.45
1:M:55:VAL:HB	1:M:90:PRO:CG	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:192:THR:HG21	1:M:212:GLY:CA	2.46	0.45
1:M:346:GLU:HG3	1:M:347:PRO:N	2.30	0.45
1:M:356:TYR:HD2	1:M:357:THR:H	1.60	0.45
1:M:554:PHE:HD1	1:M:562:ARG:CZ	2.29	0.45
2:N:195:LEU:O	2:N:197:SER:N	2.50	0.45
1:A:273:PRO:HB2	1:A:276:GLU:H	1.80	0.45
1:A:405:LEU:O	1:A:409:GLN:HG2	2.16	0.45
1:A:515:ALA:C	1:A:517:CYS:N	2.66	0.45
5:A:702:FLC:CAC	6:A:703:FAD:C2	2.95	0.45
4:D:1:ILE:O	4:D:2:ASN:C	2.54	0.45
1:M:115:ARG:HH21	1:M:279:ASN:HB2	1.82	0.45
1:M:124:THR:HG22	1:M:125:TRP:H	1.80	0.45
1:M:334:LEU:HD23	1:M:338:TYR:CE1	2.52	0.45
1:A:151:ARG:HH11	1:A:151:ARG:HD2	1.50	0.45
1:A:514:VAL:H	1:A:514:VAL:HG23	1.46	0.45
1:M:41:MET:HE3	1:M:42:ARG:HG3	1.98	0.45
1:M:106:ARG:CB	1:M:112:ASN:HD22	2.30	0.45
1:M:223:LEU:HD12	1:M:360:GLY:O	2.17	0.45
1:M:260:TYR:CE2	1:M:262:TYR:HA	2.51	0.45
2:N:196:ASN:HA	2:N:201:VAL:HG11	1.97	0.45
3:O:30:GLY:C	3:O:32:ALA:N	2.70	0.45
3:O:127:ALA:O	3:O:128:LEU:HD23	2.17	0.45
1:A:94:THR:O	1:A:97:GLU:N	2.48	0.45
1:A:433:GLU:O	1:A:434:GLN:C	2.54	0.45
1:M:264:GLN:C	1:M:266:TYR:H	2.19	0.45
1:M:382:SER:O	1:M:383:VAL:C	2.55	0.45
1:M:542:ARG:NH2	1:M:544:ASP:OD1	2.49	0.45
2:N:196:ASN:HB3	2:N:231:SER:CB	2.47	0.45
3:O:126:VAL:HG11	10:P:800:MQ7:H141	1.99	0.45
3:C:49:LEU:HB2	3:C:56:TRP:CE3	2.51	0.45
4:D:13:PHE:CE1	4:D:101:TYR:CG	3.05	0.45
4:D:18:GLY:O	4:D:19:ALA:C	2.55	0.45
1:M:509:GLY:O	1:M:512:LEU:HD12	2.17	0.45
1:M:560:THR:HG22	1:M:561:THR:N	2.31	0.45
2:N:241:LYS:CB	2:N:242:PRO:HD3	2.45	0.45
3:O:33:VAL:O	3:O:36:VAL:HG22	2.16	0.45
3:O:50:LYS:NZ	4:P:117:THR:OG1	2.48	0.45
1:A:12:ALA:CB	1:A:34:LEU:HD21	2.46	0.45
1:A:36:SER:OG	1:A:37:LYS:N	2.47	0.45
1:A:50:GLY:N	6:A:703:FAD:O4	2.49	0.45
1:A:154:GLU:O	1:A:175:MET:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:GLU:OE2	2:B:25:PHE:CZ	2.70	0.45
3:C:62:PHE:CZ	3:C:68:ILE:CD1	3.00	0.45
1:M:242:LEU:HD12	5:M:802:FLC:OB1	2.17	0.45
2:N:36:LEU:N	2:N:76:ALA:O	2.42	0.45
2:B:155:TYR:CZ	2:B:169:GLY:HA3	2.52	0.44
2:B:175:LEU:HD12	2:B:175:LEU:HA	1.79	0.44
2:B:211:SER:OG	2:B:219:ASP:HA	2.17	0.44
3:C:30:GLY:C	3:C:32:ALA:N	2.70	0.44
1:M:60:ASP:HB2	1:M:123:ARG:NH2	2.31	0.44
1:M:91:THR:O	1:M:95:GLN:N	2.50	0.44
1:M:146:PHE:O	1:M:149:ILE:HG13	2.18	0.44
1:M:232:HIS:ND1	1:M:233:PRO:HD2	2.32	0.44
1:M:248:ARG:HG2	1:M:248:ARG:NH1	2.28	0.44
4:P:75:LEU:HD23	4:P:75:LEU:HA	1.80	0.44
1:A:49:GLN:HG2	1:A:129:ASP:O	2.17	0.44
1:A:319:LEU:O	1:A:320:GLY:O	2.35	0.44
1:A:437:LYS:HE3	1:A:441:ASN:OD1	2.18	0.44
2:B:8:ILE:HD12	2:B:28:VAL:HG21	1.99	0.44
4:D:73:LEU:HB2	4:D:74:PRO:CD	2.42	0.44
4:D:113:ILE:O	4:D:116:VAL:N	2.50	0.44
1:M:32:ILE:CG2	1:M:149:ILE:HA	2.47	0.44
1:M:74:ASP:O	1:M:529:ARG:NH2	2.51	0.44
2:N:31:ASP:N	2:N:34:THR:HG21	2.32	0.44
2:N:178:ARG:NH1	2:N:179:TYR:CE1	2.85	0.44
3:O:62:PHE:CE1	3:O:68:ILE:CG1	2.99	0.44
3:O:80:LEU:HD23	3:O:80:LEU:HA	1.87	0.44
1:A:413:ARG:HH11	1:A:413:ARG:HA	1.83	0.44
1:A:504:TYR:N	1:A:504:TYR:CD2	2.81	0.44
1:A:532:HIS:CD2	1:A:532:HIS:O	2.70	0.44
4:D:7:ARG:O	4:D:7:ARG:CG	2.65	0.44
1:M:78:GLU:CB	1:M:224:ARG:HH22	2.30	0.44
1:M:227:GLU:CG	1:M:463:CYS:SG	2.88	0.44
1:M:243:MET:CE	1:M:348:ILE:HG21	2.46	0.44
1:A:37:LYS:CG	1:A:38:VAL:HG13	2.47	0.44
1:A:115:ARG:NH1	1:A:115:ARG:CG	2.74	0.44
1:A:168:ARG:HD2	1:A:186:ASN:OD1	2.18	0.44
2:B:97:PRO:C	2:B:104:VAL:CG2	2.82	0.44
1:M:1:GLN:O	1:M:182:GLN:HG2	2.18	0.44
1:M:105:ARG:NH1	2:N:134:GLN:HB2	2.32	0.44
1:M:156:PHE:O	1:M:173:MET:N	2.50	0.44
1:M:160:ILE:HD12	1:M:170:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:248:ARG:HH11	1:M:248:ARG:CG	2.24	0.44
2:N:98:ILE:CD1	3:O:9:ARG:HE	2.30	0.44
2:N:173:ILE:HG23	2:N:195:LEU:HD21	1.99	0.44
3:O:19:LEU:HA	3:O:20:PRO:HD3	1.79	0.44
4:P:61:PHE:O	4:P:64:ARG:N	2.44	0.44
1:A:307:PRO:CD	1:A:308:ARG:H	2.26	0.44
2:B:151:CYS:SG	2:B:153:LEU:HG	2.58	0.44
3:C:50:LYS:CE	3:C:50:LYS:CA	2.86	0.44
2:N:153:LEU:HD12	2:N:215:PRO:HD3	2.00	0.44
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.81	0.44
1:A:89:CYS:O	1:A:93:MET:HG2	2.16	0.44
1:A:92:GLU:HG3	1:A:400:VAL:HG12	1.99	0.44
2:B:15:PRO:HB3	3:C:5:LYS:N	2.31	0.44
3:C:48:ALA:O	3:C:50:LYS:N	2.50	0.44
3:C:72:ASN:HD22	3:C:72:ASN:HA	1.59	0.44
3:C:90:ALA:N	3:C:91:PRO:CD	2.72	0.44
1:M:104:SER:OG	1:M:127:ALA:HA	2.17	0.44
1:M:253:ILE:HA	1:M:283:GLU:CD	2.38	0.44
1:M:467:ARG:CZ	1:M:533:GLN:H	2.31	0.44
4:P:27:ILE:O	4:P:27:ILE:CG2	2.65	0.44
4:P:40:PRO:HG2	4:P:41:LEU:H	1.83	0.44
4:P:82:MET:O	4:P:86:MET:HG2	2.18	0.44
1:A:232:HIS:HE1	5:A:702:FLC:HG2	1.83	0.44
1:A:356:TYR:HE1	6:A:703:FAD:O3'	1.99	0.44
1:A:450:LYS:HD3	1:A:450:LYS:HA	1.67	0.44
3:C:50:LYS:C	3:C:52:GLY:N	2.69	0.44
3:C:121:ILE:C	3:C:123:ILE:N	2.70	0.44
1:M:89:CYS:N	1:M:90:PRO:CD	2.81	0.44
1:M:191:ALA:CB	1:M:377:VAL:O	2.65	0.44
1:M:236:LEU:HD23	1:M:239:SER:OG	2.17	0.44
3:O:86:TRP:CH2	4:P:21:GLY:HA3	2.53	0.44
3:O:125:PHE:HD1	3:O:129:TYR:HB2	1.83	0.44
1:A:202:ASN:HB3	1:A:354:ALA:HB3	1.99	0.44
1:A:335:ALA:O	1:A:339:VAL:HG22	2.18	0.44
2:B:105:ASP:OD1	2:B:105:ASP:O	2.36	0.44
2:B:112:SER:O	2:B:113:LEU:C	2.54	0.44
3:C:9:ARG:HG2	3:C:9:ARG:NH1	2.31	0.44
1:M:162:VAL:O	1:M:163:ASP:HB2	2.17	0.44
1:M:250:GLU:OE2	1:M:327:ARG:HG3	2.17	0.44
1:M:261:ARG:NH2	1:M:283:GLU:OE1	2.51	0.44
2:N:36:LEU:O	2:N:39:ALA:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:51:LEU:HD12	2:N:51:LEU:O	2.18	0.44
2:N:120:ILE:HA	2:N:185:ASP:OD1	2.18	0.44
4:P:111:THR:O	4:P:115:VAL:HG23	2.17	0.44
1:A:390:ARG:CD	1:A:395:SER:HB2	2.46	0.44
1:A:391:LEU:HA	1:A:391:LEU:HD12	1.47	0.44
1:A:495:SER:OG	2:B:100:ARG:NH1	2.49	0.44
3:C:46:LEU:HD12	3:C:46:LEU:HA	1.75	0.44
3:C:105:PRO:HD2	3:C:106:GLU:H	1.83	0.44
4:D:2:ASN:HA	4:D:3:PRO:HD3	1.75	0.44
1:M:81:VAL:HG11	1:M:383:VAL:O	2.18	0.44
1:M:160:ILE:HD11	1:M:188:VAL:HG11	1.99	0.44
1:M:229:VAL:HG21	1:M:464:GLY:O	2.18	0.44
1:M:466:TYR:CD2	1:M:466:TYR:N	2.84	0.44
2:N:150:ASN:OD1	2:N:150:ASN:N	2.51	0.44
3:O:32:ALA:HB2	4:P:81:ARG:HD2	1.99	0.44
4:P:27:ILE:C	4:P:29:PRO:HD2	2.37	0.44
1:A:446:GLU:HB2	1:A:489:VAL:CA	2.48	0.43
3:C:89:LEU:C	3:C:91:PRO:HD2	2.37	0.43
1:M:162:VAL:HG22	1:M:219:HIS:NE2	2.33	0.43
1:M:199:TYR:HE1	1:M:459:MET:O	2.01	0.43
1:M:356:TYR:HE1	1:M:395:SER:OG	2.01	0.43
3:O:32:ALA:O	3:O:33:VAL:C	2.57	0.43
1:A:92:GLU:HG3	1:A:400:VAL:CG1	2.49	0.43
1:A:427:ALA:HA	1:A:430:ALA:CB	2.48	0.43
4:D:0:MET:CG	4:D:1:ILE:N	2.77	0.43
1:M:92:GLU:O	1:M:96:LEU:N	2.45	0.43
1:M:242:LEU:HD23	1:M:243:MET:N	2.33	0.43
3:O:105:PRO:CG	3:O:106:GLU:H	2.31	0.43
3:O:106:GLU:HB2	3:O:107:PRO:CD	2.48	0.43
1:A:97:GLU:OE1	1:A:105:ARG:NH2	2.52	0.43
1:A:562:ARG:NH1	1:A:562:ARG:CG	2.73	0.43
2:B:29:PRO:HG3	2:B:42:TYR:CE1	2.53	0.43
3:C:36:VAL:O	3:C:39:SER:N	2.52	0.43
1:M:232:HIS:NE2	1:M:242:LEU:HD12	2.34	0.43
1:M:295:TRP:CD1	1:M:296:HIS:N	2.86	0.43
1:M:346:GLU:CG	1:M:347:PRO:HD2	2.44	0.43
3:O:2:THR:HG22	3:O:4:ARG:N	2.04	0.43
1:A:27:ASN:HA	1:A:28:PRO:HD3	1.42	0.43
1:A:253:ILE:HG23	1:A:255:VAL:HG13	2.00	0.43
1:A:500:THR:HB	1:A:504:TYR:CE2	2.52	0.43
1:M:4:GLN:OE1	1:M:31:LYS:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:13:GLY:C	1:M:15:ALA:H	2.20	0.43
1:M:65:HIS:O	1:M:67:HIS:N	2.51	0.43
1:M:145:GLN:HA	2:N:119:TYR:CZ	2.53	0.43
1:M:171:VAL:HB	1:M:432:VAL:HG11	2.00	0.43
1:M:268:MET:O	1:M:269:GLY:C	2.56	0.43
1:M:467:ARG:NH2	1:M:531:ALA:O	2.52	0.43
1:M:554:PHE:O	1:M:555:ARG:CG	2.66	0.43
3:O:50:LYS:CE	4:P:117:THR:OG1	2.66	0.43
3:O:50:LYS:C	3:O:52:GLY:N	2.71	0.43
3:O:91:PRO:O	3:O:93:ALA:N	2.49	0.43
1:A:279:ASN:O	1:A:280:LYS:CB	2.65	0.43
2:B:126:THR:O	2:B:129:GLN:HB2	2.18	0.43
1:M:43:SER:OG	1:M:44:HIS:N	2.52	0.43
1:M:77:CYS:O	1:M:568:VAL:CG1	2.65	0.43
1:M:112:ASN:O	1:M:126:PHE:CE2	2.71	0.43
1:M:243:MET:HE3	1:M:331:ILE:HG23	2.00	0.43
1:M:452:ARG:NE	1:M:508:LEU:HD22	2.32	0.43
1:M:527:GLU:OE2	1:M:529:ARG:HG3	2.18	0.43
2:N:48:ALA:HA	2:N:49:PRO:HD3	1.78	0.43
2:N:100:ARG:O	2:N:102:LEU:N	2.52	0.43
2:N:160:GLN:HA	2:N:160:GLN:HE21	1.84	0.43
1:A:15:ALA:C	1:A:17:LEU:N	2.71	0.43
1:A:306:THR:CB	1:A:307:PRO:HD2	2.38	0.43
1:A:510:HIS:O	1:A:513:ASN:N	2.51	0.43
1:M:106:ARG:HD2	1:M:108:ASP:OD1	2.18	0.43
2:N:43:ILE:HG21	2:N:51:LEU:HD21	2.01	0.43
3:O:26:MET:O	3:O:29:GLU:HB2	2.18	0.43
3:O:32:ALA:HA	3:O:35:ALA:HB3	2.00	0.43
3:O:56:TRP:CD1	3:O:56:TRP:C	2.91	0.43
1:A:119:MET:HE2	1:A:391:LEU:HD23	2.00	0.43
1:A:227:GLU:OE1	1:A:525:ARG:NE	2.49	0.43
1:A:255:VAL:CG2	1:A:259:GLY:HA2	2.48	0.43
1:A:362:GLU:OE1	1:A:370:ARG:NE	2.52	0.43
2:B:4:LYS:HZ1	2:B:4:LYS:H	1.67	0.43
3:C:31:THR:CG2	3:C:82:HIS:HB2	2.42	0.43
4:D:96:GLY:O	4:D:97:LYS:C	2.55	0.43
1:M:52:SER:HB2	1:M:396:LEU:HD23	2.01	0.43
1:M:106:ARG:HB2	1:M:107:PRO:CD	2.48	0.43
1:M:253:ILE:HG22	1:M:255:VAL:HG13	2.00	0.43
4:P:4:ASN:HA	4:P:5:PRO:HD3	1.77	0.43
4:P:35:VAL:O	4:P:40:PRO:HD3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:O	1:A:428:GLN:NE2	2.52	0.43
1:A:194:GLY:O	1:A:208:VAL:HG12	2.19	0.43
2:B:26:TYR:CG	2:B:43:ILE:HD13	2.54	0.43
2:B:39:ALA:O	2:B:40:LEU:C	2.56	0.43
4:D:103:LEU:HD23	4:D:103:LEU:C	2.39	0.43
1:M:242:LEU:CD2	1:M:242:LEU:C	2.75	0.43
2:N:54:ARG:HH11	2:N:54:ARG:CG	2.19	0.43
2:N:117:LYS:C	2:N:119:TYR:H	2.22	0.43
3:O:89:LEU:C	3:O:91:PRO:HD2	2.38	0.43
1:A:483:GLN:CA	1:A:483:GLN:OE1	2.67	0.43
1:A:503:LEU:O	1:A:504:TYR:C	2.53	0.43
1:A:504:TYR:N	1:A:504:TYR:HD2	2.17	0.43
2:B:231:SER:O	2:B:234:ASP:HB3	2.19	0.43
3:C:124:LEU:CD2	4:D:34:LEU:HD21	2.41	0.43
1:M:60:ASP:OD1	1:M:60:ASP:N	2.52	0.43
1:M:113:VAL:HG23	1:M:123:ARG:HA	1.97	0.43
1:M:126:PHE:N	1:M:126:PHE:CD2	2.87	0.43
1:M:243:MET:HE1	1:M:348:ILE:HD13	2.00	0.43
2:N:167:PHE:HD1	2:N:199:ASN:C	2.22	0.43
2:N:232:SER:C	2:N:234:ASP:N	2.72	0.43
3:O:126:VAL:HG12	10:P:800:MQ7:H141	1.99	0.43
1:A:280:LYS:O	1:A:281:TYR:HD1	2.01	0.43
1:A:330:PHE:CZ	2:B:61:ILE:CG1	3.02	0.43
3:C:15:TRP:CE3	3:C:16:TRP:N	2.87	0.43
4:D:37:ILE:N	4:D:37:ILE:CD1	2.82	0.43
1:M:162:VAL:HG13	1:M:219:HIS:HE1	1.84	0.43
1:M:225:ASP:HB2	1:M:550:HIS:CG	2.54	0.43
1:M:446:GLU:CB	1:M:488:ARG:O	2.67	0.43
1:M:473:GLN:OE1	1:M:473:GLN:HA	2.19	0.43
2:N:28:VAL:HG12	2:N:29:PRO:CD	2.48	0.43
2:N:158:CYS:HB2	8:N:245:F3S:S4	2.58	0.43
2:N:239:THR:HG22	2:N:239:THR:O	2.17	0.43
4:P:81:ARG:HH11	4:P:81:ARG:HG3	1.83	0.43
1:A:37:LYS:C	1:A:38:VAL:CG1	2.86	0.42
1:A:211:ASP:HB3	6:A:703:FAD:N6A	2.30	0.42
1:A:211:ASP:O	1:A:215:MET:HG3	2.19	0.42
1:A:230:GLN:CD	1:A:287:ARG:HH21	2.22	0.42
2:B:164:ASN:C	2:B:164:ASN:OD1	2.57	0.42
3:C:116:THR:HA	4:D:26:ILE:HG23	2.01	0.42
1:M:129:ASP:OD1	1:M:129:ASP:O	2.37	0.42
1:M:189:VAL:CG1	1:M:377:VAL:HG23	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:452:ARG:CD	1:M:452:ARG:N	2.82	0.42
2:N:29:PRO:HD2	2:N:42:TYR:HB3	2.01	0.42
1:A:27:ASN:ND2	1:A:29:ASN:H	2.17	0.42
1:A:551:THR:HG23	1:A:565:TYR:CE2	2.53	0.42
2:B:193:ALA:O	4:D:5:PRO:HG2	2.19	0.42
1:M:474:LYS:HA	1:M:474:LYS:HD3	1.86	0.42
2:N:6:LEU:HD22	2:N:81:LEU:HD21	2.00	0.42
2:N:117:LYS:HD2	2:N:190:GLU:O	2.18	0.42
3:O:91:PRO:HA	3:O:108:ILE:HD12	2.01	0.42
4:P:28:ALA:N	4:P:29:PRO:CD	2.82	0.42
1:A:62:PHE:CD2	1:A:86:VAL:HG13	2.45	0.42
1:A:319:LEU:HD12	1:A:323:LYS:HE2	2.02	0.42
1:A:371:ILE:HG21	1:A:371:ILE:HD13	1.60	0.42
3:C:128:LEU:HA	3:C:128:LEU:HD23	1.77	0.42
1:M:124:THR:HG22	1:M:125:TRP:N	2.34	0.42
1:M:276:GLU:N	1:M:277:PRO:HD3	2.35	0.42
3:O:91:PRO:C	3:O:93:ALA:H	2.22	0.42
4:P:72:VAL:HG23	4:P:73:LEU:H	1.83	0.42
2:B:12:ARG:NH2	2:B:50:ASP:OD1	2.43	0.42
2:B:34:THR:HG22	2:B:81:LEU:HG	2.01	0.42
2:B:170:PRO:HA	2:B:224:ILE:HD11	2.00	0.42
3:C:108:ILE:O	3:C:109:ILE:C	2.56	0.42
4:D:4:ASN:C	4:D:4:ASN:HD22	2.22	0.42
4:D:19:ALA:O	4:D:20:GLY:C	2.58	0.42
4:D:31:MET:HE3	4:D:31:MET:HB3	1.81	0.42
1:M:17:LEU:HD21	1:M:139:LEU:HB2	2.00	0.42
1:M:243:MET:O	1:M:244:THR:O	2.38	0.42
2:N:105:ASP:C	2:N:107:THR:H	2.22	0.42
2:N:188:LYS:H	2:N:188:LYS:HG2	1.37	0.42
1:A:122:GLU:OE2	1:A:122:GLU:N	2.35	0.42
1:A:334:LEU:HD23	1:A:334:LEU:HA	1.93	0.42
1:A:392:GLY:O	1:A:393:SER:CB	2.64	0.42
1:A:478:LYS:O	1:A:481:GLU:HB3	2.19	0.42
2:B:68:MET:HE1	2:B:73:PRO:N	2.35	0.42
1:M:53:ALA:HA	1:M:125:TRP:CB	2.49	0.42
1:M:224:ARG:HA	1:M:551:THR:O	2.19	0.42
1:M:228:PHE:HE2	1:M:388:ALA:HA	1.80	0.42
1:M:266:TYR:CE2	1:M:296:HIS:CB	3.02	0.42
1:M:455:MET:HB2	1:M:482:LEU:CD2	2.49	0.42
2:N:133:ILE:O	2:N:133:ILE:CG2	2.66	0.42
2:N:193:ALA:HB1	4:P:5:PRO:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:27:LEU:O	3:O:29:GLU:N	2.52	0.42
3:O:30:GLY:C	3:O:32:ALA:H	2.22	0.42
1:A:437:LYS:HA	1:A:440:VAL:CG2	2.46	0.42
2:B:132:ASN:HD22	2:B:184:ARG:HD3	1.84	0.42
2:B:135:THR:O	2:B:136:PRO:C	2.57	0.42
2:B:135:THR:C	2:B:137:ALA:H	2.22	0.42
3:C:106:GLU:CG	3:C:107:PRO:HD3	2.50	0.42
1:M:45:THR:O	1:M:132:GLY:O	2.37	0.42
1:M:211:ASP:OD2	1:M:510:HIS:HB2	2.19	0.42
2:N:177:HIS:CA	2:N:180:ASN:HB2	2.46	0.42
4:P:85:ALA:O	4:P:89:LEU:HD12	2.20	0.42
4:P:95:ALA:O	4:P:99:VAL:HG23	2.20	0.42
1:A:34:LEU:HA	1:A:34:LEU:HD12	1.81	0.42
4:D:13:PHE:HB3	4:D:80:HIS:ND1	2.35	0.42
1:M:35:ILE:HG23	1:M:155:HIS:HB2	2.02	0.42
1:M:40:PRO:O	1:M:41:MET:C	2.57	0.42
1:M:329:PRO:O	1:M:333:GLU:N	2.47	0.42
1:M:377:VAL:HG21	1:M:406:ALA:HB1	2.01	0.42
1:M:389:ASN:O	1:M:391:LEU:N	2.53	0.42
1:M:555:ARG:NE	1:M:559:GLY:HA2	2.34	0.42
2:N:59:MET:O	2:N:59:MET:SD	2.77	0.42
4:P:80:HIS:HD2	4:P:84:HIS:CD2	2.32	0.42
4:P:81:ARG:HG3	4:P:81:ARG:NH1	2.35	0.42
1:A:48:ALA:HA	6:A:703:FAD:C5X	2.50	0.42
1:A:61:SER:OG	1:A:62:PHE:N	2.49	0.42
1:A:222:PRO:HB3	1:A:554:PHE:CE2	2.55	0.42
1:A:236:LEU:HA	1:A:237:PRO:HD3	1.89	0.42
1:A:543:ASP:OD1	1:A:546:ASN:N	2.41	0.42
3:C:21:PHE:CD2	3:C:21:PHE:C	2.93	0.42
4:D:117:THR:O	4:D:118:ILE:HG12	2.19	0.42
1:M:233:PRO:CG	1:M:234:THR:H	2.31	0.42
2:N:37:LEU:HD12	2:N:55:TRP:CB	2.50	0.42
2:N:57:CYS:SG	2:N:61:ILE:HG22	2.60	0.42
3:O:28:ARG:O	3:O:31:THR:CG2	2.68	0.42
3:O:67:VAL:O	3:O:69:VAL:N	2.53	0.42
4:P:13:PHE:HE2	4:P:97:LYS:HD3	1.85	0.42
1:A:1:GLN:O	1:A:181:VAL:HA	2.20	0.42
1:A:27:ASN:HD22	1:A:28:PRO:N	2.01	0.42
1:A:89:CYS:N	1:A:90:PRO:CD	2.83	0.42
1:A:330:PHE:O	1:A:331:ILE:C	2.58	0.42
1:A:369:THR:HG23	1:A:374:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:ARG:NH2	2:B:51:LEU:HA	2.35	0.42
2:B:80:PHE:CD1	2:B:82:ARG:NH2	2.88	0.42
2:B:109:PHE:CZ	2:B:113:LEU:HD21	2.55	0.42
3:C:27:LEU:O	3:C:30:GLY:N	2.53	0.42
4:D:37:ILE:O	4:D:40:PRO:HD2	2.20	0.42
1:M:372:LYS:O	1:M:413:ARG:HG2	2.20	0.42
3:O:27:LEU:C	3:O:29:GLU:N	2.71	0.42
4:P:28:ALA:O	4:P:32:ILE:HG13	2.20	0.42
1:A:261:ARG:NH1	1:A:283:GLU:OE1	2.51	0.42
1:A:554:PHE:HE1	1:A:564:GLU:HB2	1.85	0.42
4:D:83:HIS:HB3	4:D:84:HIS:H	1.59	0.42
4:D:98:TRP:O	4:D:102:GLY:N	2.52	0.42
1:M:11:GLY:HA2	6:M:803:FAD:C1B	2.50	0.42
1:M:73:GLY:C	1:M:388:ALA:H	2.24	0.42
1:M:129:ASP:HB2	1:M:328:LEU:CB	2.50	0.42
1:M:182:GLN:HE22	1:M:429:ALA:HB1	1.84	0.42
1:M:335:ALA:O	1:M:339:VAL:HB	2.20	0.42
1:A:320:GLY:O	1:A:321:GLU:C	2.58	0.41
1:A:413:ARG:HA	1:A:413:ARG:NH1	2.35	0.41
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.55	0.41
1:A:469:PRO:HA	1:A:523:MET:HE3	2.02	0.41
2:B:66:GLY:HA2	2:B:74:LYS:O	2.20	0.41
2:B:227:GLY:O	2:B:230:GLU:N	2.51	0.41
3:C:49:LEU:CD2	4:D:55:LEU:HD12	2.50	0.41
3:C:78:ALA:O	3:C:79:ALA:C	2.58	0.41
3:C:106:GLU:H	3:C:106:GLU:HG3	1.65	0.41
1:M:92:GLU:HA	1:M:95:GLN:CB	2.40	0.41
1:M:99:TRP:CZ3	1:M:142:THR:HG21	2.55	0.41
1:M:526:LYS:HE3	1:M:547:PHE:CE1	2.55	0.41
1:M:555:ARG:HD3	1:M:559:GLY:HA2	2.00	0.41
2:N:44:LYS:O	2:N:46:ASN:N	2.53	0.41
2:N:60:ALA:N	2:N:77:CYS:SG	2.87	0.41
2:N:224:ILE:H	2:N:224:ILE:HG13	1.74	0.41
4:P:73:LEU:HB2	4:P:74:PRO:HD3	2.02	0.41
1:A:70:VAL:CG1	1:A:573:LEU:HD23	2.49	0.41
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.82	0.41
1:A:173:MET:CE	1:A:173:MET:CG	2.95	0.41
1:A:211:ASP:HA	1:A:510:HIS:CD2	2.54	0.41
1:A:368:GLU:HG3	1:A:375:PHE:CE2	2.55	0.41
1:A:486:PHE:HA	1:A:489:VAL:HG12	2.01	0.41
1:A:532:HIS:CD2	1:A:532:HIS:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:PHE:CD1	3:C:129:TYR:CD2	3.08	0.41
4:D:61:PHE:C	4:D:63:GLY:H	2.22	0.41
4:D:73:LEU:O	4:D:74:PRO:C	2.55	0.41
4:D:76:TRP:O	4:D:77:CYS:C	2.58	0.41
1:M:135:MET:SD	1:M:396:LEU:HG	2.60	0.41
1:M:219:HIS:HB3	1:M:371:ILE:CD1	2.51	0.41
1:M:265:ASP:C	1:M:266:TYR:CD1	2.94	0.41
3:O:68:ILE:O	3:O:68:ILE:CG2	2.65	0.41
1:A:71:ALA:O	1:A:72:GLY:C	2.58	0.41
1:A:482:LEU:HA	1:A:482:LEU:HD23	1.57	0.41
3:C:40:ILE:O	3:C:41:GLU:C	2.58	0.41
4:D:1:ILE:O	4:D:2:ASN:O	2.38	0.41
1:M:74:ASP:O	1:M:529:ARG:NE	2.54	0.41
1:M:355:HIS:CD2	5:M:802:FLC:OHB	2.73	0.41
2:N:5:ASN:ND2	2:N:29:PRO:HA	2.35	0.41
2:N:175:LEU:HD12	2:N:178:ARG:HB3	2.02	0.41
2:N:214:CYS:SG	2:N:218:VAL:CG2	2.96	0.41
4:P:66:PHE:HD2	4:P:67:LEU:N	2.18	0.41
4:P:100:PHE:CD1	4:P:100:PHE:N	2.87	0.41
1:A:471:LEU:HA	1:A:471:LEU:HD23	1.64	0.41
2:B:168:ILE:HD13	2:B:168:ILE:HG21	1.84	0.41
4:D:101:TYR:HA	4:D:104:ALA:HB3	2.02	0.41
1:M:108:ASP:O	2:N:133:ILE:HG13	2.20	0.41
1:M:139:LEU:C	1:M:141:GLN:H	2.23	0.41
1:M:250:GLU:O	1:M:319:LEU:HD11	2.20	0.41
1:M:334:LEU:HD23	1:M:338:TYR:HE1	1.84	0.41
3:O:53:PRO:HD3	4:P:51:TYR:OH	2.20	0.41
1:A:20:ALA:HB1	1:A:149:ILE:HD13	2.02	0.41
1:A:55:VAL:HG21	1:A:62:PHE:CE2	2.55	0.41
1:A:194:GLY:C	1:A:208:VAL:HG12	2.41	0.41
4:D:59:GLN:HB2	4:D:59:GLN:HE21	1.63	0.41
1:M:42:ARG:HG2	2:N:62:CYS:O	2.20	0.41
1:M:127:ALA:N	1:M:131:THR:OG1	2.54	0.41
1:M:144:LEU:HD22	2:N:114:GLU:HG3	2.02	0.41
1:M:156:PHE:CG	1:M:503:LEU:HD22	2.55	0.41
1:M:199:TYR:CE1	1:M:459:MET:HB3	2.56	0.41
1:M:204:ASN:OD1	1:M:208:VAL:HB	2.21	0.41
1:M:228:PHE:HD1	1:M:228:PHE:HA	1.56	0.41
1:M:262:TYR:CB	1:M:297:GLU:OE2	2.68	0.41
1:M:334:LEU:O	1:M:338:TYR:N	2.46	0.41
1:M:396:LEU:HD13	6:M:803:FAD:C2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:556:ASP:HB3	1:M:557:ALA:H	1.65	0.41
2:N:53:TYR:N	2:N:53:TYR:CD1	2.87	0.41
3:O:28:ARG:NH2	3:O:89:LEU:HD11	2.35	0.41
1:A:335:ALA:HB1	1:A:341:VAL:O	2.20	0.41
2:B:110:ILE:H	2:B:110:ILE:HG12	1.54	0.41
4:D:94:PRO:HA	2:N:243:ARG:O	2.20	0.41
2:N:68:MET:HE1	2:N:73:PRO:HB3	2.00	0.41
2:N:158:CYS:SG	2:N:160:GLN:HB2	2.61	0.41
3:O:67:VAL:O	3:O:68:ILE:C	2.57	0.41
3:O:91:PRO:HB3	3:O:108:ILE:HD12	2.01	0.41
4:P:9:ASP:O	4:P:12:VAL:HG23	2.21	0.41
4:P:17:PHE:O	4:P:18:GLY:C	2.59	0.41
1:A:97:GLU:CD	2:B:131:THR:HB	2.41	0.41
1:A:177:GLU:OE2	1:A:177:GLU:CA	2.60	0.41
1:A:232:HIS:CE1	5:A:702:FLC:HG2	2.55	0.41
1:A:526:LYS:HZ2	1:A:534:ARG:HH12	1.69	0.41
1:A:527:GLU:CG	1:A:547:PHE:HB3	2.43	0.41
2:B:241:LYS:O	2:B:243:ARG:HG3	2.20	0.41
4:D:16:LEU:O	4:D:18:GLY:N	2.54	0.41
1:M:42:ARG:HG2	2:N:63:GLY:O	2.20	0.41
1:M:49:GLN:HE22	6:M:803:FAD:H6	1.85	0.41
2:N:34:THR:O	2:N:34:THR:HG23	2.20	0.41
3:O:60:VAL:HG12	3:O:60:VAL:O	2.21	0.41
4:P:41:LEU:HD23	4:P:41:LEU:HA	1.72	0.41
4:P:95:ALA:O	4:P:96:GLY:C	2.58	0.41
1:A:55:VAL:HG21	1:A:62:PHE:CD2	2.56	0.41
1:A:141:GLN:O	1:A:144:LEU:HB2	2.21	0.41
1:A:227:GLU:HB3	1:A:521:SER:CB	2.51	0.41
1:A:262:TYR:OH	1:A:312:VAL:HG11	2.21	0.41
1:A:355:HIS:NE2	5:A:702:FLC:OHB	2.54	0.41
1:A:445:GLY:H	1:A:490:ARG:HB3	1.86	0.41
1:A:502:LEU:O	1:A:503:LEU:C	2.56	0.41
2:B:40:LEU:HD23	2:B:40:LEU:HA	1.74	0.41
3:C:50:LYS:HD3	4:D:118:ILE:CG1	2.50	0.41
1:M:471:LEU:HD12	1:M:472:MET:H	1.76	0.41
1:M:526:LYS:HA	1:M:534:ARG:CD	2.51	0.41
2:N:36:LEU:CB	2:N:76:ALA:O	2.65	0.41
2:N:137:ALA:N	2:N:139:MET:SD	2.94	0.41
3:O:128:LEU:HB3	4:P:45:PRO:HG2	2.02	0.41
10:P:800:MQ7:H141	10:P:800:MQ7:H17	2.02	0.41
1:A:52:SER:HB3	1:A:93:MET:CE	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLY:O	1:A:74:ASP:CB	2.54	0.41
1:A:115:ARG:NH1	1:A:122:GLU:OE1	2.53	0.41
1:A:253:ILE:HG21	1:A:253:ILE:HD13	1.67	0.41
1:A:513:ASN:OD1	1:A:555:ARG:CZ	2.69	0.41
2:B:109:PHE:CE1	2:B:113:LEU:HD11	2.55	0.41
3:C:21:PHE:HD2	3:C:21:PHE:C	2.23	0.41
3:C:78:ALA:O	3:C:81:LEU:N	2.54	0.41
4:D:16:LEU:HA	4:D:16:LEU:HD23	1.69	0.41
1:M:5:ALA:O	1:M:185:ALA:CA	2.68	0.41
1:M:103:TRP:HZ3	1:M:131:THR:CG2	2.31	0.41
1:M:205:GLY:HA2	2:N:58:ARG:HD2	2.02	0.41
1:M:226:MET:O	1:M:227:GLU:C	2.59	0.41
1:M:228:PHE:CE2	1:M:388:ALA:CA	3.01	0.41
1:M:273:PRO:HG3	1:M:276:GLU:OE1	2.21	0.41
1:M:452:ARG:HD2	1:M:508:LEU:HD22	2.02	0.41
2:N:36:LEU:CB	2:N:76:ALA:HB1	2.49	0.41
2:N:37:LEU:HD22	2:N:77:CYS:CA	2.49	0.41
2:N:68:MET:HE2	2:N:73:PRO:HB3	2.00	0.41
2:N:123:ASN:OD1	2:N:124:SER:N	2.48	0.41
2:N:124:SER:O	2:N:125:ARG:C	2.59	0.41
2:N:142:TYR:O	2:N:143:HIS:C	2.59	0.41
2:N:160:GLN:HG3	2:N:203:SER:O	2.21	0.41
2:N:179:TYR:HA	2:N:182:ASP:HB2	2.03	0.41
3:O:121:ILE:O	3:O:124:LEU:N	2.54	0.41
4:P:13:PHE:CE2	4:P:97:LYS:HD3	2.56	0.41
4:P:95:ALA:O	4:P:98:TRP:N	2.49	0.41
1:A:79:GLN:HG3	1:A:569:LYS:O	2.21	0.41
1:A:452:ARG:NH2	2:B:45:ASP:OD2	2.50	0.41
2:B:68:MET:HE2	2:B:68:MET:HB3	1.93	0.41
1:M:89:CYS:N	1:M:90:PRO:HD2	2.36	0.41
1:M:190:MET:H	1:M:376:ALA:HA	1.86	0.41
1:M:456:GLY:O	1:M:457:LEU:C	2.58	0.41
2:N:240:LEU:N	2:N:240:LEU:CD2	2.78	0.41
1:A:171:VAL:HG11	1:A:432:VAL:HG11	2.03	0.40
1:A:312:VAL:HG22	1:A:350:VAL:O	2.21	0.40
3:C:9:ARG:HA	3:C:10:PRO:HD3	1.82	0.40
4:D:117:THR:C	4:D:118:ILE:HG12	2.41	0.40
1:M:1:GLN:O	1:M:182:GLN:CG	2.69	0.40
1:M:10:VAL:HG11	1:M:157:VAL:HG21	2.03	0.40
1:M:161:LEU:HB2	1:M:169:GLY:O	2.21	0.40
1:M:198:VAL:O	1:M:456:GLY:HA2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:263:LEU:HD21	1:M:290:VAL:HG13	2.03	0.40
1:M:433:GLU:HG3	1:M:434:GLN:HG3	2.03	0.40
1:M:497:VAL:O	1:M:498:PHE:C	2.59	0.40
1:M:516:GLU:OE1	1:M:516:GLU:CA	2.68	0.40
2:N:37:LEU:HD13	2:N:77:CYS:HB3	2.03	0.40
4:P:22:MET:O	4:P:26:ILE:HD13	2.21	0.40
4:P:39:LEU:HA	4:P:39:LEU:HD12	1.79	0.40
1:A:41:MET:HE3	2:B:150:ASN:HD22	1.85	0.40
1:A:341:VAL:O	1:A:343:PRO:HD3	2.21	0.40
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.57	0.40
3:C:9:ARG:HH11	3:C:9:ARG:CG	2.32	0.40
3:C:50:LYS:HZ3	4:D:118:ILE:CD1	2.11	0.40
4:D:112:LEU:O	4:D:116:VAL:HG22	2.21	0.40
1:M:32:ILE:CG1	1:M:33:ALA:N	2.83	0.40
1:M:100:GLY:HA2	2:N:184:ARG:HH21	1.85	0.40
1:M:225:ASP:CA	1:M:550:HIS:HB3	2.51	0.40
1:M:554:PHE:CD2	1:M:560:THR:HB	2.51	0.40
2:N:37:LEU:HD12	2:N:55:TRP:HB2	2.03	0.40
2:N:109:PHE:CE1	2:N:113:LEU:CD1	3.04	0.40
2:N:235:PHE:O	2:N:238:ALA:N	2.55	0.40
4:P:23:TRP:HE1	4:P:70:MET:HE3	1.85	0.40
4:P:93:VAL:HA	4:P:94:PRO:HD2	1.74	0.40
1:A:147:PRO:O	1:A:149:ILE:N	2.54	0.40
1:A:182:GLN:HE22	1:A:184:ARG:NH1	2.16	0.40
1:A:257:LYS:HA	1:A:304:ILE:HD11	2.03	0.40
1:A:262:TYR:CD1	1:A:263:LEU:HD23	2.57	0.40
1:A:319:LEU:CD1	1:A:323:LYS:HE3	2.52	0.40
2:B:219:ASP:OD2	3:C:92:LYS:HE2	2.22	0.40
1:M:144:LEU:HD22	2:N:114:GLU:HA	2.03	0.40
1:M:146:PHE:HA	1:M:147:PRO:HD2	1.82	0.40
1:M:226:MET:HB3	1:M:517:CYS:O	2.22	0.40
2:N:73:PRO:O	2:N:74:LYS:CG	2.68	0.40
3:O:46:LEU:HA	3:O:46:LEU:HD12	1.75	0.40
3:O:66:PRO:HG2	3:O:67:VAL:H	1.85	0.40
4:P:40:PRO:HG2	4:P:41:LEU:N	2.36	0.40
3:C:53:PRO:CA	4:D:51:TYR:CE1	3.04	0.40
3:C:65:ASN:OD1	3:C:66:PRO:CD	2.68	0.40
1:M:41:MET:HE2	1:M:42:ARG:HG3	2.03	0.40
1:M:89:CYS:HA	1:M:401:VAL:CG2	2.51	0.40
1:M:151:ARG:NH1	1:M:153:ASP:OD2	2.55	0.40
1:M:184:ARG:HG2	1:M:184:ARG:HH11	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:211:ASP:OD1	1:M:507:GLU:HA	2.22	0.40
1:M:214:GLY:HA3	1:M:510:HIS:ND1	2.36	0.40
1:M:229:VAL:O	1:M:531:ALA:HB1	2.20	0.40
1:M:263:LEU:CD1	1:M:283:GLU:CA	2.99	0.40
2:N:73:PRO:C	2:N:74:LYS:HG3	2.40	0.40
3:O:105:PRO:HG2	3:O:106:GLU:H	1.86	0.40
4:P:111:THR:O	4:P:115:VAL:CG2	2.69	0.40
1:A:70:VAL:O	1:A:71:ALA:C	2.58	0.40
2:B:54:ARG:CD	2:B:103:VAL:HG13	2.51	0.40
2:B:68:MET:HG2	2:B:93:LEU:HA	2.03	0.40
3:C:53:PRO:N	4:D:51:TYR:CE1	2.89	0.40
1:M:114:ARG:HB2	1:M:114:ARG:HH11	1.85	0.40
1:M:175:MET:O	1:M:498:PHE:HA	2.20	0.40
1:M:229:VAL:HG13	1:M:230:GLN:N	2.37	0.40
2:N:1:ALA:O	2:N:2:GLU:C	2.60	0.40
2:N:80:PHE:CB	2:N:82:ARG:HG2	2.51	0.40
2:N:108:HIS:NE2	2:N:112:SER:OG	2.54	0.40
2:N:232:SER:O	2:N:235:PHE:HB2	2.21	0.40
3:O:127:ALA:C	3:O:128:LEU:HD23	2.42	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	575/602 (96%)	492 (86%)	69 (12%)	14 (2%)	6	28
1	M	570/602 (95%)	402 (70%)	103 (18%)	65 (11%)	0	2
2	B	241/243 (99%)	207 (86%)	30 (12%)	4 (2%)	9	35
2	N	241/243 (99%)	126 (52%)	79 (33%)	36 (15%)	0	1
3	C	128/130 (98%)	99 (77%)	25 (20%)	4 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	128/130 (98%)	103 (80%)	18 (14%)	7 (6%)	2	11
4	D	117/119 (98%)	68 (58%)	35 (30%)	14 (12%)	0	2
4	P	117/119 (98%)	76 (65%)	26 (22%)	15 (13%)	0	1
All	All	2117/2188 (97%)	1573 (74%)	385 (18%)	159 (8%)	1	7

All (159) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLY
1	A	270	PRO
1	A	321	GLU
2	B	242	PRO
3	C	31	THR
4	D	61	PHE
1	M	25	GLN
1	M	29	ASN
1	M	47	ALA
1	M	58	ASP
1	M	62	PHE
1	M	111	VAL
1	M	219	HIS
1	M	226	MET
1	M	227	GLU
1	M	244	THR
1	M	282	MET
1	M	284	LEU
1	M	394	ASN
1	M	464	GLY
1	M	530	GLY
2	N	19	THR
2	N	65	CYS
2	N	76	ALA
2	N	121	ILE
2	N	135	THR
2	N	150	ASN
2	N	189	LYS
2	N	190	GLU
2	N	219	ASP
3	O	18	LYS
3	O	31	THR
3	O	92	LYS

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Mol	Chain	Res	Type
4	P	10	GLU
4	P	34	LEU
4	P	61	PHE
4	P	99	VAL
1	A	287	ARG
1	A	343	PRO
1	A	389	ASN
2	B	32	ALA
4	D	2	ASN
4	D	17	PHE
4	D	88	ASP
1	M	40	PRO
1	M	49	GLN
1	M	50	GLY
1	M	74	ASP
1	M	79	GLN
1	M	122	GLU
1	M	127	ALA
1	M	166	HIS
1	M	175	MET
1	M	188	VAL
1	M	217	LEU
1	M	230	GLN
1	M	238	GLY
1	M	277	PRO
1	M	287	ARG
1	M	293	ALA
1	M	387	GLY
1	M	390	ARG
1	M	395	SER
1	M	498	PHE
1	M	555	ARG
2	N	2	GLU
2	N	57	CYS
2	N	61	ILE
2	N	141	LYS
2	N	155	TYR
2	N	186	HIS
2	N	187	GLY
2	N	197	SER
2	N	201	VAL
2	N	218	VAL

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Mol	Chain	Res	Type
2	N	236	LEU
4	P	20	GLY
4	P	43	LEU
4	P	46	GLY
4	P	114	GLY
1	A	282	MET
4	D	20	GLY
4	D	24	SER
4	D	51	TYR
4	D	99	VAL
1	M	63	GLU
1	M	66	PHE
1	M	107	PRO
1	M	174	ASN
1	M	269	GLY
1	M	446	GLU
2	N	15	PRO
2	N	53	TYR
2	N	60	ALA
2	N	101	ASP
2	N	115	ALA
2	N	128	ASP
2	N	137	ALA
2	N	196	ASN
4	P	95	ALA
1	A	271	GLU
1	A	329	PRO
1	A	347	PRO
3	C	49	LEU
4	D	16	LEU
1	M	26	ALA
1	M	59	HIS
1	M	77	CYS
1	M	200	ARG
1	M	262	TYR
1	M	317	ARG
1	M	343	PRO
1	M	460	GLU
2	N	47	LEU
4	P	1	ILE
1	A	320	GLY
1	A	530	GLY

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Mol	Chain	Res	Type
1	A	575	PRO
2	B	170	PRO
2	B	183	SER
4	D	5	PRO
4	D	85	ALA
1	M	43	SER
1	M	65	HIS
1	M	148	GLN
1	M	233	PRO
1	M	286	PRO
1	M	456	GLY
1	M	461	GLU
2	N	45	ASP
4	P	100	PHE
4	P	113	ILE
3	C	53	PRO
4	D	113	ILE
1	M	271	GLU
1	M	276	GLU
1	M	373	GLY
2	N	195	LEU
2	N	220	PRO
3	O	49	LEU
4	P	83	HIS
1	M	208	VAL
3	O	53	PRO
4	P	2	ASN
1	A	107	PRO
3	C	67	VAL
4	D	114	GLY
1	M	509	GLY
4	P	21	GLY
4	D	72	VAL
2	N	136	PRO
2	N	162	GLY
3	O	122	VAL
1	M	383	VAL
2	N	49	PRO
1	M	100	GLY
1	M	121	ILE
2	N	149	ILE
3	O	106	GLU

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	460/475 (97%)	349 (76%)	111 (24%)	0	2
1	M	456/475 (96%)	406 (89%)	50 (11%)	6	24
2	B	205/205 (100%)	171 (83%)	34 (17%)	2	10
2	N	205/205 (100%)	175 (85%)	30 (15%)	3	14
3	C	111/111 (100%)	89 (80%)	22 (20%)	1	5
3	O	111/111 (100%)	81 (73%)	30 (27%)	0	1
4	D	97/97 (100%)	79 (81%)	18 (19%)	1	7
4	P	97/97 (100%)	75 (77%)	22 (23%)	1	3
All	All	1742/1776 (98%)	1425 (82%)	317 (18%)	1	7

All (317) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	6	ASP
1	A	7	LEU
1	A	17	LEU
1	A	18	ARG
1	A	25	GLN
1	A	27	ASN
1	A	28	PRO
1	A	29	ASN
1	A	31	LYS
1	A	36	SER
1	A	41	MET
1	A	42	ARG
1	A	49	GLN
1	A	58	ASP
1	A	63	GLU
1	A	76	LEU
1	A	77	CYS
1	A	79	GLN

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Mol	Chain	Res	Type
1	A	86	VAL
1	A	90	PRO
1	A	91	THR
1	A	92	GLU
1	A	96	LEU
1	A	104	SER
1	A	107	PRO
1	A	112	ASN
1	A	115	ARG
1	A	116	PHE
1	A	119	MET
1	A	122	GLU
1	A	123	ARG
1	A	133	PHE
1	A	138	THR
1	A	150	GLN
1	A	168	ARG
1	A	170	LEU
1	A	175	MET
1	A	180	LEU
1	A	181	VAL
1	A	184	ARG
1	A	197	ARG
1	A	217	LEU
1	A	218	SER
1	A	222	PRO
1	A	223	LEU
1	A	224	ARG
1	A	230	GLN
1	A	241	ILE
1	A	253	ILE
1	A	257	LYS
1	A	258	ASN
1	A	260	TYR
1	A	261	ARG
1	A	263	LEU
1	A	265	ASP
1	A	278	LYS
1	A	280	LYS
1	A	287	ARG
1	A	288	ASP
1	A	289	LYS

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Mol	Chain	Res	Type
1	A	299	ARG
1	A	310	ASP
1	A	314	LEU
1	A	317	ARG
1	A	319	LEU
1	A	321	GLU
1	A	322	LYS
1	A	325	HIS
1	A	327	ARG
1	A	328	LEU
1	A	332	CYS
1	A	336	LYS
1	A	344	VAL
1	A	358	MET
1	A	372	LYS
1	A	391	LEU
1	A	404	ARG
1	A	412	GLU
1	A	413	ARG
1	A	416	THR
1	A	422	GLU
1	A	438	ASP
1	A	440	VAL
1	A	441	ASN
1	A	442	GLN
1	A	450	LYS
1	A	465	ILE
1	A	466	TYR
1	A	476	ILE
1	A	487	LYS
1	A	489	VAL
1	A	490	ARG
1	A	508	LEU
1	A	512	LEU
1	A	518	MET
1	A	523	MET
1	A	527	GLU
1	A	529	ARG
1	A	532	HIS
1	A	534	ARG
1	A	536	ASP
1	A	537	GLU

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Mol	Chain	Res	Type
1	A	539	CYS
1	A	541	GLU
1	A	542	ARG
1	A	543	ASP
1	A	546	ASN
1	A	558	ASP
1	A	560	THR
1	A	562	ARG
2	B	4	LYS
2	B	5	ASN
2	B	12	ARG
2	B	38	ASP
2	B	45	ASP
2	B	46	ASN
2	B	47	LEU
2	B	50	ASP
2	B	52	SER
2	B	61	ILE
2	B	68	MET
2	B	78	LYS
2	B	86	ASP
2	B	93	LEU
2	B	105	ASP
2	B	106	MET
2	B	107	THR
2	B	110	ILE
2	B	117	LYS
2	B	124	SER
2	B	125	ARG
2	B	128	ASP
2	B	132	ASN
2	B	141	LYS
2	B	178	ARG
2	B	183	SER
2	B	184	ARG
2	B	190	GLU
2	B	197	SER
2	B	203	SER
2	B	206	PHE
2	B	212	GLU
2	B	237	ILE
2	B	241	LYS

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Mol	Chain	Res	Type
3	C	1	THR
3	C	9	ARG
3	C	11	MET
3	C	12	THR
3	C	19	LEU
3	C	21	PHE
3	C	31	THR
3	C	36	VAL
3	C	37	TRP
3	C	39	SER
3	C	42	LEU
3	C	50	LYS
3	C	54	GLU
3	C	64	GLN
3	C	70	ILE
3	C	72	ASN
3	C	74	ILE
3	C	100	ASP
3	C	103	MET
3	C	106	GLU
3	C	111	SER
3	C	116	THR
4	D	1	ILE
4	D	4	ASN
4	D	7	ARG
4	D	12	VAL
4	D	30	VAL
4	D	31	MET
4	D	39	LEU
4	D	43	LEU
4	D	47	ASP
4	D	50	SER
4	D	59	GLN
4	D	75	LEU
4	D	82	MET
4	D	83	HIS
4	D	86	MET
4	D	115	VAL
4	D	117	THR
4	D	118	ILE
1	M	6	ASP
1	M	18	ARG

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Mol	Chain	Res	Type
1	M	49	GLN
1	M	52	SER
1	M	57	GLN
1	M	76	LEU
1	M	90	PRO
1	M	97	GLU
1	M	105	ARG
1	M	116	PHE
1	M	122	GLU
1	M	126	PHE
1	M	146	PHE
1	M	151	ARG
1	M	152	PHE
1	M	160	ILE
1	M	192	THR
1	M	200	ARG
1	M	207	ILE
1	M	219	HIS
1	M	223	LEU
1	M	226	MET
1	M	227	GLU
1	M	228	PHE
1	M	229	VAL
1	M	231	TYR
1	M	248	ARG
1	M	254	LEU
1	M	262	TYR
1	M	277	PRO
1	M	279	ASN
1	M	287	ARG
1	M	295	TRP
1	M	328	LEU
1	M	330	PHE
1	M	332	CYS
1	M	343	PRO
1	M	351	ARG
1	M	356	TYR
1	M	386	HIS
1	M	398	GLU
1	M	463	CYS
1	M	490	ARG
1	M	499	ASN

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Mol	Chain	Res	Type
1	M	505	THR
1	M	526	LYS
1	M	549	LYS
1	M	556	ASP
1	M	567	ASP
1	M	570	ILE
2	N	25	PHE
2	N	27	GLU
2	N	36	LEU
2	N	37	LEU
2	N	43	ILE
2	N	51	LEU
2	N	53	TYR
2	N	54	ARG
2	N	55	TRP
2	N	57	CYS
2	N	58	ARG
2	N	69	VAL
2	N	75	LEU
2	N	133	ILE
2	N	139	MET
2	N	144	GLN
2	N	150	ASN
2	N	153	LEU
2	N	158	CYS
2	N	178	ARG
2	N	183	SER
2	N	186	HIS
2	N	188	LYS
2	N	192	MET
2	N	196	ASN
2	N	206	PHE
2	N	213	VAL
2	N	216	LYS
2	N	235	PHE
2	N	240	LEU
3	O	1	THR
3	O	4	ARG
3	O	9	ARG
3	O	11	MET
3	O	12	THR
3	O	17	LYS

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Mol	Chain	Res	Type
3	O	19	LEU
3	O	31	THR
3	O	37	TRP
3	O	39	SER
3	O	42	LEU
3	O	47	PHE
3	O	54	GLU
3	O	61	ASP
3	O	68	ILE
3	O	70	ILE
3	O	72	ASN
3	O	85	THR
3	O	92	LYS
3	O	96	ILE
3	O	98	VAL
3	O	99	LYS
3	O	100	ASP
3	O	102	LYS
3	O	103	MET
3	O	110	LYS
3	O	111	SER
3	O	117	VAL
3	O	123	ILE
3	O	130	TRP
4	P	4	ASN
4	P	6	LYS
4	P	7	ARG
4	P	12	VAL
4	P	16	LEU
4	P	23	TRP
4	P	43	LEU
4	P	52	GLU
4	P	53	ARG
4	P	65	VAL
4	P	66	PHE
4	P	75	LEU
4	P	82	MET
4	P	87	HIS
4	P	89	LEU
4	P	93	VAL
4	P	97	LYS
4	P	103	LEU

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Mol	Chain	Res	Type
4	P	112	LEU
4	P	115	VAL
4	P	116	VAL
4	P	117	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	27	ASN
1	A	57	GLN
1	A	95	GLN
1	A	182	GLN
1	A	204	ASN
1	A	219	HIS
1	A	232	HIS
1	A	279	ASN
1	A	318	HIS
1	A	366	ASN
1	A	409	GLN
1	A	421	ASN
1	A	434	GLN
1	A	499	ASN
1	A	510	HIS
1	A	532	HIS
2	B	95	ASN
2	B	123	ASN
2	B	144	GLN
2	B	150	ASN
2	B	160	GLN
2	B	180	ASN
2	B	194	GLN
2	B	199	ASN
3	C	72	ASN
4	D	4	ASN
4	D	59	GLN
1	M	44	HIS
1	M	49	GLN
1	M	65	HIS
1	M	79	GLN
1	M	112	ASN
1	M	137	HIS

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Mol	Chain	Res	Type
1	M	166	HIS
1	M	174	ASN
1	M	182	GLN
1	M	230	GLN
1	M	279	ASN
1	M	302	ASN
1	M	355	HIS
1	M	394	ASN
1	M	442	GLN
1	M	520	HIS
1	M	532	HIS
1	M	533	GLN
1	M	550	HIS
2	N	5	ASN
2	N	138	GLN
2	N	144	GLN
2	N	160	GLN
2	N	196	ASN
2	N	226	GLN
3	O	64	GLN
3	O	65	ASN
3	O	72	ASN
3	O	82	HIS
3	O	95	ASN
4	P	4	ASN
4	P	59	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	FAD	A	703	-	51,57,58	3.82	26 (50%)	59,87,89	1.95	10 (16%)
8	F3S	B	245	2	0,9,9	-	-	-	-	-
10	MQ7	D	700	-	34,34,49	3.40	15 (44%)	42,45,63	2.34	14 (33%)
10	MQ7	P	800	-	34,34,49	3.42	16 (47%)	42,45,63	2.54	13 (30%)
9	SF4	N	246	2	0,12,12	-	-	-	-	-
9	SF4	B	246	2	0,12,12	-	-	-	-	-
6	FAD	M	803	-	51,57,58	3.98	22 (43%)	59,87,89	1.86	9 (15%)
7	FES	N	244	2	0,4,4	-	-	-	-	-
7	FES	B	244	2	0,4,4	-	-	-	-	-
5	FLC	M	802	-	3,12,12	4.90	2 (66%)	3,17,17	5.77	2 (66%)
5	FLC	A	702	-	3,12,12	3.30	2 (66%)	3,17,17	8.57	2 (66%)
8	F3S	N	245	2	0,9,9	-	-	-	-	-

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
6	FAD	A	703	-	-	9/30/46/50	0/6/6/6
10	MQ7	D	700	-	-	7/23/43/61	0/2/2/2
8	F3S	B	245	2	-	-	0/3/3/3
9	SF4	N	246	2	-	-	0/6/5/5
9	SF4	B	246	2	-	-	0/6/5/5
6	FAD	M	803	-	-	7/30/46/50	0/6/6/6
7	FES	N	244	2	-	-	0/1/1/1
7	FES	B	244	2	-	-	0/1/1/1
8	F3S	N	245	2	-	-	0/3/3/3
5	FLC	M	802	-	-	3/6/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FLC	A	702	-	-	1/6/16/16	-
10	MQ7	P	800	-	-	9/23/43/61	0/2/2/2

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	FAD	C4X-N5	10.47	1.48	1.33
6	M	803	FAD	C10-N1	9.73	1.45	1.33
6	M	803	FAD	C4X-C10	9.71	1.48	1.38
6	M	803	FAD	C4X-N5	9.68	1.47	1.33
6	M	803	FAD	C9A-N10	9.52	1.51	1.38
6	A	703	FAD	C9A-N10	9.17	1.50	1.38
6	A	703	FAD	C10-N1	8.88	1.44	1.33
10	P	800	MQ7	C12-C13	8.84	1.54	1.33
6	M	803	FAD	C1'-N10	8.81	1.57	1.48
10	D	700	MQ7	C12-C13	8.76	1.54	1.33
6	A	703	FAD	C4X-C10	7.69	1.46	1.38
10	P	800	MQ7	C17-C18	7.35	1.50	1.33
6	M	803	FAD	C2A-N3A	7.07	1.43	1.32
6	A	703	FAD	C4A-N3A	7.07	1.45	1.35
6	M	803	FAD	C4A-N3A	7.05	1.45	1.35
10	D	700	MQ7	C17-C18	7.01	1.49	1.33
6	M	803	FAD	C4-N3	6.68	1.44	1.33
6	A	703	FAD	C4-N3	6.49	1.44	1.33
10	P	800	MQ7	C22-C23	6.39	1.48	1.33
10	D	700	MQ7	C22-C23	6.34	1.48	1.33
6	A	703	FAD	C1'-N10	5.97	1.54	1.48
5	M	802	FLC	CG-CB	5.94	1.63	1.54
10	P	800	MQ7	C27-C28	5.88	1.49	1.32
5	M	802	FLC	CA-CB	5.88	1.63	1.54
10	D	700	MQ7	C27-C28	5.66	1.48	1.32
6	A	703	FAD	C2A-N3A	5.50	1.41	1.32
6	A	703	FAD	C8-C7	5.24	1.54	1.40
10	D	700	MQ7	C9-C10	5.08	1.48	1.39
6	M	803	FAD	C9A-C5X	4.89	1.52	1.42
10	P	800	MQ7	C9-C10	4.88	1.47	1.39
6	M	803	FAD	C6-C7	4.79	1.49	1.37
6	M	803	FAD	C8-C7	4.71	1.52	1.40
10	D	700	MQ7	C11-C12	-4.65	1.43	1.50
10	D	700	MQ7	C7-C6	4.57	1.48	1.38
10	P	800	MQ7	C7-C6	4.54	1.48	1.38
6	A	703	FAD	C5X-N5	4.51	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	FAD	C6-C7	4.46	1.49	1.37
10	P	800	MQ7	C2-C1	4.36	1.57	1.48
10	P	800	MQ7	C8-C7	4.30	1.49	1.38
6	A	703	FAD	C9-C9A	4.23	1.49	1.40
10	D	700	MQ7	C8-C7	4.23	1.49	1.38
10	D	700	MQ7	C5-C4	4.19	1.56	1.48
5	A	702	FLC	CA-CB	4.17	1.60	1.54
6	M	803	FAD	C4-C4X	4.15	1.48	1.41
10	D	700	MQ7	C2-C1	4.12	1.56	1.48
6	M	803	FAD	C9-C8	4.12	1.48	1.37
6	A	703	FAD	C7M-C7	-4.03	1.43	1.51
6	A	703	FAD	C9A-C5X	4.00	1.50	1.42
6	A	703	FAD	C4-C4X	3.92	1.48	1.41
6	M	803	FAD	C9-C9A	3.89	1.48	1.40
10	P	800	MQ7	C11-C12	-3.88	1.45	1.50
6	A	703	FAD	C2B-C3B	-3.83	1.42	1.52
6	A	703	FAD	C9-C8	3.80	1.47	1.37
5	A	702	FLC	CG-CB	3.63	1.60	1.54
6	M	803	FAD	C7M-C7	-3.63	1.43	1.51
10	P	800	MQ7	C3-C4	3.60	1.56	1.47
6	A	703	FAD	C4'-C3'	-3.59	1.46	1.53
10	P	800	MQ7	C5-C4	3.59	1.55	1.48
6	A	703	FAD	C5A-C4A	-3.45	1.31	1.40
6	M	803	FAD	C5X-N5	3.12	1.40	1.35
10	P	800	MQ7	C8-C9	3.10	1.45	1.38
10	D	700	MQ7	C3-C4	3.09	1.54	1.47
10	D	700	MQ7	C8-C9	3.09	1.45	1.38
6	M	803	FAD	C5A-C4A	-3.04	1.32	1.40
6	M	803	FAD	C5'-C4'	3.02	1.56	1.51
10	P	800	MQ7	C6-C5	2.97	1.44	1.39
6	M	803	FAD	C6-C5X	2.94	1.46	1.41
10	D	700	MQ7	C6-C5	2.92	1.44	1.39
10	P	800	MQ7	C15-C13	2.81	1.57	1.51
6	A	703	FAD	C2'-C3'	-2.75	1.48	1.53
6	A	703	FAD	C6-C5X	2.65	1.46	1.41
6	M	803	FAD	C2B-C3B	-2.62	1.45	1.52
10	D	700	MQ7	O4-C4	2.55	1.28	1.23
6	A	703	FAD	P-O5'	-2.50	1.49	1.59
6	M	803	FAD	C8A-N7A	-2.44	1.30	1.34
6	A	703	FAD	C8A-N7A	-2.37	1.30	1.34
6	A	703	FAD	O4-C4	-2.18	1.19	1.24
10	P	800	MQ7	C19-C18	2.14	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	700	MQ7	C19-C18	2.11	1.56	1.50
6	M	803	FAD	C2A-N1A	2.05	1.37	1.33
6	A	703	FAD	C3B-C4B	2.04	1.58	1.53
6	A	703	FAD	O2'-C2'	-2.03	1.39	1.43
10	P	800	MQ7	O4-C4	2.02	1.27	1.23

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	702	FLC	CB-CA-CAC	14.66	138.46	114.98
10	P	800	MQ7	C16-C15-C13	9.16	143.11	112.98
5	M	802	FLC	CB-CA-CAC	8.36	128.37	114.98
10	D	700	MQ7	C12-C11-C3	6.94	130.77	112.05
10	D	700	MQ7	C16-C15-C13	6.82	135.43	112.98
6	M	803	FAD	C4-N3-C2	6.66	120.76	115.14
6	A	703	FAD	C4-C4X-C10	-6.33	115.76	119.95
6	M	803	FAD	C4X-N5-C5X	6.32	123.09	116.77
6	A	703	FAD	C4-N3-C2	6.26	120.43	115.14
6	A	703	FAD	C4X-N5-C5X	6.25	123.02	116.77
6	M	803	FAD	C4-C4X-C10	-5.67	116.20	119.95
10	P	800	MQ7	C12-C11-C3	5.65	127.28	112.05
5	M	802	FLC	CB-CG-CGC	5.36	123.56	114.98
10	D	700	MQ7	C11-C3-C4	-5.11	113.03	118.50
6	A	703	FAD	C4-C4X-N5	4.57	123.82	118.60
10	P	800	MQ7	C11-C3-C4	-4.49	113.70	118.50
10	P	800	MQ7	C14-C13-C15	4.04	122.07	115.27
10	P	800	MQ7	C21-C20-C18	-3.82	100.40	112.98
6	M	803	FAD	C4-C4X-N5	3.77	122.90	118.60
10	P	800	MQ7	C11-C12-C13	3.70	132.96	126.79
10	D	700	MQ7	C21-C20-C18	-3.52	101.39	112.98
10	P	800	MQ7	O1-C1-C10	-3.41	116.04	121.56
6	M	803	FAD	N3A-C2A-N1A	-3.20	123.67	128.68
6	A	703	FAD	N3A-C2A-N1A	-3.17	123.72	128.68
10	D	700	MQ7	O1-C1-C10	-3.16	116.44	121.56
6	M	803	FAD	C4X-C10-N10	-2.88	117.34	120.30
6	A	703	FAD	C4X-C10-N10	-2.78	117.45	120.30
10	D	700	MQ7	C26-C25-C23	2.72	121.93	112.98
10	P	800	MQ7	C26-C25-C23	2.71	121.88	112.98
6	A	703	FAD	O3'-C3'-C2'	-2.70	102.30	108.81
10	P	800	MQ7	C5-C10-C1	-2.69	117.77	120.68
10	D	700	MQ7	C25-C23-C22	-2.67	115.72	121.12
10	P	800	MQ7	C25-C23-C22	-2.60	115.86	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	700	MQ7	C5-C10-C1	-2.57	117.89	120.68
6	M	803	FAD	C1'-N10-C9A	2.49	120.25	118.29
10	D	700	MQ7	C19-C18-C20	2.45	119.39	115.27
6	A	703	FAD	O4'-C4'-C5'	-2.44	104.43	109.92
10	D	700	MQ7	C14-C13-C15	2.43	119.36	115.27
6	M	803	FAD	O4'-C4'-C5'	-2.40	104.52	109.92
10	P	800	MQ7	C24-C23-C25	2.34	119.21	115.27
10	D	700	MQ7	C20-C18-C17	-2.33	116.40	121.12
10	D	700	MQ7	C2M-C2-C1	-2.29	112.47	116.27
5	A	702	FLC	CG-CB-CA	-2.28	103.23	109.33
10	D	700	MQ7	C24-C23-C25	2.25	119.06	115.27
10	P	800	MQ7	C2M-C2-C1	-2.23	112.57	116.27
6	A	703	FAD	C1'-N10-C9A	2.18	120.01	118.29
6	A	703	FAD	P-O3P-PA	-2.11	125.58	132.83
10	D	700	MQ7	C29-C28-C27	-2.09	116.60	122.65
6	M	803	FAD	O5'-C5'-C4'	2.06	114.86	109.36
10	P	800	MQ7	C20-C18-C17	-2.05	116.96	121.12

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	802	FLC	CA-CB-CG-CGC
5	M	802	FLC	CBC-CB-CG-CGC
5	M	802	FLC	OHB-CB-CG-CGC
6	A	703	FAD	N10-C1'-C2'-O2'
6	A	703	FAD	N10-C1'-C2'-C3'
6	A	703	FAD	C3'-C4'-C5'-O5'
6	A	703	FAD	O4'-C4'-C5'-O5'
6	A	703	FAD	C5'-O5'-P-O1P
6	A	703	FAD	C5'-O5'-P-O2P
6	A	703	FAD	PA-O3P-P-O5'
6	M	803	FAD	C3'-C4'-C5'-O5'
6	M	803	FAD	O4'-C4'-C5'-O5'
6	M	803	FAD	C5'-O5'-P-O1P
6	M	803	FAD	PA-O3P-P-O5'
10	P	800	MQ7	C22-C23-C25-C26
10	P	800	MQ7	C24-C23-C25-C26
10	D	700	MQ7	C14-C13-C15-C16
10	P	800	MQ7	C14-C13-C15-C16
10	D	700	MQ7	C12-C13-C15-C16
10	P	800	MQ7	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
10	D	700	MQ7	C18-C20-C21-C22
10	P	800	MQ7	C23-C25-C26-C27
5	A	702	FLC	CA-CB-CG-CGC
10	P	800	MQ7	C13-C15-C16-C17
10	D	700	MQ7	C13-C15-C16-C17
10	P	800	MQ7	C12-C11-C3-C4
6	M	803	FAD	O4B-C4B-C5B-O5B
6	A	703	FAD	C5'-O5'-P-O3P
6	M	803	FAD	C5'-O5'-P-O3P
6	A	703	FAD	O4B-C4B-C5B-O5B
6	M	803	FAD	PA-O3P-P-O1P
10	D	700	MQ7	C15-C16-C17-C18
10	P	800	MQ7	C15-C16-C17-C18
10	D	700	MQ7	C25-C26-C27-C28
10	D	700	MQ7	C3-C11-C12-C13
10	P	800	MQ7	C3-C11-C12-C13

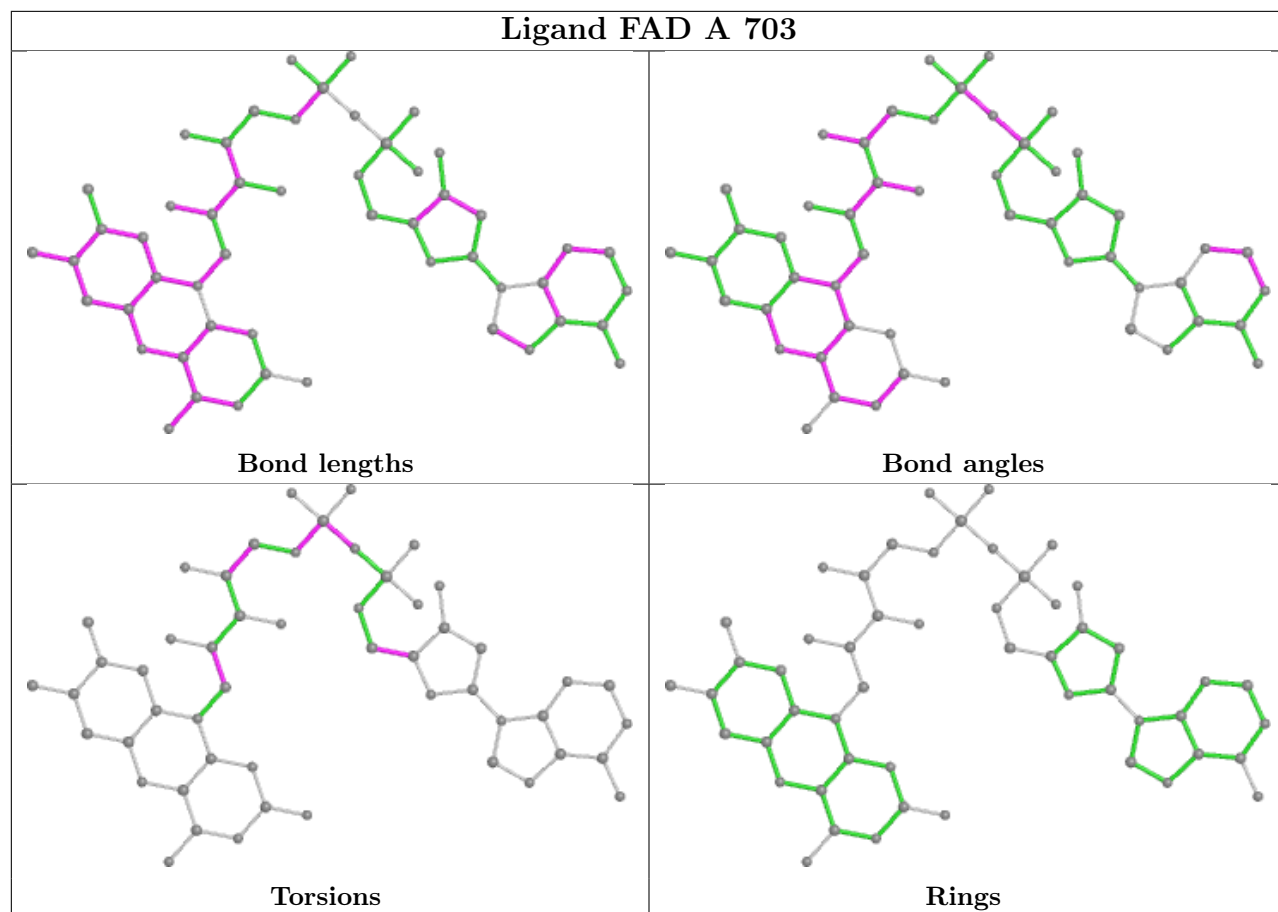
There are no ring outliers.

8 monomers are involved in 67 short contacts:

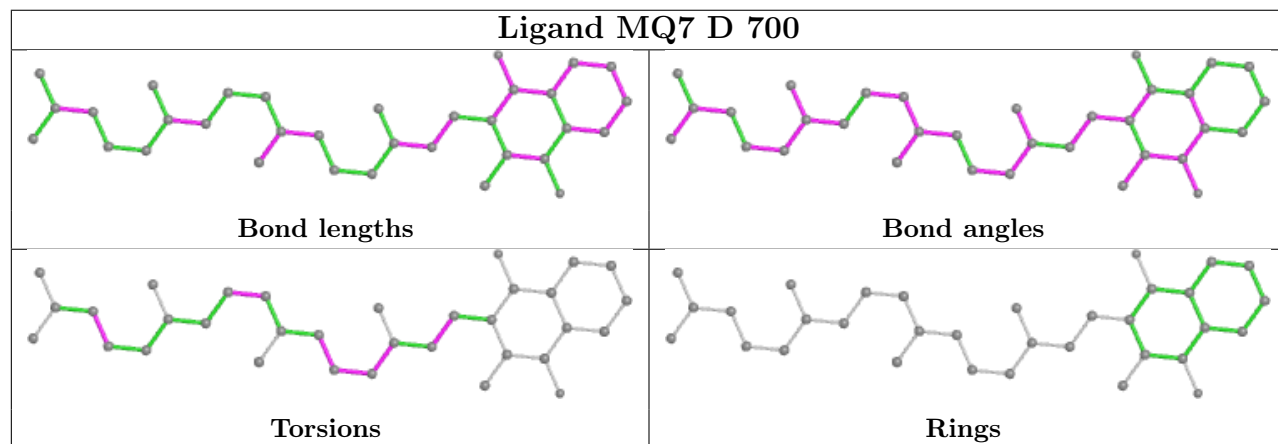
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	703	FAD	17	0
10	D	700	MQ7	7	0
10	P	800	MQ7	12	0
9	N	246	SF4	3	0
6	M	803	FAD	14	0
5	M	802	FLC	3	0
5	A	702	FLC	14	0
8	N	245	F3S	1	0

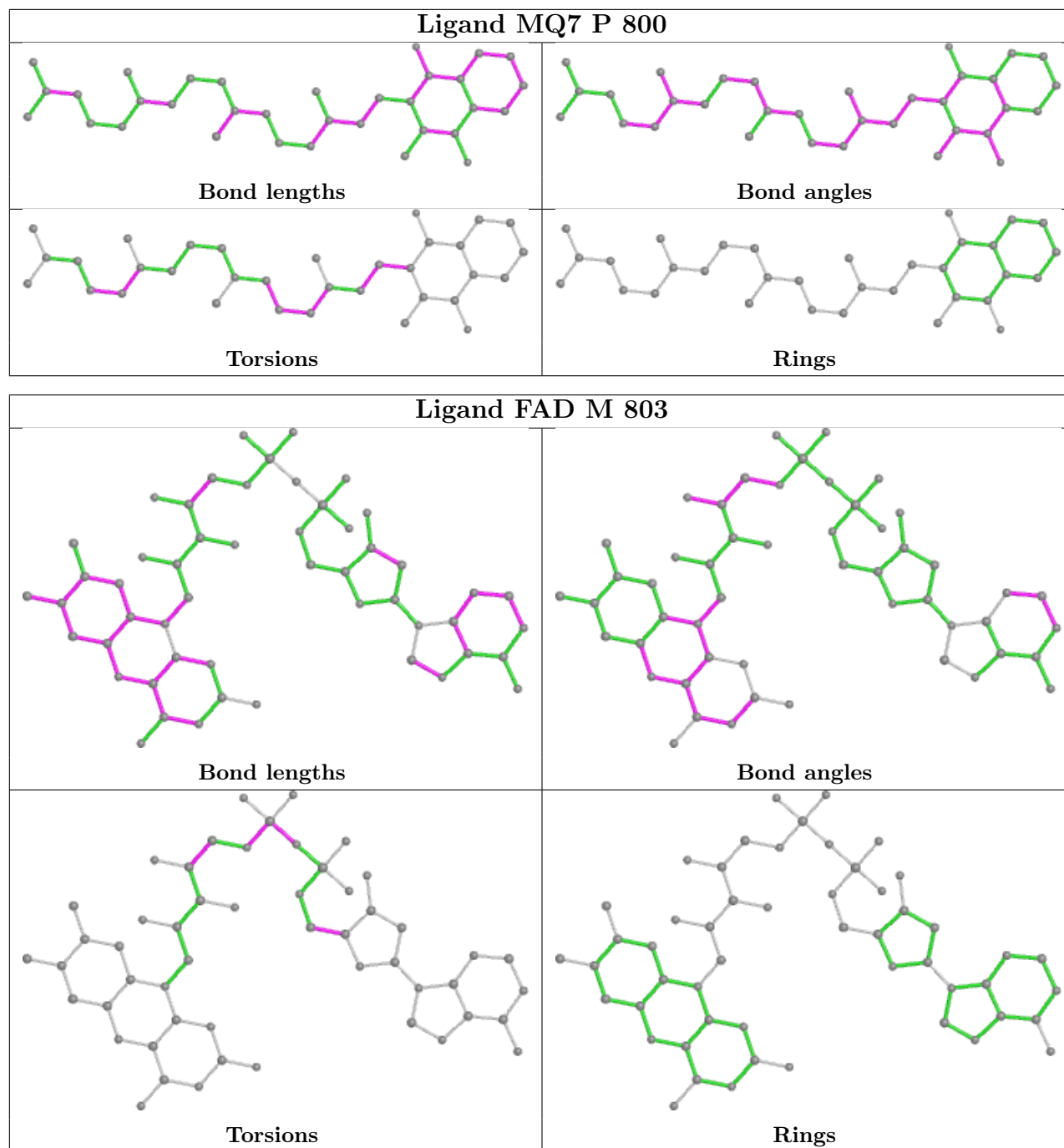
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 703



Ligand MQ7 D 700





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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	577/602 (95%)	-0.47	0 100 100	9, 14, 62, 85	0
1	M	572/602 (95%)	0.93	96 (16%) 1 1	30, 92, 127, 142	0
2	B	243/243 (100%)	-0.57	2 (0%) 86 86	9, 15, 36, 85	0
2	N	243/243 (100%)	0.28	13 (5%) 26 24	9, 62, 119, 147	0
3	C	130/130 (100%)	-0.47	0 100 100	10, 32, 59, 76	0
3	O	130/130 (100%)	-0.08	3 (2%) 60 59	24, 55, 106, 123	0
4	D	119/119 (100%)	-0.60	0 100 100	18, 36, 61, 70	0
4	P	119/119 (100%)	-0.34	1 (0%) 86 86	27, 49, 80, 118	0
All	All	2133/2188 (97%)	0.00	115 (5%) 25 24	9, 45, 114, 147	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	17	VAL	8.5
1	M	484	GLU	6.2
1	M	557	ALA	6.0
1	M	392	GLY	5.7
1	M	159	ASP	4.8
1	M	218	SER	4.7
3	O	1	THR	4.7
1	M	219	HIS	4.6
1	M	325	HIS	4.4
1	M	188	VAL	4.4
1	M	8	ALA	4.3
1	M	434	GLN	4.2
1	M	556	ASP	4.1
1	M	545	VAL	4.1
1	M	373	GLY	4.1
1	M	544	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	M	546	ASN	4.1
1	M	411	THR	4.0
1	M	63	GLU	4.0
1	M	270	PRO	3.9
2	N	1	ALA	3.8
1	M	253	ILE	3.7
2	N	16	GLU	3.7
2	N	98	ILE	3.7
1	M	31	LYS	3.7
1	M	77	CYS	3.6
2	B	242	PRO	3.6
1	M	393	SER	3.6
1	M	378	GLY	3.6
1	M	571	THR	3.5
3	O	2	THR	3.5
1	M	473	GLN	3.5
2	N	25	PHE	3.5
1	M	548	LEU	3.4
2	N	46	ASN	3.4
1	M	475	THR	3.3
1	M	307	PRO	3.3
1	M	229	VAL	3.3
1	M	206	GLY	3.2
1	M	447	ASN	3.2
1	M	482	LEU	3.2
1	M	379	GLU	3.2
1	M	27	ASN	3.1
1	M	147	PRO	3.1
2	N	2	GLU	3.0
1	M	171	VAL	3.0
2	N	128	ASP	3.0
1	M	24	ALA	3.0
1	M	371	ILE	3.0
1	M	359	GLY	3.0
1	M	189	VAL	2.9
1	M	320	GLY	2.9
1	M	358	MET	2.9
1	M	559	GLY	2.9
1	M	445	GLY	2.9
1	M	513	ASN	2.9
1	M	163	ASP	2.8
1	M	99	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	124	THR	2.8
1	M	451	ILE	2.8
1	M	156	PHE	2.8
2	B	1	ALA	2.7
1	M	169	GLY	2.7
1	M	381	SER	2.7
1	M	366	ASN	2.7
4	P	0	MET	2.6
1	M	84	TYR	2.6
2	N	40	LEU	2.6
1	M	549	LYS	2.6
1	M	216	ALA	2.6
1	M	59	HIS	2.6
1	M	563	LEU	2.6
1	M	444	GLY	2.6
1	M	403	GLY	2.5
1	M	318	HIS	2.5
1	M	172	ALA	2.5
1	M	377	VAL	2.5
1	M	220	GLY	2.5
1	M	360	GLY	2.5
1	M	558	ASP	2.5
1	M	526	LYS	2.5
1	M	493	ASP	2.4
1	M	64	TYR	2.4
1	M	180	LEU	2.4
1	M	88	HIS	2.4
2	N	8	ILE	2.4
1	M	280	LYS	2.3
2	N	122	GLY	2.3
2	N	26	TYR	2.3
1	M	222	PRO	2.3
1	M	157	VAL	2.3
1	M	185	ALA	2.3
1	M	367	CYS	2.2
1	M	319	LEU	2.2
1	M	223	LEU	2.2
1	M	191	ALA	2.2
1	M	305	SER	2.2
2	N	30	TYR	2.2
1	M	160	ILE	2.2
1	M	251	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	230	GLN	2.2
3	O	100	ASP	2.2
1	M	182	GLN	2.1
1	M	390	ARG	2.1
1	M	181	VAL	2.1
1	M	207	ILE	2.1
1	M	376	ALA	2.1
1	M	250	GLU	2.1
1	M	477	ASP	2.1
1	M	510	HIS	2.1
1	M	203	THR	2.1
1	M	23	ALA	2.0
1	M	394	ASN	2.0
1	M	306	THR	2.0
1	M	55	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

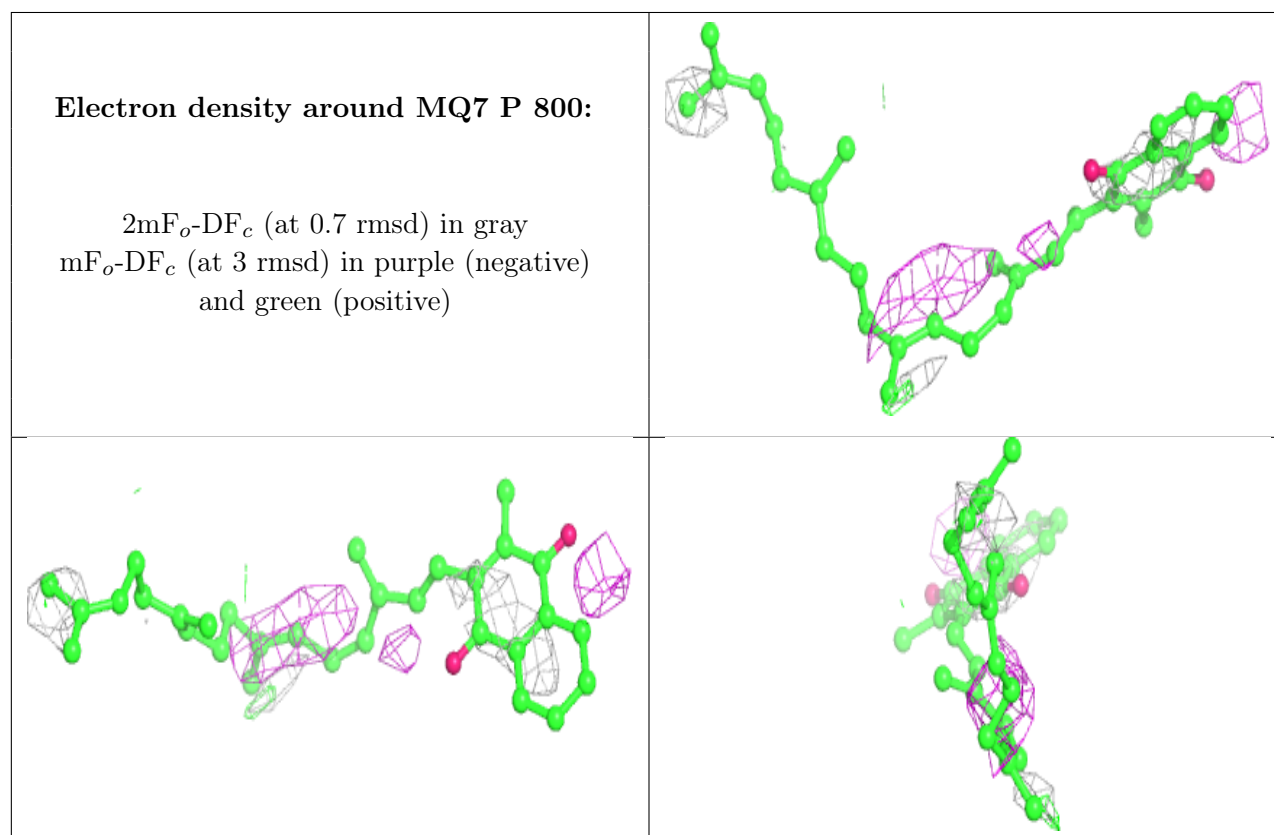
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	MQ7	P	800	33/48	0.60	1.16	83,106,120,123	0
10	MQ7	D	700	33/48	0.64	0.79	59,100,117,127	0
5	FLC	M	802	13/13	0.71	0.42	60,74,92,97	0
5	FLC	A	702	13/13	0.85	0.29	31,37,38,39	0
6	FAD	M	803	52/53	0.86	0.45	23,87,158,164	0
7	FES	N	244	4/4	0.96	0.14	21,24,44,53	0
6	FAD	A	703	52/53	0.97	0.21	0,1,17,36	0
9	SF4	N	246	8/8	0.97	0.15	20,29,49,53	0

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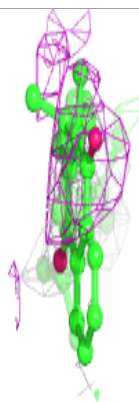
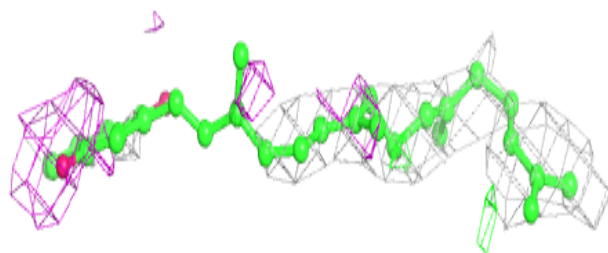
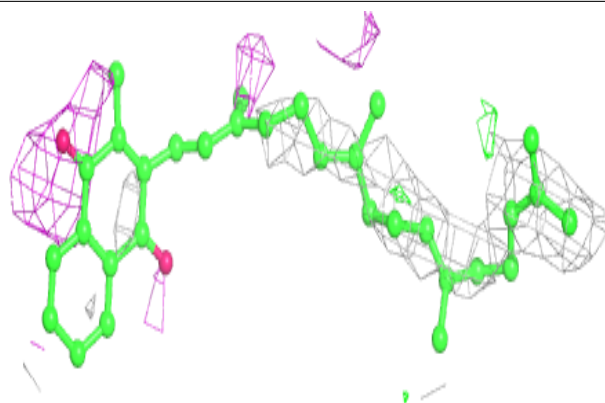
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	FES	B	244	4/4	0.98	0.18	0,4,5,8	0
9	SF4	B	246	8/8	0.99	0.19	9,21,27,27	0
8	F3S	N	245	7/7	0.99	0.09	14,16,29,49	0
8	F3S	B	245	7/7	1.00	0.13	7,11,15,24	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

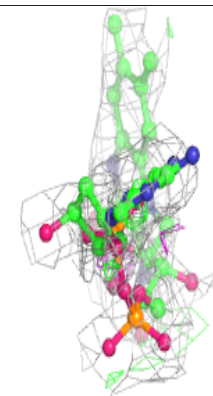
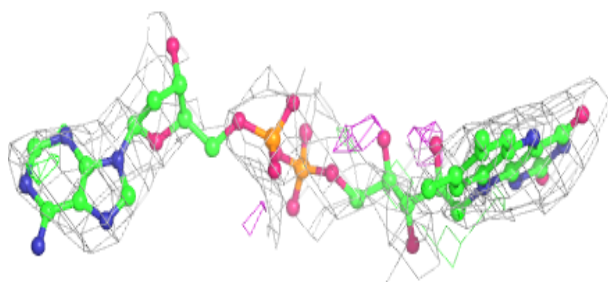
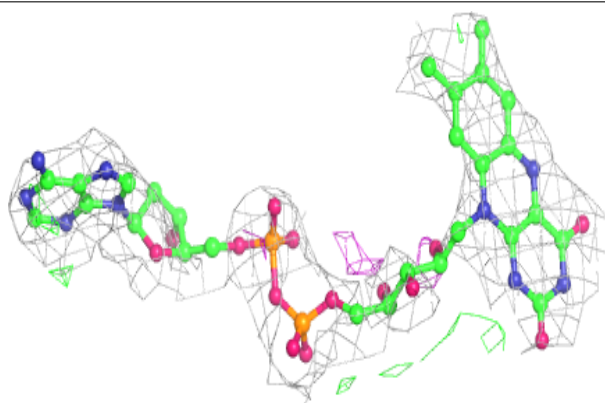


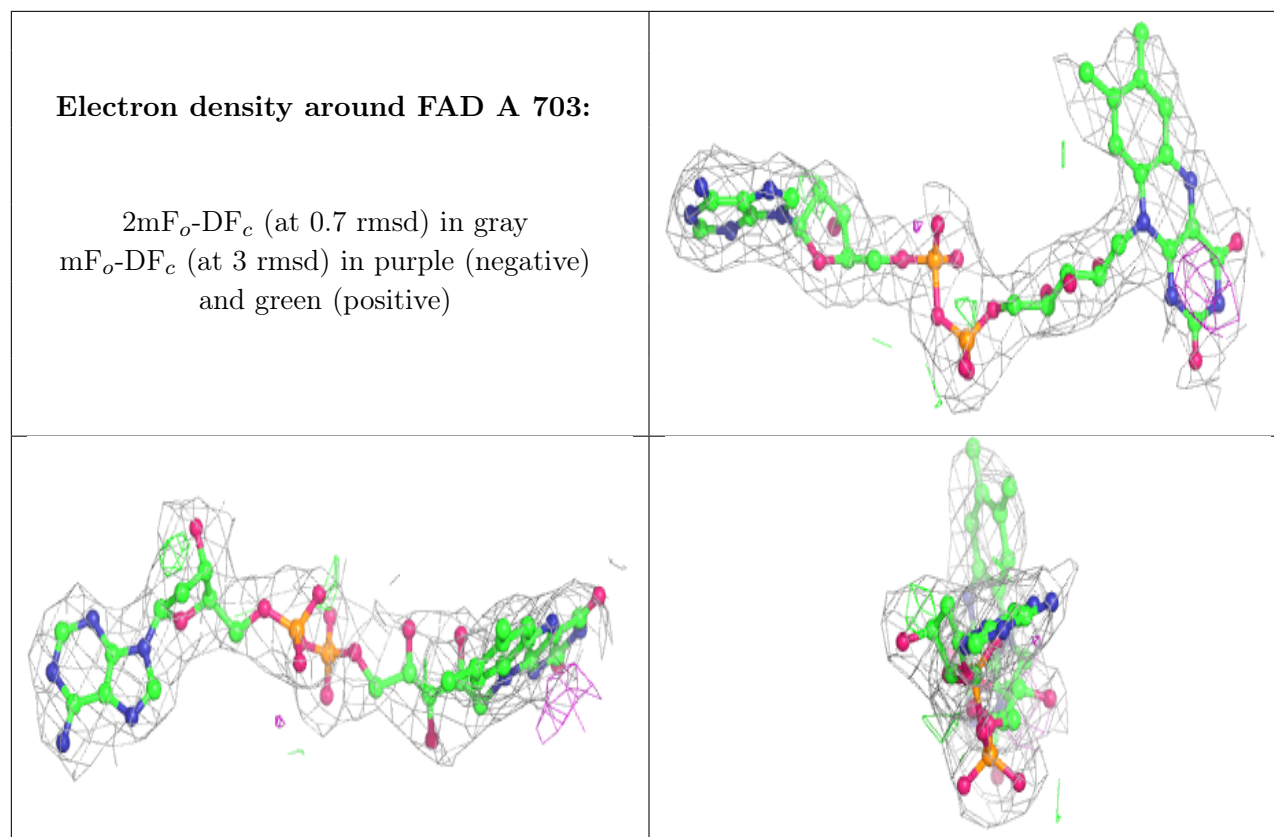
Electron density around MQ7 D 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD M 803:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.