



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:20 PM UTC

PDB ID : 2B76 / pdb_00002b76
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

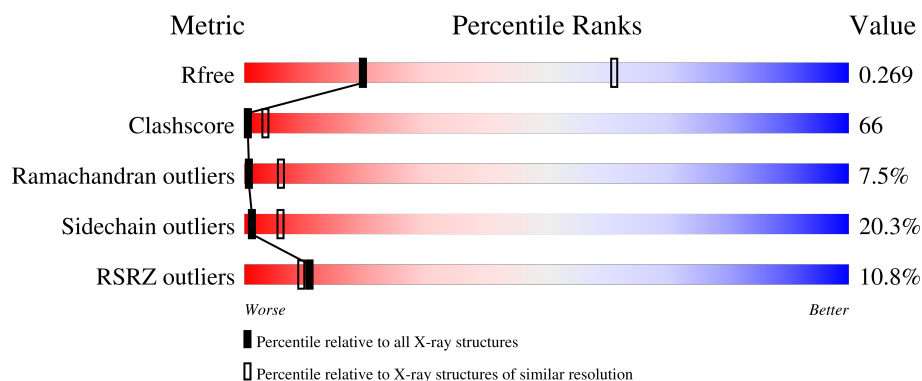
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	18% 37% 30% 10% .
1	M	602	33% 20% 56% 15% 5%
2	B	243	27% 49% 21% .
2	N	243	8% 19% 57% 22% .
3	C	130	24% 52% 22% .

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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
5	FLC	A	702	-	-	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.

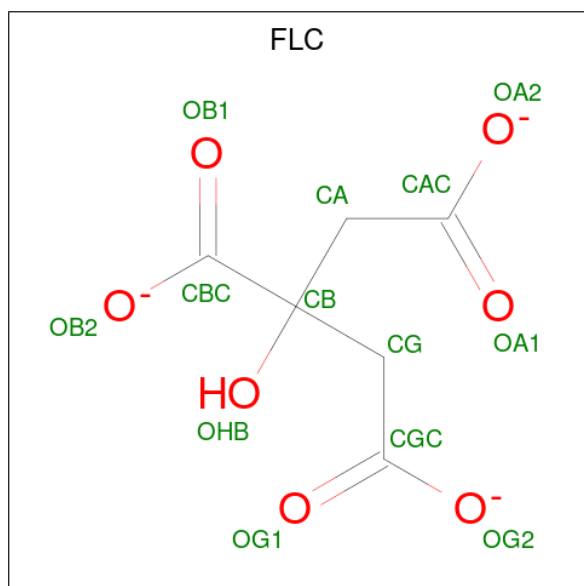
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

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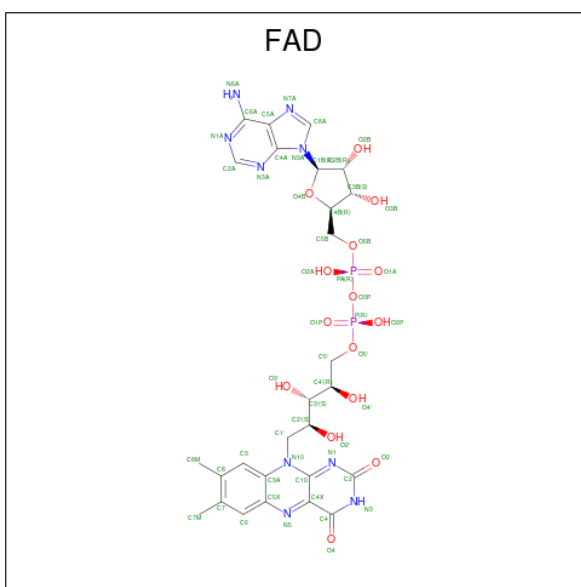
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



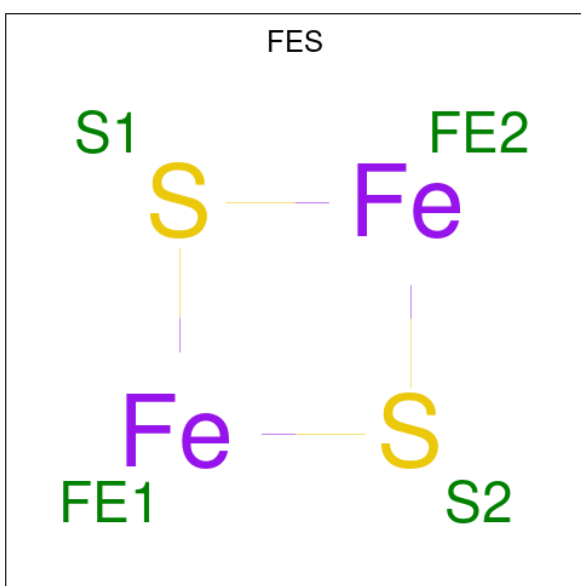
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		
5	M	1	Total	C	O	0	0
			13	6	7		

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



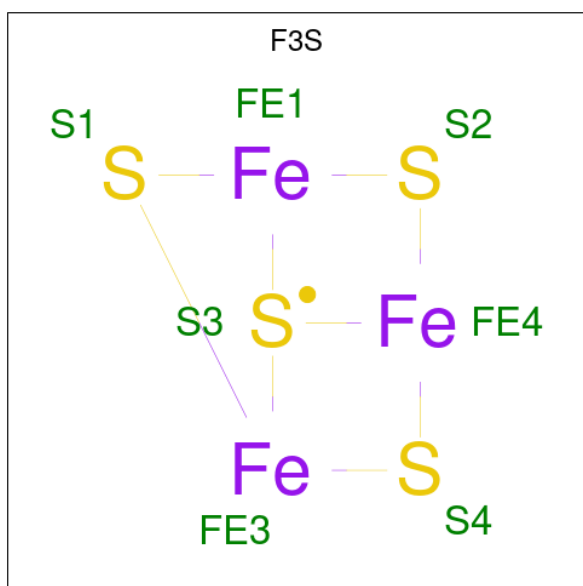
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 52	C 27	N 9	O 14	P 2	0	0
6	M	1	Total 52	C 27	N 9	O 14	P 2	0	0

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



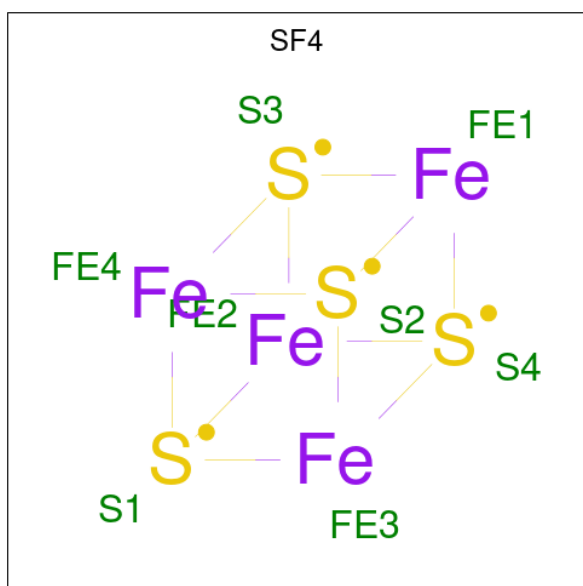
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 4	Fe 2	S 2	0	0
7	N	1	Total 4	Fe 2	S 2	0	0

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: 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 (CCD ID: SF4) (formula: Fe_4S_4).



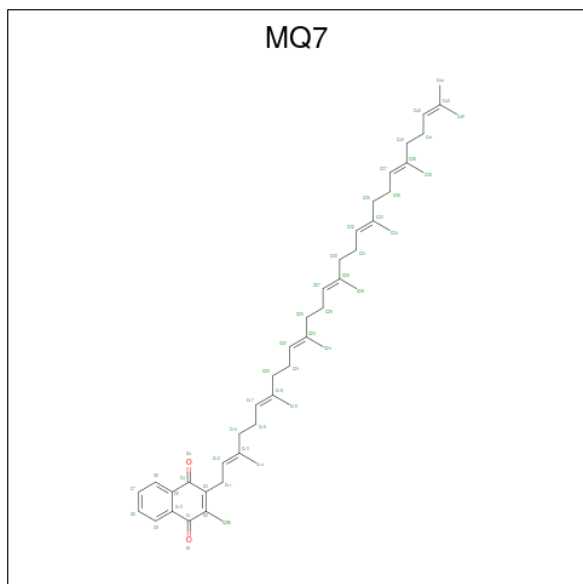
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		

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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 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).

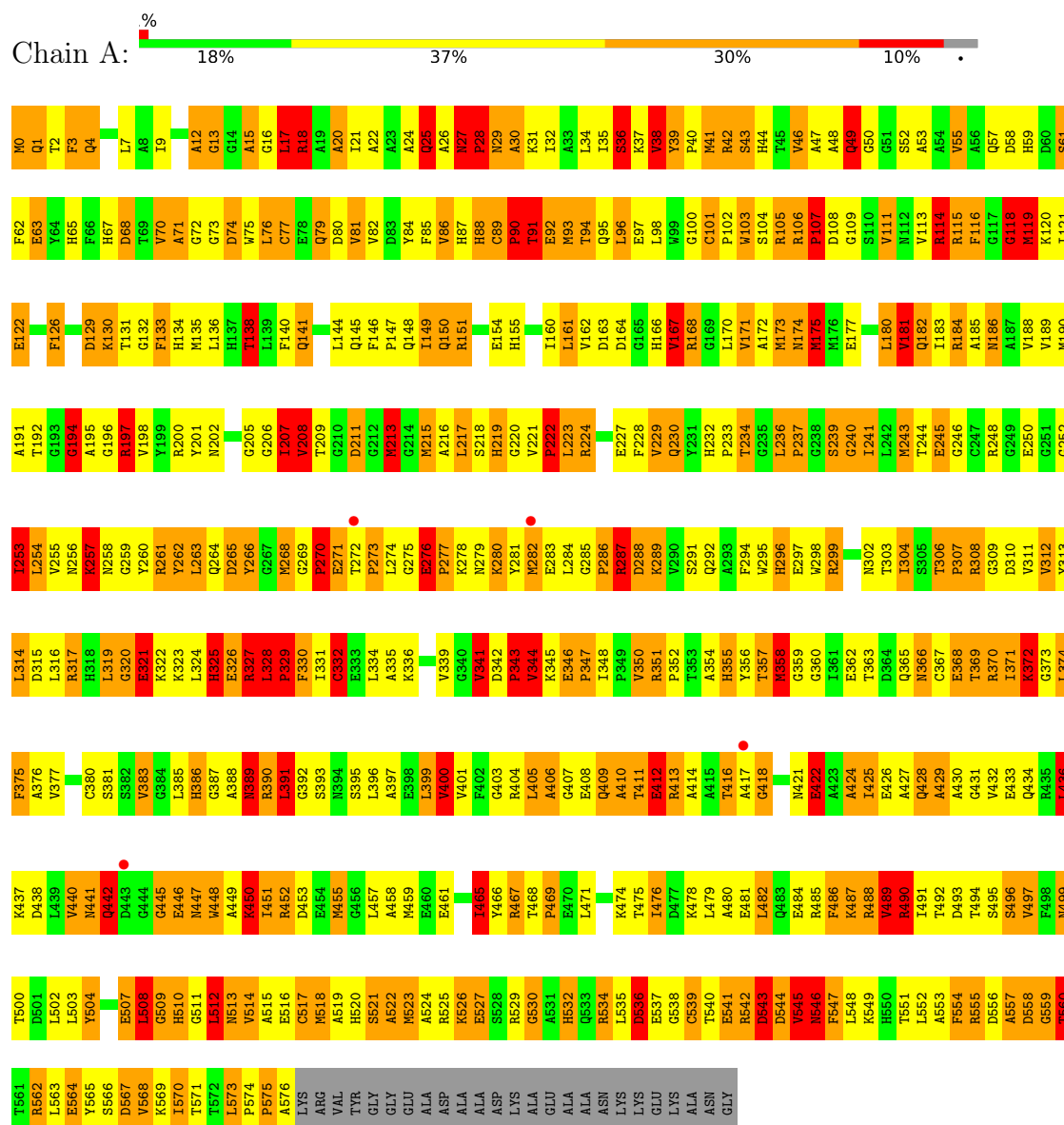


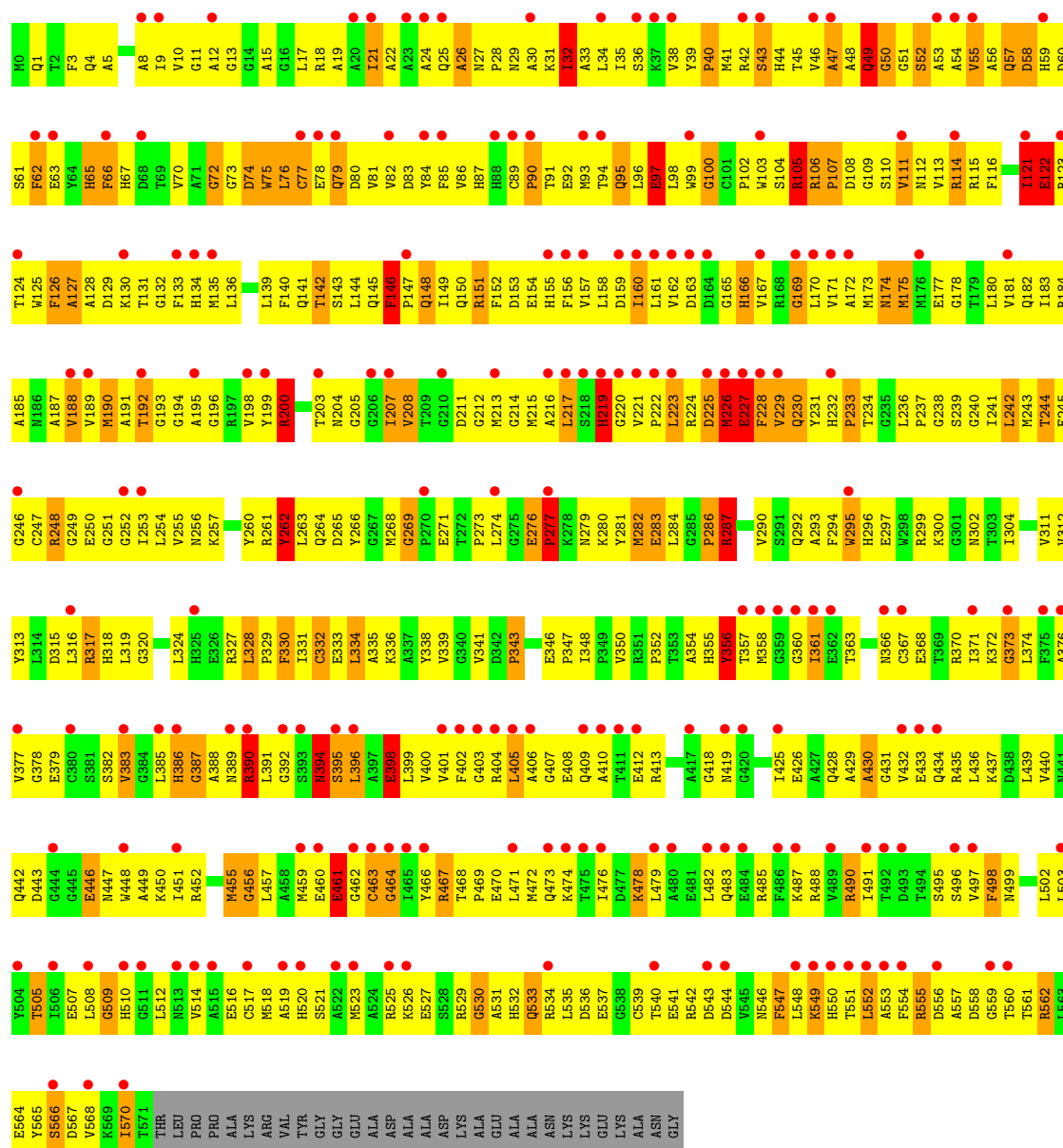
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	C	O	0	0
			33	31	2		
10	P	1	Total	C	O	0	0
			33	31	2		

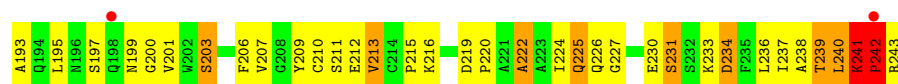
3 Residue-property plots

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.

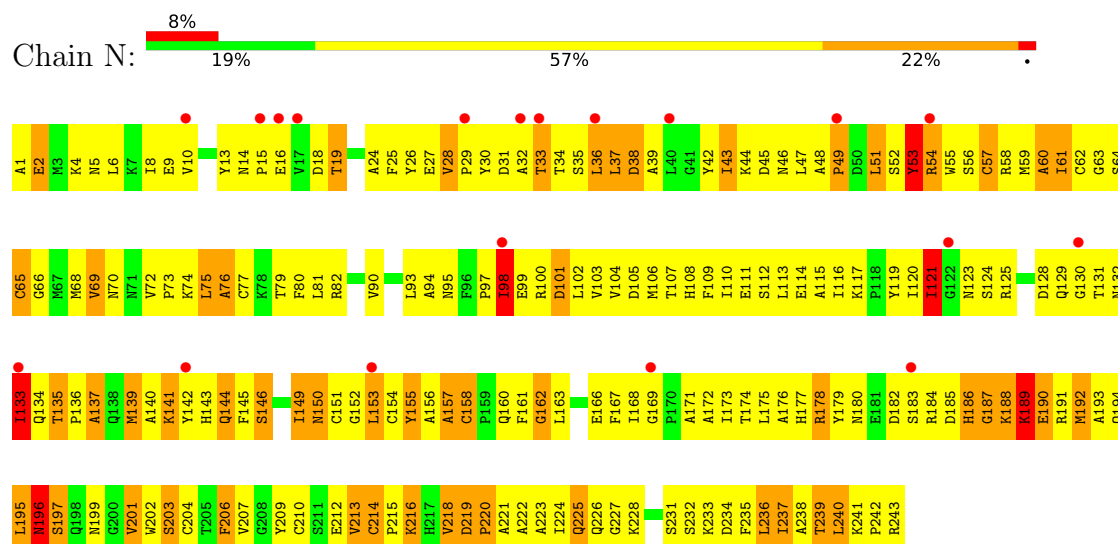
• Molecule 1: Fumarate reductase flavoprotein subunit



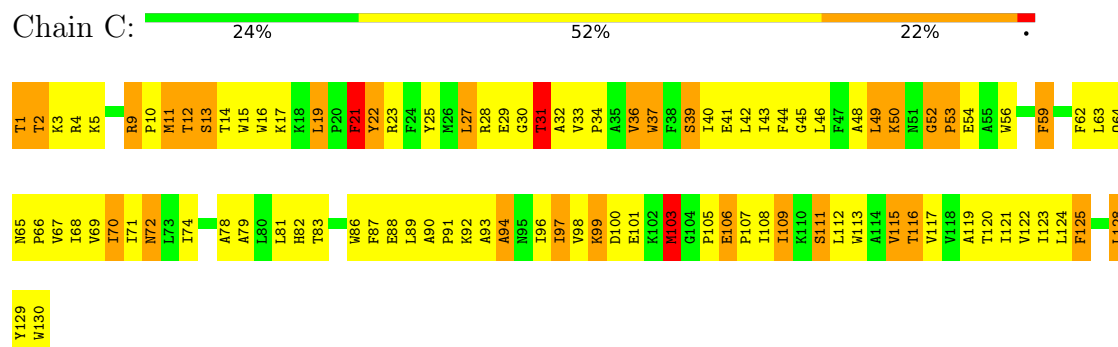




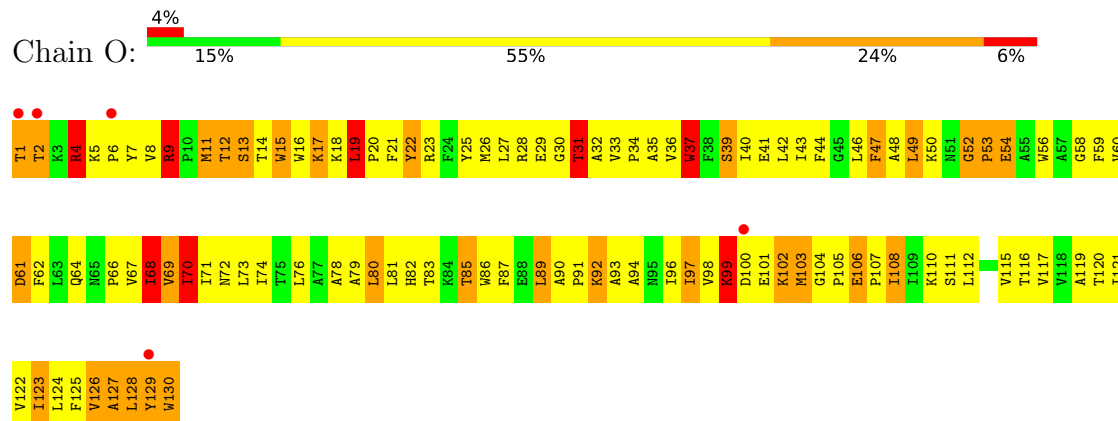
• Molecule 2: Fumarate reductase iron-sulfur protein



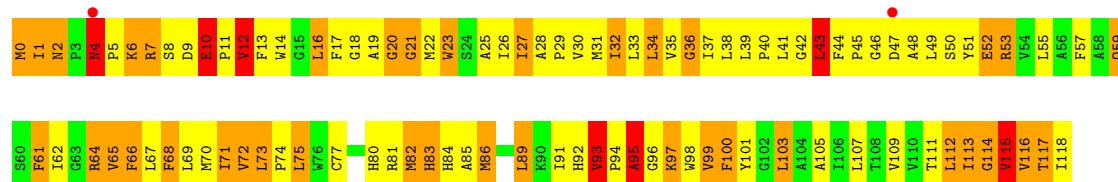
• Molecule 3: Fumarate reductase subunit C



• Molecule 3: Fumarate reductase subunit C



• 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 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	83.5 (20.00-3.30) 83.1 (20.00-3.30)	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 0.238 , 0.269	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)	0.26 , 50.9	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	0.87	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: F3S, FAD, SF4, MQ7, FES, FLC

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	2.28	189/4540 (4.2%)	2.34	287/6139 (4.7%)
1	M	0.43	0/4504	1.15	47/6087 (0.8%)
2	B	1.43	16/1931 (0.8%)	1.70	52/2617 (2.0%)
2	N	0.49	0/1931	1.10	15/2617 (0.6%)
3	C	1.22	0/1094	1.59	25/1496 (1.7%)
3	O	1.22	3/1094 (0.3%)	1.68	30/1496 (2.0%)
4	D	1.03	3/956 (0.3%)	1.48	21/1303 (1.6%)
4	P	0.96	2/956 (0.2%)	1.64	27/1303 (2.1%)
All	All	1.41	213/17006 (1.3%)	1.70	504/23058 (2.2%)

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 (213) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	277	PRO	CA-C	17.34	1.71	1.52
1	A	465	ILE	CA-CB	-13.60	1.39	1.54
1	A	352	PRO	CA-C	13.11	1.68	1.52
1	A	63	GLU	C-O	-13.06	1.09	1.24
1	A	371	ILE	CA-CB	11.77	1.67	1.53
1	A	270	PRO	CA-C	11.29	1.68	1.52
1	A	119	MET	CA-C	10.88	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	VAL	C-O	-10.83	1.11	1.24
1	A	173	MET	SD-CE	10.74	2.06	1.79
1	A	287	ARG	C-O	-10.41	1.10	1.24
1	A	221	VAL	CA-CB	-10.35	1.40	1.54
2	B	207	VAL	CA-CB	-10.27	1.42	1.54
1	A	425	ILE	CA-CB	10.23	1.65	1.54
1	A	410	ALA	C-O	-9.94	1.12	1.24
1	A	543	ASP	CA-CB	9.92	1.69	1.53
1	A	183	ILE	CA-CB	9.91	1.66	1.54
1	A	39	TYR	CA-C	-9.89	1.43	1.53
2	B	56	SER	C-O	-9.78	1.11	1.24
1	A	328	LEU	N-CA	9.77	1.57	1.46
1	A	90	PRO	CA-CB	-9.66	1.40	1.53
1	A	22	ALA	CA-CB	-9.66	1.38	1.53
1	A	138	THR	CA-CB	9.61	1.68	1.53
1	A	240	GLY	C-O	-9.54	1.10	1.24
1	A	484	GLU	CA-C	-9.30	1.40	1.52
1	A	469	PRO	CA-C	-9.15	1.39	1.52
1	A	514	VAL	CA-CB	-9.14	1.43	1.54
1	A	386	HIS	C-O	-9.06	1.12	1.24
1	A	276	GLU	CA-CB	8.95	1.67	1.53
1	A	574	PRO	CA-CB	-8.93	1.41	1.54
1	A	253	ILE	CA-CB	8.87	1.66	1.54
1	A	276	GLU	N-CA	-8.86	1.33	1.46
1	A	372	LYS	CB-CG	8.77	1.78	1.52
1	A	272	THR	CA-C	8.73	1.65	1.53
1	A	312	VAL	CA-CB	-8.70	1.42	1.54
1	A	136	LEU	C-O	-8.64	1.13	1.24
1	A	220	GLY	C-O	-8.60	1.12	1.23
1	A	450	LYS	CD-CE	8.57	1.78	1.52
1	A	190	MET	SD-CE	-8.55	1.58	1.79
1	A	325	HIS	CA-C	-8.55	1.41	1.52
1	A	557	ALA	CA-C	8.47	1.63	1.52
1	A	545	VAL	C-O	-8.30	1.14	1.24
1	A	400	VAL	CA-CB	-8.28	1.43	1.54
1	A	172	ALA	CA-CB	-8.24	1.39	1.53
1	A	369	THR	CA-CB	8.23	1.65	1.53
1	A	192	THR	CA-C	-8.22	1.41	1.52
1	A	327	ARG	CA-C	8.09	1.63	1.52
1	A	424	ALA	CA-CB	8.09	1.66	1.53
1	A	391	LEU	C-O	-8.07	1.14	1.24
2	B	234	ASP	C-O	-7.95	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	GLN	C-O	-7.90	1.11	1.24
1	A	422	GLU	C-O	-7.80	1.14	1.24
1	A	243	MET	C-O	-7.79	1.14	1.24
1	A	344	VAL	CA-C	7.69	1.60	1.52
1	A	219	HIS	CA-C	-7.67	1.42	1.52
1	A	269	GLY	N-CA	-7.66	1.34	1.44
1	A	90	PRO	CA-C	-7.64	1.41	1.52
1	A	357	THR	CA-CB	-7.63	1.41	1.52
1	A	445	GLY	C-N	-7.62	1.23	1.33
1	A	35	ILE	C-O	-7.58	1.13	1.24
1	A	28	PRO	CA-C	-7.53	1.41	1.52
1	A	467	ARG	CA-C	-7.51	1.43	1.52
1	A	391	LEU	CA-CB	-7.46	1.42	1.53
1	A	461	GLU	CA-CB	7.42	1.65	1.53
1	A	138	THR	C-O	-7.41	1.15	1.24
1	A	17	LEU	CA-C	-7.39	1.43	1.53
4	P	95	ALA	CA-CB	-7.36	1.41	1.53
1	A	368	GLU	CA-CB	-7.31	1.42	1.53
1	A	351	ARG	CA-C	7.29	1.61	1.52
1	A	544	ASP	C-O	-7.28	1.13	1.23
1	A	219	HIS	CA-CB	-7.26	1.43	1.53
1	A	175	MET	SD-CE	7.26	1.97	1.79
1	A	191	ALA	CA-CB	-7.23	1.47	1.53
1	A	539	CYS	CA-C	-7.21	1.43	1.53
1	A	546	ASN	CA-CB	7.20	1.64	1.53
1	A	351	ARG	CA-CB	7.19	1.63	1.54
1	A	522	ALA	CA-CB	7.18	1.64	1.53
1	A	146	PHE	C-O	-7.17	1.19	1.25
1	A	575	PRO	C-N	-7.13	1.23	1.33
1	A	390	ARG	CA-C	-7.11	1.43	1.52
1	A	28	PRO	N-CA	-7.08	1.38	1.47
1	A	372	LYS	CG-CD	7.08	1.73	1.52
1	A	195	ALA	CA-C	7.04	1.62	1.52
1	A	207	ILE	CG1-CD1	7.00	1.79	1.51
1	A	129	ASP	CB-CG	6.96	1.69	1.52
1	A	480	ALA	CA-C	-6.81	1.44	1.52
2	B	69	VAL	CA-CB	-6.81	1.45	1.54
1	A	24	ALA	CA-C	-6.79	1.43	1.52
1	A	451	ILE	CA-CB	-6.70	1.47	1.54
1	A	91	THR	CA-CB	6.66	1.64	1.53
1	A	575	PRO	CA-C	-6.64	1.43	1.52
1	A	113	VAL	CA-C	6.62	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	ILE	CA-C	6.61	1.59	1.53
1	A	409	GLN	CA-C	-6.60	1.43	1.52
1	A	53	ALA	CA-C	-6.59	1.44	1.52
1	A	535	LEU	CA-C	-6.56	1.44	1.52
1	A	330	PHE	CA-CB	6.54	1.64	1.53
1	A	490	ARG	CA-CB	-6.50	1.43	1.53
1	A	186	ASN	CA-C	-6.46	1.44	1.53
1	A	36	SER	CA-CB	-6.44	1.43	1.53
2	B	98	ILE	CA-CB	-6.44	1.46	1.54
1	A	167	VAL	CA-C	-6.42	1.44	1.52
2	B	31	ASP	C-O	-6.41	1.15	1.23
1	A	229	VAL	CA-CB	6.35	1.61	1.54
1	A	192	THR	C-O	-6.34	1.15	1.24
1	A	372	LYS	C-O	-6.33	1.16	1.23
1	A	89	CYS	CA-CB	6.31	1.63	1.54
1	A	188	VAL	CA-CB	6.30	1.62	1.54
3	O	1	THR	C-O	6.22	1.35	1.23
1	A	484	GLU	C-O	-6.21	1.16	1.24
1	A	347	PRO	CA-C	6.20	1.61	1.52
1	A	455	MET	SD-CE	-6.16	1.64	1.79
1	A	136	LEU	CA-C	-6.13	1.45	1.52
2	B	130	GLY	N-CA	6.13	1.52	1.45
1	A	326	GLU	N-CA	6.06	1.53	1.46
1	A	399	LEU	CA-C	-6.05	1.44	1.52
2	B	242	PRO	C-N	-6.05	1.24	1.33
1	A	396	LEU	CA-CB	6.04	1.62	1.53
1	A	429	ALA	CA-C	6.04	1.60	1.52
1	A	549	LYS	CG-CD	6.03	1.70	1.52
1	A	135	MET	CA-C	-6.02	1.44	1.52
1	A	563	LEU	CA-CB	-5.96	1.44	1.53
1	A	36	SER	CA-C	5.96	1.59	1.52
1	A	195	ALA	N-CA	5.94	1.53	1.46
1	A	512	LEU	C-O	-5.94	1.16	1.24
1	A	90	PRO	N-CD	-5.93	1.39	1.47
2	B	130	GLY	CA-C	5.93	1.58	1.52
1	A	223	LEU	CA-C	-5.92	1.45	1.52
1	A	71	ALA	C-O	-5.92	1.17	1.24
1	A	119	MET	N-CA	5.91	1.52	1.45
1	A	185	ALA	CA-C	-5.91	1.45	1.52
2	B	39	ALA	CA-CB	-5.88	1.44	1.53
1	A	120	LYS	N-CA	5.87	1.53	1.46
1	A	389	ASN	CA-CB	-5.84	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	213	VAL	CA-CB	-5.80	1.48	1.54
1	A	421	ASN	CA-C	-5.79	1.45	1.52
1	A	545	VAL	CA-CB	5.79	1.61	1.54
1	A	35	ILE	C-N	-5.78	1.26	1.33
1	A	547	PHE	CA-CB	5.77	1.62	1.53
1	A	253	ILE	CA-C	5.73	1.59	1.52
4	D	0	MET	SD-CE	5.73	1.93	1.79
1	A	237	PRO	C-O	-5.72	1.17	1.23
1	A	20	ALA	CA-CB	5.72	1.62	1.53
1	A	421	ASN	CA-CB	5.72	1.60	1.52
1	A	504	TYR	C-O	-5.71	1.17	1.24
1	A	494	THR	C-O	-5.69	1.16	1.24
1	A	228	PHE	CA-CB	5.67	1.59	1.52
1	A	391	LEU	CB-CG	-5.65	1.42	1.53
1	A	451	ILE	CA-C	-5.63	1.46	1.52
4	D	93	VAL	CA-CB	-5.63	1.48	1.53
1	A	211	ASP	C-N	-5.61	1.26	1.33
1	A	542	ARG	CA-C	-5.61	1.45	1.52
1	A	171	VAL	CA-CB	-5.60	1.46	1.55
1	A	459	MET	CA-CB	-5.60	1.44	1.53
1	A	299	ARG	CA-CB	5.59	1.63	1.53
1	A	213	MET	SD-CE	-5.58	1.65	1.79
1	A	76	LEU	CA-C	-5.57	1.45	1.52
1	A	489	VAL	CA-C	-5.53	1.45	1.52
4	P	86	MET	SD-CE	5.52	1.93	1.79
1	A	216	ALA	CA-CB	5.49	1.62	1.53
1	A	465	ILE	C-O	-5.48	1.18	1.24
1	A	461	GLU	C-O	-5.47	1.17	1.24
1	A	475	THR	CA-C	-5.47	1.45	1.52
1	A	436	LEU	N-CA	-5.47	1.39	1.46
1	A	189	VAL	CA-CB	5.45	1.60	1.54
2	B	5	ASN	CA-C	5.45	1.58	1.52
1	A	474	LYS	CA-CB	5.45	1.61	1.53
1	A	114	ARG	C-O	-5.44	1.16	1.23
1	A	389	ASN	C-O	-5.44	1.17	1.24
1	A	100	GLY	C-O	-5.42	1.16	1.24
1	A	510	HIS	C-O	-5.42	1.17	1.24
1	A	453	ASP	C-O	-5.41	1.17	1.24
1	A	61	SER	CA-CB	-5.39	1.44	1.53
1	A	146	PHE	CA-C	-5.38	1.46	1.52
1	A	213	MET	CG-SD	5.37	1.94	1.80
1	A	43	SER	CA-C	5.35	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	GLY	C-O	5.34	1.28	1.23
1	A	82	VAL	CA-C	-5.33	1.46	1.52
3	O	5	LYS	C-O	-5.31	1.18	1.24
1	A	85	PHE	C-O	-5.30	1.18	1.24
1	A	545	VAL	CA-C	-5.29	1.46	1.52
2	B	236	LEU	C-O	-5.27	1.18	1.24
1	A	84	TYR	CA-CB	5.26	1.62	1.53
1	A	576	ALA	CA-CB	5.26	1.70	1.52
1	A	484	GLU	CG-CD	5.26	1.65	1.52
1	A	410	ALA	CA-C	-5.23	1.46	1.52
1	A	53	ALA	CA-CB	-5.22	1.45	1.53
1	A	183	ILE	CA-C	-5.22	1.46	1.52
1	A	296	HIS	C-O	-5.21	1.18	1.24
1	A	181	VAL	CA-C	5.20	1.59	1.52
1	A	120	LYS	CA-CB	5.20	1.61	1.53
1	A	270	PRO	N-CD	5.20	1.55	1.47
2	B	136	PRO	C-O	-5.17	1.17	1.24
1	A	513	ASN	C-O	-5.13	1.17	1.24
1	A	370	ARG	CA-C	-5.13	1.45	1.52
1	A	499	ASN	CA-CB	5.12	1.59	1.52
2	B	42	TYR	C-O	-5.12	1.18	1.24
3	O	4	ARG	C-O	5.12	1.30	1.23
1	A	0	MET	SD-CE	5.11	1.92	1.79
1	A	67	HIS	CA-CB	-5.10	1.45	1.53
1	A	82	VAL	C-O	-5.09	1.18	1.24
1	A	553	ALA	CA-CB	-5.09	1.44	1.53
1	A	557	ALA	N-CA	5.08	1.52	1.46
1	A	207	ILE	C-O	-5.08	1.17	1.24
1	A	25	GLN	CA-CB	-5.08	1.47	1.54
1	A	94	THR	CA-C	5.08	1.59	1.52
4	D	95	ALA	CA-CB	5.07	1.61	1.53
2	B	241	LYS	CA-CB	5.05	1.61	1.53
1	A	332	CYS	CA-C	5.05	1.59	1.52
1	A	390	ARG	C-O	-5.05	1.17	1.23
1	A	141	GLN	CA-CB	5.04	1.61	1.53
1	A	277	PRO	N-CA	5.02	1.52	1.47
1	A	372	LYS	CA-CB	5.01	1.61	1.53
1	A	309	GLY	CA-C	5.01	1.57	1.52

All (504) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	70	ILE	N-CA-C	-16.21	95.18	110.42
1	A	269	GLY	O-C-N	15.49	137.26	121.77
1	A	269	GLY	CA-C-N	13.12	136.24	119.84
1	A	269	GLY	C-N-CA	13.12	136.24	119.84
4	P	12	VAL	N-CA-C	-12.74	99.57	111.67
2	B	14	ASN	CA-C-N	-12.09	106.38	119.19
2	B	14	ASN	C-N-CA	-12.09	106.38	119.19
3	C	70	ILE	N-CA-C	-11.71	100.08	110.74
1	A	266	TYR	N-CA-CB	-11.22	95.94	111.65
3	C	99	LYS	N-CA-C	-11.11	91.55	108.00
1	A	545	VAL	CB-CA-C	-11.03	97.57	112.02
1	A	262	TYR	N-CA-C	10.94	126.14	113.01
1	A	12	ALA	N-CA-C	10.77	124.66	110.88
2	B	13	TYR	CB-CA-C	-10.62	98.27	111.43
1	A	269	GLY	N-CA-C	10.53	133.82	112.34
2	B	28	VAL	N-CA-C	10.38	119.20	107.89
1	A	270	PRO	CB-CA-C	10.13	128.27	111.56
2	B	124	SER	N-CA-C	9.98	123.19	111.71
1	A	27	ASN	CA-C-N	9.94	129.58	119.24
1	A	27	ASN	C-N-CA	9.94	129.58	119.24
1	A	105	ARG	N-CA-C	9.94	123.30	109.18
1	A	325	HIS	CA-C-N	-9.89	100.58	121.64
1	A	325	HIS	C-N-CA	-9.89	100.58	121.64
1	A	538	GLY	CA-C-N	-9.87	108.66	122.87
1	A	538	GLY	C-N-CA	-9.87	108.66	122.87
1	A	410	ALA	N-CA-C	-9.78	100.31	110.97
1	A	277	PRO	N-CA-C	-9.55	92.88	111.69
4	P	27	ILE	N-CA-C	9.42	124.44	113.42
1	M	540	THR	N-CA-C	-9.37	102.94	114.75
1	A	229	VAL	O-C-N	-9.35	112.65	123.03
3	O	58	GLY	N-CA-C	-9.32	103.11	114.66
1	A	492	THR	N-CA-C	9.24	122.19	111.11
1	A	76	LEU	N-CA-C	-9.23	102.03	113.38
4	D	39	LEU	CA-C-N	-9.22	110.21	120.45
4	D	39	LEU	C-N-CA	-9.22	110.21	120.45
1	A	223	LEU	N-CA-C	-9.14	94.87	109.59
1	A	341	VAL	N-CA-C	8.96	122.30	107.24
1	M	487	LYS	N-CA-C	8.96	123.52	112.23
1	A	544	ASP	N-CA-C	-8.95	101.89	113.17
3	O	61	ASP	N-CA-C	-8.94	101.50	111.07
4	D	32	ILE	N-CA-C	-8.89	101.68	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	103	MET	N-CA-C	8.88	121.79	110.24
1	A	118	GLY	O-C-N	-8.85	112.86	122.41
3	C	1	THR	CA-C-N	-8.62	107.60	123.03
3	C	1	THR	C-N-CA	-8.62	107.60	123.03
1	A	321	GLU	N-CA-C	8.53	128.98	110.80
1	A	360	GLY	N-CA-C	8.52	123.49	110.88
1	A	266	TYR	N-CA-C	-8.52	99.96	110.61
4	P	93	VAL	CA-C-N	8.49	128.50	119.76
4	P	93	VAL	C-N-CA	8.49	128.50	119.76
1	A	465	ILE	CB-CA-C	-8.47	100.85	111.70
1	A	270	PRO	N-CA-C	-8.42	95.12	112.47
1	A	15	ALA	N-CA-C	8.38	120.10	110.97
4	P	48	ALA	N-CA-C	8.37	121.33	111.71
1	A	26	ALA	N-CA-C	-8.33	102.13	111.71
2	N	239	THR	N-CA-C	-8.31	102.17	113.30
4	P	4	ASN	CA-C-N	8.26	130.17	119.84
4	P	4	ASN	C-N-CA	8.26	130.17	119.84
1	A	269	GLY	C-N-CD	-8.26	91.12	125.00
1	A	120	LYS	CA-CB-CG	8.24	130.57	114.10
1	A	63	GLU	N-CA-C	-8.13	102.11	110.97
1	A	544	ASP	N-CA-CB	8.13	122.52	110.49
1	A	13	GLY	N-CA-C	-8.07	98.73	112.77
1	A	296	HIS	N-CA-C	-8.02	102.23	110.97
1	A	556	ASP	CA-C-N	-8.01	109.55	120.28
1	A	556	ASP	C-N-CA	-8.01	109.55	120.28
1	M	546	ASN	N-CA-C	7.95	121.47	111.69
4	P	72	VAL	N-CA-C	7.95	117.89	110.42
4	P	4	ASN	N-CA-C	-7.92	97.00	109.04
1	A	560	THR	N-CA-C	7.91	120.74	110.53
1	M	552	LEU	N-CA-C	7.91	118.99	108.07
1	M	396	LEU	N-CA-C	-7.91	102.27	112.23
1	A	370	ARG	NE-CZ-NH1	-7.87	113.63	121.50
1	A	391	LEU	CB-CA-C	-7.87	96.11	109.72
1	A	18	ARG	CG-CD-NE	-7.82	94.79	112.00
1	A	386	HIS	N-CA-C	7.82	122.64	113.18
1	A	1	GLN	N-CA-C	-7.79	96.55	109.24
1	A	446	GLU	CA-C-N	-7.69	106.85	121.54
1	A	446	GLU	C-N-CA	-7.69	106.85	121.54
1	A	494	THR	N-CA-C	-7.69	103.46	112.92
1	A	136	LEU	N-CA-C	-7.69	102.02	111.40
2	B	239	THR	N-CA-C	-7.67	103.72	113.23
1	A	286	PRO	CA-C-O	-7.66	112.97	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	LEU	N-CA-C	-7.65	102.59	112.23
3	O	13	SER	N-CA-C	-7.64	103.76	113.23
1	A	28	PRO	CA-C-N	-7.63	107.05	122.31
1	A	28	PRO	C-N-CA	-7.63	107.05	122.31
4	P	32	ILE	N-CA-C	-7.63	103.36	110.53
1	A	16	GLY	N-CA-C	-7.63	105.85	115.31
2	B	8	ILE	N-CA-C	7.63	119.58	109.21
1	A	555	ARG	CA-C-N	-7.62	109.14	122.64
1	A	555	ARG	C-N-CA	-7.62	109.14	122.64
2	N	146	SER	N-CA-C	-7.62	103.05	111.36
1	A	372	LYS	CB-CG-CD	7.61	128.79	111.30
3	C	2	THR	N-CA-C	-7.58	98.21	109.81
1	A	38	VAL	CA-C-O	-7.57	113.39	121.19
1	A	545	VAL	N-CA-CB	7.54	120.22	110.57
1	A	219	HIS	CA-CB-CG	-7.52	106.28	113.80
4	P	36	GLY	N-CA-C	7.52	121.22	112.50
1	A	276	GLU	O-C-N	7.51	129.96	121.32
3	C	97	ILE	N-CA-C	7.46	118.81	107.77
3	O	68	ILE	CA-C-N	-7.46	111.03	121.77
3	O	68	ILE	C-N-CA	-7.46	111.03	121.77
4	P	115	VAL	N-CA-C	7.46	118.19	110.36
1	A	233	PRO	N-CA-C	7.43	123.86	113.53
1	A	106	ARG	CB-CA-C	-7.43	97.24	108.61
1	A	381	SER	N-CA-C	7.43	120.70	109.41
3	O	128	LEU	N-CA-C	7.40	123.45	113.97
1	A	538	GLY	N-CA-C	-7.39	105.68	114.48
1	A	265	ASP	N-CA-C	7.35	119.27	110.44
4	P	8	SER	N-CA-C	7.33	120.85	110.23
1	A	401	VAL	CB-CA-C	-7.31	102.61	111.97
3	O	19	LEU	N-CA-C	7.30	119.10	109.83
1	A	30	ALA	N-CA-C	7.28	121.26	110.48
1	A	556	ASP	O-C-N	-7.27	113.27	122.43
1	A	488	ARG	CA-C-N	-7.25	112.92	122.99
1	A	488	ARG	C-N-CA	-7.25	112.92	122.99
2	B	15	PRO	CA-C-N	-7.23	108.49	121.14
2	B	15	PRO	C-N-CA	-7.23	108.49	121.14
1	A	206	GLY	N-CA-C	7.23	122.71	113.24
2	N	237	ILE	N-CA-C	-7.23	105.59	111.81
2	B	3	MET	N-CA-C	7.22	121.44	109.46
1	A	396	LEU	N-CA-C	-7.16	103.47	111.28
1	A	131	THR	N-CA-C	7.15	123.17	111.37
1	M	97	GLU	N-CA-C	-7.12	104.20	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	21	PHE	N-CA-C	-7.10	104.75	113.41
1	A	291	SER	N-CA-C	-7.10	101.82	112.04
1	A	573	LEU	N-CA-C	7.09	121.42	108.94
1	M	95	GLN	N-CA-C	-7.09	103.29	112.23
1	A	567	ASP	N-CA-C	7.08	120.49	110.50
2	N	226	GLN	N-CA-C	-7.08	104.79	113.50
1	A	547	PHE	N-CA-C	7.08	122.01	112.88
3	O	9	ARG	N-CA-C	7.04	120.01	110.29
1	A	306	THR	CA-C-N	6.99	127.95	120.47
1	A	306	THR	C-N-CA	6.99	127.95	120.47
1	A	366	ASN	CB-CA-C	-6.98	98.92	110.72
1	A	221	VAL	CA-C-N	-6.98	113.32	120.85
1	A	221	VAL	C-N-CA	-6.98	113.32	120.85
1	A	341	VAL	CA-C-O	6.96	127.14	120.31
3	O	97	ILE	CB-CA-C	-6.95	102.46	110.73
1	A	284	LEU	N-CA-C	-6.94	104.12	112.59
3	C	2	THR	CA-C-N	-6.90	111.60	122.65
3	C	2	THR	C-N-CA	-6.90	111.60	122.65
1	A	326	GLU	CB-CG-CD	-6.87	100.92	112.60
2	N	98	ILE	N-CA-C	6.86	113.55	106.21
1	A	192	THR	N-CA-C	-6.85	104.67	113.16
1	A	508	LEU	N-CA-C	-6.84	103.05	111.40
1	A	418	GLY	N-CA-C	-6.83	97.00	113.18
1	A	194	GLY	N-CA-C	6.83	129.35	113.18
3	C	117	VAL	CB-CA-C	-6.81	103.16	111.88
3	C	94	ALA	N-CA-C	-6.79	98.66	109.59
3	C	103	MET	N-CA-C	6.75	118.72	110.41
3	O	127	ALA	N-CA-C	6.74	119.46	111.71
2	B	76	ALA	N-CA-C	-6.73	103.14	111.75
1	A	302	ASN	N-CA-C	6.72	121.70	112.90
1	A	401	VAL	N-CA-C	6.70	116.85	110.42
3	C	59	PHE	N-CA-C	-6.68	103.61	111.03
1	A	557	ALA	N-CA-C	6.68	118.56	111.28
1	A	285	GLY	CA-C-N	6.67	127.07	119.93
1	A	285	GLY	C-N-CA	6.67	127.07	119.93
2	B	163	LEU	N-CA-C	-6.67	105.70	114.31
1	A	574	PRO	CB-CA-C	6.67	119.06	110.92
3	O	54	GLU	N-CA-C	-6.67	103.94	111.07
3	O	99	LYS	N-CA-C	-6.65	96.84	108.08
1	A	276	GLU	CB-CA-C	-6.62	97.12	110.17
1	A	376	ALA	CA-C-N	-6.62	112.78	122.58
1	A	376	ALA	C-N-CA	-6.62	112.78	122.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	23	SER	N-CA-C	6.61	118.54	110.41
4	P	10	GLU	N-CA-C	6.60	124.40	109.81
1	A	9	ILE	N-CA-C	6.60	116.91	106.88
1	A	3	PHE	N-CA-C	-6.58	97.88	108.55
2	B	46	ASN	N-CA-C	6.58	123.59	113.19
2	B	66	GLY	N-CA-C	6.56	119.04	111.36
1	M	190	MET	N-CA-C	6.56	119.02	107.61
1	A	68	ASP	CB-CA-C	-6.55	99.86	110.74
1	A	146	PHE	CA-C-N	-6.55	113.06	119.87
1	A	146	PHE	C-N-CA	-6.55	113.06	119.87
1	A	76	LEU	CA-C-N	-6.53	111.59	120.87
1	A	76	LEU	C-N-CA	-6.53	111.59	120.87
1	A	113	VAL	CB-CA-C	6.53	120.31	110.90
1	A	197	ARG	CA-C-N	-6.51	110.25	121.97
1	A	197	ARG	C-N-CA	-6.51	110.25	121.97
1	M	356	TYR	N-CA-C	6.51	118.42	110.41
2	B	154	CYS	N-CA-C	-6.49	104.29	111.36
3	O	37	TRP	N-CA-C	-6.46	104.24	111.28
1	A	563	LEU	N-CA-C	6.46	120.43	110.42
1	M	245	GLU	N-CA-C	-6.45	105.27	113.01
1	A	517	CYS	N-CA-CB	-6.45	99.89	110.40
1	M	249	GLY	N-CA-C	6.43	121.67	113.24
1	M	105	ARG	N-CA-C	6.42	119.66	109.65
2	N	227	GLY	N-CA-C	-6.38	106.75	114.66
1	A	352	PRO	O-C-N	-6.37	115.22	123.00
1	A	312	VAL	N-CA-C	-6.37	96.09	109.34
1	A	329	PRO	N-CA-C	6.35	125.55	112.47
4	P	47	ASP	N-CA-C	6.35	120.73	112.92
1	A	573	LEU	CA-C-N	6.33	126.90	120.38
1	A	573	LEU	C-N-CA	6.33	126.90	120.38
1	A	160	ILE	CB-CA-C	-6.31	104.64	111.59
1	A	189	VAL	N-CA-C	-6.28	99.38	108.36
1	A	273	PRO	CB-CA-C	-6.26	103.22	111.23
1	M	398	GLU	N-CA-C	-6.25	104.91	112.54
2	B	191	ARG	N-CA-C	6.22	121.15	113.50
1	A	269	GLY	CA-C-O	6.22	130.41	121.52
2	B	231	SER	N-CA-C	-6.20	103.45	111.02
1	A	63	GLU	CA-C-O	-6.20	114.49	121.00
3	O	104	GLY	CA-C-N	6.20	127.58	119.84
3	O	104	GLY	C-N-CA	6.20	127.58	119.84
1	A	431	GLY	CA-C-N	-6.18	111.81	120.53
1	A	431	GLY	C-N-CA	-6.18	111.81	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	445	GLY	N-CA-C	6.18	127.83	113.18
2	B	13	TYR	CA-CB-CG	-6.18	102.78	113.90
1	A	486	PHE	CA-C-O	6.17	126.97	119.38
1	M	75	TRP	N-CA-C	6.17	120.07	111.74
1	A	88	HIS	CA-C-N	-6.17	112.71	120.06
1	A	88	HIS	C-N-CA	-6.17	112.71	120.06
1	A	330	PHE	CB-CA-C	6.17	121.15	110.79
1	A	571	THR	CA-C-N	-6.17	112.27	122.08
1	A	571	THR	C-N-CA	-6.17	112.27	122.08
1	A	234	THR	N-CA-C	6.16	120.79	107.49
1	A	239	SER	CB-CA-C	-6.16	100.38	110.85
1	A	161	LEU	CA-CB-CG	-6.15	94.78	116.30
2	B	54	ARG	N-CA-C	6.15	119.26	109.24
1	A	517	CYS	CB-CA-C	6.15	122.84	109.99
4	P	53	ARG	N-CA-C	6.14	119.25	111.69
1	A	448	TRP	CB-CA-C	-6.14	98.21	110.42
1	A	559	GLY	CA-C-O	-6.13	112.54	119.04
2	B	13	TYR	O-C-N	-6.13	117.37	123.62
1	A	474	LYS	N-CA-C	-6.13	104.68	111.36
3	C	14	THR	N-CA-C	-6.13	105.90	113.19
1	M	478	LYS	N-CA-C	-6.12	105.97	113.50
1	A	222	PRO	N-CA-C	6.10	121.89	111.03
3	C	21	PHE	N-CA-C	-6.10	106.37	113.88
1	M	27	ASN	CA-C-N	6.09	125.98	119.28
1	M	27	ASN	C-N-CA	6.09	125.98	119.28
3	C	13	SER	N-CA-C	-6.09	105.68	113.23
2	B	30	TYR	N-CA-C	6.08	117.79	108.42
2	N	38	ASP	N-CA-C	-6.08	104.57	111.14
2	B	25	PHE	N-CA-C	6.08	118.30	108.34
1	M	169	GLY	N-CA-C	6.08	122.60	111.12
1	A	519	ALA	CA-C-N	-6.07	111.67	120.29
1	A	519	ALA	C-N-CA	-6.07	111.67	120.29
1	A	195	ALA	N-CA-C	6.07	120.71	112.88
1	A	277	PRO	CB-CA-C	-6.06	100.61	110.25
1	A	514	VAL	CB-CA-C	-6.06	104.10	112.04
1	A	326	GLU	CA-C-O	6.06	127.39	120.00
1	A	383	VAL	N-CA-C	-6.06	103.52	111.09
3	O	52	GLY	CA-C-N	6.05	127.41	119.84
3	O	52	GLY	C-N-CA	6.05	127.41	119.84
1	M	114	ARG	CB-CA-C	-6.05	108.36	117.07
1	A	566	SER	N-CA-C	-6.04	100.34	109.95
2	N	133	ILE	N-CA-C	6.04	116.40	107.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	PHE	N-CA-C	-6.02	104.06	111.40
2	B	240	LEU	N-CA-C	-6.02	105.59	113.17
1	M	431	GLY	N-CA-C	-6.02	105.52	112.50
1	A	119	MET	CA-C-N	6.00	130.73	120.71
1	A	119	MET	C-N-CA	6.00	130.73	120.71
1	A	442	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	A	311	VAL	CB-CA-C	-5.98	101.48	111.29
1	M	21	ILE	N-CA-C	5.97	116.15	110.42
3	O	126	VAL	N-CA-C	-5.97	104.81	110.42
1	A	380	CYS	N-CA-C	-5.96	105.99	113.20
1	A	272	THR	CA-C-N	5.95	125.91	119.78
1	A	272	THR	C-N-CA	5.95	125.91	119.78
1	A	304	ILE	CB-CA-C	-5.95	102.75	110.84
1	A	453	ASP	N-CA-CB	5.95	118.87	110.12
2	B	241	LYS	N-CA-C	5.95	122.96	109.81
1	A	307	PRO	N-CA-C	-5.95	104.64	114.75
4	D	53	ARG	N-CA-C	5.94	117.56	111.14
1	A	345	LYS	N-CA-C	5.93	120.68	113.38
2	B	88	MET	N-CA-C	5.93	117.92	107.61
1	A	544	ASP	CA-C-N	-5.92	112.98	120.56
1	A	544	ASP	C-N-CA	-5.92	112.98	120.56
1	A	522	ALA	N-CA-C	5.92	117.40	111.07
1	M	378	GLY	N-CA-C	5.91	118.01	110.20
3	O	15	TRP	N-CA-C	5.91	118.23	111.02
1	A	149	ILE	CB-CA-C	-5.91	102.38	110.77
4	P	10	GLU	CA-C-N	-5.90	114.22	120.94
4	P	10	GLU	C-N-CA	-5.90	114.22	120.94
2	B	129	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	M	72	GLY	N-CA-C	-5.89	105.48	113.37
1	M	361	ILE	N-CA-C	5.88	116.41	108.17
3	C	128	LEU	N-CA-C	5.88	121.12	113.88
1	A	326	GLU	N-CA-C	5.88	120.62	112.45
1	A	448	TRP	N-CA-CB	5.87	120.41	110.49
1	A	558	ASP	CA-CB-CG	-5.87	106.73	112.60
1	A	459	MET	CA-C-N	5.87	128.14	120.28
1	A	459	MET	C-N-CA	5.87	128.14	120.28
4	D	108	THR	N-CA-C	-5.86	105.02	111.82
4	P	59	GLN	N-CA-C	5.85	119.68	112.54
1	A	180	LEU	CB-CA-C	-5.84	100.60	110.19
2	N	214	CYS	CA-C-N	5.84	125.71	119.28
2	N	214	CYS	C-N-CA	5.84	125.71	119.28
1	A	32	ILE	CB-CA-C	-5.84	103.67	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	ASN	CA-C-N	5.83	127.13	119.84
4	D	2	ASN	C-N-CA	5.83	127.13	119.84
1	A	79	GLN	N-CA-C	5.83	117.71	111.36
1	A	375	PHE	CA-C-N	-5.83	113.29	122.73
1	A	375	PHE	C-N-CA	-5.83	113.29	122.73
1	M	55	VAL	N-CA-C	5.82	115.92	108.12
3	O	97	ILE	N-CA-C	5.82	117.01	107.24
1	M	114	ARG	CA-C-O	5.81	121.31	117.94
4	D	56	ALA	CA-C-N	5.80	128.86	120.79
4	D	56	ALA	C-N-CA	5.80	128.86	120.79
4	P	64	ARG	N-CA-C	-5.79	102.70	111.56
1	A	32	ILE	N-CA-C	5.78	116.91	108.58
4	D	44	PHE	CA-C-N	5.78	127.07	119.84
4	D	44	PHE	C-N-CA	5.78	127.07	119.84
1	M	106	ARG	CA-C-N	5.78	127.07	119.84
1	M	106	ARG	C-N-CA	5.78	127.07	119.84
1	A	61	SER	CB-CA-C	-5.78	98.92	110.42
1	A	17	LEU	N-CA-C	-5.77	103.73	112.04
1	A	277	PRO	CA-N-CD	-5.76	103.93	112.00
4	P	92	HIS	N-CA-C	5.76	117.68	108.41
4	D	41	LEU	N-CA-C	-5.75	106.11	113.02
1	A	243	MET	N-CA-C	-5.75	99.36	108.73
4	D	35	VAL	N-CA-C	5.73	117.16	110.62
1	A	141	GLN	CB-CG-CD	5.73	122.34	112.60
1	A	49	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	A	188	VAL	CA-C-N	-5.70	115.75	122.93
1	A	188	VAL	C-N-CA	-5.70	115.75	122.93
1	A	560	THR	CB-CA-C	-5.69	98.63	110.40
2	B	11	VAL	N-CA-C	5.69	116.60	107.73
3	C	19	LEU	N-CA-C	5.69	117.86	109.50
3	C	52	GLY	CA-C-N	5.68	126.94	119.84
3	C	52	GLY	C-N-CA	5.68	126.94	119.84
1	A	428	GLN	OE1-CD-NE2	-5.66	116.94	122.60
1	A	424	ALA	CA-C-N	5.66	128.18	120.77
1	A	424	ALA	C-N-CA	5.66	128.18	120.77
1	A	486	PHE	N-CA-CB	-5.66	101.00	110.39
1	M	467	ARG	N-CA-C	5.65	117.26	107.93
1	M	405	LEU	N-CA-C	-5.65	106.93	113.88
4	P	86	MET	N-CA-C	-5.65	104.59	112.45
3	O	94	ALA	N-CA-C	-5.65	99.20	108.41
1	A	74	ASP	N-CA-C	5.64	119.48	111.92
1	A	424	ALA	O-C-N	5.64	128.12	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	68	PHE	N-CA-C	-5.64	104.83	110.97
2	B	104	VAL	N-CA-C	5.63	117.53	108.85
2	B	24	ALA	CA-C-N	-5.62	114.84	122.77
2	B	24	ALA	C-N-CA	-5.62	114.84	122.77
1	M	566	SER	N-CA-C	5.62	117.66	108.55
1	A	545	VAL	CA-C-O	-5.62	114.81	121.05
2	B	128	ASP	N-CA-C	-5.62	105.25	111.71
3	O	47	PHE	N-CA-C	5.62	119.39	112.54
1	A	465	ILE	N-CA-C	5.61	116.06	110.23
2	B	169	GLY	N-CA-C	5.60	123.77	112.34
4	D	72	VAL	N-CA-C	5.59	120.98	109.34
1	A	274	LEU	N-CA-C	-5.59	105.09	111.07
1	A	406	ALA	N-CA-C	-5.58	104.04	111.24
3	O	89	LEU	N-CA-C	5.58	120.09	113.12
1	A	4	GLN	N-CA-C	-5.57	101.09	109.95
1	A	182	GLN	CA-C-N	-5.57	115.91	122.93
1	A	182	GLN	C-N-CA	-5.57	115.91	122.93
1	M	370	ARG	N-CA-C	5.57	117.82	111.02
1	A	113	VAL	N-CA-CB	-5.57	103.11	112.47
1	A	535	LEU	CA-C-N	-5.56	112.82	120.71
1	A	535	LEU	C-N-CA	-5.56	112.82	120.71
3	O	115	VAL	CB-CA-C	-5.55	104.65	112.14
1	A	49	GLN	N-CA-C	5.54	120.53	113.55
1	A	103	TRP	CA-C-O	-5.54	115.46	121.44
1	M	225	ASP	N-CA-C	5.54	119.62	112.86
1	A	447	ASN	CA-C-N	-5.53	110.97	121.54
1	A	447	ASN	C-N-CA	-5.53	110.97	121.54
1	A	355	HIS	N-CA-C	5.53	122.57	110.80
1	A	326	GLU	CA-C-N	5.52	131.03	122.26
1	A	326	GLU	C-N-CA	5.52	131.03	122.26
1	A	329	PRO	N-CA-CB	-5.52	97.45	103.25
2	N	157	ALA	N-CA-C	-5.52	104.67	111.40
1	A	497	VAL	N-CA-C	5.51	116.42	106.61
2	B	78	LYS	N-CA-C	5.51	117.05	110.44
2	B	233	LYS	N-CA-C	-5.51	105.43	111.82
1	A	484	GLU	N-CA-C	-5.50	104.69	111.40
1	A	209	THR	N-CA-C	5.50	120.67	113.30
1	A	265	ASP	CB-CA-C	-5.50	99.24	111.77
4	D	66	PHE	N-CA-C	5.50	117.71	111.11
1	A	365	GLN	OE1-CD-NE2	-5.49	117.11	122.60
2	N	206	PHE	N-CA-C	5.49	119.14	111.74
1	M	533	GLN	N-CA-C	5.48	117.15	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	ARG	NE-CZ-NH1	-5.48	116.02	121.50
2	B	16	GLU	CA-CB-CG	5.47	125.05	114.10
2	N	33	THR	N-CA-C	-5.47	105.97	113.30
2	B	121	ILE	N-CA-C	5.44	115.79	108.17
1	A	126	PHE	N-CA-C	5.44	117.36	108.76
2	B	132	ASN	CA-C-N	-5.44	114.52	122.68
2	B	132	ASN	C-N-CA	-5.44	114.52	122.68
1	A	118	GLY	CA-C-N	-5.43	111.16	122.07
1	A	118	GLY	C-N-CA	-5.43	111.16	122.07
1	M	430	ALA	N-CA-C	-5.42	105.80	112.90
3	O	108	ILE	CB-CA-C	-5.42	105.03	111.81
1	A	172	ALA	N-CA-C	5.42	117.31	109.07
1	A	244	THR	N-CA-C	5.42	118.14	110.50
1	A	304	ILE	N-CA-C	5.42	116.11	108.36
3	C	22	TYR	N-CA-C	-5.41	105.03	111.69
1	A	46	VAL	CB-CA-C	-5.41	104.75	112.22
1	A	185	ALA	CA-C-O	-5.41	115.49	121.33
2	B	203	SER	N-CA-C	-5.40	106.28	112.92
1	A	248	ARG	CG-CD-NE	-5.39	100.15	112.00
2	B	222	ALA	N-CA-C	-5.39	105.44	112.23
1	M	366	ASN	N-CA-C	-5.39	104.98	112.30
1	A	150	GLN	N-CA-CB	-5.38	101.54	110.47
1	A	254	LEU	N-CA-CB	5.37	119.20	110.77
1	A	233	PRO	N-CD-CG	-5.37	95.15	103.20
1	A	268	MET	O-C-N	5.36	128.86	122.21
2	N	203	SER	N-CA-C	-5.36	106.12	113.30
1	A	208	VAL	CA-C-N	-5.36	114.19	122.49
1	A	208	VAL	C-N-CA	-5.36	114.19	122.49
1	A	521	SER	CA-CB-OG	-5.36	100.39	111.10
2	B	132	ASN	N-CA-C	-5.36	102.06	110.36
1	M	412	GLU	N-CA-C	-5.35	106.72	113.20
2	B	98	ILE	N-CA-C	5.35	116.59	109.37
2	N	189	LYS	N-CA-C	5.35	122.19	110.80
1	A	487	LYS	N-CA-C	-5.34	106.72	113.18
1	A	344	VAL	N-CA-C	5.34	116.60	112.12
3	C	70	ILE	CB-CA-C	-5.33	104.90	111.94
1	A	87	HIS	CA-C-N	-5.33	113.74	122.54
1	A	87	HIS	C-N-CA	-5.33	113.74	122.54
3	O	22	TYR	N-CA-C	-5.33	104.90	111.40
2	B	113	LEU	N-CA-C	-5.33	104.88	111.33
2	B	201	VAL	CB-CA-C	-5.32	103.91	112.16
4	D	61	PHE	N-CA-C	5.32	122.14	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ASN	O-C-N	5.32	129.01	122.20
1	M	32	ILE	N-CA-C	5.32	117.04	108.85
4	P	71	ILE	N-CA-C	5.31	115.57	110.74
1	A	81	VAL	CB-CA-C	-5.29	105.11	111.88
1	A	429	ALA	N-CA-C	-5.29	104.93	111.33
1	A	174	ASN	N-CA-C	-5.29	102.09	109.96
4	D	4	ASN	CA-C-N	5.29	126.45	119.84
4	D	4	ASN	C-N-CA	5.29	126.45	119.84
3	O	73	LEU	N-CA-C	-5.28	105.43	111.14
2	B	14	ASN	CA-CB-CG	5.28	117.88	112.60
1	A	536	ASP	O-C-N	5.28	129.36	122.87
2	B	143	HIS	N-CA-C	5.27	120.02	111.37
1	A	286	PRO	N-CA-C	5.26	119.83	111.26
1	A	542	ARG	N-CA-C	-5.26	101.89	110.20
1	A	219	HIS	CB-CA-C	-5.25	102.48	111.46
1	A	215	MET	N-CA-C	-5.25	105.03	111.75
1	A	77	CYS	CB-CA-C	-5.24	100.69	109.65
1	A	452	ARG	N-CA-C	5.24	117.40	111.11
1	A	453	ASP	CB-CA-C	-5.24	102.10	110.79
1	A	113	VAL	N-CA-C	5.24	117.16	108.99
1	A	130	LYS	CG-CD-CE	5.22	123.31	111.30
1	A	39	TYR	N-CA-CB	5.22	118.17	109.98
1	A	163	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	36	SER	O-C-N	-5.21	117.84	123.42
1	A	93	MET	N-CA-CB	5.20	117.94	110.20
4	P	73	LEU	CA-C-N	-5.19	114.26	119.56
4	P	73	LEU	C-N-CA	-5.19	114.26	119.56
1	A	509	GLY	CA-C-N	-5.19	113.69	120.44
1	A	509	GLY	C-N-CA	-5.19	113.69	120.44
1	A	343	PRO	N-CA-C	5.19	123.16	112.47
2	B	103	VAL	N-CA-C	5.18	115.37	108.11
1	A	308	ARG	N-CA-C	-5.18	106.47	112.89
2	B	200	GLY	N-CA-C	-5.17	105.11	112.55
1	A	451	ILE	CA-C-N	-5.17	113.57	120.54
1	A	451	ILE	C-N-CA	-5.17	113.57	120.54
1	A	555	ARG	O-C-N	-5.17	116.59	122.89
1	A	167	VAL	N-CA-C	-5.16	100.97	108.97
1	A	358	MET	N-CA-C	-5.16	106.25	112.54
2	B	74	LYS	N-CA-C	5.16	115.86	108.74
1	A	207	ILE	CB-CG1-CD1	5.16	124.63	113.80
1	A	151	ARG	NE-CZ-NH1	-5.15	116.35	121.50
2	B	99	GLU	N-CA-C	-5.15	105.83	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	16	LEU	N-CA-C	-5.14	105.12	111.40
1	A	111	VAL	N-CA-C	5.14	116.15	108.54
3	C	3	LYS	N-CA-C	-5.14	106.60	112.92
1	M	394	ASN	N-CA-C	5.14	121.74	110.80
1	A	164	ASP	N-CA-CB	-5.14	104.10	111.91
1	A	390	ARG	CA-C-O	-5.14	115.96	121.56
1	A	116	PHE	N-CA-C	5.12	117.03	108.99
4	D	27	ILE	N-CA-C	5.12	120.79	113.16
4	D	73	LEU	CA-C-N	-5.12	113.44	119.84
4	D	73	LEU	C-N-CA	-5.12	113.44	119.84
1	A	554	PHE	CA-C-O	-5.12	114.81	120.24
3	C	130	TRP	N-CA-C	5.12	125.32	111.00
1	M	547	PHE	N-CA-C	5.10	121.67	110.80
1	A	245	GLU	N-CA-CB	5.10	118.08	110.22
2	B	225	GLN	CB-CA-C	-5.10	102.87	110.88
1	A	122	GLU	N-CA-C	5.10	117.69	110.50
1	A	39	TYR	N-CA-C	-5.10	103.17	109.64
1	A	186	ASN	N-CA-CB	5.10	119.53	111.17
1	A	476	ILE	CB-CA-C	-5.10	105.44	111.81
1	A	268	MET	CA-C-N	-5.09	113.88	121.87
1	A	268	MET	C-N-CA	-5.09	113.88	121.87
1	A	257	LYS	N-CA-CB	5.09	118.05	110.22
1	A	276	GLU	N-CA-C	5.09	121.05	109.81
1	A	370	ARG	CD-NE-CZ	-5.08	117.29	124.40
1	M	146	PHE	CA-C-N	5.08	126.18	119.84
1	M	146	PHE	C-N-CA	5.08	126.18	119.84
1	A	101	CYS	N-CA-C	-5.07	103.65	109.93
1	A	482	LEU	N-CA-C	-5.07	105.65	111.07
1	M	227	GLU	N-CA-C	5.06	121.59	110.80
1	A	70	VAL	CB-CA-C	-5.05	105.36	111.87
1	A	385	LEU	N-CA-C	-5.04	105.25	111.40
1	A	412	GLU	CG-CD-OE2	-5.04	106.80	118.40
1	A	489	VAL	N-CA-C	-5.04	100.86	108.12
1	A	390	ARG	N-CA-C	-5.04	103.40	110.50
1	M	142	THR	N-CA-C	-5.03	107.82	114.31
1	M	354	ALA	N-CA-C	5.03	116.95	109.25
1	A	507	GLU	CB-CA-C	-5.03	101.33	110.63
3	C	125	PHE	N-CA-C	-5.03	105.90	112.23
3	C	14	THR	CB-CA-C	-5.02	100.52	110.27
1	M	262	TYR	N-CA-C	5.01	118.86	112.34
1	M	57	GLN	N-CA-C	5.01	114.77	108.45
1	A	457	LEU	CB-CA-C	5.00	119.20	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	SER	N-CA-CB	-5.00	102.92	110.92

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	484	0
1	M	4414	0	4300	785	0
2	B	1888	0	1837	184	0
2	N	1888	0	1837	334	0
3	C	1058	0	1108	129	0
3	O	1058	0	1108	141	0
4	D	926	0	971	147	0
4	P	926	0	971	136	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	13	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
9	N	8	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	33	0	37	7	0
10	P	33	0	37	11	0
All	All	16840	0	16611	2214	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 66.

All (2214) 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:C8M	1.81	1.42
1:A:44:HIS:NE2	6:A:703:FAD:HM82	1.06	1.39
1:A:44:HIS:NE2	6:A:703:FAD:C8M	1.86	1.36
1:A:27:ASN:C	1:A:27:ASN:HD22	1.35	1.21
1:M:44:HIS:NE2	6:M:803:FAD:HM82	0.88	1.20
1:A:253:ILE:HG22	1:A:315:ASP:CB	1.72	1.18
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:236:LEU:HD21	1:A:243:MET:HE2	1.21	1.14
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:261:ARG:NH1	1:A:282:MET:HE3	1.66	1.10
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:A:261:ARG:HH11	1:A:282:MET:HE3	1.18	1.06
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ARG:NH1	1:A:92:GLU:OE1	1.88	1.05
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:A:44:HIS:CD2	6:A:703:FAD:HM82	1.94	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
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:115:ARG:HH11	1:A:115:ARG:HG3	1.24	0.96
1:A:236:LEU:HD21	1:A:243:MET:CE	1.95	0.96
1:A:253:ILE:CG2	1:A:315:ASP:CB	2.39	0.96
1:A:27:ASN:C	1:A:27:ASN:ND2	2.09	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
1:M:44:HIS:CD2	6:M:803:FAD:HM82	1.99	0.95
1:A:263:LEU:HB3	1:A:268:MET:HE3	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:M:44:HIS:CE1	6:M:803:FAD:HM82	2.02	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:M:273:PRO:HG2	1:M:276:GLU:HB2	1.49	0.92
1:A:236:LEU:CD2	1:A:243:MET:HE2	2.00	0.91
3:O:4:ARG:NE	3:O:6:PRO:HG3	1.86	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
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
1:A:44:HIS:CE1	6:A:703:FAD:HM82	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:263:LEU:CB	1:A:268:MET:HE3	2.03	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
1:M:391:LEU:HG	1:M:392:GLY:N	1.86	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
2:N:68:MET:HE1	2:N:73:PRO:HB3	1.57	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: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:A:261:ARG:HH11	1:A:282:MET:CE	1.88	0.84
2:B:50:ASP:C	2:B:50:ASP:OD1	2.19	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
1:M:242:LEU:C	1:M:242:LEU:HD23	2.03	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:M:243:MET:HE2	1:M:348:ILE:HG21	1.61	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
2:B:97:PRO:C	2:B:104:VAL:HG23	2.05	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
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:A:198:VAL:HG23	1:A:455:MET:HE3	1.61	0.80
1:M:180:LEU:HD13	1:M:433:GLU:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:N:106:MET:HE3	2:N:109:PHE:CD2	2.17	0.80
1:A:155:HIS:CD2	1:A:174:ASN:HA	2.17	0.80
1:A:103:TRP:O	2:B:139:MET:HE1	1.81	0.79
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: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
1:A:282:MET:HE3	1:A:283:GLU:OE1	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:MET:HE3	1:A:348:ILE:HD12	1.64	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
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:41:MET:HE2	2:B:150:ASN:HD22	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:227:GLU:CG	1:M:518:MET:HB3	2.15	0.76
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
2:N:241:LYS:C	2:N:243:ARG:H	1.94	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
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
2:B:4:LYS:HB2	2:B:4:LYS:HZ2	1.52	0.74
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
2:N:144:GLN:HG3	3:O:102:LYS:HZ2	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
1:A:436:LEU:HD23	1:A:436:LEU:C	2.14	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:295:TRP:CD1	1:M:299:ARG:HE	2.08	0.71
1:M:399:LEU:HD21	6:M:803:FAD:H5'2	1.71	0.71
2:B:105:ASP:C	2:B:105:ASP:OD1	2.32	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
4:D:50:SER:O	4:D:51:TYR:C	2.34	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:166:HIS:HD2	1:M:413:ARG:HH21	1.39	0.71
1:A:529:ARG:O	1:A:530:GLY:C	2.34	0.70
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
2:N:235:PHE:C	2:N:237:ILE:H	1.98	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
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
2:B:65:CYS:O	2:B:67:MET:HE3	1.91	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
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
2:B:68:MET:HE3	2:B:72:VAL:O	1.92	0.70
3:C:48:ALA:C	3:C:50:LYS:H	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:36:GLY:C	4:D:37:ILE:HD12	2.18	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:455:MET:HE1	1:M:508:LEU:HD21	1.76	0.68
1:M:22:ALA:HB2	1:M:404:ARG:HA	1.74	0.68
1:M:264:GLN:HB3	1:M:282:MET:HE1	1.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:27:ASN:ND2	1:A:30:ALA:N	2.42	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
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:4:LYS:C	2:N:5:ASN:HD22	2.02	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
2:N:192:MET:O	2:N:193:ALA:C	2.38	0.67
1:A:262:TYR:CE1	1:A:263:LEU:HD23	2.30	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
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
4:P:23:TRP:HE1	4:P:70:MET:HE3	1.59	0.66
2:N:75:LEU:HD21	2:N:215:PRO:CB	2.23	0.66
2:N:144:GLN:HG3	3:O:102:LYS:HZ1	1.60	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:455:MET:HE2	1:M:482:LEU:HD13	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:A:447:ASN:O	1:A:448:TRP:C	2.36	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
4:P:23:TRP:C	4:P:23:TRP:CD1	2.74	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:48:ALA:C	3:O:50:LYS:H	2.03	0.65
3:O:50:LYS:CE	4:P:118:ILE:HG22	2.22	0.65
1:A:441:ASN:O	1:A:442:GLN:C	2.37	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:A:545:VAL:HG12	1:A:546:ASN:CG	2.20	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
1:A:198:VAL:CG2	1:A:455:MET:HE3	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:56:ALA:C	1:M:57:GLN:HG2	2.21	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
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
4:P:32:ILE:O	4:P:33:LEU:C	2.38	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
2:N:239:THR:C	2:N:240:LEU:HD23	2.22	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
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
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:212:GLY:HA2	1:M:215:MET:HE2	1.78	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
2:N:241:LYS:C	2:N:243:ARG:N	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:214:GLY:HA3	1:M:510:HIS:HB3	1.81	0.63
2:N:68:MET:HE3	2:N:93:LEU:HD12	1.80	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
2:B:67:MET:CE	2:B:76:ALA:HB2	2.29	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
4:P:113:ILE:O	4:P:114:GLY:C	2.42	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:213:MET:HE1	1:A:357:THR:HG21	1.79	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
1:M:403:GLY:HA2	1:M:406:ALA:CB	2.27	0.63
1:M:537:GLU:H	1:M:537:GLU:CD	2.06	0.63
4:D:23:TRP:C	4:D:25:ALA:H	2.06	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:68:MET:HE3	2:B:72:VAL:C	2.24	0.62
1:M:83:ASP:O	1:M:87:HIS:ND1	2.33	0.62
1:M:147:PRO:C	1:M:149:ILE:H	2.07	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
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
4:D:87:HIS:C	4:D:89:LEU:H	2.07	0.62
1:M:92:GLU:CD	1:M:400:VAL:HG12	2.25	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
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
4:D:9:ASP:C	4:D:11:PRO:HD2	2.24	0.62
1:M:53:ALA:H	1:M:394:ASN:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:149:ILE:O	2:N:150:ASN:C	2.42	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
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
2:B:31:ASP:C	2:B:31:ASP:OD2	2.43	0.61
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
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: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:151:ARG:HH12	1:M:153:ASP:CG	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:263:LEU:HB2	1:A:268:MET:HE3	1.83	0.60
2:B:26:TYR:CD2	2:B:47:LEU:CD1	2.85	0.60
2:B:68:MET:CE	2:B:72:VAL:C	2.74	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: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
1:A:324:LEU:C	1:A:326:GLU:N	2.56	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:M:72:GLY:HA3	1:M:391:LEU:CD2	2.20	0.60
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:A:44:HIS:CD2	6:A:703:FAD:C8M	2.69	0.60
2:B:67:MET:HE3	2:B:76:ALA:HB2	1.84	0.60
1:M:55:VAL:HG22	1:M:65:HIS:HD2	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:GLN:NE2	1:A:3:PHE:CZ	2.69	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:57:GLN:C	1:M:60:ASP:OD1	2.45	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
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
1:A:65:HIS:HD1	1:A:86:VAL:HG22	1.67	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
2:N:54:ARG:C	2:N:55:TRP:CD1	2.81	0.59
4:D:67:LEU:HD13	10:D:700:MQ7:H6	1.83	0.59
1:M:52:SER:C	1:M:125:TRP:HB2	2.27	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
1:A:429:ALA:O	1:A:430:ALA:C	2.45	0.59
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
2:N:106:MET:HE3	2:N:109:PHE:HD2	1.67	0.59
4:D:113:ILE:O	4:D:114:GLY:C	2.45	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
1:M:225:ASP:O	1:M:225:ASP:CG	2.44	0.59
2:B:75:LEU:C	2:B:77:CYS:N	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:135:THR:C	2:B:137:ALA:N	2.58	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:B:75:LEU:C	2:B:77:CYS:H	2.06	0.59
1:M:276:GLU:O	1:M:277:PRO:C	2.44	0.59
2:N:154:CYS:C	2:N:156:ALA:H	2.10	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:M:175:MET:HE3	1:M:503:LEU:CD1	2.33	0.58
2:N:175:LEU:O	2:N:176:ALA:C	2.44	0.58
3:O:50:LYS:C	3:O:52:GLY:H	2.11	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
2:B:241:LYS:O	2:B:242:PRO:C	2.46	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
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
1:A:91:THR:HG22	1:A:92:GLU:N	2.17	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:51:LEU:C	2:N:51:LEU:HD12	2.28	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
1:A:106:ARG:O	1:A:107:PRO:C	2.45	0.58
4:D:87:HIS:C	4:D:89:LEU:N	2.59	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:54:ALA:H	1:M:125:TRP:CD1	2.21	0.58
1:M:216:ALA:O	1:M:217:LEU:C	2.47	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: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
2:N:44:LYS:C	2:N:46:ASN:H	2.10	0.58
2:N:70:ASN:C	2:N:72:VAL:H	2.11	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
2:N:219:ASP:CG	2:N:222:ALA:HB3	2.29	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:A:273:PRO:HG2	1:A:276:GLU:HB2	1.85	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
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
1:A:224:ARG:HB2	1:A:552:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:ALA:HA	4:D:70:MET:HE1	1.85	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
2:N:235:PHE:C	2:N:237:ILE:N	2.62	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:110:SER:O	1:M:111:VAL:C	2.47	0.57
1:M:194:GLY:N	1:M:208:VAL:CG1	2.67	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:227:GLU:HB2	1:M:518:MET:C	2.30	0.57
1:M:256:ASN:HD22	1:M:262:TYR:HB3	1.69	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:A:417:ALA:C	1:A:418:GLY:O	2.40	0.57
1:M:363:THR:HB	1:M:367:CYS:C	2.30	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:211:ASP:CG	1:M:507:GLU:HA	2.30	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
1:M:40:PRO:HG3	1:M:140:PHE:CE1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:79:GLN:CD	1:M:570:ILE:HG23	2.30	0.56
2:N:112:SER:O	2:N:116:ILE:HG23	2.05	0.56
4:P:50:SER:O	4:P:51:TYR:C	2.48	0.56
1:A:102:PRO:O	1:A:103:TRP:C	2.48	0.56
1:A:230:GLN:NE2	1:A:287:ARG:HE	2.03	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:357:THR:HB	1:M:518:MET:HE1	1.87	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:M:469:PRO:O	1:M:523:MET:HE1	2.06	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
1:M:162:VAL:HG12	1:M:163:ASP:N	2.20	0.56
2:N:68:MET:CE	2:N:73:PRO:HB3	2.33	0.56
3:O:28:ARG:O	3:O:31:THR:HB	2.06	0.56
1:A:410:ALA:O	1:A:411:THR:C	2.47	0.56
2:B:180:ASN:HD21	2:B:188:LYS:HG3	1.68	0.56
1:M:58:ASP:C	1:M:60:ASP:H	2.13	0.56
1:M:78:GLU:C	1:M:80:ASP:H	2.11	0.56
4:P:66:PHE:C	4:P:66:PHE:CD2	2.84	0.56
1:A:416:THR:O	1:A:416:THR:HG22	2.01	0.56
3:C:123:ILE:HG23	10:D:700:MQ7:H161	1.88	0.56
1:M:295:TRP:CD1	1:M:295:TRP:C	2.83	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:A:493:ASP:CG	1:A:499:ASN:ND2	2.64	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:31:ASP:CG	2:N:32:ALA:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:252:GLY:O	1:M:283:GLU:HG2	2.06	0.55
2:N:162:GLY:O	3:O:11:MET:HE3	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
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: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
2:N:108:HIS:O	2:N:109:PHE:C	2.49	0.55
1:A:280:LYS:C	1:A:281:TYR:HD1	2.15	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
4:D:86:MET:HE2	4:D:91:ILE:HG21	1.88	0.55
1:M:264:GLN:HB3	1:M:282:MET:CE	2.36	0.55
1:A:93:MET:HE1	1:A:397:ALA:HA	1.87	0.55
1:A:254:LEU:HA	1:A:313:TYR:O	2.07	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
1:A:540:THR:C	1:A:541:GLU:OE2	2.49	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:94:PRO:O	4:P:95:ALA:C	2.50	0.55
4:P:112:LEU:O	4:P:112:LEU:HG	2.07	0.55
1:M:175:MET:HE3	1:M:503:LEU:HD13	1.88	0.55
1:M:279:ASN:HD22	1:M:280:LYS:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:386:HIS:O	1:M:387:GLY:O	2.25	0.55
2:N:31:ASP:CG	2:N:32:ALA:N	2.64	0.55
2:N:120:ILE:C	2:N:121:ILE:HG13	2.32	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
1:A:557:ALA:C	1:A:559:GLY:H	2.15	0.55
2:N:6:LEU:CD1	2:N:81:LEU:HD21	2.33	0.55
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
2:B:176:ALA:O	2:B:177:HIS:C	2.48	0.54
3:C:65:ASN:OD1	3:C:66:PRO:HD2	2.06	0.54
1:M:78:GLU:N	1:M:224:ARG:NH2	2.55	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
3:C:50:LYS:C	3:C:52:GLY:H	2.14	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
1:M:279:ASN:HD22	1:M:279:ASN:C	2.15	0.54
1:A:245:GLU:O	1:A:246:GLY:C	2.47	0.54
2:B:128:ASP:OD1	2:B:128:ASP:N	2.40	0.54
2:B:142:TYR:CD1	2:B:142:TYR:C	2.86	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:A:133:PHE:C	1:A:133:PHE:CD2	2.86	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:72:GLY:C	1:M:74:ASP:H	2.14	0.54
1:M:82:VAL:CG2	1:M:385:LEU:HA	2.30	0.54
1:M:257:LYS:HB2	1:M:302:ASN:C	2.32	0.54
2:N:192:MET:O	2:N:196:ASN:ND2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:19:ALA:O	4:P:20:GLY:C	2.50	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:135:MET:HE1	1:M:396:LEU:HG	1.89	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
3:C:121:ILE:O	3:C:122:VAL:C	2.47	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
4:P:23:TRP:C	4:P:25:ALA:H	2.15	0.54
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:23:TRP:C	4:D:25:ALA:N	2.64	0.54
4:D:37:ILE:HD12	4:D:37:ILE:N	2.22	0.54
4:D:98:TRP:O	4:D:99:VAL:C	2.51	0.54
1:M:78:GLU:C	1:M:80:ASP:N	2.66	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:52:SER:C	2:N:53:TYR:HD1	2.15	0.54
2:N:125:ARG:HA	2:N:129:GLN:OE1	2.08	0.54
2:B:26:TYR:CD2	2:B:47:LEU:HD13	2.33	0.53
4:D:51:TYR:O	4:D:52:GLU:C	2.49	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:412:GLU:HG3	1:A:413:ARG:N	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:182:ASP:C	2:B:182:ASP:OD2	2.51	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
1:M:461:GLU:CD	1:M:461:GLU:H	2.16	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
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
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
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
1:M:529:ARG:O	1:M:530:GLY:C	2.52	0.53
3:O:79:ALA:O	3:O:80:LEU:C	2.50	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
4:D:66:PHE:C	4:D:66:PHE:CD2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:46:VAL:C	1:M:48:ALA:H	2.16	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: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
1:A:109:GLY:C	2:B:133:ILE:HG23	2.34	0.52
1:A:270:PRO:O	1:A:271:GLU:C	2.50	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
2:N:101:ASP:O	2:N:102:LEU:HD23	2.09	0.52
1:A:390:ARG:NH2	5:A:702:FLL: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
3:C:27:LEU:O	3:C:28:ARG:C	2.49	0.52
4:D:4:ASN:C	4:D:4:ASN:ND2	2.67	0.52
1:M:78:GLU:HB2	1:M:224:ARG:HH22	1.74	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:A:230:GLN:CD	1:A:287:ARG:HE	2.17	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: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
1:M:470:GLU:O	1:M:470:GLU:CD	2.53	0.52
3:O:48:ALA:C	3:O:50:LYS:N	2.68	0.52
2:B:242:PRO:O	2:B:243:ARG:C	2.51	0.52
3:C:22:TYR:O	3:C:25:TYR:HB3	2.10	0.52
1:M:455:MET:HE1	1:M:508:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:511:GLY:O	1:A:512:LEU:C	2.50	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:A:282:MET:CE	1:A:283:GLU:OE1	2.54	0.51
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:N:4:LYS:C	2:N:5:ASN:ND2	2.67	0.51
1:A:386:HIS:O	1:A:387:GLY:C	2.49	0.51
2:B:209:TYR:O	2:B:213:VAL:HG13	2.10	0.51
4:D:84:HIS:C	4:D:86:MET:H	2.18	0.51
4:D:105:ALA:O	4:D:106:ILE:C	2.53	0.51
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:213:MET:HE1	1:M:361:ILE:HD11	1.93	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:229:VAL:HG22	1:A:518:MET:HE2	1.91	0.51
1:A:292:GLN:HG2	1:A:466:TYR:CZ	2.45	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
3:O:43:ILE:O	3:O:44:PHE:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ALA:C	1:A:430:ALA:HB3	2.35	0.51
2:B:70:ASN:O	2:B:71:ASN:HB2	2.09	0.51
3:C:27:LEU:C	3:C:29:GLU:N	2.65	0.51
4:D:10:GLU:C	4:D:12:VAL:H	2.18	0.51
1:M:49:GLN:O	1:M:50:GLY:C	2.54	0.51
1:M:84:TYR:HE2	1:M:405:LEU:HD11	1.76	0.51
1:M:194:GLY:HA3	1:M:379:GLU:CD	2.35	0.51
1:M:418:GLY:O	1:M:419:ASN:CG	2.53	0.51
1:M:467:ARG:NH2	1:M:533:GLN:H	2.07	0.51
1:A:12:ALA:HB1	1:A:40:PRO:HB3	1.92	0.51
1:A:256:ASN:OD1	1:A:259:GLY:N	2.42	0.51
1:A:261:ARG:HB3	1:A:282:MET:HE1	1.93	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: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
1:A:324:LEU:C	1:A:326:GLU:H	2.18	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:434:GLN:HA	1:M:437:LYS:HB2	1.93	0.51
1:M:503:LEU:C	1:M:505:THR:H	2.18	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:A:469:PRO:HB3	1:A:523:MET:HE1	1.93	0.51
1:M:3:PHE:HB3	1:M:183:ILE:HG23	1.93	0.51
1:M:191:ALA:HB2	1:M:377:VAL:O	2.10	0.51
2:N:189:LYS:C	2:N:191:ARG:H	2.15	0.51
3:O:67:VAL:C	3:O:69:VAL:N	2.66	0.51
1:A:391:LEU:O	1:A:392:GLY:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:88:GLU:HA	3:C:109:ILE:HD13	1.93	0.51
1:M:13:GLY:C	1:M:15:ALA:N	2.67	0.51
1:M:53:ALA:HB3	1:M:394:ASN:ND2	2.26	0.51
1:M:61:SER:O	1:M:62:PHE:C	2.54	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
1:M:360:GLY:C	1:M:361:ILE:HD12	2.36	0.51
2:N:37:LEU:CD2	2:N:77:CYS:HA	2.41	0.51
2:N:54:ARG:C	2:N:55:TRP:HD1	2.18	0.51
4:P:103:LEU:HD21	4:P:107:LEU:HD11	1.93	0.51
4:D:28:ALA:O	4:D:32:ILE:HG13	2.11	0.50
4:D:75:LEU:O	4:D:76:TRP:C	2.54	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
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
4:P:18:GLY:O	4:P:19:ALA:C	2.53	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:425:ILE:O	1:A:426:GLU:C	2.53	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
3:O:27:LEU:O	3:O:28:ARG:C	2.52	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:207:VAL:HG22	3:O:25:TYR:CZ	2.46	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:527:GLU:HG2	1:A:547:PHE:HB2	1.90	0.50
4:D:84:HIS:C	4:D:86:MET:N	2.69	0.50
1:M:266:TYR:HE2	1:M:296:HIS:HB3	1.77	0.50
2:N:134:GLN:OE1	2:N:184:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ARG:CZ	1:A:413:ARG:HB2	2.41	0.50
1:A:515:ALA:O	1:A:516:GLU:C	2.55	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:196:ASN:HB3	2:N:231:SER:OG	2.12	0.50
4:P:98:TRP:O	4:P:99:VAL:C	2.52	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:A:167:VAL:HG11	1:A:373:GLY:C	2.37	0.50
3:C:30:GLY:C	3:C:32:ALA:H	2.19	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
2:N:241:LYS:O	2:N:243:ARG:N	2.44	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
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
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:433:GLU:O	1:A:434:GLN:C	2.54	0.49
1:A:567:ASP:OD1	1:A:568:VAL:N	2.45	0.49
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
1:A:515:ALA:C	1:A:517:CYS:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:ILE:O	4:D:2:ASN:C	2.54	0.49
1:M:203:THR:HA	1:M:240:GLY:O	2.12	0.49
1:M:382:SER:O	1:M:383:VAL:C	2.55	0.49
2:B:184:ARG:HH11	2:B:184:ARG:HG3	1.77	0.49
4:D:18:GLY:O	4:D:19:ALA:C	2.55	0.49
1:M:21:ILE:CD1	1:M:139:LEU:HD22	2.41	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
3:O:15:TRP:CE3	3:O:16:TRP:N	2.80	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:264:GLN:C	1:M:266:TYR:H	2.19	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
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
3:C:30:GLY:C	3:C:32:ALA:N	2.70	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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:27:ILE:C	4:P:29:PRO:HD2	2.37	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
3:O:53:PRO:HB3	4:P:51:TYR:CG	2.47	0.49
1:A:243:MET:HE3	1:A:348:ILE:CD1	2.37	0.49
1:M:41:MET:HE2	1:M:42:ARG:HG3	1.94	0.49
1:M:53:ALA:HA	1:M:125:TRP:HB2	1.94	0.49
1:M:358:MET:HE1	1:M:390:ARG:H	1.78	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:97:PRO:C	2:B:104:VAL:CG2	2.82	0.48
2:B:111:GLU:OE1	4:D:0:MET:HB2	2.13	0.48
3:C:121:ILE:C	3:C:123:ILE:N	2.70	0.48
1:M:35:ILE:CG2	1:M:36:SER:N	2.75	0.48
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
2:N:192:MET:HE3	2:N:195:LEU:HB2	1.94	0.48
4:P:37:ILE:HG22	4:P:38:LEU:N	2.26	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:112:SER:O	2:B:113:LEU:C	2.54	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:165:GLY:O	1:M:166:HIS:HB3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:50:LYS:C	3:C:52:GLY:N	2.69	0.48
3:C:89:LEU:C	3:C:91:PRO:HD2	2.37	0.48
4:D:0:MET:CG	4:D:1:ILE:H	2.21	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:M:253:ILE:HA	1:M:283:GLU:CD	2.38	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
3:O:32:ALA:O	3:O:33:VAL:C	2.57	0.48
4:P:0:MET:O	4:P:1:ILE:HG12	2.12	0.48
3:C:36:VAL:CG1	3:C:37:TRP:N	2.75	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:A:37:LYS:C	1:A:38:VAL:CG1	2.86	0.48
1:M:13:GLY:C	1:M:15:ALA:H	2.20	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
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:57:CYS:O	2:B:58:ARG:HB2	2.12	0.48
2:B:121:ILE:O	2:B:186:HIS:N	2.47	0.48
3:C:63:LEU:CB	4:D:40:PRO:HG3	2.36	0.48
4:D:100:PHE:C	4:D:102:GLY:N	2.68	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.94	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:50:LYS:C	3:O:52:GLY:N	2.71	0.48
3:C:124:LEU:O	3:C:128:LEU:HB2	2.14	0.48
2:N:196:ASN:N	2:N:196:ASN:ND2	2.47	0.48
3:O:56:TRP:CD1	3:O:56:TRP:C	2.91	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:268:MET:O	1:M:269:GLY:C	2.56	0.48
1:M:440:VAL:HA	1:M:491:ILE:HD12	1.96	0.48
3:O:89:LEU:C	3:O:91:PRO:HD2	2.38	0.48
1:A:17:LEU:HD11	1:A:140:PHE:HA	1.95	0.47
1:A:253:ILE:HG22	1:A:315:ASP:N	2.29	0.47
1:A:503:LEU:O	1:A:504:TYR:C	2.53	0.47
2:B:39:ALA:O	2:B:40:LEU:C	2.56	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:117:LYS:C	2:N:119:TYR:H	2.22	0.47
2:N:216:LYS:HA	2:N:216:LYS:NZ	2.29	0.47
1:A:15:ALA:C	1:A:17:LEU:N	2.71	0.47
1:A:427:ALA:HA	1:A:430:ALA:HB2	1.97	0.47
4:D:10:GLU:N	4:D:11:PRO:HD2	2.29	0.47
4:D:103:LEU:HD23	4:D:103:LEU:C	2.39	0.47
2:N:31:ASP:H	2:N:34:THR:CG2	2.27	0.47
2:N:167:PHE:HD1	2:N:199:ASN:C	2.22	0.47
2:N:232:SER:C	2:N:234:ASP:N	2.72	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: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
1:A:558:ASP:OD2	1:A:560:THR:OG1	2.32	0.47
2:B:164:ASN:OD1	2:B:164:ASN:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:230:GLN:CD	1:A:287:ARG:HH21	2.22	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
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: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
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
3:O:30:GLY:C	3:O:32:ALA:H	2.22	0.47
3:O:91:PRO:C	3:O:93:ALA:H	2.22	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
2:B:180:ASN:OD1	2:B:191:ARG:HD2	2.14	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
3:C:108:ILE:O	3:C:109:ILE:C	2.56	0.47
4:D:4:ASN:C	4:D:4:ASN:HD22	2.22	0.47
4:D:19:ALA:O	4:D:20:GLY:C	2.58	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: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
2:B:75:LEU:HB3	2:B:77:CYS:HB3	1.97	0.47
2:B:135:THR:O	2:B:136:PRO:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:4:LYS:O	2:N:5:ASN:ND2	2.41	0.47
2:N:44:LYS:C	2:N:46:ASN:N	2.68	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
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:40:PRO:O	1:M:41:MET:C	2.57	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
4:D:61:PHE:HA	4:D:64:ARG:HB2	1.97	0.47
1:M:230:GLN:HG2	1:M:390:ARG:NH2	2.25	0.47
1:A:330:PHE:O	1:A:331:ILE:C	2.58	0.46
3:C:88:GLU:HA	3:C:109:ILE:CD1	2.45	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
4:P:65:VAL:O	4:P:69:LEU:HG	2.16	0.46
1:A:44:HIS:NE2	6:A:703:FAD:HM81	2.12	0.46
2:B:135:THR:C	2:B:137:ALA:H	2.22	0.46
3:C:21:PHE:C	3:C:21:PHE:CD2	2.93	0.46
1:M:73:GLY:C	1:M:388:ALA:H	2.24	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
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:320:GLY:O	1:A:321:GLU:C	2.58	0.46
1:A:520:HIS:O	1:A:521:SER:C	2.53	0.46
3:C:78:ALA:O	3:C:79:ALA:C	2.58	0.46
4:D:1:ILE:O	4:D:1:ILE:CG2	2.56	0.46
4:D:61:PHE:C	4:D:63:GLY:H	2.22	0.46
4:D:73:LEU:O	4:D:74:PRO:C	2.55	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
3:O:49:LEU:HD11	4:P:55:LEU:HB2	1.98	0.46
1:A:71:ALA:O	1:A:72:GLY:C	2.58	0.46
1:A:504:TYR:HA	1:A:507:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:HIS:C	1:A:532:HIS:CD2	2.94	0.46
4:D:76:TRP:O	4:D:77:CYS:C	2.58	0.46
1:M:103:TRP:CE3	1:M:127:ALA:HB2	2.51	0.46
1:M:139:LEU:C	1:M:141:GLN:H	2.23	0.46
1:M:237:PRO:O	1:M:239:SER:N	2.37	0.46
1:M:265:ASP:C	1:M:266:TYR:CD1	2.94	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
2:N:105:ASP:C	2:N:107:THR:H	2.22	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
2:B:97:PRO:O	2:B:104:VAL:CG2	2.62	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
2:B:127:ALA:C	2:B:129:GLN:N	2.68	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:147:PRO:C	1:M:149:ILE:N	2.69	0.46
4:P:17:PHE:O	4:P:18:GLY:C	2.59	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:194:GLY:C	1:A:208:VAL:HG12	2.41	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:358:MET:HE2	1:A:358:MET:HB2	1.83	0.46
1:A:541:GLU:OE2	1:A:541:GLU:CA	2.63	0.46
3:C:49:LEU:HD21	4:D:55:LEU:HD12	1.98	0.46
1:M:143:SER:O	1:M:149:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:67:VAL:O	3:O:68:ILE:C	2.57	0.46
4:P:72:VAL:O	4:P:75:LEU:CB	2.64	0.46
1:A:97:GLU:CD	2:B:131:THR:HB	2.41	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
4:D:96:GLY:O	4:D:97:LYS:C	2.55	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
4:P:95:ALA:O	4:P:96:GLY:C	2.58	0.46
1:A:38:VAL:O	1:A:38:VAL:HG22	2.14	0.46
1:A:502:LEU:O	1:A:503:LEU:C	2.56	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
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:HD2	3:C:21:PHE:C	2.23	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
2:N:124:SER:O	2:N:125:ARG:C	2.59	0.45
2:N:142:TYR:O	2:N:143:HIS:C	2.59	0.45
1:A:332:CYS:HA	1:A:343:PRO:HG2	1.97	0.45
3:C:15:TRP:CE3	3:C:16:TRP:HA	2.51	0.45
3:C:103:MET:HE3	3:C:103:MET:HB2	1.84	0.45
4:D:55:LEU:CG	4:D:59:GLN:NE2	2.61	0.45
1:M:170:LEU:O	1:M:182:GLN:HA	2.16	0.45
1:M:226:MET:O	1:M:227:GLU:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:456:GLY:O	1:M:457:LEU:C	2.58	0.45
1:M:497:VAL:O	1:M:498:PHE:C	2.59	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
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: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
4:D:117:THR:C	4:D:118:ILE:HG12	2.41	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:73:PRO:C	2:N:74:LYS:HG3	2.40	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: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
3:C:40:ILE:O	3:C:41:GLU:C	2.58	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:A:702:FLC:CAC	6:A:703:FAD:C2	2.95	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:223:LEU:HD23	1:M:226:MET:HE2	1.98	0.45
1:M:334:LEU:HD23	1:M:338:TYR:CE1	2.52	0.45
3:O:30:GLY:C	3:O:32:ALA:N	2.70	0.45
1:A:151:ARG:HH11	1:A:151:ARG:HD2	1.50	0.45
1:A:469:PRO:CB	1:A:523:MET:HE1	2.46	0.45
1:A:514:VAL:H	1:A:514:VAL:HG23	1.46	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: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:350:VAL:CG2	1:A:350:VAL:O	2.61	0.45
1:M:542:ARG:NH2	1:M:544:ASP:OD1	2.49	0.45
2:N:1:ALA:O	2:N:2:GLU:C	2.60	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
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
3:O:127:ALA:C	3:O:128:LEU:HD23	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:48:ALA:C	3:C:50:LYS:N	2.66	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
1:M:295:TRP:O	1:M:296:HIS:C	2.61	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:198:VAL:CG2	1:A:455:MET:CE	2.88	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:103:TRP:O	2:B:139:MET:CE	2.60	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
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: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
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
1:M:243:MET:O	1:M:244:THR:C	2.59	0.44
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:143:HIS:O	2:N:144:GLN:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:O:27:LEU:C	3:O:29:GLU:N	2.71	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
1:M:262:TYR:CD1	1:M:262:TYR:C	2.96	0.44
1:M:382:SER:HG	1:M:386:HIS:CE1	2.32	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
2:B:241:LYS:C	2:B:243:ARG:N	2.74	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:467:ARG:CZ	1:M:533:GLN:H	2.31	0.44
3:O:99:LYS:C	3:O:100:ASP:OD1	2.61	0.44
4:P:27:ILE:O	4:P:27:ILE:CG2	2.65	0.44
4:P:39:LEU:O	4:P:40:PRO:C	2.60	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:43:ILE:O	3:C:44:PHE:C	2.61	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:195:ALA:O	1:M:196:GLY:C	2.59	0.44
1:M:236:LEU:HD23	1:M:239:SER:OG	2.17	0.44
1:M:407:GLY:C	1:M:409:GLN:H	2.26	0.44
2:N:154:CYS:C	2:N:156:ALA:N	2.76	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
4:P:34:LEU:O	4:P:35:VAL:C	2.61	0.44
4:P:73:LEU:O	4:P:74:PRO:C	2.58	0.44
1:A:202:ASN:HB3	1:A:354:ALA:HB3	1.99	0.44
1:A:261:ARG:HD2	1:A:282:MET:HE1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:M:279:ASN:C	1:M:280:LYS:HG2	2.43	0.44
2:N:36:LEU:O	2:N:39:ALA:N	2.51	0.44
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
4:D:87:HIS:O	4:D:88:ASP:C	2.61	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
1:A:446:GLU:HB2	1:A:489:VAL:CA	2.48	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
2:N:225:GLN:CD	2:N:225:GLN:N	2.75	0.43
1:A:92:GLU:HG3	1:A:400:VAL:CG1	2.49	0.43
1:A:94:THR:O	1:A:95:GLN:C	2.60	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:394:ASN:C	1:M:396:LEU:H	2.26	0.43
2:N:219:ASP:CG	2:N:222:ALA:CB	2.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:PHE:CD2	2:B:206:PHE:C	2.95	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
2:B:144:GLN:C	2:B:146:SER:H	2.25	0.43
1:M:4:GLN:OE1	1:M:31:LYS:HD3	2.19	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: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
2:N:81:LEU:HD23	2:N:81:LEU:C	2.41	0.43
3:O:50:LYS:CE	4:P:117:THR:OG1	2.66	0.43
3:O:76:LEU:HD12	3:O:76:LEU:C	2.43	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: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
4:P:23:TRP:C	4:P:25:ALA:N	2.76	0.43
1:A:70:VAL:O	1:A:71:ALA:C	2.58	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
2:B:68:MET:HE2	2:B:68:MET:HB3	1.90	0.43
1:M:65:HIS:C	1:M:67:HIS:N	2.76	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
2:N:52:SER:C	2:N:53:TYR:CD1	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:446:GLU:O	1:A:447:ASN:C	2.56	0.43
3:C:31:THR:CG2	3:C:82:HIS:HB2	2.42	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
2:N:18:ASP:O	2:N:19:THR:C	2.60	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
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:206:PHE:HD2	2:B:206:PHE:C	2.27	0.43
2:N:54:ARG:HH11	2:N:54:ARG:CG	2.19	0.43
4:P:44:PHE:C	4:P:44:PHE:CD1	2.96	0.43
1:A:15:ALA:C	1:A:17:LEU:H	2.25	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
4:D:15:GLY:O	4:D:16:LEU:C	2.62	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
2:N:163:LEU:HG	3:O:11:MET:HE3	2.01	0.43
2:N:187:GLY:C	2:N:189:LYS:H	2.26	0.43
3:O:82:HIS:CD2	3:O:82:HIS:C	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:116:THR:HA	4:D:26:ILE:HG23	2.01	0.42
1:M:58:ASP:C	1:M:60:ASP:N	2.77	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
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
2:N:149:ILE:C	2:N:151:CYS:N	2.74	0.42
4:P:51:TYR:O	4:P:52:GLU:C	2.62	0.42
1:A:2:THR:C	1:A:3:PHE:CD1	2.96	0.42
1:A:27:ASN:ND2	1:A:29:ASN:H	2.17	0.42
1:A:182:GLN:CD	1:A:184:ARG:HH12	2.27	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:30:GLY:O	3:C:31:THR:C	2.61	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
2:N:209:TYR:O	2:N:210:CYS:C	2.62	0.42
4:P:72:VAL:HG23	4:P:73:LEU:H	1.83	0.42
1:A:106:ARG:C	1:A:108:ASP:N	2.77	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
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
1:M:316:LEU:C	1:M:318:HIS:H	2.27	0.42
2:N:188:LYS:H	2:N:188:LYS:HG2	1.37	0.42
1:A:37:LYS:C	1:A:38:VAL:HG13	2.41	0.42
1:A:80:ASP:O	1:A:81:VAL:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:37:ILE:O	4:D:38:LEU:C	2.60	0.42
1:M:53:ALA:HA	1:M:125:TRP:CB	2.49	0.42
1:M:72:GLY:C	1:M:74:ASP:N	2.76	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
2:N:223:ALA:O	2:N:224:ILE:C	2.63	0.42
3:O:27:LEU:O	3:O:29:GLU:N	2.52	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
3:C:106:GLU:CG	3:C:107:PRO:HD3	2.50	0.42
3:C:119:ALA:O	3:C:120:THR:C	2.63	0.42
4:D:100:PHE:C	4:D:102:GLY:H	2.27	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
1:A:294:PHE:CD2	1:A:294:PHE:C	2.97	0.42
1:A:508:LEU:O	1:A:509:GLY:C	2.61	0.42
2:B:166:GLU:CD	2:B:199:ASN:HD21	2.27	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: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
3:O:40:ILE:O	3:O:41:GLU:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ASP:OD1	1:A:546:ASN:N	2.41	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
2:N:160:GLN:O	2:N:161:PHE:C	2.61	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:369:THR:HG23	1:A:374:LEU:O	2.20	0.42
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
4:P:28:ALA:O	4:P:32:ILE:HG13	2.20	0.42
1:A:196:GLY:C	1:A:198:VAL:H	2.27	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: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
3:O:78:ALA:O	3:O:79:ALA:C	2.62	0.42
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
2:B:66:GLY:HA2	2:B:74:LYS:O	2.20	0.41
2:B:111:GLU:HG2	4:D:0:MET:HE3	2.02	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:O:29:GLU:O	3:O:30:GLY:C	2.61	0.41
4:P:9:ASP:C	4:P:11:PRO:HD3	2.45	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
2:B:238:ALA:C	2:B:241:LYS:HB3	2.44	0.41
3:C:125:PHE:CD1	3:C:129:TYR:CD2	3.08	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:242:LEU:CD2	1:M:242:LEU:C	2.75	0.41
1:M:244:THR:C	1:M:246:GLY:N	2.75	0.41
3:O:68:ILE:O	3:O:68:ILE:CG2	2.65	0.41
1:A:482:LEU:HA	1:A:482:LEU:HD23	1.57	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
1:M:392:GLY:C	1:M:394:ASN:H	2.28	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:406:ALA:O	1:A:407:GLY:C	2.60	0.41
1:A:471:LEU:HA	1:A:471:LEU:HD23	1.64	0.41
1:A:493:ASP:C	1:A:499:ASN:HD21	2.28	0.41
2:B:44:LYS:HA	2:B:48:ALA:C	2.40	0.41
2:B:159:PRO:C	2:B:161:PHE:N	2.77	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:244:THR:C	1:M:246:GLY:H	2.28	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
2:N:75:LEU:C	2:N:77:CYS:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:366:ASN:C	1:A:367:CYS:SG	3.02	0.41
2:B:174:THR:O	2:B:175:LEU:C	2.63	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
1:M:556:ASP:HB3	1:M:557:ALA:H	1.65	0.41
2:N:53:TYR:CD1	2:N:53:TYR:N	2.87	0.41
3:O:28:ARG:NH2	3:O:89:LEU:HD11	2.35	0.41
3:O:119:ALA:O	3:O:120:THR:C	2.62	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:7:ARG:O	4:D:7:ARG:CG	2.65	0.41
4:D:94:PRO:HA	2:N:243:ARG:O	2.20	0.41
2:N:158:CYS:SG	2:N:160:GLN:HB2	2.61	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
1:A:232:HIS:CE1	5:A:702:FLC:HG2	2.55	0.41
1:A:261:ARG:NH1	1:A:282:MET:HE2	2.30	0.41
1:A:522:ALA:C	1:A:524:ALA:H	2.29	0.41
1:A:527:GLU:CG	1:A:547:PHE:HB3	2.43	0.41
2:B:75:LEU:O	2:B:76:ALA:C	2.61	0.41
2:B:166:GLU:CD	2:B:199:ASN:ND2	2.78	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
4:D:111:THR:O	4:D:112:LEU:C	2.60	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
1:M:503:LEU:C	1:M:505:THR:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:41:LEU:HD23	4:P:41:LEU:HA	1.72	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:177:GLU:OE2	1:A:177:GLU:CA	2.60	0.41
1:A:194:GLY:C	1:A:208:VAL:CG1	2.94	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:481:GLU:O	1:A:482:LEU:C	2.63	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
3:C:90:ALA:O	3:C:91:PRO:C	2.64	0.41
1:M:139:LEU:C	1:M:141:GLN:N	2.78	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
2:N:236:LEU:C	2:N:240:LEU:HD21	2.46	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:25:GLN:C	1:A:27:ASN:N	2.74	0.41
1:A:44:HIS:C	1:A:46:VAL:N	2.77	0.41
1:A:52:SER:HB3	1:A:93:MET:CE	2.51	0.41
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:280:LYS:C	1:A:281:TYR:CD1	2.98	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: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:228:PHE:CE2	1:M:388:ALA:CA	3.01	0.41
1:M:269:GLY:O	1:M:282:MET:HE3	2.20	0.41
1:M:273:PRO:HG3	1:M:276:GLU:OE1	2.21	0.41
1:M:292:GLN:C	1:M:294:PHE:H	2.29	0.41
1:M:382:SER:OG	1:M:386:HIS:NE2	2.46	0.41
1:M:452:ARG:HD2	1:M:508:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:123:ASN:OD1	2:N:124:SER:N	2.48	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
2:N:193:ALA:O	2:N:194:GLN:C	2.64	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
3:C:65:ASN:OD1	3:C:65:ASN:C	2.64	0.41
3:C:111:SER:C	3:C:113:TRP:N	2.75	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:242:LEU:HD23	1:M:243:MET:N	2.33	0.41
1:M:434:GLN:O	1:M:435:ARG:C	2.63	0.41
2:N:240:LEU:N	2:N:240:LEU:CD2	2.78	0.41
1:A:122:GLU:H	1:A:122:GLU:CD	2.26	0.40
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
2:B:225:GLN:O	2:B:226:GLN:C	2.59	0.40
3:C:9:ARG:HA	3:C:10:PRO:HD3	1.82	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:28:PRO:C	1:M:30:ALA:N	2.79	0.40
1:M:85:PHE:CD1	1:M:85:PHE:C	2.98	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
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:471:LEU:O	1:M:472:MET:C	2.63	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
4:P:84:HIS:C	4:P:86:MET:H	2.28	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
2:B:226:GLN:O	2:B:227:GLY:C	2.64	0.40
3:C:9:ARG:HH11	3:C:9:ARG:CG	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:LYS:HZ3	4:D:118:ILE:CD1	2.11	0.40
4:D:61:PHE:C	4:D:63:GLY:N	2.79	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:93:VAL:HA	4:P:94:PRO:HD2	1.74	0.40
1:A:88:HIS:C	1:A:90:PRO:HD2	2.47	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:100:ARG:O	2:B:101:ASP:C	2.62	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
1:M:470:GLU:CD	1:M:470:GLU:C	2.89	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: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
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
1:M:462:GLY:C	1:M:464:GLY:H	2.29	0.40
2:N:161:PHE:C	2:N:163:LEU:H	2.29	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:196:GLY:C	1:A:198:VAL:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:C	1:A:255:VAL:CG1	2.94	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
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:140:ALA:O	2:N:141:LYS:C	2.65	0.40
2:N:232:SER:O	2:N:235:PHE:HB2	2.21	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%)	4	24
1	M	570/602 (95%)	402 (70%)	103 (18%)	65 (11%)	0	2
2	B	241/243 (99%)	207 (86%)	30 (12%)	4 (2%)	7	30
2	N	241/243 (99%)	126 (52%)	79 (33%)	36 (15%)	0	1
3	C	128/130 (98%)	99 (77%)	25 (20%)	4 (3%)	3	20
3	O	128/130 (98%)	103 (80%)	18 (14%)	7 (6%)	1	10
4	D	117/119 (98%)	68 (58%)	35 (30%)	14 (12%)	0	1
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	6

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	337 (73%)	123 (27%)	0	2
1	M	456/475 (96%)	404 (89%)	52 (11%)	5	21
2	B	205/205 (100%)	167 (82%)	38 (18%)	1	7
2	N	205/205 (100%)	176 (86%)	29 (14%)	3	14
3	C	111/111 (100%)	84 (76%)	27 (24%)	1	3
3	O	111/111 (100%)	76 (68%)	35 (32%)	0	1
4	D	97/97 (100%)	71 (73%)	26 (27%)	0	2
4	P	97/97 (100%)	74 (76%)	23 (24%)	1	4
All	All	1742/1776 (98%)	1389 (80%)	353 (20%)	1	6

All (353) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	7	LEU
1	A	17	LEU
1	A	18	ARG
1	A	21	ILE
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	38	VAL
1	A	41	MET
1	A	42	ARG
1	A	49	GLN
1	A	55	VAL
1	A	58	ASP
1	A	63	GLU
1	A	76	LEU
1	A	77	CYS
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

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Mol	Chain	Res	Type
1	A	111	VAL
1	A	114	ARG
1	A	115	ARG
1	A	116	PHE
1	A	119	MET
1	A	130	LYS
1	A	133	PHE
1	A	138	THR
1	A	150	GLN
1	A	167	VAL
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	207	ILE
1	A	208	VAL
1	A	213	MET
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	236	LEU
1	A	241	ILE
1	A	253	ILE
1	A	257	LYS
1	A	258	ASN
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
1	A	310	ASP
1	A	314	LEU
1	A	317	ARG

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Mol	Chain	Res	Type
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	346	GLU
1	A	350	VAL
1	A	358	MET
1	A	372	LYS
1	A	374	LEU
1	A	391	LEU
1	A	400	VAL
1	A	411	THR
1	A	412	GLU
1	A	413	ARG
1	A	416	THR
1	A	422	GLU
1	A	436	LEU
1	A	438	ASP
1	A	440	VAL
1	A	441	ASN
1	A	442	GLN
1	A	450	LYS
1	A	451	ILE
1	A	465	ILE
1	A	468	THR
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	526	LYS
1	A	527	GLU
1	A	532	HIS
1	A	534	ARG

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Mol	Chain	Res	Type
1	A	536	ASP
1	A	537	GLU
1	A	539	CYS
1	A	541	GLU
1	A	543	ASP
1	A	545	VAL
1	A	546	ASN
1	A	560	THR
1	A	562	ARG
1	A	564	GLU
1	A	568	VAL
1	A	570	ILE
2	B	4	LYS
2	B	5	ASN
2	B	12	ARG
2	B	28	VAL
2	B	43	ILE
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	103	VAL
2	B	105	ASP
2	B	106	MET
2	B	107	THR
2	B	110	ILE
2	B	116	ILE
2	B	117	LYS
2	B	120	ILE
2	B	124	SER
2	B	125	ARG
2	B	128	ASP
2	B	132	ASN
2	B	141	LYS
2	B	173	ILE
2	B	183	SER

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Mol	Chain	Res	Type
2	B	184	ARG
2	B	190	GLU
2	B	197	SER
2	B	203	SER
2	B	237	ILE
2	B	239	THR
2	B	240	LEU
2	B	241	LYS
3	C	1	THR
3	C	2	THR
3	C	9	ARG
3	C	11	MET
3	C	12	THR
3	C	19	LEU
3	C	21	PHE
3	C	27	LEU
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	71	ILE
3	C	72	ASN
3	C	74	ILE
3	C	100	ASP
3	C	103	MET
3	C	106	GLU
3	C	109	ILE
3	C	111	SER
3	C	115	VAL
3	C	116	THR
4	D	1	ILE
4	D	4	ASN
4	D	7	ARG
4	D	12	VAL
4	D	26	ILE
4	D	30	VAL
4	D	31	MET

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Mol	Chain	Res	Type
4	D	35	VAL
4	D	37	ILE
4	D	39	LEU
4	D	43	LEU
4	D	47	ASP
4	D	50	SER
4	D	59	GLN
4	D	62	ILE
4	D	65	VAL
4	D	73	LEU
4	D	75	LEU
4	D	82	MET
4	D	86	MET
4	D	91	ILE
4	D	99	VAL
4	D	113	ILE
4	D	115	VAL
4	D	117	THR
4	D	118	ILE
1	M	32	ILE
1	M	49	GLN
1	M	52	SER
1	M	76	LEU
1	M	90	PRO
1	M	97	GLU
1	M	105	ARG
1	M	121	ILE
1	M	122	GLU
1	M	126	PHE
1	M	146	PHE
1	M	151	ARG
1	M	154	GLU
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

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Mol	Chain	Res	Type
1	M	231	TYR
1	M	242	LEU
1	M	248	ARG
1	M	254	LEU
1	M	262	TYR
1	M	274	LEU
1	M	277	PRO
1	M	283	GLU
1	M	286	PRO
1	M	287	ARG
1	M	295	TRP
1	M	328	LEU
1	M	330	PHE
1	M	332	CYS
1	M	334	LEU
1	M	343	PRO
1	M	356	TYR
1	M	386	HIS
1	M	390	ARG
1	M	398	GLU
1	M	455	MET
1	M	461	GLU
1	M	463	CYS
1	M	490	ARG
1	M	505	THR
1	M	549	LYS
1	M	562	ARG
1	M	567	ASP
1	M	570	ILE
2	N	25	PHE
2	N	27	GLU
2	N	28	VAL
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	69	VAL
2	N	75	LEU
2	N	98	ILE
2	N	121	ILE

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Mol	Chain	Res	Type
2	N	133	ILE
2	N	139	MET
2	N	144	GLN
2	N	146	SER
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	213	VAL
2	N	216	LYS
2	N	225	GLN
2	N	240	LEU
3	O	1	THR
3	O	2	THR
3	O	4	ARG
3	O	8	VAL
3	O	9	ARG
3	O	11	MET
3	O	12	THR
3	O	17	LYS
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	69	VAL
3	O	70	ILE
3	O	72	ASN
3	O	74	ILE
3	O	80	LEU
3	O	85	THR
3	O	92	LYS
3	O	96	ILE
3	O	98	VAL

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Mol	Chain	Res	Type
3	O	99	LYS
3	O	102	LYS
3	O	103	MET
3	O	110	LYS
3	O	111	SER
3	O	116	THR
3	O	117	VAL
3	O	123	ILE
3	O	130	TRP
4	P	0	MET
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	89	LEU
4	P	91	ILE
4	P	93	VAL
4	P	97	LYS
4	P	103	LEU
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 (65) 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	137	HIS
1	A	182	GLN

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Mol	Chain	Res	Type
1	A	204	ASN
1	A	219	HIS
1	A	230	GLN
1	A	232	HIS
1	A	279	ASN
1	A	318	HIS
1	A	409	GLN
1	A	421	ASN
1	A	434	GLN
1	A	442	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	180	ASN
2	B	186	HIS
2	B	194	GLN
2	B	199	ASN
3	C	51	ASN
3	C	64	GLN
3	C	72	ASN
4	D	4	ASN
4	D	59	GLN
4	D	83	HIS
1	M	49	GLN
1	M	65	HIS
1	M	79	GLN
1	M	112	ASN
1	M	137	HIS
1	M	166	HIS
1	M	174	ASN
1	M	182	GLN
1	M	204	ASN
1	M	219	HIS
1	M	230	GLN
1	M	279	ASN
1	M	302	ASN
1	M	394	ASN
1	M	419	ASN

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Mol	Chain	Res	Type
1	M	434	GLN
1	M	442	GLN
1	M	520	HIS
1	M	533	GLN
1	M	550	HIS
2	N	5	ASN
2	N	70	ASN
2	N	71	ASN
2	N	144	GLN
2	N	160	GLN
2	N	196	ASN
3	O	64	GLN
3	O	65	ASN
3	O	82	HIS
3	O	95	ASN
4	P	4	ASN
4	P	59	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	M	803	-	57,57,58	4.25	23 (40%)	83,87,89	1.73	18 (21%)
5	FLC	A	702	-	12,12,12	4.42	5 (41%)	17,17,17	2.73	4 (23%)
8	F3S	B	245	2	0,9,9	-	-	-	-	-
10	MQ7	D	700	-	34,34,49	3.54	15 (44%)	43,45,63	2.36	14 (32%)
8	F3S	N	245	2	0,9,9	-	-	-	-	-
9	SF4	N	246	2	0,12,12	-	-	-	-	-
9	SF4	B	246	2	0,12,12	-	-	-	-	-
5	FLC	M	802	-	12,12,12	4.45	4 (33%)	17,17,17	2.31	5 (29%)
7	FES	B	244	2	0,4,4	-	-	-	-	-
10	MQ7	P	800	-	34,34,49	3.57	16 (47%)	43,45,63	2.52	12 (27%)
7	FES	N	244	2	0,4,4	-	-	-	-	-
6	FAD	A	703	-	57,57,58	3.97	27 (47%)	83,87,89	1.84	18 (21%)

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
10	MQ7	D	700	-	-	7/23/43/61	0/2/2/2
5	FLC	A	702	-	-	4/16/16/16	-
6	FAD	M	803	-	-	7/34/46/50	0/6/6/6
8	F3S	B	245	2	-	-	0/3/3/3
8	F3S	N	245	2	-	-	0/3/3/3
9	SF4	N	246	2	-	-	0/6/5/5
9	SF4	B	246	2	-	-	0/6/5/5
5	FLC	M	802	-	-	5/16/16/16	-
7	FES	B	244	2	-	-	0/1/1/1
10	MQ7	P	800	-	-	8/23/43/61	0/2/2/2
7	FES	N	244	2	-	-	0/1/1/1
6	FAD	A	703	-	-	9/34/46/50	0/6/6/6

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	803	FAD	PA-O3P	20.51	1.81	1.59
6	A	703	FAD	PA-O3P	15.93	1.76	1.59
5	A	702	FLC	CB-CBC	11.01	1.64	1.53
5	M	802	FLC	CB-CBC	10.40	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	800	MQ7	C12-C13	9.18	1.54	1.33
10	D	700	MQ7	C12-C13	9.09	1.54	1.33
6	A	703	FAD	P-O3P	-8.23	1.50	1.59
6	A	703	FAD	C4X-N5	8.12	1.48	1.30
10	P	800	MQ7	C17-C18	7.62	1.50	1.33
6	M	803	FAD	C4X-N5	7.60	1.47	1.30
6	M	803	FAD	C6-C7	7.58	1.49	1.39
5	M	802	FLC	CG-CB	7.53	1.63	1.54
5	M	802	FLC	CA-CB	7.46	1.63	1.54
10	D	700	MQ7	C17-C18	7.27	1.49	1.33
6	M	803	FAD	C9A-C5X	6.97	1.52	1.41
6	A	703	FAD	C6-C7	6.95	1.49	1.39
6	M	803	FAD	C10-N10	6.85	1.52	1.37
10	P	800	MQ7	C22-C23	6.63	1.48	1.33
10	D	700	MQ7	C22-C23	6.57	1.48	1.33
5	A	702	FLC	CG-CGC	-6.54	1.30	1.50
6	M	803	FAD	C9-C8	6.33	1.48	1.39
6	M	803	FAD	C10-N1	6.18	1.45	1.33
6	A	703	FAD	C9-C9A	5.91	1.49	1.39
6	M	803	FAD	C9A-N10	5.90	1.51	1.41
6	A	703	FAD	C4A-N3A	5.88	1.45	1.34
6	M	803	FAD	C4A-N3A	5.87	1.45	1.34
6	A	703	FAD	C9A-C5X	5.86	1.50	1.41
6	A	703	FAD	C10-N10	5.75	1.49	1.37
6	A	703	FAD	C9-C8	5.71	1.47	1.39
6	A	703	FAD	C10-N1	5.64	1.44	1.33
10	D	700	MQ7	C7-C6	5.63	1.48	1.38
6	A	703	FAD	C9A-N10	5.63	1.50	1.41
10	P	800	MQ7	C27-C28	5.63	1.49	1.32
10	P	800	MQ7	C7-C6	5.60	1.48	1.38
5	A	702	FLC	CA-CB	5.51	1.60	1.54
6	M	803	FAD	C9-C9A	5.48	1.48	1.39
10	D	700	MQ7	C27-C28	5.42	1.48	1.32
6	A	703	FAD	C8-C7	5.40	1.54	1.40
6	M	803	FAD	C2A-N3A	5.39	1.43	1.33
10	D	700	MQ7	C9-C10	5.31	1.48	1.39
10	P	800	MQ7	C9-C10	5.10	1.47	1.39
6	M	803	FAD	P-O3P	-5.08	1.54	1.59
10	P	800	MQ7	C8-C7	5.08	1.49	1.38
10	D	700	MQ7	C8-C7	5.00	1.49	1.38
5	A	702	FLC	CG-CB	4.90	1.60	1.54
6	M	803	FAD	C8-C7	4.85	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	FAD	C7M-C7	-4.30	1.43	1.51
10	P	800	MQ7	C2-C1	4.28	1.57	1.47
6	M	803	FAD	C6-C5X	4.24	1.46	1.40
10	D	700	MQ7	C11-C12	-4.22	1.43	1.50
10	D	700	MQ7	C5-C4	4.12	1.56	1.48
6	A	703	FAD	C5A-C4A	-4.08	1.31	1.39
10	D	700	MQ7	C2-C1	4.05	1.56	1.47
6	A	703	FAD	C2B-C3B	-3.98	1.42	1.52
6	A	703	FAD	C2A-N3A	3.96	1.41	1.33
6	A	703	FAD	C6-C5X	3.94	1.46	1.40
6	M	803	FAD	C1'-N10	3.90	1.57	1.47
6	M	803	FAD	C7M-C7	-3.87	1.43	1.51
6	A	703	FAD	C4'-C3'	-3.84	1.46	1.53
10	P	800	MQ7	C8-C9	3.83	1.45	1.38
10	D	700	MQ7	C8-C9	3.81	1.45	1.38
10	P	800	MQ7	C3-C4	3.61	1.56	1.47
10	P	800	MQ7	C5-C4	3.53	1.55	1.48
10	P	800	MQ7	C11-C12	-3.51	1.45	1.50
6	M	803	FAD	C5A-C4A	-3.47	1.32	1.39
6	A	703	FAD	C1'-C2'	-3.45	1.47	1.52
6	M	803	FAD	C5'-C4'	3.14	1.56	1.51
6	M	803	FAD	C4-N3	3.11	1.44	1.38
10	D	700	MQ7	C3-C4	3.10	1.54	1.47
10	P	800	MQ7	C6-C5	3.09	1.44	1.39
10	D	700	MQ7	C6-C5	3.03	1.44	1.39
6	A	703	FAD	C2'-C3'	-2.94	1.48	1.53
6	M	803	FAD	C8A-N9A	2.94	1.42	1.37
6	A	703	FAD	C4-N3	2.93	1.44	1.38
10	P	800	MQ7	C15-C13	2.83	1.57	1.51
6	A	703	FAD	C8A-N9A	2.75	1.42	1.37
6	M	803	FAD	C2B-C3B	-2.73	1.45	1.52
6	A	703	FAD	C1'-N10	2.69	1.54	1.47
6	A	703	FAD	P-O5'	-2.61	1.49	1.59
10	D	700	MQ7	O4-C4	2.57	1.28	1.23
5	M	802	FLC	CA-CAC	2.41	1.58	1.50
6	A	703	FAD	O4-C4	-2.37	1.19	1.23
6	M	803	FAD	C6A-N1A	2.30	1.42	1.35
5	A	702	FLC	OA2-CAC	-2.25	1.23	1.30
10	P	800	MQ7	C19-C18	2.24	1.56	1.50
10	D	700	MQ7	C19-C18	2.21	1.56	1.50
6	M	803	FAD	C2A-N1A	2.13	1.37	1.33
6	A	703	FAD	C3B-C4B	2.13	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	703	FAD	O2'-C2'	-2.05	1.39	1.43
10	P	800	MQ7	O4-C4	2.04	1.27	1.23

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	800	MQ7	C16-C15-C13	9.03	143.11	113.19
5	A	702	FLC	CB-CA-CAC	8.98	138.46	113.92
10	D	700	MQ7	C12-C11-C3	7.59	130.77	112.08
10	D	700	MQ7	C16-C15-C13	6.71	135.43	113.19
10	P	800	MQ7	C12-C11-C3	6.17	127.28	112.08
6	M	803	FAD	C4A-N9A-C8A	-5.38	100.09	105.74
5	M	802	FLC	CB-CA-CAC	5.28	128.37	113.92
10	D	700	MQ7	C11-C3-C4	-5.26	113.03	118.58
6	A	703	FAD	C4A-N9A-C8A	-5.22	100.26	105.74
6	A	703	FAD	C5A-C4A-N9A	5.01	111.27	105.81
6	M	803	FAD	C5A-C4A-N9A	4.95	111.21	105.81
10	P	800	MQ7	C11-C3-C4	-4.63	113.70	118.58
6	M	803	FAD	N3A-C4A-N9A	-4.51	119.49	127.17
6	A	703	FAD	N3A-C4A-N9A	-4.37	119.74	127.17
6	A	703	FAD	O3P-PA-O1A	4.31	123.67	110.70
6	M	803	FAD	O3P-PA-O1A	4.17	123.26	110.70
6	A	703	FAD	C4-C4X-N5	4.06	123.82	118.21
10	P	800	MQ7	C14-C13-C15	3.94	122.07	115.23
5	M	802	FLC	OB2-CBC-CB	3.89	120.59	113.14
10	P	800	MQ7	C21-C20-C18	-3.86	100.40	113.19
6	A	703	FAD	O2A-PA-O3P	-3.69	97.31	107.27
10	D	700	MQ7	C21-C20-C18	-3.56	101.39	113.19
10	P	800	MQ7	C11-C12-C13	3.56	132.96	126.83
5	M	802	FLC	CB-CG-CGC	3.53	123.56	113.92
6	A	703	FAD	O3P-P-O1P	-3.48	100.24	110.70
10	P	800	MQ7	O1-C1-C10	-3.46	116.04	121.57
5	A	702	FLC	OB2-CBC-CB	3.45	119.75	113.14
6	M	803	FAD	C4-C4X-N5	3.40	122.90	118.21
6	M	803	FAD	N3A-C2A-N1A	-3.24	123.67	128.58
5	A	702	FLC	OHB-CB-CBC	3.22	113.52	108.96
6	A	703	FAD	N3A-C2A-N1A	-3.21	123.72	128.58
10	D	700	MQ7	O1-C1-C10	-3.21	116.44	121.57
6	A	703	FAD	C4X-C4-N3	3.16	121.29	113.25
6	M	803	FAD	C4X-C4-N3	3.14	121.24	113.25
6	M	803	FAD	O3P-P-O1P	-3.14	101.27	110.70
6	M	803	FAD	C5X-N5-C4X	3.09	123.09	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	703	FAD	C5X-N5-C4X	3.05	123.02	118.09
5	M	802	FLC	OA1-CAC-CA	-3.01	114.43	122.95
6	A	703	FAD	C4-N3-C2	-2.94	120.43	125.64
6	A	703	FAD	O3'-C3'-C2'	-2.92	102.30	108.93
6	A	703	FAD	C9A-C5X-N5	-2.84	119.44	122.45
6	A	703	FAD	C10-N1-C2	2.83	122.98	116.85
6	A	703	FAD	O4-C4-C4X	-2.82	119.09	126.53
5	M	802	FLC	OA2-CAC-CA	2.82	123.27	114.35
6	M	803	FAD	C4-N3-C2	-2.75	120.76	125.64
10	P	800	MQ7	C5-C10-C1	-2.74	117.77	120.71
6	M	803	FAD	O4-C4-C4X	-2.72	119.34	126.53
6	M	803	FAD	C10-N1-C2	2.70	122.69	116.85
10	D	700	MQ7	C26-C25-C23	2.64	121.93	113.19
10	P	800	MQ7	C26-C25-C23	2.62	121.88	113.19
10	D	700	MQ7	C5-C10-C1	-2.62	117.89	120.71
6	A	703	FAD	O4'-C4'-C5'	-2.52	104.43	109.99
6	M	803	FAD	O4'-C4'-C5'	-2.48	104.52	109.99
10	D	700	MQ7	C25-C23-C22	-2.43	115.72	121.17
10	D	700	MQ7	C19-C18-C20	2.40	119.39	115.23
10	D	700	MQ7	C14-C13-C15	2.38	119.36	115.23
5	A	702	FLC	CG-CB-CA	-2.37	103.23	109.31
6	M	803	FAD	O2A-PA-O3P	-2.37	100.87	107.27
10	P	800	MQ7	C25-C23-C22	-2.36	115.86	121.17
10	P	800	MQ7	C24-C23-C25	2.29	119.21	115.23
10	D	700	MQ7	C2M-C2-C1	-2.28	112.47	116.68
6	A	703	FAD	O2P-P-O3P	2.24	113.32	107.27
10	P	800	MQ7	C2M-C2-C1	-2.23	112.57	116.68
10	D	700	MQ7	C24-C23-C25	2.20	119.06	115.23
6	M	803	FAD	C9A-C5X-N5	-2.20	120.12	122.45
6	M	803	FAD	C4X-C10-N1	-2.17	119.27	124.59
6	A	703	FAD	C10-C4X-N5	-2.15	120.41	124.81
10	D	700	MQ7	C20-C18-C17	-2.12	116.40	121.17
6	M	803	FAD	C9-C9A-N10	2.09	124.66	121.85
6	M	803	FAD	O5'-C5'-C4'	2.06	114.86	109.36
10	D	700	MQ7	C29-C28-C27	-2.02	116.60	122.66

There are no chirality outliers.

All (40) 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

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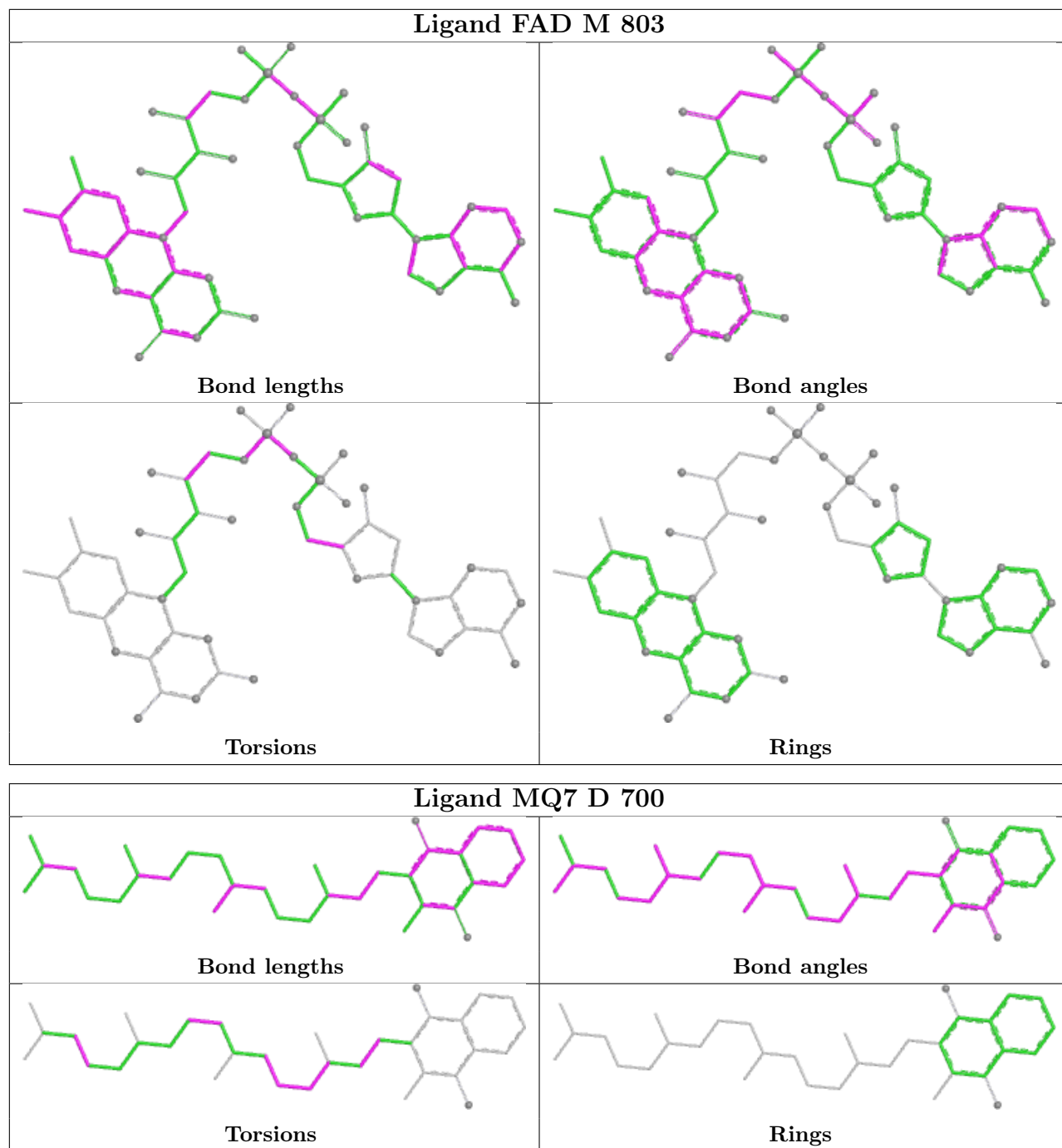
Mol	Chain	Res	Type	Atoms
6	A	703	FAD	N10-C1'-C2'-O2'
6	A	703	FAD	N10-C1'-C2'-C3'
6	A	703	FAD	C3'-C4'-C5'-O5'
6	A	703	FAD	O4'-C4'-C5'-O5'
6	A	703	FAD	C5'-O5'-P-O1P
6	A	703	FAD	C5'-O5'-P-O2P
6	A	703	FAD	C5'-O5'-P-O3P
6	A	703	FAD	PA-O3P-P-O5'
6	M	803	FAD	C3'-C4'-C5'-O5'
6	M	803	FAD	O4'-C4'-C5'-O5'
6	M	803	FAD	C5'-O5'-P-O1P
6	M	803	FAD	C5'-O5'-P-O3P
6	M	803	FAD	PA-O3P-P-O5'
10	P	800	MQ7	C24-C23-C25-C26
10	P	800	MQ7	C22-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
10	D	700	MQ7	C18-C20-C21-C22
5	M	802	FLC	OHB-CB-CG-CGC
10	P	800	MQ7	C23-C25-C26-C27
10	P	800	MQ7	C13-C15-C16-C17
5	A	702	FLC	CB-CG-CGC-OG1
5	A	702	FLC	CB-CG-CGC-OG2
5	M	802	FLC	CB-CA-CAC-OA1
5	A	702	FLC	CA-CB-CG-CGC
5	M	802	FLC	CB-CA-CAC-OA2
10	D	700	MQ7	C13-C15-C16-C17
5	A	702	FLC	CBC-CB-CG-CGC
6	M	803	FAD	PA-O3P-P-O1P
10	P	800	MQ7	C15-C16-C17-C18
10	D	700	MQ7	C15-C16-C17-C18
10	D	700	MQ7	C3-C11-C12-C13
10	P	800	MQ7	C3-C11-C12-C13
10	D	700	MQ7	C25-C26-C27-C28
6	A	703	FAD	PA-O3P-P-O1P
6	M	803	FAD	O4B-C4B-C5B-O5B

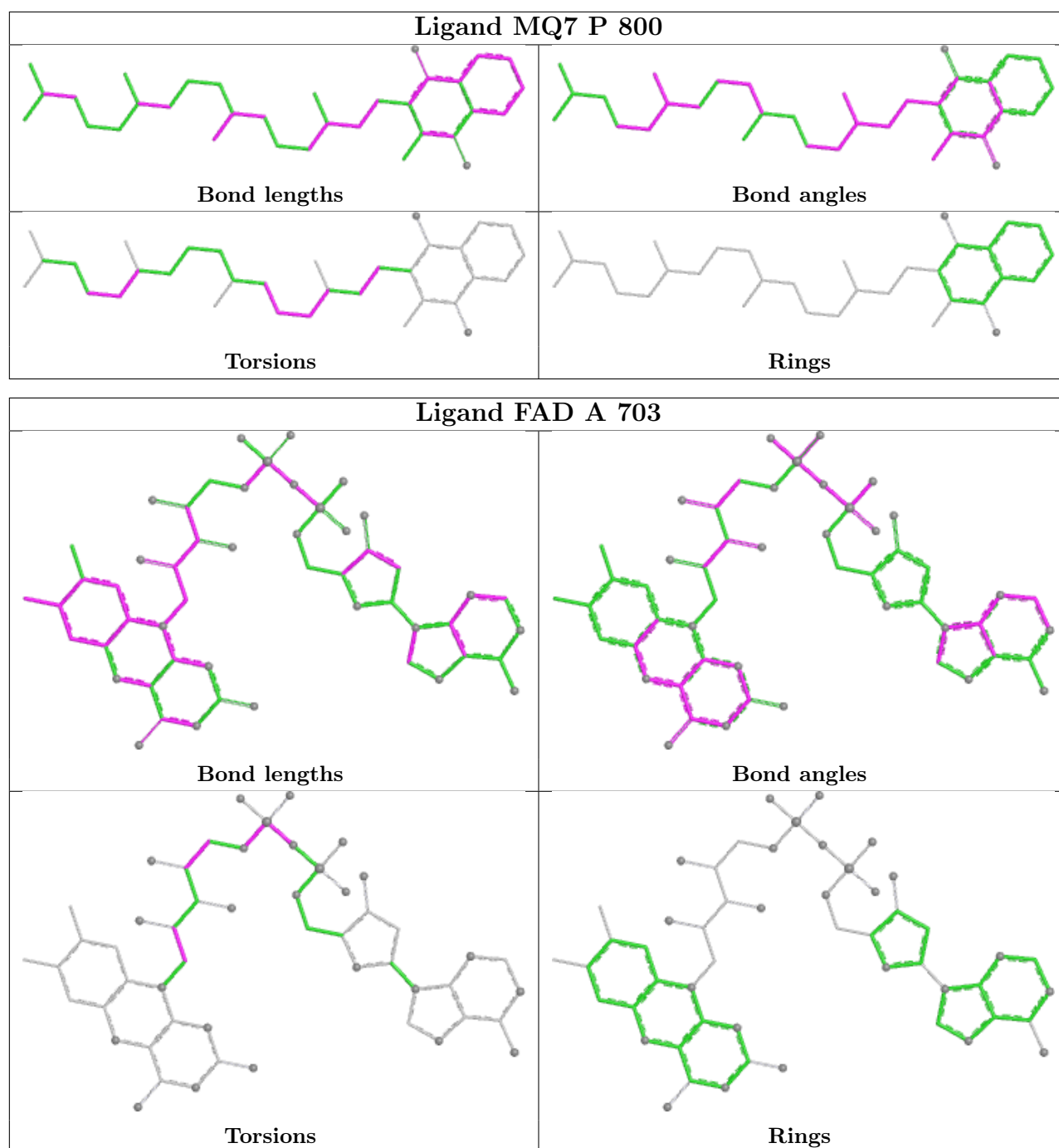
There are no ring outliers.

8 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	M	803	FAD	13	0
5	A	702	FLC	14	0
10	D	700	MQ7	7	0
8	N	245	F3S	1	0
9	N	246	SF4	3	0
5	M	802	FLC	3	0
10	P	800	MQ7	11	0
6	A	703	FAD	17	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.21	4 (0%) 84 70	9, 14, 62, 85	0
1	M	572/602 (95%)	1.67	199 (34%) 1 1	30, 92, 127, 142	0
2	B	243/243 (100%)	-0.29	2 (0%) 82 68	9, 15, 36, 85	0
2	N	243/243 (100%)	0.69	19 (7%) 19 14	9, 62, 119, 147	0
3	C	130/130 (100%)	-0.09	0 100 100	10, 32, 59, 76	0
3	O	130/130 (100%)	0.32	5 (3%) 44 30	24, 55, 106, 123	0
4	D	119/119 (100%)	-0.01	0 100 100	18, 36, 61, 70	0
4	P	119/119 (100%)	0.31	2 (1%) 69 50	27, 49, 80, 118	0
All	All	2133/2188 (97%)	0.47	231 (10%) 11 9	9, 45, 114, 147	0

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	189	VAL	7.5
1	M	229	VAL	7.4
1	M	403	GLY	7.2
1	M	385	LEU	7.1
1	M	188	VAL	6.0
1	M	359	GLY	5.5
1	M	392	GLY	5.2
1	M	514	VAL	5.2
1	M	393	SER	5.2
2	N	17	VAL	5.0
1	M	411	THR	5.0
1	M	544	ASP	4.9
1	M	225	ASP	4.9
1	M	376	ALA	4.8
1	M	358	MET	4.8
3	O	1	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	M	383	VAL	4.6
1	M	367	CYS	4.6
1	M	553	ALA	4.6
1	M	223	LEU	4.5
1	M	568	VAL	4.4
1	M	206	GLY	4.4
1	M	405	LEU	4.4
4	P	4	ASN	4.2
1	M	361	ILE	4.2
1	M	491	ILE	4.2
3	O	6	PRO	4.2
2	N	169	GLY	4.2
1	M	162	VAL	4.1
1	M	513	ASN	4.1
1	M	77	CYS	4.1
1	M	482	LEU	4.0
1	M	207	ILE	3.9
1	M	550	HIS	3.9
1	M	375	PHE	3.9
1	M	515	ALA	3.9
1	M	226	MET	3.8
1	M	216	ALA	3.8
1	M	124	THR	3.8
1	M	20	ALA	3.7
1	M	218	SER	3.7
1	M	46	VAL	3.7
1	M	90	PRO	3.7
1	M	84	TYR	3.6
1	M	406	ALA	3.6
1	M	219	HIS	3.6
1	M	511	GLY	3.6
1	M	164	ASP	3.6
1	M	23	ALA	3.6
1	M	402	PHE	3.5
2	N	133	ILE	3.5
1	M	492	THR	3.5
1	M	8	ALA	3.5
2	N	153	LEU	3.5
1	M	549	LYS	3.5
1	M	552	LEU	3.5
1	M	371	ILE	3.5
1	M	161	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	425	ILE	3.4
1	M	30	ALA	3.4
1	M	484	GLU	3.4
1	M	157	VAL	3.4
1	M	37	LYS	3.4
1	M	111	VAL	3.4
1	M	476	ILE	3.4
1	M	99	TRP	3.3
1	M	217	LEU	3.3
2	N	40	LEU	3.3
1	M	373	GLY	3.3
1	M	198	VAL	3.3
1	M	543	ASP	3.2
1	M	479	LEU	3.2
2	B	242	PRO	3.2
1	M	221	VAL	3.2
1	M	88	HIS	3.2
1	M	227	GLU	3.2
1	M	159	ASP	3.2
1	M	377	VAL	3.2
1	M	93	MET	3.1
1	M	42	ARG	3.1
1	M	222	PRO	3.1
1	M	522	ALA	3.1
1	M	133	PHE	3.1
1	M	433	GLU	3.1
1	M	506	ILE	3.1
1	M	55	VAL	3.0
1	M	489	VAL	3.0
2	N	54	ARG	3.0
1	M	156	PHE	3.0
1	M	295	TRP	3.0
1	M	176	MET	3.0
1	M	38	VAL	3.0
1	M	163	ASP	3.0
1	M	121	ILE	3.0
1	M	160	ILE	3.0
1	M	508	LEU	3.0
1	M	525	ARG	3.0
1	M	410	ALA	3.0
1	M	497	VAL	3.0
1	M	551	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	62	PHE	2.9
1	M	486	PHE	2.9
1	M	554	PHE	2.9
1	M	274	LEU	2.9
1	M	560	THR	2.9
1	M	43	SER	2.9
1	M	451	ILE	2.9
1	M	79	GLN	2.9
1	M	82	VAL	2.9
1	M	464	GLY	2.9
2	N	142	TYR	2.9
1	M	232	HIS	2.8
1	M	94	THR	2.8
1	M	85	PHE	2.8
1	M	170	LEU	2.8
1	M	466	TYR	2.8
1	M	325	HIS	2.8
1	M	47	ALA	2.8
1	M	147	PRO	2.8
2	B	198	GLN	2.8
1	M	181	VAL	2.8
1	M	504	TYR	2.7
1	M	459	MET	2.7
1	A	282	MET	2.7
1	M	417	ALA	2.7
1	M	519	ALA	2.7
1	M	409	GLN	2.7
1	M	566	SER	2.7
1	M	171	VAL	2.7
1	M	25	GLN	2.7
2	N	122	GLY	2.7
1	M	34	LEU	2.7
1	M	89	CYS	2.6
1	M	228	PHE	2.6
1	M	526	LYS	2.6
1	M	444	GLY	2.6
1	M	172	ALA	2.6
2	N	15	PRO	2.6
1	M	103	TRP	2.6
1	M	390	ARG	2.6
3	O	2	THR	2.6
1	M	362	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	213	MET	2.5
1	M	496	SER	2.5
1	M	66	PHE	2.5
1	M	534	ARG	2.5
1	A	417	ALA	2.5
1	M	270	PRO	2.5
1	M	487	LYS	2.5
1	M	503	LEU	2.5
1	M	167	VAL	2.5
1	M	463	CYS	2.4
1	M	570	ILE	2.4
1	M	357	THR	2.4
1	M	483	GLN	2.4
2	N	32	ALA	2.4
1	M	465	ILE	2.4
1	M	36	SER	2.4
1	M	517	CYS	2.4
1	M	475	THR	2.4
1	M	134	HIS	2.4
2	N	16	GLU	2.4
1	M	401	VAL	2.4
1	M	210	GLY	2.4
1	M	510	HIS	2.4
2	N	10	VAL	2.4
1	M	493	ASP	2.4
1	M	559	GLY	2.4
1	M	523	MET	2.4
1	M	199	TYR	2.3
1	M	556	ASP	2.3
1	M	434	GLN	2.3
2	N	183	SER	2.3
1	M	386	HIS	2.3
1	M	169	GLY	2.3
1	M	252	GLY	2.3
1	M	203	THR	2.3
3	O	129	TYR	2.3
1	M	192	THR	2.3
1	M	419	ASN	2.3
1	M	220	GLY	2.3
1	M	316	LEU	2.3
1	M	366	ASN	2.3
1	M	389	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	443	ASP	2.3
1	M	412	GLU	2.2
1	M	396	LEU	2.2
1	M	123	ARG	2.2
1	M	380	CYS	2.2
1	M	63	GLU	2.2
1	M	59	HIS	2.2
1	M	474	LYS	2.2
2	N	33	THR	2.2
1	M	395	SER	2.2
1	M	9	ILE	2.2
2	N	98	ILE	2.2
1	M	53	ALA	2.2
1	M	246	GLY	2.2
1	M	471	LEU	2.2
4	P	47	ASP	2.2
1	M	155	HIS	2.2
1	M	135	MET	2.2
1	M	277	PRO	2.2
1	M	360	GLY	2.2
2	N	130	GLY	2.2
1	A	272	THR	2.1
1	M	24	ALA	2.1
1	M	195	ALA	2.1
2	N	29	PRO	2.1
1	M	432	VAL	2.1
1	M	253	ILE	2.1
2	N	36	LEU	2.1
1	M	54	ALA	2.1
1	M	473	GLN	2.1
1	M	78	GLU	2.1
1	M	460	GLU	2.1
1	M	130	LYS	2.1
1	M	21	ILE	2.1
1	M	548	LEU	2.1
3	O	100	ASP	2.1
1	M	404	ARG	2.1
1	M	12	ALA	2.1
1	M	462	GLY	2.1
1	M	114	ARG	2.1
1	M	448	TRP	2.1
1	M	480	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	420	GLY	2.1
1	M	520	HIS	2.0
1	M	540	THR	2.0
1	M	68	ASP	2.0
2	N	49	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

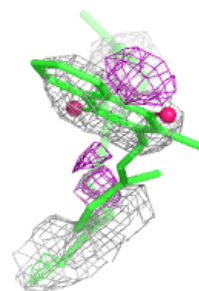
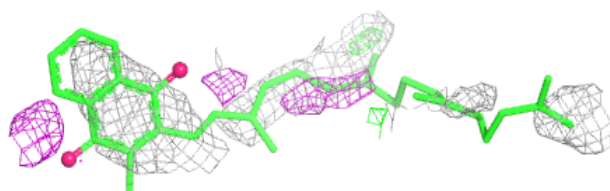
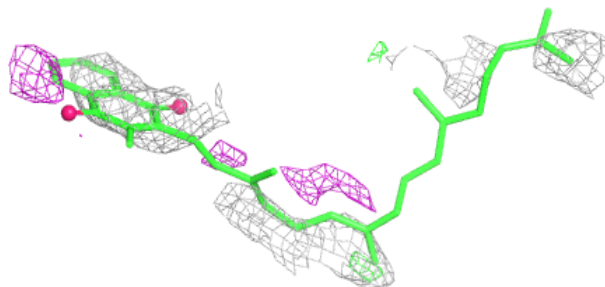
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FLC	A	702	13/13	0.68	0.28	31,37,38,39	0
10	MQ7	P	800	33/48	0.69	0.32	83,106,120,123	0
5	FLC	M	802	13/13	0.70	0.21	60,74,92,97	0
10	MQ7	D	700	33/48	0.76	0.35	59,100,117,127	0
6	FAD	M	803	52/53	0.81	0.23	23,87,158,164	0
9	SF4	N	246	8/8	0.96	0.07	20,29,49,53	0
7	FES	N	244	4/4	0.97	0.05	21,24,44,53	0
6	FAD	A	703	52/53	0.98	0.08	0,1,17,36	0
7	FES	B	244	4/4	0.99	0.04	0,4,5,8	0
8	F3S	N	245	7/7	0.99	0.05	14,16,29,49	0
9	SF4	B	246	8/8	0.99	0.09	9,21,27,27	0
8	F3S	B	245	7/7	1.00	0.05	7,11,15,24	0

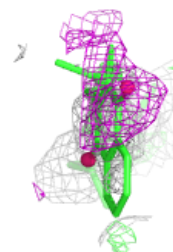
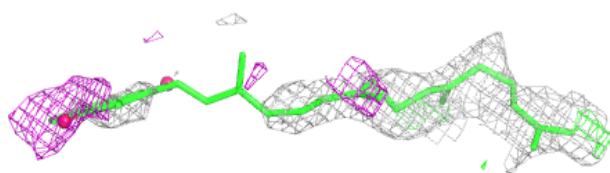
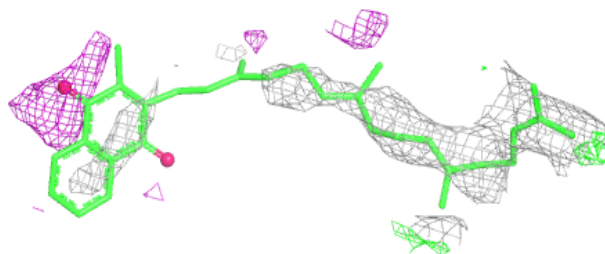
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MQ7 P 800:

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

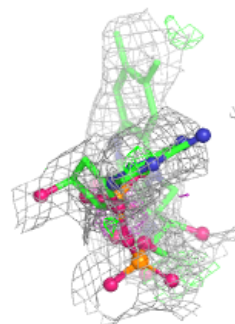
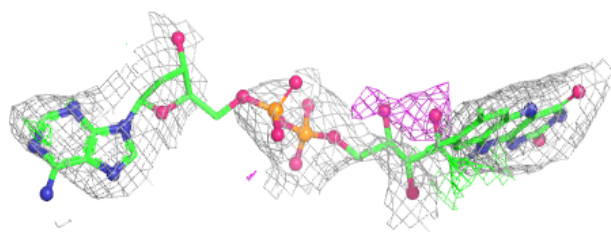
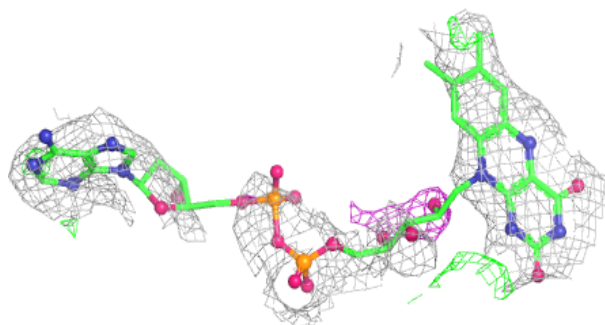
**Electron density around MQ7 D 700:**

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

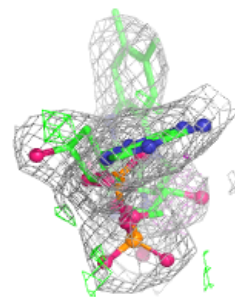
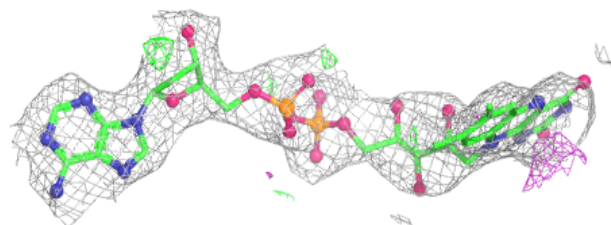
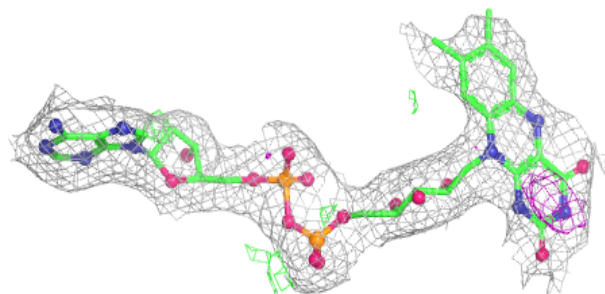


Electron density around FAD M 803:

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

**Electron density around FAD A 703:**

$2mF_o-DF_c$ (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.