



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:12 PM UTC

PDB ID : 3CIR / pdb_00003cir
Title : E. coli Quinol fumarate reductase FrdA T234A mutation
Authors : Tomasiak, T.M.; Maklashina, E.; Cecchini, G.; Iverson, T.M.
Deposited on : 2008-03-11
Resolution : 3.65 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

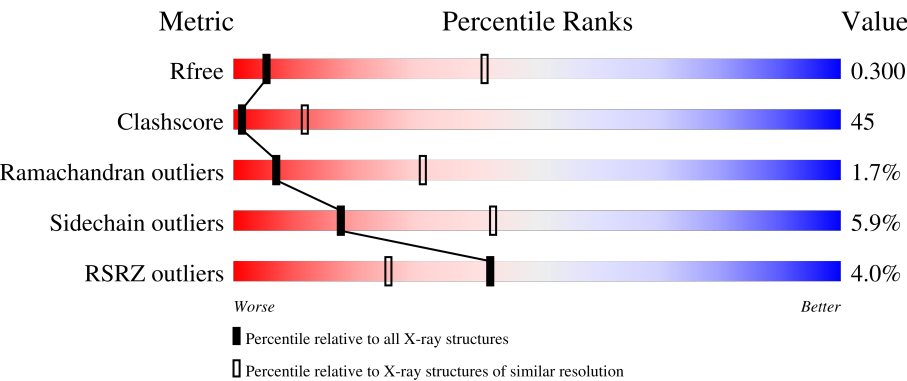
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

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	5% 40% 43% 7% 10%
1	M	602	7% 26% 50% 6% 16%
2	B	243	% 47% 45% 8%
2	N	243	3% 42% 52% 5%
3	C	130	2% 41% 50% 8%

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Mol	Chain	Length	Quality of chain
3	O	130	% 45% 51% • •
4	D	119	39% 52% 8%
4	P	119	39% 58% •

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	FAD	M	601	-	-	X	-
8	SF4	B	246	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15746 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	541	Total	C	N	O	S	0	0	0
			4140	2576	752	783	29			
1	M	504	Total	C	N	O	S	0	0	0
			3718	2295	682	715	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ALA	THR	engineered mutation	UNP P00363
M	234	ALA	THR	engineered mutation	UNP P00363

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

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.

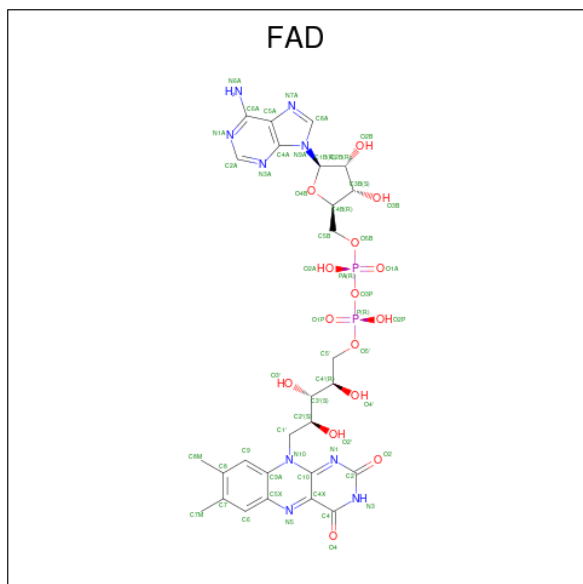
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

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



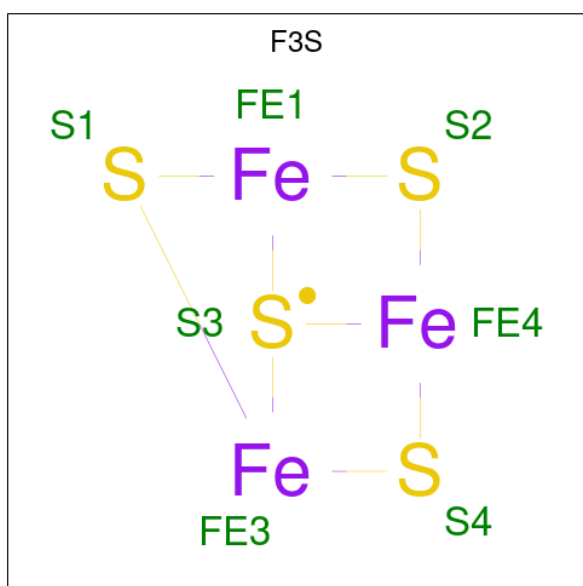
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	M	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



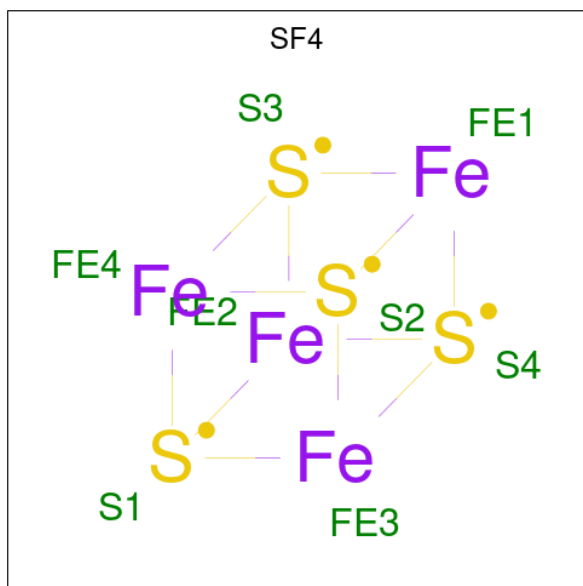
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		
6	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



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

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

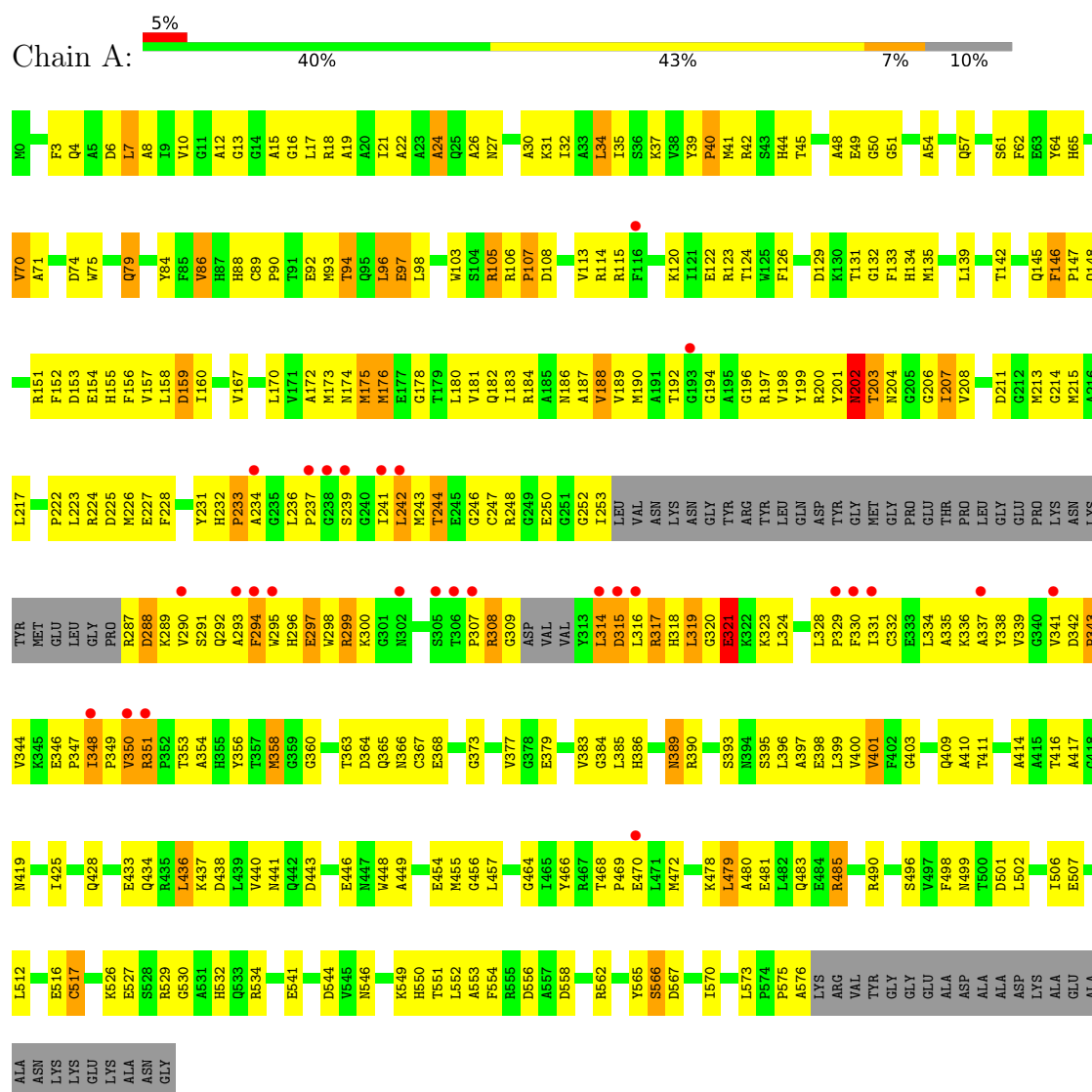


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	N	1	Total	Fe	S	0	0
			8	4	4		

3 Residue-property plots

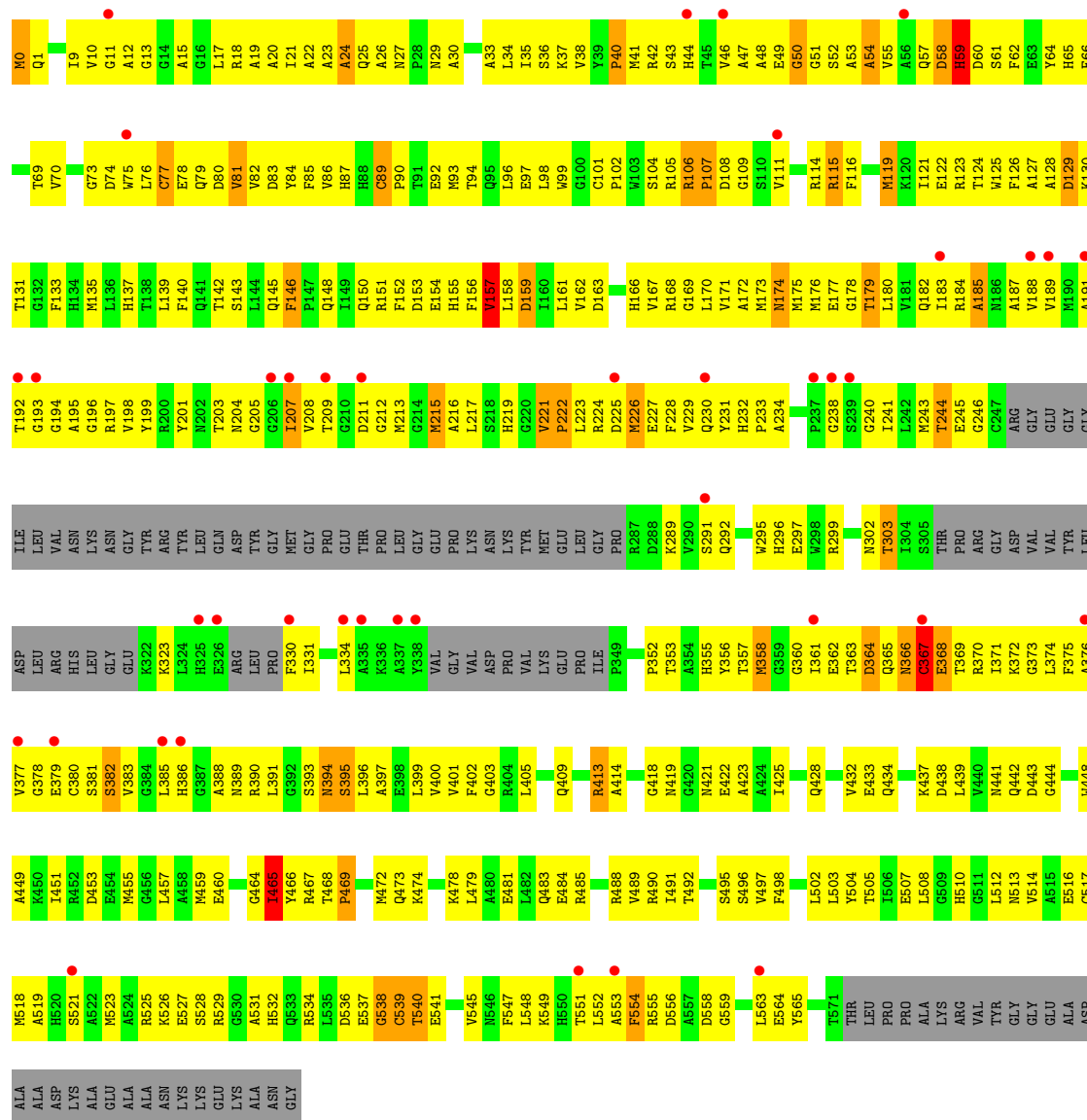
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Fumarate reductase flavoprotein subunit

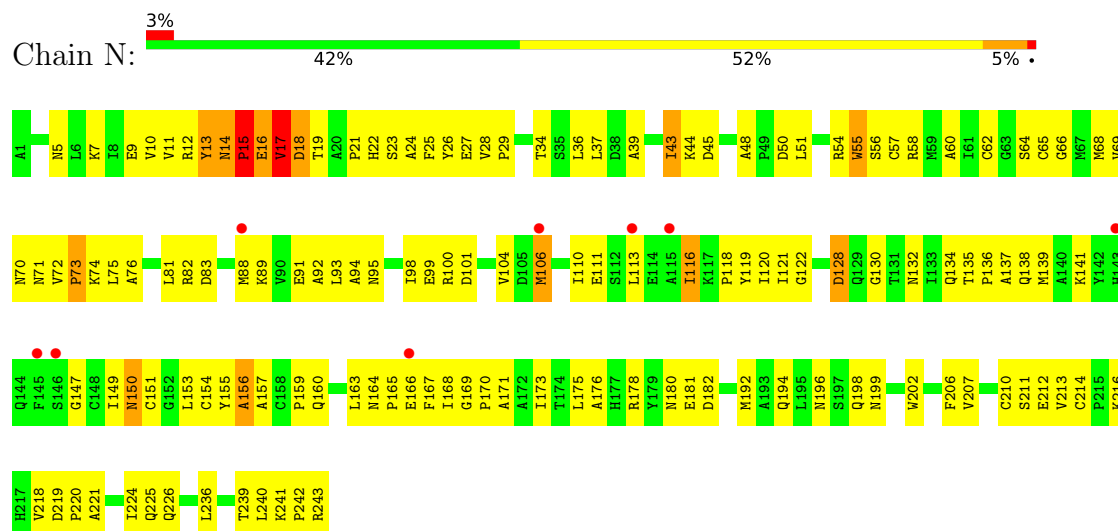


• Molecule 1: Fumarate reductase flavoprotein subunit

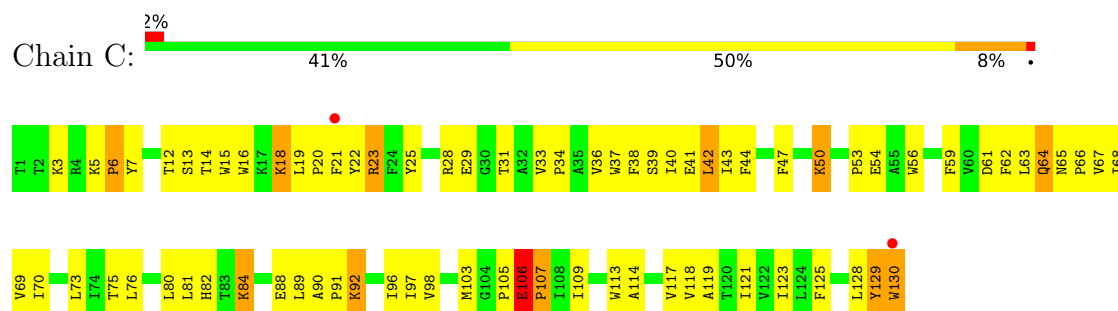




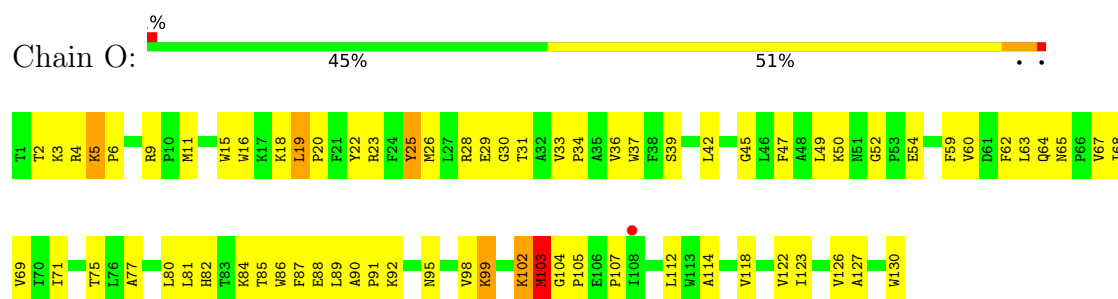
- Molecule 2: Fumarate reductase iron-sulfur subunit



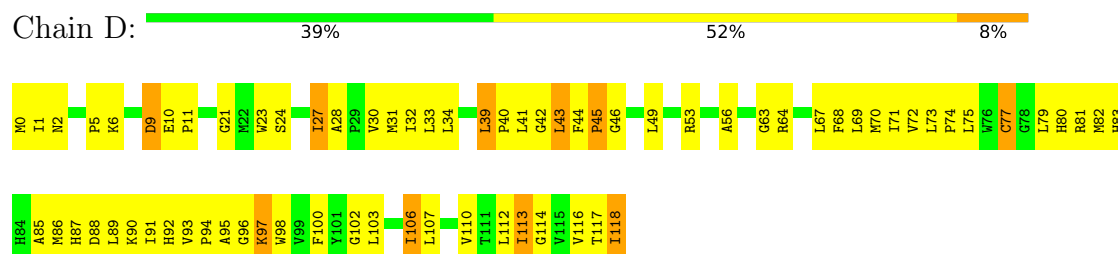
- Molecule 3: Fumarate reductase subunit C



- Molecule 3: Fumarate reductase subunit C



- Molecule 4: Fumarate reductase subunit D

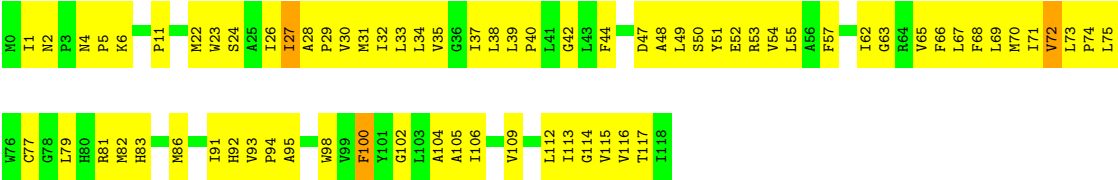


- Molecule 4: Fumarate reductase subunit D

Chain P:

39%

58%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.86Å 135.47Å 266.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	266.00 – 3.65 133.01 – 3.65	Depositor EDS
% Data completeness (in resolution range)	80.8 (266.00-3.65) 80.8 (133.01-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.39	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.296 0.252 , 0.300	Depositor DCC
R_{free} test set	1038 reflections (1.96%)	wwPDB-VP
Wilson B-factor (Å ²)	79.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 80.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	15746	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: FES, FAD, SF4, F3S

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.81	5/4221 (0.1%)	1.24	43/5705 (0.8%)
1	M	0.78	4/3778 (0.1%)	1.28	44/5107 (0.9%)
2	B	0.80	6/1931 (0.3%)	1.28	30/2617 (1.1%)
2	N	0.63	1/1931 (0.1%)	1.11	10/2617 (0.4%)
3	C	0.77	3/1094 (0.3%)	1.11	7/1496 (0.5%)
3	O	0.68	0/1094	1.17	11/1496 (0.7%)
4	D	0.71	1/956 (0.1%)	1.15	2/1303 (0.2%)
4	P	0.60	0/956	1.06	6/1303 (0.5%)
All	All	0.76	20/15961 (0.1%)	1.21	153/21644 (0.7%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	299	ARG	CA-C	11.83	1.69	1.52
1	A	300	LYS	N-CA	10.60	1.60	1.45
3	C	106	GLU	C-N	10.45	1.46	1.34
1	A	315	ASP	CA-C	-8.92	1.42	1.52
1	M	466	TYR	CA-C	8.43	1.63	1.52
1	M	539	CYS	CA-C	8.06	1.62	1.52
2	B	241	LYS	C-N	7.62	1.41	1.33
2	N	164	ASN	CA-C	-6.97	1.45	1.52
2	B	163	LEU	CA-C	-6.76	1.43	1.52
1	A	307	PRO	CA-C	6.72	1.62	1.52
1	M	366	ASN	CA-C	6.62	1.61	1.52
2	B	93	LEU	CA-C	-6.47	1.44	1.52
2	B	214	CYS	C-O	-6.35	1.15	1.24
1	M	540	THR	N-CA	6.22	1.54	1.46
3	C	6	PRO	CA-C	5.43	1.60	1.52
2	B	215	PRO	N-CD	-5.25	1.40	1.47
1	A	189	VAL	N-CA	-5.24	1.40	1.46
4	D	45	PRO	CA-C	5.24	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	241	LYS	CA-C	5.24	1.59	1.52
3	C	106	GLU	CA-C	5.09	1.59	1.52

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	323	LYS	N-CA-C	17.83	134.62	112.86
2	B	213	VAL	N-CA-C	10.36	122.85	112.90
1	A	308	ARG	N-CA-C	9.98	126.46	113.18
1	M	303	THR	N-CA-C	-9.85	94.09	109.76
1	A	39	TYR	CA-C-N	8.69	130.71	119.84
1	A	39	TYR	C-N-CA	8.69	130.71	119.84
2	N	17	VAL	N-CA-C	-8.54	100.09	112.04
1	M	548	LEU	N-CA-C	-8.45	101.23	112.72
2	B	164	ASN	CA-C-N	8.25	127.91	119.82
2	B	164	ASN	C-N-CA	8.25	127.91	119.82
1	M	296	HIS	N-CA-C	-7.93	101.94	111.69
1	M	365	GLN	N-CA-C	-7.92	103.07	112.89
1	M	367	CYS	N-CA-C	7.73	122.34	111.52
3	C	106	GLU	CA-C-N	7.71	127.25	118.85
3	C	106	GLU	C-N-CA	7.71	127.25	118.85
1	M	540	THR	N-CA-C	7.67	122.41	112.89
1	M	358	MET	CA-C-N	-7.60	114.31	122.67
1	M	358	MET	C-N-CA	-7.60	114.31	122.67
2	N	156	ALA	N-CA-C	-7.49	104.17	113.38
1	M	556	ASP	N-CA-C	7.41	120.09	110.53
2	B	203	SER	N-CA-C	-7.40	103.39	113.30
2	B	158	CYS	CA-C-N	7.37	127.23	119.05
2	B	158	CYS	C-N-CA	7.37	127.23	119.05
4	P	35	VAL	N-CA-C	7.23	117.32	110.53
3	O	103	MET	CA-C-N	7.20	133.18	121.87
3	O	103	MET	C-N-CA	7.20	133.18	121.87
1	M	545	VAL	N-CA-C	7.16	119.17	111.58
1	M	492	THR	N-CA-C	7.09	119.86	111.71
1	A	348	ILE	N-CA-C	7.08	114.00	107.56
1	A	27	ASN	CA-C-N	6.91	126.88	119.28
1	A	27	ASN	C-N-CA	6.91	126.88	119.28
3	O	52	GLY	CA-C-N	6.83	128.38	119.84
3	O	52	GLY	C-N-CA	6.83	128.38	119.84
2	B	146	SER	N-CA-C	6.82	121.19	113.01
1	M	106	ARG	N-CA-C	-6.77	101.54	110.07
3	O	103	MET	CB-CA-C	6.76	120.71	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	107	PRO	CA-N-CD	-6.71	102.61	112.00
3	C	81	LEU	N-CA-C	-6.67	103.93	111.07
1	A	246	GLY	N-CA-C	-6.67	106.59	115.32
1	M	244	THR	N-CA-C	-6.59	100.68	110.23
1	M	178	GLY	N-CA-C	-6.48	106.78	115.21
1	M	418	GLY	N-CA-C	-6.42	97.97	113.18
1	M	545	VAL	CB-CA-C	-6.37	103.92	111.94
3	O	25	TYR	N-CA-C	-6.33	104.30	111.14
1	M	221	VAL	CA-C-N	6.32	126.83	120.14
1	M	221	VAL	C-N-CA	6.32	126.83	120.14
1	A	299	ARG	CA-C-N	6.31	132.30	122.26
1	A	299	ARG	C-N-CA	6.31	132.30	122.26
1	A	297	GLU	N-CA-C	-6.31	105.41	113.23
1	M	403	GLY	N-CA-C	-6.25	105.22	112.73
1	A	299	ARG	CA-C-O	-6.22	111.59	119.31
4	D	27	ILE	N-CA-C	6.21	121.11	112.35
2	N	198	GLN	N-CA-C	-6.21	105.67	113.18
3	O	105	PRO	N-CA-C	6.14	122.06	113.53
1	A	146	PHE	CA-C-N	6.09	125.65	119.19
1	A	146	PHE	C-N-CA	6.09	125.65	119.19
1	M	174	ASN	N-CA-C	-6.09	101.02	110.10
4	P	83	HIS	N-CA-C	-6.06	104.59	111.07
2	N	19	THR	N-CA-C	-6.03	106.25	113.97
2	B	93	LEU	O-C-N	6.00	130.33	122.89
4	P	100	PHE	N-CA-C	5.96	117.57	111.14
1	M	81	VAL	N-CA-C	-5.91	107.05	112.96
1	A	32	ILE	CA-C-N	-5.90	115.17	122.84
1	A	32	ILE	C-N-CA	-5.90	115.17	122.84
1	A	159	ASP	N-CA-C	5.88	117.18	108.60
2	B	173	ILE	CB-CA-C	-5.85	104.40	111.88
2	B	163	LEU	CA-C-N	-5.83	115.25	122.42
2	B	163	LEU	C-N-CA	-5.83	115.25	122.42
2	N	15	PRO	CA-N-CD	-5.80	103.87	112.00
1	A	419	ASN	N-CA-C	5.80	118.19	110.53
1	A	314	LEU	N-CA-C	-5.79	99.28	108.73
2	B	198	GLN	N-CA-C	-5.76	105.52	112.54
4	P	72	VAL	N-CA-C	5.72	115.85	110.30
1	A	79	GLN	N-CA-C	5.70	119.05	111.75
3	C	73	LEU	N-CA-C	-5.67	105.10	111.28
1	A	346	GLU	CA-C-N	5.66	126.10	119.99
1	A	346	GLU	C-N-CA	5.66	126.10	119.99
2	B	28	VAL	CA-C-N	5.64	125.61	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	28	VAL	C-N-CA	5.64	125.61	120.03
1	A	320	GLY	CA-C-N	5.63	132.30	121.54
1	A	320	GLY	C-N-CA	5.63	132.30	121.54
2	B	93	LEU	CA-C-O	5.62	126.17	120.88
1	A	242	LEU	N-CA-C	5.59	117.75	110.43
1	A	532	HIS	N-CA-C	5.56	117.77	107.99
2	B	93	LEU	CA-C-N	5.54	128.98	121.05
2	B	93	LEU	C-N-CA	5.54	128.98	121.05
1	M	464	GLY	CA-C-O	-5.54	116.49	122.47
1	A	384	GLY	N-CA-C	-5.53	107.13	115.32
1	M	538	GLY	N-CA-C	-5.52	107.58	115.64
2	B	213	VAL	CB-CA-C	-5.50	104.38	111.20
2	B	163	LEU	CA-C-O	5.48	125.68	119.27
1	M	303	THR	N-CA-CB	5.46	118.41	109.95
1	A	350	VAL	N-CA-C	5.46	117.96	108.90
1	A	189	VAL	N-CA-C	-5.43	100.65	108.53
1	M	243	MET	N-CA-C	5.41	117.78	109.07
1	M	466	TYR	CA-C-N	5.38	131.01	122.62
1	M	466	TYR	C-N-CA	5.38	131.01	122.62
1	M	441	ASN	N-CA-C	-5.36	106.74	113.28
4	P	47	ASP	N-CA-C	5.36	118.83	112.72
1	M	75	TRP	CB-CA-C	-5.36	103.97	111.80
2	B	151	CYS	N-CA-C	5.36	119.53	112.89
3	O	19	LEU	CA-C-N	5.35	126.53	119.84
3	O	19	LEU	C-N-CA	5.35	126.53	119.84
3	O	103	MET	O-C-N	5.34	129.49	122.93
1	A	343	PRO	CA-C-N	-5.33	115.50	121.85
1	A	343	PRO	C-N-CA	-5.33	115.50	121.85
1	A	401	VAL	N-CA-C	5.31	115.41	110.42
2	B	169	GLY	CA-C-N	5.31	126.47	119.84
2	B	169	GLY	C-N-CA	5.31	126.47	119.84
1	M	22	ALA	N-CA-C	-5.30	106.76	113.18
1	M	537	GLU	N-CA-C	5.30	118.00	110.10
2	B	107	THR	N-CA-C	5.30	116.74	111.07
1	M	157	VAL	N-CA-C	5.29	117.31	109.17
2	N	14	ASN	CA-C-N	5.27	126.43	119.84
2	N	14	ASN	C-N-CA	5.27	126.43	119.84
1	A	233	PRO	N-CA-C	5.26	120.85	113.53
1	M	222	PRO	N-CA-C	5.26	120.47	111.68
1	M	368	GLU	N-CA-C	5.26	117.41	109.41
2	B	154	CYS	CA-C-N	-5.25	112.84	120.29
2	B	154	CYS	C-N-CA	-5.25	112.84	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	65	CYS	N-CA-C	5.24	119.30	113.01
3	C	96	ILE	N-CA-C	5.24	115.40	107.75
1	M	489	VAL	CB-CA-C	-5.24	105.58	111.23
1	A	566	SER	CA-C-N	-5.21	115.38	122.93
1	A	566	SER	C-N-CA	-5.21	115.38	122.93
1	M	24	ALA	N-CA-C	-5.19	105.24	112.45
3	C	129	TYR	CA-CB-CG	5.15	123.17	113.90
1	M	364	ASP	N-CA-C	5.15	117.82	109.79
1	A	105	ARG	N-CA-C	5.15	117.36	109.95
1	A	202	ASN	N-CA-C	5.14	115.84	108.74
2	N	14	ASN	N-CA-C	-5.14	99.44	108.69
4	D	106	ILE	N-CA-C	5.13	115.36	110.53
2	B	153	LEU	N-CA-C	5.13	117.61	111.71
1	A	86	VAL	N-CA-C	5.12	116.46	110.62
1	M	146	PHE	CA-C-N	5.12	125.41	119.47
1	M	146	PHE	C-N-CA	5.12	125.41	119.47
1	A	24	ALA	N-CA-C	-5.12	105.39	110.97
2	B	144	GLN	N-CA-C	5.11	117.24	111.11
1	M	215	MET	N-CA-C	-5.10	107.61	113.88
1	A	321	GLU	N-CA-C	5.09	121.64	110.80
4	P	27	ILE	N-CA-C	5.09	120.74	113.16
1	M	159	ASP	N-CA-C	5.08	116.25	108.42
2	N	43	ILE	N-CA-C	-5.08	105.65	110.42
1	A	175	MET	N-CA-C	5.06	117.45	111.33
1	M	331	ILE	N-CA-C	-5.05	108.91	113.71
1	M	465	ILE	N-CA-C	5.05	119.84	109.34
1	A	107	PRO	N-CA-C	-5.04	107.28	113.84
2	B	48	ALA	CA-C-N	5.04	124.76	119.82
2	B	48	ALA	C-N-CA	5.04	124.76	119.82
1	A	134	HIS	N-CA-C	5.04	116.77	111.28
1	A	299	ARG	N-CA-C	5.03	119.13	112.89
2	N	45	ASP	N-CA-C	5.03	116.45	111.07
3	O	127	ALA	N-CA-C	5.00	119.23	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4140	0	4014	364	0
1	M	3718	0	3461	466	0
2	B	1888	0	1837	179	0
2	N	1888	0	1837	179	0
3	C	1058	0	1108	110	1
3	O	1058	0	1108	87	1
4	D	926	0	971	90	0
4	P	926	0	971	80	0
5	A	53	0	31	11	0
5	M	53	0	31	27	0
6	B	4	0	0	1	0
6	N	4	0	0	1	0
7	B	7	0	0	1	0
7	N	7	0	0	1	0
8	B	8	0	0	2	0
8	N	8	0	0	1	0
All	All	15746	0	15369	1395	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (1395) 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:44:HIS:NE2	5:A:601:FAD:C8M	1.77	1.48
1:M:44:HIS:NE2	5:M:601:FAD:C8M	1.78	1.44
1:A:243:MET:SD	1:A:331:ILE:HG23	1.61	1.41
2:B:4:LYS:H	2:B:4:LYS:NZ	1.17	1.38
2:B:4:LYS:HZ2	2:B:4:LYS:N	1.20	1.35
1:A:330:PHE:CE2	2:B:59:MET:CE	2.13	1.31
1:A:330:PHE:HE2	2:B:59:MET:CE	1.44	1.30
1:M:44:HIS:CE1	5:M:601:FAD:HM82	1.75	1.20
1:M:119:MET:SD	1:M:123:ARG:NH1	2.16	1.19
1:M:44:HIS:NE2	5:M:601:FAD:HM82	0.84	1.17
1:A:332:CYS:HA	1:A:343:PRO:HG2	1.22	1.15
1:A:106:ARG:HG3	1:A:107:PRO:HD2	1.27	1.14
1:A:294:PHE:CE1	1:A:351:ARG:HG3	1.82	1.14
2:N:106:MET:HE2	2:N:106:MET:HA	1.31	1.12
1:A:44:HIS:NE2	5:A:601:FAD:HM82	0.80	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:NH1	2:B:134:GLN:HB3	1.65	1.10
1:A:237:PRO:CG	1:A:308:ARG:CB	2.29	1.10
1:A:330:PHE:CE2	2:B:59:MET:HE3	1.83	1.10
1:M:497:VAL:HG21	2:N:15:PRO:HG3	1.18	1.09
1:A:44:HIS:CE1	5:A:601:FAD:HM82	1.87	1.09
1:M:291:SER:CB	1:M:465:ILE:HD13	1.84	1.07
2:B:96:PHE:HB3	2:B:104:VAL:HG21	1.25	1.07
1:A:294:PHE:HE1	1:A:351:ARG:HG3	0.90	1.06
1:A:237:PRO:HG3	1:A:308:ARG:CB	1.85	1.06
2:B:68:MET:HE2	2:B:94:ALA:HB2	1.37	1.06
1:M:395:SER:OG	5:M:601:FAD:H2'	1.55	1.05
1:A:330:PHE:CE2	2:B:59:MET:HE2	1.89	1.05
1:A:243:MET:SD	1:A:331:ILE:CG2	2.45	1.04
1:M:358:MET:HE3	1:M:389:ASN:HA	1.36	1.03
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.40	1.02
1:M:166:HIS:HB3	1:M:168:ARG:HH12	1.20	1.02
1:M:115:ARG:CG	1:M:115:ARG:HH11	1.73	1.02
3:C:50:LYS:HD3	4:D:118:ILE:HG13	1.40	1.01
1:A:44:HIS:CD2	5:A:601:FAD:HM82	1.96	1.01
1:A:294:PHE:HE1	1:A:351:ARG:CG	1.72	1.01
1:M:35:ILE:HG12	1:M:152:PHE:HB2	1.43	1.01
1:A:203:THR:HG21	1:A:242:LEU:HD21	1.42	1.00
4:D:72:VAL:HA	4:D:75:LEU:HD12	1.43	1.00
1:M:115:ARG:HH11	1:M:115:ARG:HG2	1.26	0.99
3:O:19:LEU:HD21	3:O:22:TYR:CE2	1.97	0.98
1:M:497:VAL:HG21	2:N:15:PRO:CG	1.91	0.98
1:M:49:GLU:OE1	1:M:330:PHE:CB	2.12	0.97
2:B:68:MET:CE	2:B:94:ALA:HB2	1.95	0.97
1:A:237:PRO:HG2	1:A:308:ARG:CB	1.93	0.96
1:M:222:PRO:HD3	1:M:370:ARG:HH11	1.30	0.96
2:B:109:PHE:HD2	2:B:110:ILE:HD13	1.31	0.96
1:A:330:PHE:CZ	2:B:59:MET:CE	2.48	0.96
1:A:247:CYS:SG	1:A:328:LEU:HD11	2.06	0.95
1:A:330:PHE:CZ	2:B:59:MET:HE2	2.01	0.94
1:M:158:LEU:HD23	1:M:432:VAL:CG1	1.97	0.94
1:A:12:ALA:HB1	1:A:17:LEU:HD21	1.49	0.94
2:N:15:PRO:O	3:O:5:LYS:NZ	1.99	0.94
2:N:116:ILE:HD12	2:N:118:PRO:HD3	1.50	0.93
1:A:41:MET:HG3	1:A:42:ARG:CD	1.98	0.93
1:A:70:VAL:HG21	1:A:573:LEU:HD23	1.48	0.93
1:A:41:MET:HG3	1:A:42:ARG:HD2	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:194:GLY:HA3	1:M:379:GLU:CD	1.93	0.93
1:M:356:TYR:CE1	1:M:379:GLU:HG3	2.04	0.93
2:N:68:MET:HE1	2:N:73:PRO:HD3	1.51	0.92
1:A:49:GLU:OE2	1:A:330:PHE:CD2	2.22	0.92
4:D:112:LEU:O	4:D:116:VAL:HG13	1.68	0.92
3:C:5:LYS:CG	3:C:5:LYS:O	2.19	0.91
2:B:206:PHE:CZ	3:C:89:LEU:HD22	2.08	0.89
1:M:115:ARG:NH1	1:M:115:ARG:CB	2.35	0.89
1:M:13:GLY:HA3	5:M:601:FAD:O1P	1.72	0.89
1:A:15:ALA:HB2	1:A:399:LEU:HD22	1.52	0.89
1:A:213:MET:HE3	1:A:360:GLY:HA2	1.53	0.89
1:A:203:THR:CG2	1:A:242:LEU:HD21	2.02	0.89
1:A:332:CYS:SG	1:A:343:PRO:HB2	2.12	0.89
1:M:177:GLU:HB3	1:M:179:THR:HG23	1.54	0.89
2:N:135:THR:HB	2:N:138:GLN:HG3	1.53	0.88
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.55	0.88
2:N:192:MET:HB3	2:N:196:ASN:HD21	1.36	0.88
1:M:527:GLU:OE2	1:M:529:ARG:NH1	2.07	0.88
3:O:19:LEU:HD21	3:O:22:TYR:CD2	2.09	0.88
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.56	0.88
2:B:97:PRO:HG2	2:B:105:ASP:HB3	1.52	0.88
3:C:125:PHE:HE1	3:C:129:TYR:CE2	1.93	0.87
1:M:104:SER:OG	1:M:127:ALA:HA	1.74	0.87
1:A:288:ASP:O	1:A:292:GLN:HB2	1.72	0.87
1:A:105:ARG:HH12	2:B:134:GLN:HB3	1.33	0.87
1:A:356:TYR:CE2	1:A:390:ARG:HD3	2.10	0.87
3:C:12:THR:HG22	3:C:14:THR:H	1.40	0.86
3:C:5:LYS:O	3:C:5:LYS:HG3	1.73	0.86
1:M:12:ALA:HA	1:M:17:LEU:HD11	1.58	0.86
4:P:51:TYR:CZ	4:P:55:LEU:HD22	2.09	0.86
2:B:12:ARG:NE	2:B:101:ASP:OD1	2.09	0.86
1:A:330:PHE:CE2	1:A:334:LEU:HD11	2.11	0.86
2:B:96:PHE:CB	2:B:104:VAL:HG21	2.05	0.86
1:M:119:MET:HE2	1:M:391:LEU:HD23	1.58	0.86
1:A:339:VAL:HA	2:B:33:THR:HG22	1.56	0.85
1:A:358:MET:HE1	1:A:389:ASN:HA	1.57	0.85
1:A:350:VAL:O	1:A:351:ARG:HD2	1.76	0.85
1:M:44:HIS:CD2	5:M:601:FAD:HM82	2.10	0.85
2:B:96:PHE:HB3	2:B:104:VAL:CG2	2.05	0.85
1:A:98:LEU:HD23	2:B:132:ASN:HD21	1.41	0.85
1:M:51:GLY:O	5:M:601:FAD:N3	2.10	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:0:MET:CE	1:M:180:LEU:HD13	2.07	0.84
3:C:15:TRP:O	3:C:18:LYS:HG2	1.77	0.84
1:A:197:ARG:HD2	1:A:206:GLY:HA2	1.59	0.84
1:A:42:ARG:NH2	2:B:63:GLY:O	2.09	0.84
1:A:433:GLU:O	1:A:437:LYS:HG3	1.77	0.84
1:A:479:LEU:HD13	1:A:516:GLU:HG2	1.59	0.84
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.58	0.84
3:C:19:LEU:HD12	3:C:20:PRO:HD2	1.59	0.83
4:P:68:PHE:CE1	4:P:72:VAL:HG21	2.13	0.83
1:M:54:ALA:N	1:M:123:ARG:O	2.12	0.83
1:A:330:PHE:CZ	1:A:334:LEU:HD11	2.12	0.83
1:M:358:MET:CE	1:M:390:ARG:H	1.91	0.83
2:N:241:LYS:O	2:N:243:ARG:HG3	1.78	0.83
1:A:330:PHE:HZ	2:B:59:MET:HB2	1.43	0.83
1:M:467:ARG:HD3	1:M:532:HIS:ND1	1.93	0.83
2:B:206:PHE:CE1	3:C:89:LEU:HB3	2.13	0.83
1:A:98:LEU:HD23	2:B:132:ASN:ND2	1.94	0.82
1:M:41:MET:HE2	2:N:150:ASN:HD22	1.43	0.82
1:A:397:ALA:O	1:A:401:VAL:HG23	1.80	0.82
1:M:366:ASN:O	1:M:409:GLN:HG3	1.79	0.82
2:B:109:PHE:CD2	2:B:110:ILE:HD13	2.13	0.82
1:M:37:LYS:HE3	1:M:207:ILE:HG22	1.61	0.81
1:A:338:TYR:O	2:B:33:THR:HB	1.80	0.81
3:O:89:LEU:C	3:O:91:PRO:HD2	2.04	0.81
1:A:244:THR:HG22	1:A:328:LEU:HD22	1.63	0.81
1:A:330:PHE:CZ	2:B:59:MET:HB2	2.15	0.81
1:M:366:ASN:HB3	1:M:409:GLN:HE21	1.44	0.81
1:A:89:CYS:HB2	1:A:90:PRO:HD3	1.61	0.81
2:B:100:ARG:NE	2:B:101:ASP:OD2	2.13	0.81
1:M:166:HIS:HB3	1:M:168:ARG:NH1	1.95	0.81
1:M:465:ILE:HG22	1:M:465:ILE:O	1.77	0.81
1:A:35:ILE:HG13	1:A:152:PHE:HB2	1.61	0.81
1:M:158:LEU:HD23	1:M:432:VAL:HG13	1.61	0.81
2:B:68:MET:SD	2:B:94:ALA:HB2	2.20	0.81
1:A:358:MET:HE1	1:A:390:ARG:H	1.46	0.80
1:A:244:THR:CG2	1:A:328:LEU:HD22	2.11	0.80
1:A:437:LYS:O	1:A:441:ASN:ND2	2.14	0.80
1:M:114:ARG:NH2	1:M:128:ALA:O	2.15	0.80
2:N:16:GLU:HG2	3:O:5:LYS:HZ3	1.45	0.80
1:M:44:HIS:N	5:M:601:FAD:O2A	2.15	0.80
1:M:444:GLY:HA3	1:M:488:ARG:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LYS:HG2	1:A:342:ASP:HA	1.65	0.79
3:O:19:LEU:H	3:O:19:LEU:HD23	1.47	0.79
4:D:9:ASP:C	4:D:11:PRO:HD2	2.08	0.79
3:C:113:TRP:O	3:C:117:VAL:HG23	1.82	0.79
1:M:363:THR:HA	1:M:368:GLU:O	1.83	0.79
1:A:129:ASP:OD2	1:A:329:PRO:HD2	1.83	0.79
1:A:330:PHE:CZ	2:B:59:MET:HE3	2.14	0.79
1:A:106:ARG:HG3	1:A:107:PRO:CD	2.11	0.78
1:M:69:THR:HG21	1:M:82:VAL:HG13	1.65	0.78
1:A:176:MET:HE3	2:B:99:GLU:HG3	1.64	0.78
4:P:69:LEU:HD22	4:P:73:LEU:HD11	1.64	0.78
1:A:287:ARG:C	1:A:289:LYS:H	1.91	0.78
1:M:370:ARG:NH2	1:M:554:PHE:HE2	1.82	0.78
2:B:109:PHE:HD2	2:B:110:ILE:CD1	1.97	0.78
1:A:556:ASP:HB2	1:A:558:ASP:OD2	1.83	0.78
1:M:551:THR:O	1:M:552:LEU:HD23	1.84	0.77
1:M:222:PRO:HA	1:M:553:ALA:O	1.85	0.77
1:A:250:GLU:HB3	1:A:323:LYS:NZ	1.98	0.77
1:A:316:LEU:O	1:A:319:LEU:N	2.16	0.77
2:B:109:PHE:CE2	2:B:113:LEU:HD11	2.19	0.77
2:N:17:VAL:HG12	2:N:18:ASP:OD2	1.84	0.77
2:N:210:CYS:SG	2:N:221:ALA:HB2	2.24	0.77
2:N:65:CYS:HB2	2:N:75:LEU:HD22	1.66	0.77
1:M:114:ARG:HG2	1:M:126:PHE:CD2	2.20	0.77
2:B:4:LYS:N	2:B:4:LYS:CE	2.48	0.77
1:M:11:GLY:HA2	5:M:601:FAD:O4B	1.85	0.77
1:M:199:TYR:OH	1:M:229:VAL:HG21	1.85	0.77
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.20	0.77
2:N:13:TYR:HA	2:N:18:ASP:OD1	1.85	0.77
2:N:37:LEU:HD21	2:N:58:ARG:HG2	1.67	0.76
1:M:115:ARG:HH11	1:M:115:ARG:CB	1.97	0.76
1:A:358:MET:HE1	1:A:390:ARG:N	2.00	0.76
1:M:0:MET:HE2	1:M:180:LEU:CD1	2.16	0.76
1:M:44:HIS:NE2	5:M:601:FAD:C8	2.48	0.76
1:M:54:ALA:HB3	1:M:125:TRP:CD1	2.19	0.76
1:A:57:GLN:NE2	1:A:122:GLU:HG2	2.00	0.76
2:B:107:THR:O	2:B:111:GLU:HG3	1.85	0.76
1:M:50:GLY:HA2	1:M:131:THR:CB	2.16	0.76
2:N:216:LYS:HE2	2:N:216:LYS:HA	1.66	0.76
3:O:50:LYS:HD2	4:P:117:THR:HG22	1.68	0.76
1:A:244:THR:HG21	1:A:328:LEU:CD2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:119:MET:HE2	1:M:391:LEU:CD2	2.16	0.76
1:M:97:GLU:OE1	2:N:132:ASN:HB2	1.86	0.76
2:N:72:VAL:O	2:N:74:LYS:HG3	1.84	0.76
1:M:222:PRO:HD3	1:M:370:ARG:NH1	2.00	0.75
2:B:134:GLN:HE21	2:B:139:MET:HE3	1.50	0.75
3:C:50:LYS:HD3	4:D:118:ILE:CG1	2.14	0.75
1:A:546:ASN:O	1:A:549:LYS:HE2	1.86	0.75
1:A:247:CYS:SG	1:A:328:LEU:CD1	2.74	0.75
1:A:337:ALA:HB1	2:B:80:PHE:CZ	2.21	0.75
1:M:50:GLY:HA2	1:M:131:THR:HB	1.69	0.75
2:N:99:GLU:OE1	3:O:4:ARG:HD2	1.86	0.75
3:O:86:TRP:HE1	4:P:22:MET:HE2	1.50	0.75
1:A:170:LEU:CD2	1:A:183:ILE:HB	2.17	0.75
1:M:370:ARG:HH22	1:M:554:PHE:HE2	1.34	0.75
1:A:330:PHE:HE2	2:B:59:MET:HE1	1.49	0.74
2:N:168:ILE:HD11	2:N:173:ILE:HG12	1.69	0.74
2:B:68:MET:HE2	2:B:94:ALA:CB	2.14	0.74
1:M:204:ASN:HB3	1:M:208:VAL:HG21	1.67	0.74
1:M:391:LEU:O	1:M:394:ASN:HB2	1.87	0.74
2:B:4:LYS:H	2:B:4:LYS:CE	1.99	0.74
1:A:170:LEU:HD23	1:A:183:ILE:HB	1.68	0.74
1:M:115:ARG:HB2	1:M:115:ARG:CZ	2.17	0.74
2:B:207:VAL:HG22	3:C:25:TYR:CE1	2.21	0.74
1:A:244:THR:CG2	1:A:328:LEU:CD2	2.66	0.74
4:D:112:LEU:HG	4:D:116:VAL:HG11	1.69	0.74
1:M:52:SER:O	1:M:125:TRP:N	2.19	0.74
4:D:71:ILE:O	4:D:75:LEU:HG	1.87	0.74
2:B:212:GLU:HG3	3:C:21:PHE:HE2	1.53	0.73
1:M:0:MET:HE2	1:M:180:LEU:HD13	1.69	0.73
1:M:177:GLU:CB	1:M:179:THR:HG23	2.17	0.73
1:A:151:ARG:NH1	1:A:153:ASP:OD1	2.19	0.73
1:A:324:LEU:CD1	1:A:344:VAL:HG22	2.19	0.73
3:C:50:LYS:HE3	3:C:50:LYS:HA	1.68	0.73
1:A:4:GLN:OE1	1:A:184:ARG:HB2	1.88	0.73
1:M:448:TRP:CH2	1:M:504:TYR:HB3	2.23	0.73
1:M:114:ARG:HG2	1:M:126:PHE:CE2	2.23	0.73
3:O:98:VAL:HG23	3:O:103:MET:HG2	1.71	0.73
1:A:446:GLU:CD	1:A:485:ARG:HD3	2.13	0.73
1:M:58:ASP:C	1:M:60:ASP:H	1.97	0.73
1:A:316:LEU:O	1:A:319:LEU:HB2	1.87	0.73
1:M:364:ASP:OD2	1:M:368:GLU:HB3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:HD13	1:A:334:LEU:HB3	1.71	0.73
1:A:358:MET:HE1	1:A:389:ASN:CA	2.18	0.73
1:A:292:GLN:HG3	1:A:466:TYR:CE1	2.24	0.72
1:A:335:ALA:O	1:A:339:VAL:HG22	1.89	0.72
2:B:40:LEU:HD11	2:B:67:MET:HE1	1.70	0.72
3:O:98:VAL:CG2	3:O:103:MET:HB3	2.20	0.72
1:A:337:ALA:HB1	2:B:80:PHE:HZ	1.55	0.72
2:N:73:PRO:O	2:N:153:LEU:HD13	1.89	0.72
2:B:4:LYS:NZ	2:B:4:LYS:N	1.99	0.72
3:C:63:LEU:HD23	3:C:68:ILE:HG21	1.72	0.72
1:M:194:GLY:HA2	1:M:379:GLU:HG2	1.71	0.72
1:A:208:VAL:HG12	1:A:208:VAL:O	1.89	0.72
1:A:105:ARG:HH12	2:B:134:GLN:CB	2.02	0.72
1:M:24:ALA:HA	1:M:148:GLN:HE22	1.54	0.72
1:M:455:MET:SD	1:M:512:LEU:HD23	2.29	0.72
2:N:169:GLY:O	2:N:173:ILE:HG13	1.90	0.72
1:M:168:ARG:HD3	1:M:425:ILE:HG12	1.72	0.72
2:N:106:MET:HA	2:N:106:MET:CE	2.17	0.72
1:M:158:LEU:HD23	1:M:432:VAL:HG12	1.68	0.72
1:M:525:ARG:HH12	1:M:547:PHE:HB3	1.55	0.71
1:M:428:GLN:O	1:M:432:VAL:HG23	1.89	0.71
1:A:42:ARG:HD2	1:A:42:ARG:N	2.05	0.71
1:M:191:ALA:O	5:M:601:FAD:H52A	1.90	0.71
1:M:0:MET:HE1	1:M:180:LEU:HD13	1.72	0.71
1:M:397:ALA:O	1:M:401:VAL:HG23	1.89	0.71
3:C:125:PHE:CE1	3:C:129:TYR:CD2	2.78	0.71
4:P:48:ALA:HA	4:P:53:ARG:HD3	1.71	0.71
2:B:94:ALA:HB3	2:B:156:ALA:HB1	1.73	0.70
1:M:21:ILE:O	1:M:25:GLN:HG3	1.91	0.70
2:N:5:ASN:HD22	2:N:27:GLU:HB3	1.55	0.70
1:M:366:ASN:HB3	1:M:409:GLN:NE2	2.05	0.70
3:O:104:GLY:O	3:O:107:PRO:HD2	1.92	0.70
1:A:236:LEU:HD11	1:A:339:VAL:HG11	1.73	0.70
2:N:104:VAL:HG23	2:N:106:MET:HE3	1.71	0.70
1:A:200:ARG:HD3	1:A:201:TYR:CE1	2.26	0.70
1:A:526:LYS:HA	1:A:534:ARG:NH1	2.07	0.70
2:B:92:ALA:HB3	2:B:98:ILE:CD1	2.22	0.70
2:N:106:MET:HE2	2:N:106:MET:CA	2.15	0.70
1:M:33:ALA:HA	1:M:150:GLN:O	1.92	0.70
1:M:360:GLY:H	1:M:382:SER:HB2	1.56	0.70
2:N:194:GLN:OE1	4:P:5:PRO:HG3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:170:LEU:C	1:M:170:LEU:HD12	2.17	0.69
1:M:439:LEU:HD12	1:M:442:GLN:OE1	1.92	0.69
1:M:525:ARG:NH1	1:M:547:PHE:HB3	2.06	0.69
1:A:328:LEU:HB3	1:A:331:ILE:HB	1.73	0.69
3:C:125:PHE:HE1	3:C:129:TYR:CD2	2.09	0.69
1:M:41:MET:HE2	2:N:150:ASN:ND2	2.07	0.69
1:M:50:GLY:HA2	1:M:131:THR:OG1	1.92	0.69
1:A:234:ALA:CB	1:A:243:MET:HB2	2.23	0.69
1:M:15:ALA:HA	1:M:399:LEU:O	1.93	0.69
1:M:438:ASP:O	1:M:442:GLN:HB2	1.91	0.69
2:N:94:ALA:HA	3:O:9:ARG:NH2	2.08	0.69
1:A:103:TRP:O	2:B:139:MET:HE1	1.93	0.69
1:M:96:LEU:HD21	1:M:139:LEU:HD21	1.74	0.69
1:M:133:PHE:HE2	2:N:147:GLY:HA2	1.58	0.69
1:M:226:MET:O	1:M:518:MET:HA	1.93	0.69
1:M:467:ARG:HH11	1:M:532:HIS:HA	1.56	0.69
2:B:215:PRO:HD2	8:B:246:SF4:S3	2.32	0.69
2:B:68:MET:CE	2:B:94:ALA:CB	2.70	0.69
3:C:50:LYS:CD	4:D:118:ILE:HG13	2.22	0.69
4:D:72:VAL:O	4:D:75:LEU:HB2	1.91	0.69
2:B:168:ILE:HD11	2:B:173:ILE:HG12	1.74	0.68
1:M:57:GLN:O	1:M:60:ASP:HB3	1.94	0.68
1:M:1:GLN:O	1:M:182:GLN:N	2.21	0.68
2:B:236:LEU:HD23	2:B:236:LEU:C	2.19	0.68
3:C:130:TRP:N	3:C:130:TRP:CD1	2.59	0.68
1:M:53:ALA:HB1	1:M:123:ARG:HG3	1.76	0.68
1:M:224:ARG:NH2	1:M:362:GLU:HG3	2.09	0.68
1:A:250:GLU:HB3	1:A:323:LYS:HZ1	1.56	0.68
1:M:163:ASP:HB3	1:M:168:ARG:HD2	1.75	0.68
1:M:212:GLY:HA2	1:M:215:MET:HE3	1.73	0.68
2:N:12:ARG:N	2:N:22:HIS:O	2.26	0.68
3:O:19:LEU:CD2	3:O:22:TYR:CD2	2.76	0.68
1:A:436:LEU:O	1:A:440:VAL:HG23	1.94	0.68
1:M:13:GLY:CA	5:M:601:FAD:O1P	2.41	0.68
1:M:177:GLU:HB3	1:M:179:THR:CG2	2.24	0.68
2:N:95:ASN:HD22	2:N:156:ALA:HA	1.58	0.68
3:C:59:PHE:O	3:C:62:PHE:HB3	1.93	0.68
3:O:87:PHE:CD2	3:O:112:LEU:HD13	2.28	0.68
2:N:166:GLU:O	2:N:199:ASN:HB3	1.93	0.67
1:M:41:MET:HB2	1:M:137:HIS:CE1	2.28	0.67
1:M:168:ARG:HH21	1:M:419:ASN:HA	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:HB3	1:A:554:PHE:CE1	2.29	0.67
4:D:97:LYS:HB2	4:D:97:LYS:NZ	2.10	0.67
2:B:68:MET:SD	2:B:94:ALA:CB	2.82	0.67
2:N:57:CYS:HB3	2:N:62:CYS:HB3	1.76	0.67
1:A:196:GLY:O	1:A:202:ASN:ND2	2.28	0.67
1:M:0:MET:CE	1:M:180:LEU:CD1	2.73	0.67
1:M:356:TYR:HE1	1:M:379:GLU:HG3	1.60	0.67
4:P:112:LEU:O	4:P:116:VAL:HG22	1.95	0.67
2:B:157:ALA:HB1	2:B:209:TYR:CD2	2.29	0.67
4:D:68:PHE:CE1	4:D:72:VAL:HG21	2.30	0.67
2:N:135:THR:HG23	2:N:136:PRO:HD2	1.76	0.67
1:A:434:GLN:HA	1:A:434:GLN:NE2	2.10	0.66
2:B:57:CYS:O	2:B:58:ARG:HB2	1.94	0.66
4:D:10:GLU:N	4:D:11:PRO:HD2	2.10	0.66
1:M:485:ARG:HG2	1:M:488:ARG:NH2	2.10	0.66
4:P:102:GLY:O	4:P:106:ILE:HG13	1.95	0.66
1:A:287:ARG:C	1:A:289:LYS:N	2.52	0.66
3:C:31:THR:HG22	4:D:81:ARG:NH1	2.09	0.66
3:C:50:LYS:NZ	4:D:118:ILE:HD12	2.11	0.66
1:A:93:MET:HE2	1:A:93:MET:N	2.09	0.66
1:M:43:SER:O	1:M:46:VAL:HG12	1.95	0.66
1:M:361:ILE:O	1:M:382:SER:HB3	1.96	0.66
1:A:287:ARG:O	1:A:289:LYS:N	2.29	0.66
2:B:155:TYR:CE2	2:B:169:GLY:HA3	2.30	0.66
4:D:41:LEU:HB2	4:D:43:LEU:CD1	2.25	0.66
1:M:27:ASN:HB3	1:M:30:ALA:HB2	1.77	0.66
2:B:119:TYR:O	2:B:121:ILE:HG13	1.96	0.66
4:D:6:LYS:HG3	4:P:6:LYS:HE2	1.78	0.66
1:M:116:PHE:CE2	1:M:245:GLU:CB	2.79	0.66
2:N:68:MET:CE	2:N:73:PRO:HD3	2.25	0.66
3:O:50:LYS:NZ	4:P:117:THR:HG21	2.11	0.66
3:O:98:VAL:HG23	3:O:103:MET:HB3	1.77	0.66
1:A:386:HIS:CE1	1:A:390:ARG:HG3	2.31	0.66
2:B:13:TYR:OH	3:C:5:LYS:HG2	1.96	0.66
1:M:196:GLY:HA3	1:M:204:ASN:OD1	1.95	0.66
3:O:86:TRP:HE1	4:P:22:MET:CE	2.08	0.66
1:A:339:VAL:HG23	1:A:341:VAL:HB	1.76	0.65
4:D:39:LEU:HB2	4:D:49:LEU:HD13	1.77	0.65
1:M:116:PHE:HE2	1:M:245:GLU:CB	2.09	0.65
1:M:168:ARG:HD3	1:M:425:ILE:CG1	2.24	0.65
1:M:413:ARG:NH1	1:M:413:ARG:HB2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:211:SER:HA	2:N:220:PRO:HD2	1.78	0.65
2:B:211:SER:HA	2:B:220:PRO:HD2	1.76	0.65
1:M:115:ARG:NH1	1:M:115:ARG:HB2	2.11	0.65
1:M:508:LEU:O	1:M:512:LEU:HG	1.97	0.65
1:A:97:GLU:HG3	1:A:98:LEU:N	2.11	0.65
1:A:351:ARG:HA	1:A:351:ARG:NE	2.09	0.65
1:A:206:GLY:HA3	2:B:55:TRP:CH2	2.31	0.65
1:M:54:ALA:HB3	1:M:125:TRP:NE1	2.11	0.65
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.30	0.65
3:O:50:LYS:HD2	4:P:117:THR:CG2	2.26	0.65
1:M:0:MET:CE	1:M:171:VAL:CG1	2.74	0.65
1:M:53:ALA:HA	1:M:124:THR:HA	1.79	0.65
1:A:213:MET:CE	1:A:360:GLY:HA2	2.24	0.65
1:A:469:PRO:HD2	1:A:470:GLU:H	1.60	0.65
4:D:93:VAL:O	2:N:243:ARG:O	2.15	0.65
4:D:106:ILE:O	4:D:110:VAL:HG23	1.96	0.65
1:M:133:PHE:CE2	2:N:147:GLY:HA2	2.32	0.65
3:C:125:PHE:CE1	3:C:129:TYR:CE2	2.81	0.65
1:M:78:GLU:O	1:M:81:VAL:HG22	1.97	0.65
2:B:57:CYS:SG	2:B:59:MET:N	2.64	0.65
1:A:98:LEU:HD21	2:B:125:ARG:HD3	1.79	0.65
1:A:204:ASN:N	1:A:204:ASN:HD22	1.95	0.64
3:C:65:ASN:ND2	3:C:67:VAL:HB	2.11	0.64
1:A:350:VAL:O	1:A:351:ARG:CD	2.45	0.64
1:A:133:PHE:CE1	2:B:149:ILE:HG22	2.32	0.64
2:B:214:CYS:HA	8:B:246:SF4:S3	2.37	0.64
1:M:241:ILE:CB	1:M:334:LEU:CB	2.75	0.64
2:N:211:SER:OG	2:N:220:PRO:HD2	1.97	0.64
3:O:28:ARG:HD2	4:P:81:ARG:NH2	2.13	0.64
1:A:386:HIS:ND1	1:A:390:ARG:HG3	2.12	0.64
1:M:145:GLN:HG3	1:M:146:PHE:CE1	2.31	0.64
1:M:176:MET:HG3	3:O:4:ARG:HD3	1.79	0.64
1:M:361:ILE:HG22	1:M:362:GLU:N	2.13	0.64
1:M:497:VAL:CG2	2:N:15:PRO:HG3	2.11	0.64
1:M:527:GLU:CD	1:M:529:ARG:NH1	2.56	0.64
1:M:151:ARG:NH1	1:M:153:ASP:OD2	2.30	0.64
1:M:194:GLY:CA	1:M:379:GLU:HG2	2.27	0.64
2:N:120:ILE:C	2:N:121:ILE:HG13	2.21	0.64
1:M:126:PHE:CD1	1:M:126:PHE:C	2.74	0.64
3:C:125:PHE:HD1	3:C:129:TYR:CE1	2.16	0.64
1:M:0:MET:CE	1:M:171:VAL:HG13	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:20:ALA:O	1:M:23:ALA:HB3	1.98	0.64
1:M:211:ASP:OD1	1:M:215:MET:HE2	1.98	0.64
1:A:42:ARG:NH2	2:B:150:ASN:O	2.31	0.64
3:O:118:VAL:O	3:O:122:VAL:HG23	1.98	0.64
1:M:194:GLY:CA	1:M:379:GLU:CD	2.71	0.63
2:N:36:LEU:HD23	2:N:76:ALA:HA	1.81	0.63
1:A:200:ARG:HB2	1:A:456:GLY:C	2.23	0.63
3:C:12:THR:HG22	3:C:13:SER:N	2.13	0.63
1:M:41:MET:HG3	2:N:150:ASN:ND2	2.14	0.63
1:M:297:GLU:O	1:M:303:THR:N	2.31	0.63
4:P:31:MET:HG3	4:P:70:MET:SD	2.39	0.63
1:M:0:MET:HE3	1:M:171:VAL:HG11	1.79	0.63
3:O:123:ILE:HD12	4:P:30:VAL:HG11	1.81	0.63
1:A:351:ARG:HA	1:A:351:ARG:HE	1.62	0.63
2:B:206:PHE:HE1	3:C:89:LEU:HB3	1.61	0.63
1:M:468:THR:O	1:M:472:MET:HB2	1.98	0.63
2:N:39:ALA:O	2:N:43:ILE:HG12	1.99	0.63
2:N:16:GLU:HG2	3:O:5:LYS:NZ	2.13	0.63
1:A:314:LEU:O	1:A:347:PRO:HA	1.98	0.63
1:M:106:ARG:HB3	1:M:108:ASP:OD2	1.99	0.63
1:M:295:TRP:O	1:M:299:ARG:CB	2.47	0.63
1:A:10:VAL:HG11	1:A:190:MET:SD	2.39	0.62
1:A:324:LEU:HD13	1:A:344:VAL:HG22	1.81	0.62
2:B:157:ALA:O	2:B:159:PRO:HD3	1.99	0.62
1:M:92:GLU:HG3	1:M:401:VAL:HA	1.80	0.62
2:N:135:THR:HG22	2:N:137:ALA:H	1.64	0.62
2:N:192:MET:HB3	2:N:196:ASN:ND2	2.11	0.62
1:A:37:LYS:HE3	1:A:207:ILE:HG22	1.80	0.62
4:D:69:LEU:O	4:D:73:LEU:HB2	2.00	0.62
4:P:65:VAL:HG23	4:P:66:PHE:N	2.15	0.62
4:P:67:LEU:O	4:P:71:ILE:HG13	1.99	0.62
1:A:364:ASP:OD1	1:A:368:GLU:N	2.33	0.62
1:M:24:ALA:HA	1:M:148:GLN:NE2	2.15	0.62
1:A:294:PHE:CE2	1:A:295:TRP:HE3	2.17	0.62
2:B:12:ARG:HE	2:B:101:ASP:CG	2.05	0.62
1:M:465:ILE:O	1:M:465:ILE:CG2	2.48	0.62
1:A:454:GLU:CD	1:A:485:ARG:HH22	2.07	0.61
2:B:4:LYS:N	2:B:4:LYS:HE3	2.15	0.61
1:A:293:ALA:O	1:A:297:GLU:HG3	2.00	0.61
1:A:330:PHE:CE2	1:A:334:LEU:CD1	2.83	0.61
1:A:332:CYS:O	1:A:336:LYS:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:42:ARG:HD2	1:M:42:ARG:N	2.15	0.61
1:M:168:ARG:HD3	1:M:425:ILE:CD1	2.29	0.61
1:A:446:GLU:OE1	1:A:485:ARG:HD3	2.00	0.61
2:B:36:LEU:O	2:B:36:LEU:HD12	2.00	0.61
2:N:211:SER:HB3	2:N:219:ASP:HA	1.83	0.61
3:O:126:VAL:HA	3:O:130:TRP:HB3	1.82	0.61
1:A:309:GLY:C	1:A:351:ARG:CD	2.72	0.61
1:M:213:MET:O	1:M:217:LEU:HB2	2.00	0.61
3:C:12:THR:HG22	3:C:14:THR:N	2.15	0.61
4:D:82:MET:O	4:D:85:ALA:HB3	2.00	0.61
1:M:421:ASN:O	1:M:425:ILE:HG13	2.00	0.61
2:B:125:ARG:HD2	2:B:132:ASN:OD1	2.00	0.61
3:C:37:TRP:O	3:C:41:GLU:HG3	2.00	0.61
3:O:29:GLU:O	3:O:31:THR:N	2.33	0.61
4:P:63:GLY:O	4:P:67:LEU:HG	2.00	0.61
2:B:57:CYS:HB3	2:B:62:CYS:CB	2.24	0.61
3:C:98:VAL:HG23	3:C:98:VAL:O	1.99	0.61
1:M:232:HIS:O	1:M:234:ALA:N	2.34	0.61
4:P:70:MET:O	4:P:74:PRO:HG2	2.00	0.61
1:M:70:VAL:HA	1:M:77:CYS:SG	2.40	0.61
1:M:504:TYR:HA	1:M:507:GLU:OE1	2.01	0.61
3:O:49:LEU:HG	4:P:55:LEU:HD13	1.81	0.61
1:A:411:THR:O	1:A:414:ALA:HB3	2.00	0.60
1:A:416:THR:O	1:A:416:THR:HG22	2.01	0.60
3:C:65:ASN:OD1	3:C:66:PRO:HD2	2.02	0.60
4:D:103:LEU:CD2	4:D:107:LEU:HD11	2.31	0.60
1:M:65:HIS:ND1	1:M:86:VAL:HG13	2.15	0.60
4:P:79:LEU:HD23	4:P:82:MET:HE3	1.81	0.60
1:A:105:ARG:NH1	2:B:134:GLN:CB	2.54	0.60
1:A:363:THR:OG1	1:A:383:VAL:HA	2.00	0.60
1:M:115:ARG:CB	1:M:115:ARG:CZ	2.79	0.60
1:M:472:MET:HE3	1:M:523:MET:CE	2.32	0.60
4:P:79:LEU:HA	4:P:82:MET:HE3	1.83	0.60
1:A:196:GLY:HA3	1:A:204:ASN:OD1	2.00	0.60
1:A:358:MET:CE	1:A:389:ASN:HA	2.31	0.60
2:B:93:LEU:HD12	2:B:94:ALA:H	1.67	0.60
1:M:0:MET:HE3	1:M:171:VAL:CG1	2.31	0.60
1:M:377:VAL:CA	1:M:381:SER:HB3	2.32	0.60
2:N:54:ARG:O	2:N:55:TRP:HB3	2.01	0.60
2:N:211:SER:CA	2:N:220:PRO:HD2	2.31	0.60
1:A:199:TYR:O	1:A:202:ASN:ND2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:208:VAL:O	1:M:208:VAL:HG12	2.01	0.60
1:M:421:ASN:HD22	1:M:422:GLU:N	1.99	0.60
3:C:90:ALA:HB3	3:C:91:PRO:HD3	1.81	0.60
1:M:35:ILE:CG2	1:M:155:HIS:HB2	2.32	0.60
1:M:157:VAL:HG12	1:M:158:LEU:N	2.17	0.60
1:A:92:GLU:HB3	1:A:400:VAL:CG1	2.32	0.60
1:A:468:THR:O	1:A:472:MET:HG3	2.02	0.60
1:M:377:VAL:HG22	1:M:378:GLY:H	1.67	0.60
1:M:413:ARG:HB2	1:M:413:ARG:HH11	1.66	0.60
1:M:209:THR:HG21	1:M:507:GLU:CA	2.32	0.60
1:M:168:ARG:HD3	1:M:425:ILE:HD11	1.83	0.60
1:M:358:MET:HE3	1:M:389:ASN:CA	2.22	0.60
1:M:395:SER:HG	5:M:601:FAD:H2'	1.64	0.60
1:M:9:ILE:HG23	1:M:189:VAL:HB	1.84	0.59
1:M:194:GLY:CA	1:M:379:GLU:CG	2.79	0.59
1:M:232:HIS:C	1:M:234:ALA:H	2.07	0.59
1:M:421:ASN:HD22	1:M:422:GLU:H	1.50	0.59
1:M:534:ARG:O	1:M:540:THR:HG22	2.02	0.59
3:O:81:LEU:HD12	3:O:85:THR:HG23	1.84	0.59
2:B:142:TYR:CD1	2:B:142:TYR:C	2.80	0.59
3:C:38:PHE:HA	3:C:41:GLU:OE1	2.01	0.59
2:N:135:THR:HB	2:N:138:GLN:CG	2.29	0.59
4:P:79:LEU:HD12	4:P:104:ALA:HB2	1.84	0.59
1:A:343:PRO:HG3	1:A:348:ILE:HD11	1.84	0.59
2:N:135:THR:CB	2:N:138:GLN:HE21	2.16	0.59
1:A:455:MET:SD	1:A:512:LEU:HD23	2.43	0.59
2:B:241:LYS:HG2	2:B:243:ARG:HB2	1.84	0.59
1:M:157:VAL:HG13	1:M:171:VAL:O	2.02	0.59
1:M:176:MET:O	1:M:497:VAL:HA	2.02	0.59
1:A:293:ALA:HA	1:A:296:HIS:CE1	2.38	0.59
3:C:13:SER:HA	4:D:90:LYS:HD3	1.85	0.59
1:M:175:MET:O	1:M:498:PHE:HA	2.03	0.59
1:A:395:SER:OG	5:A:601:FAD:H2'	2.03	0.59
1:M:197:ARG:HB2	1:M:208:VAL:O	2.03	0.59
4:P:95:ALA:HB1	4:P:98:TRP:HB2	1.83	0.59
2:B:134:GLN:HA	2:B:138:GLN:OE1	2.03	0.59
2:B:206:PHE:C	2:B:206:PHE:CD2	2.80	0.59
1:M:230:GLN:O	1:M:355:HIS:HB3	2.02	0.59
2:B:8:ILE:HD11	2:B:81:LEU:HD13	1.85	0.58
1:M:48:ALA:HA	5:M:601:FAD:C5X	2.33	0.58
2:N:116:ILE:HD12	2:N:118:PRO:CD	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:98:VAL:CG2	3:O:103:MET:HG2	2.32	0.58
1:A:366:ASN:HB3	1:A:409:GLN:HG3	1.86	0.58
4:D:117:THR:O	4:D:118:ILE:HG23	2.04	0.58
1:M:74:ASP:HB2	1:M:388:ALA:HB3	1.85	0.58
1:M:193:GLY:C	1:M:379:GLU:HB3	2.28	0.58
1:M:503:LEU:O	1:M:507:GLU:HG3	2.02	0.58
3:C:31:THR:CG2	4:D:81:ARG:NH1	2.67	0.58
1:M:37:LYS:CE	1:M:207:ILE:HG22	2.32	0.58
1:M:527:GLU:CD	1:M:529:ARG:HH11	2.09	0.58
2:N:73:PRO:CB	2:N:153:LEU:HD22	2.33	0.58
1:A:288:ASP:O	1:A:292:GLN:CB	2.49	0.58
1:A:292:GLN:CG	1:A:466:TYR:CE1	2.86	0.58
2:B:6:LEU:HD23	2:B:81:LEU:HD13	1.85	0.58
2:B:242:PRO:HG2	4:P:94:PRO:N	2.18	0.58
3:O:84:LYS:HG3	3:O:85:THR:N	2.19	0.58
1:A:316:LEU:O	1:A:317:ARG:C	2.47	0.58
4:D:31:MET:HG3	4:D:70:MET:SD	2.44	0.58
1:M:0:MET:HE1	1:M:171:VAL:HG13	1.86	0.58
2:B:92:ALA:HB3	2:B:98:ILE:HD11	1.84	0.58
1:M:18:ARG:NH1	1:M:99:TRP:HH2	2.02	0.58
1:A:433:GLU:HG2	1:A:437:LYS:HE3	1.85	0.58
2:B:104:VAL:HG22	2:B:105:ASP:N	2.18	0.58
4:D:2:ASN:HD21	4:P:4:ASN:HD22	1.51	0.58
1:M:201:TYR:CE2	1:M:238:GLY:HA2	2.39	0.58
1:M:413:ARG:HH11	1:M:413:ARG:CB	2.17	0.58
1:A:236:LEU:HD12	1:A:349:PRO:O	2.03	0.57
1:M:223:LEU:HB3	1:M:226:MET:CG	2.34	0.57
2:N:167:PHE:CE2	2:N:169:GLY:HA2	2.39	0.57
4:P:42:GLY:HA2	4:P:44:PHE:CE2	2.39	0.57
1:A:501:ASP:HB2	2:B:49:PRO:O	2.04	0.57
1:A:236:LEU:HD21	1:A:339:VAL:HG13	1.87	0.57
1:A:469:PRO:CD	1:A:470:GLU:H	2.17	0.57
1:A:550:HIS:HB2	1:A:566:SER:OG	2.05	0.57
2:B:57:CYS:SG	2:B:60:ALA:N	2.77	0.57
2:B:68:MET:O	2:B:90:VAL:HA	2.04	0.57
2:B:197:SER:HB3	4:D:5:PRO:HB2	1.87	0.57
1:M:43:SER:HB3	5:M:601:FAD:O2A	2.05	0.57
1:M:467:ARG:HB3	1:M:472:MET:HE2	1.85	0.57
2:N:175:LEU:O	2:N:178:ARG:HB3	2.03	0.57
1:A:7:LEU:C	1:A:7:LEU:HD12	2.29	0.57
1:A:437:LYS:C	1:A:441:ASN:ND2	2.62	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:176:MET:HE3	2:N:99:GLU:HG3	1.86	0.57
4:P:33:LEU:HA	4:P:37:ILE:HD12	1.86	0.57
1:A:203:THR:OG1	5:A:601:FAD:HM83	2.05	0.57
2:B:166:GLU:O	2:B:199:ASN:HB3	2.03	0.57
1:M:157:VAL:HG22	1:M:172:ALA:HB2	1.87	0.57
2:B:104:VAL:CG2	2:B:105:ASP:N	2.67	0.57
3:C:117:VAL:O	3:C:121:ILE:HD13	2.04	0.57
1:M:50:GLY:CA	1:M:131:THR:HB	2.33	0.57
1:M:54:ALA:O	1:M:123:ARG:HB2	2.04	0.57
4:P:28:ALA:HB3	4:P:29:PRO:HD3	1.86	0.57
1:M:433:GLU:HG2	1:M:437:LYS:NZ	2.20	0.57
3:O:114:ALA:O	3:O:118:VAL:HG23	2.04	0.57
4:P:95:ALA:O	4:P:98:TRP:HB2	2.04	0.57
1:A:232:HIS:ND1	1:A:233:PRO:HD2	2.20	0.57
4:D:33:LEU:HG	4:D:34:LEU:N	2.20	0.57
4:D:95:ALA:HB2	2:N:239:THR:HG22	1.87	0.57
1:A:92:GLU:HB3	1:A:400:VAL:HG12	1.87	0.57
1:A:142:THR:O	1:A:145:GLN:HG2	2.04	0.57
1:M:0:MET:HE1	1:M:171:VAL:CG1	2.35	0.57
1:M:377:VAL:HA	1:M:381:SER:CB	2.34	0.57
2:N:206:PHE:O	2:N:206:PHE:CD2	2.57	0.57
3:C:114:ALA:O	3:C:118:VAL:HG23	2.06	0.56
1:M:13:GLY:HA3	5:M:601:FAD:P	2.44	0.56
1:M:168:ARG:HA	1:M:185:ALA:O	2.05	0.56
1:M:231:TYR:CD2	1:M:352:PRO:HB2	2.40	0.56
3:O:11:MET:HE3	3:O:15:TRP:CG	2.40	0.56
1:A:57:GLN:HE21	1:A:122:GLU:HG2	1.69	0.56
1:A:113:VAL:HG21	1:A:123:ARG:HA	1.86	0.56
1:A:498:PHE:CD2	2:B:103:VAL:HG21	2.40	0.56
3:C:42:LEU:HB3	4:D:71:ILE:HG12	1.87	0.56
3:O:90:ALA:N	3:O:91:PRO:CD	2.68	0.56
1:A:114:ARG:HG2	1:A:126:PHE:CD2	2.41	0.56
1:M:157:VAL:HG12	1:M:158:LEU:H	1.70	0.56
1:M:157:VAL:HG12	1:M:159:ASP:H	1.69	0.56
2:N:16:GLU:HA	2:N:18:ASP:O	2.05	0.56
2:N:241:LYS:HG3	2:N:242:PRO:N	2.19	0.56
1:M:96:LEU:CD1	1:M:135:MET:HE3	2.35	0.56
1:M:201:TYR:HE2	1:M:238:GLY:HA2	1.70	0.56
1:M:521:SER:OG	1:M:551:THR:HG21	2.05	0.56
1:M:528:SER:OG	1:M:539:CYS:O	2.23	0.56
2:N:135:THR:CG2	2:N:136:PRO:HD2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:77:CYS:O	4:P:81:ARG:HG3	2.05	0.56
4:D:112:LEU:HG	4:D:116:VAL:CG1	2.35	0.56
1:A:30:ALA:O	1:A:148:GLN:HB3	2.06	0.56
1:M:478:LYS:O	1:M:481:GLU:HB3	2.06	0.56
1:A:156:PHE:C	1:A:156:PHE:CD2	2.84	0.56
3:C:125:PHE:CD1	3:C:129:TYR:CD1	2.94	0.56
2:N:178:ARG:HD3	2:N:178:ARG:C	2.31	0.56
3:O:67:VAL:O	3:O:71:ILE:HG13	2.06	0.56
1:A:35:ILE:HG23	1:A:155:HIS:HB2	1.88	0.56
1:M:176:MET:CG	3:O:4:ARG:HD3	2.35	0.56
2:N:12:ARG:HH22	2:N:50:ASP:CG	2.14	0.56
2:N:181:GLU:OE2	2:N:181:GLU:HA	2.05	0.56
3:C:12:THR:CG2	3:C:13:SER:N	2.68	0.56
4:D:113:ILE:HA	4:D:116:VAL:HG22	1.87	0.56
2:N:14:ASN:HA	2:N:100:ARG:HD3	1.87	0.56
2:N:73:PRO:HB3	2:N:153:LEU:HD22	1.88	0.56
2:B:198:GLN:O	2:B:203:SER:OG	2.24	0.55
3:O:65:ASN:O	3:O:69:VAL:HG23	2.06	0.55
1:A:133:PHE:HE1	2:B:149:ILE:HG22	1.70	0.55
2:B:50:ASP:O	2:B:100:ARG:NH2	2.33	0.55
1:M:0:MET:HE2	1:M:180:LEU:HD12	1.88	0.55
1:M:41:MET:HG3	2:N:150:ASN:HD22	1.69	0.55
1:M:356:TYR:CG	1:M:357:THR:N	2.74	0.55
1:M:497:VAL:O	2:N:100:ARG:NH1	2.40	0.55
1:M:502:LEU:O	1:M:505:THR:HB	2.06	0.55
1:M:532:HIS:HE2	1:M:534:ARG:HD2	1.72	0.55
1:A:106:ARG:CG	1:A:107:PRO:HD2	2.19	0.55
3:C:125:PHE:CD1	3:C:129:TYR:CE1	2.94	0.55
1:M:451:ILE:HB	1:M:508:LEU:HD21	1.89	0.55
3:O:89:LEU:C	3:O:91:PRO:CD	2.77	0.55
1:A:158:LEU:HD11	1:A:173:MET:HG3	1.86	0.55
1:A:309:GLY:HA3	1:A:351:ARG:HB2	1.88	0.55
3:C:50:LYS:HD3	4:D:118:ILE:CD1	2.36	0.55
1:M:29:ASN:OD1	1:M:29:ASN:O	2.24	0.55
1:M:66:PHE:HD1	1:M:82:VAL:HG12	1.71	0.55
1:M:84:TYR:CE2	1:M:405:LEU:HD22	2.41	0.55
1:M:373:GLY:HA2	1:M:413:ARG:HG2	1.89	0.55
1:A:204:ASN:OD1	1:A:208:VAL:HG11	2.07	0.55
1:A:395:SER:HB3	5:A:601:FAD:N1	2.21	0.55
2:N:111:GLU:CD	4:P:1:ILE:HG13	2.32	0.55
4:D:24:SER:O	4:D:28:ALA:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:70:MET:HE3	4:D:70:MET:O	2.07	0.55
1:M:364:ASP:H	1:M:368:GLU:H	1.55	0.55
2:N:37:LEU:CD2	2:N:58:ARG:HG2	2.37	0.55
2:N:155:TYR:CZ	2:N:169:GLY:HA3	2.42	0.55
1:A:366:ASN:O	1:A:367:CYS:HB2	2.06	0.55
2:N:99:GLU:OE2	3:O:6:PRO:HB3	2.07	0.55
2:B:134:GLN:NE2	2:B:139:MET:HE3	2.22	0.55
1:M:295:TRP:O	1:M:299:ARG:N	2.37	0.55
1:A:478:LYS:O	1:A:481:GLU:HB3	2.06	0.55
2:B:75:LEU:HD21	2:B:153:LEU:HD11	1.88	0.55
3:C:5:LYS:O	3:C:5:LYS:HG2	2.05	0.55
1:M:162:VAL:HG21	1:M:371:ILE:HD13	1.89	0.55
1:M:192:THR:HA	5:M:601:FAD:O4B	2.07	0.55
1:A:176:MET:HE3	2:B:99:GLU:CG	2.36	0.54
1:M:232:HIS:C	1:M:234:ALA:N	2.62	0.54
1:M:291:SER:CB	1:M:465:ILE:HG21	2.37	0.54
4:P:65:VAL:CG2	4:P:66:PHE:N	2.69	0.54
2:B:157:ALA:HB1	2:B:209:TYR:HD2	1.72	0.54
1:M:10:VAL:HG12	1:M:192:THR:HG22	1.89	0.54
1:M:41:MET:CE	2:N:150:ASN:HD22	2.19	0.54
1:M:183:ILE:HD12	1:M:183:ILE:N	2.23	0.54
1:M:213:MET:HB3	1:M:223:LEU:HD21	1.88	0.54
1:A:48:ALA:HB3	1:A:132:GLY:HA3	1.89	0.54
1:A:204:ASN:N	1:A:204:ASN:ND2	2.54	0.54
1:A:198:VAL:HG13	1:A:199:TYR:CD1	2.42	0.54
1:M:358:MET:SD	1:M:390:ARG:N	2.81	0.54
1:M:490:ARG:HG2	1:M:491:ILE:N	2.21	0.54
1:M:547:PHE:C	1:M:549:LYS:H	2.16	0.54
1:A:575:PRO:O	1:A:576:ALA:HB2	2.07	0.54
1:M:106:ARG:O	1:M:108:ASP:N	2.41	0.54
1:M:356:TYR:CE1	1:M:379:GLU:CG	2.86	0.54
2:B:206:PHE:O	3:C:28:ARG:NH2	2.41	0.54
1:M:104:SER:HG	1:M:127:ALA:HA	1.69	0.54
1:M:549:LYS:HD2	1:M:565:TYR:CD2	2.42	0.54
4:D:39:LEU:N	4:D:40:PRO:HD2	2.22	0.54
1:A:234:ALA:HB3	1:A:243:MET:HB2	1.88	0.54
1:M:59:HIS:ND1	1:M:59:HIS:C	2.66	0.54
2:N:12:ARG:HH22	2:N:50:ASP:C	2.15	0.54
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.90	0.54
1:A:294:PHE:CD2	1:A:295:TRP:N	2.76	0.54
3:C:19:LEU:HD12	3:C:20:PRO:CD	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:204:ASN:N	1:M:204:ASN:HD22	2.05	0.54
2:N:73:PRO:C	2:N:153:LEU:HD22	2.33	0.54
2:B:11:VAL:CG2	2:B:91:GLU:HG2	2.38	0.54
2:B:93:LEU:HD12	2:B:94:ALA:N	2.23	0.54
1:M:188:VAL:O	1:M:374:LEU:HD12	2.08	0.54
3:O:29:GLU:C	3:O:31:THR:H	2.16	0.54
1:A:324:LEU:HD12	1:A:344:VAL:HG22	1.91	0.53
2:B:126:THR:H	2:B:129:GLN:HG3	1.73	0.53
4:D:63:GLY:O	4:D:67:LEU:HD23	2.09	0.53
1:M:396:LEU:HA	1:M:399:LEU:HD12	1.90	0.53
1:M:497:VAL:CG2	2:N:15:PRO:CG	2.78	0.53
1:A:167:VAL:HG21	1:A:188:VAL:CG2	2.38	0.53
2:B:81:LEU:HD22	2:B:88:MET:SD	2.49	0.53
1:M:358:MET:SD	1:M:390:ARG:HB2	2.48	0.53
2:N:70:ASN:O	2:N:71:ASN:HB2	2.08	0.53
1:A:92:GLU:C	1:A:93:MET:HE2	2.32	0.53
2:B:242:PRO:HG2	4:P:93:VAL:C	2.33	0.53
3:C:63:LEU:HD23	3:C:68:ILE:CG2	2.37	0.53
1:M:11:GLY:HA3	1:M:191:ALA:O	2.08	0.53
1:M:379:GLU:HG2	1:M:379:GLU:O	2.08	0.53
1:A:527:GLU:CD	1:A:529:ARG:HH11	2.16	0.53
1:M:161:LEU:HD22	1:M:428:GLN:HB3	1.90	0.53
3:O:50:LYS:HZ3	4:P:117:THR:HG21	1.72	0.53
1:M:555:ARG:HE	1:M:559:GLY:HA2	1.73	0.53
2:N:157:ALA:HB2	2:N:213:VAL:HG21	1.91	0.53
1:M:58:ASP:C	1:M:60:ASP:N	2.67	0.53
3:O:2:THR:OG1	3:O:4:ARG:HG2	2.09	0.53
1:A:89:CYS:O	1:A:93:MET:HG2	2.08	0.53
1:A:186:ASN:HB3	1:A:417:ALA:CB	2.39	0.53
1:M:55:VAL:HG13	1:M:60:ASP:OD1	2.08	0.53
2:N:44:LYS:HD3	2:N:51:LEU:O	2.09	0.53
1:M:184:ARG:O	1:M:185:ALA:HB2	2.09	0.53
2:N:211:SER:CB	2:N:220:PRO:HD2	2.39	0.53
1:A:122:GLU:H	1:A:122:GLU:CD	2.16	0.52
1:A:201:TYR:C	1:A:353:THR:HG1	2.17	0.52
4:D:94:PRO:HA	2:N:243:ARG:HA	1.92	0.52
1:M:194:GLY:N	1:M:379:GLU:HB3	2.23	0.52
1:M:209:THR:HG21	1:M:507:GLU:HA	1.91	0.52
1:M:361:ILE:CG2	1:M:362:GLU:N	2.72	0.52
1:A:241:ILE:HG21	1:A:334:LEU:HB3	1.90	0.52
1:M:115:ARG:O	1:M:115:ARG:HG3	2.01	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:145:GLN:HB3	2:N:119:TYR:CZ	2.45	0.52
2:N:211:SER:CB	2:N:219:ASP:HA	2.39	0.52
1:A:35:ILE:HD12	1:A:35:ILE:N	2.25	0.52
1:A:243:MET:HE1	1:A:331:ILE:O	2.10	0.52
1:M:201:TYR:HB2	1:M:460:GLU:OE2	2.09	0.52
2:N:55:TRP:HA	2:N:64:SER:OG	2.10	0.52
1:A:396:LEU:HG	5:A:601:FAD:C2	2.40	0.52
2:B:11:VAL:HG21	2:B:91:GLU:HG2	1.91	0.52
2:B:207:VAL:HG22	3:C:25:TYR:CZ	2.44	0.52
2:N:173:ILE:O	2:N:176:ALA:HB3	2.09	0.52
4:P:27:ILE:HG22	4:P:31:MET:HG2	1.91	0.52
1:A:434:GLN:HA	1:A:434:GLN:HE21	1.74	0.52
4:D:30:VAL:O	4:D:33:LEU:HB3	2.09	0.52
1:M:554:PHE:N	1:M:554:PHE:CD1	2.78	0.52
1:A:319:LEU:HG	1:A:324:LEU:HD21	1.91	0.52
4:D:95:ALA:CB	2:N:239:THR:HG22	2.40	0.52
1:M:360:GLY:N	1:M:382:SER:HB2	2.24	0.52
4:P:115:VAL:HG22	4:P:115:VAL:O	2.10	0.52
1:A:22:ALA:O	1:A:26:ALA:N	2.36	0.52
3:C:13:SER:CA	4:D:90:LYS:HD3	2.39	0.52
1:M:44:HIS:C	1:M:46:VAL:N	2.65	0.52
1:M:192:THR:C	5:M:601:FAD:H51A	2.34	0.52
1:M:378:GLY:C	1:M:380:CYS:H	2.16	0.52
1:M:468:THR:O	1:M:472:MET:HG3	2.08	0.52
1:A:61:SER:HB3	1:A:64:TYR:HD1	1.75	0.52
2:B:110:ILE:HD13	2:B:110:ILE:N	2.23	0.52
4:D:70:MET:O	4:D:74:PRO:HG2	2.09	0.52
1:M:216:ALA:O	1:M:221:VAL:HB	2.10	0.52
3:C:76:LEU:HD23	3:C:76:LEU:C	2.34	0.52
1:M:226:MET:HB2	1:M:517:CYS:O	2.09	0.52
2:N:12:ARG:NH2	2:N:50:ASP:OD1	2.42	0.52
2:N:69:VAL:CG1	2:N:88:MET:HE3	2.39	0.52
1:M:209:THR:O	1:M:209:THR:HG22	2.09	0.51
1:M:377:VAL:HA	1:M:381:SER:HB3	1.92	0.51
1:A:222:PRO:HB3	1:A:554:PHE:CZ	2.45	0.51
1:A:527:GLU:OE2	1:A:529:ARG:NH1	2.42	0.51
3:C:130:TRP:N	3:C:130:TRP:HD1	2.08	0.51
1:M:523:MET:HA	1:M:523:MET:HE3	1.92	0.51
3:O:29:GLU:C	3:O:31:THR:N	2.67	0.51
1:A:8:ALA:O	1:A:188:VAL:HA	2.09	0.51
1:A:294:PHE:CE1	1:A:351:ARG:CD	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:34:LEU:O	1:M:151:ARG:HA	2.11	0.51
1:M:60:ASP:CG	1:M:121:ILE:HG21	2.36	0.51
4:P:86:MET:HE3	4:P:91:ILE:HB	1.91	0.51
1:A:96:LEU:CD2	1:A:135:MET:HE3	2.41	0.51
1:A:97:GLU:OE2	2:B:132:ASN:N	2.44	0.51
1:A:170:LEU:HD21	1:A:183:ILE:HB	1.90	0.51
1:M:563:LEU:O	1:M:564:GLU:HG3	2.10	0.51
1:M:142:THR:O	1:M:145:GLN:HG2	2.11	0.51
1:M:527:GLU:OE1	1:M:529:ARG:NH1	2.44	0.51
2:N:98:ILE:HD11	3:O:9:ARG:CZ	2.41	0.51
1:M:377:VAL:HG22	1:M:378:GLY:N	2.24	0.51
4:D:0:MET:HG3	4:D:1:ILE:N	2.25	0.51
1:M:54:ALA:C	1:M:123:ARG:HB2	2.35	0.51
1:M:205:GLY:C	1:M:207:ILE:N	2.69	0.51
2:B:232:SER:HA	4:D:11:PRO:HB3	1.92	0.51
3:C:105:PRO:O	3:C:109:ILE:HG13	2.10	0.51
1:M:472:MET:HE3	1:M:523:MET:HE1	1.93	0.51
4:P:51:TYR:OH	4:P:55:LEU:HD22	2.10	0.51
1:A:44:HIS:NE2	5:A:601:FAD:C8	2.67	0.51
1:A:54:ALA:HB2	1:A:93:MET:HG3	1.93	0.51
1:M:35:ILE:HG23	1:M:155:HIS:HB2	1.93	0.51
1:M:55:VAL:HG22	1:M:123:ARG:HE	1.76	0.51
1:M:85:PHE:HB2	1:M:402:PHE:CZ	2.46	0.51
1:A:79:GLN:NE2	1:A:570:ILE:HD13	2.26	0.50
1:A:114:ARG:O	1:A:122:GLU:HB2	2.11	0.50
1:M:130:LYS:O	1:M:133:PHE:HB3	2.12	0.50
3:O:98:VAL:HG23	3:O:103:MET:CG	2.38	0.50
3:O:98:VAL:HG21	3:O:103:MET:HB3	1.91	0.50
1:A:96:LEU:HD21	1:A:135:MET:HE3	1.93	0.50
1:A:217:LEU:HD11	1:A:517:CYS:SG	2.52	0.50
1:A:225:ASP:HA	1:A:227:GLU:OE2	2.11	0.50
2:B:28:VAL:HG12	2:B:29:PRO:O	2.10	0.50
3:C:31:THR:CG2	4:D:81:ARG:HH12	2.25	0.50
1:M:156:PHE:O	1:M:173:MET:N	2.40	0.50
1:M:395:SER:HB3	5:M:601:FAD:N1	2.25	0.50
1:M:526:LYS:HA	1:M:534:ARG:NH1	2.26	0.50
1:A:194:GLY:O	1:A:208:VAL:HG13	2.11	0.50
1:A:425:ILE:O	1:A:428:GLN:HB3	2.12	0.50
2:B:75:LEU:HD11	2:B:215:PRO:HG3	1.94	0.50
3:C:18:LYS:HD3	3:C:18:LYS:N	2.26	0.50
4:D:98:TRP:O	4:D:102:GLY:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:512:LEU:O	1:M:516:GLU:HG3	2.12	0.50
3:O:98:VAL:HG23	3:O:103:MET:CB	2.42	0.50
4:P:62:ILE:O	4:P:65:VAL:HG22	2.10	0.50
2:B:110:ILE:O	2:B:114:GLU:HG3	2.12	0.50
1:M:52:SER:O	1:M:124:THR:HA	2.12	0.50
1:M:93:MET:HB3	1:M:125:TRP:CD2	2.46	0.50
1:A:37:LYS:NZ	1:A:507:GLU:OE2	2.40	0.50
1:A:552:LEU:HB3	1:A:554:PHE:HE1	1.76	0.50
2:B:222:ALA:HB2	3:C:92:LYS:HE3	1.93	0.50
1:M:115:ARG:NH1	1:M:115:ARG:HB3	2.23	0.50
1:M:197:ARG:HG2	1:M:208:VAL:HB	1.94	0.50
1:M:199:TYR:CZ	1:M:229:VAL:HG21	2.46	0.50
3:O:47:PHE:HE2	4:P:114:GLY:CA	2.24	0.50
1:A:309:GLY:C	1:A:351:ARG:HD2	2.34	0.50
4:D:0:MET:HE2	4:D:1:ILE:O	2.12	0.50
1:M:17:LEU:HD12	1:M:17:LEU:N	2.26	0.50
1:M:73:GLY:O	1:M:388:ALA:HB3	2.12	0.50
2:N:10:VAL:O	2:N:23:SER:HA	2.12	0.50
2:N:111:GLU:OE2	4:P:1:ILE:N	2.45	0.50
4:P:70:MET:O	4:P:70:MET:HE3	2.12	0.50
2:B:106:MET:O	2:B:110:ILE:HG12	2.12	0.50
1:M:65:HIS:CE1	1:M:86:VAL:HG22	2.47	0.50
1:M:114:ARG:O	1:M:124:THR:HB	2.11	0.50
2:N:151:CYS:N	8:N:246:SF4:S4	2.85	0.50
2:N:239:THR:HG22	2:N:239:THR:O	2.11	0.50
3:O:28:ARG:HD2	4:P:81:ARG:HH22	1.75	0.50
4:P:24:SER:O	4:P:28:ALA:HB3	2.12	0.50
1:A:61:SER:HB3	1:A:64:TYR:CD1	2.46	0.50
1:A:338:TYR:O	2:B:33:THR:CB	2.58	0.50
2:B:113:LEU:O	2:B:118:PRO:HD3	2.12	0.50
2:N:94:ALA:HA	3:O:9:ARG:CZ	2.42	0.50
2:N:240:LEU:O	2:N:243:ARG:HG2	2.12	0.50
3:C:38:PHE:HB2	3:C:75:THR:HG21	1.93	0.50
1:M:159:ASP:OD1	1:M:219:HIS:NE2	2.44	0.50
2:B:16:GLU:OE2	3:C:3:LYS:HD2	2.12	0.49
4:D:80:HIS:O	4:D:83:HIS:HB3	2.12	0.49
1:M:11:GLY:HA2	5:M:601:FAD:C4B	2.42	0.49
1:M:228:PHE:O	1:M:358:MET:HB2	2.12	0.49
1:A:92:GLU:HG3	1:A:401:VAL:HA	1.94	0.49
1:A:309:GLY:CA	1:A:351:ARG:HG2	2.42	0.49
3:C:31:THR:HG21	3:C:82:HIS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:211:ASP:CG	1:M:510:HIS:CD2	2.90	0.49
4:P:113:ILE:HA	4:P:116:VAL:CG2	2.41	0.49
1:A:93:MET:HE2	1:A:93:MET:CA	2.41	0.49
2:B:125:ARG:HH11	2:B:125:ARG:HG3	1.76	0.49
1:M:213:MET:SD	1:M:223:LEU:HD22	2.52	0.49
1:M:479:LEU:O	1:M:483:GLN:HG2	2.12	0.49
3:O:75:THR:HG22	4:P:32:ILE:HD13	1.94	0.49
3:O:88:GLU:O	3:O:91:PRO:HD2	2.13	0.49
1:A:18:ARG:HD3	1:A:400:VAL:HG13	1.94	0.49
1:A:224:ARG:HA	1:A:551:THR:O	2.12	0.49
1:A:330:PHE:HZ	2:B:59:MET:CE	2.19	0.49
2:B:93:LEU:HD11	2:B:156:ALA:CB	2.43	0.49
2:N:159:PRO:HB3	3:O:15:TRP:CZ3	2.47	0.49
2:B:19:THR:HA	3:C:5:LYS:NZ	2.28	0.49
4:D:97:LYS:HB2	4:D:97:LYS:HZ3	1.78	0.49
1:M:496:SER:HB2	3:O:3:LYS:HD3	1.95	0.49
1:A:21:ILE:O	1:A:24:ALA:HB3	2.12	0.49
2:B:155:TYR:CZ	2:B:169:GLY:HA3	2.47	0.49
3:C:119:ALA:O	3:C:123:ILE:HD13	2.12	0.49
4:D:23:TRP:CE2	4:D:27:ILE:HD12	2.46	0.49
1:A:17:LEU:CD2	1:A:34:LEU:HD11	2.43	0.49
1:M:44:HIS:CE1	5:M:601:FAD:C8M	2.61	0.49
1:M:53:ALA:HA	1:M:123:ARG:O	2.12	0.49
3:O:95:ASN:ND2	3:O:102:LYS:HD2	2.27	0.49
1:A:145:GLN:HB3	2:B:119:TYR:CE2	2.47	0.49
1:A:156:PHE:C	1:A:156:PHE:HD2	2.21	0.49
1:M:289:LYS:HA	1:M:292:GLN:CB	2.42	0.49
1:M:495:SER:HB3	2:N:14:ASN:HD21	1.78	0.49
2:N:34:THR:HG22	2:N:81:LEU:HD13	1.95	0.49
1:A:234:ALA:HB1	1:A:243:MET:HB2	1.93	0.49
1:A:434:GLN:HE21	1:A:434:GLN:CA	2.26	0.49
1:A:517:CYS:HB3	1:A:553:ALA:CB	2.43	0.49
3:C:50:LYS:HZ3	4:D:118:ILE:HD12	1.77	0.49
1:M:201:TYR:C	1:M:353:THR:HG23	2.38	0.49
2:N:104:VAL:HG23	2:N:106:MET:CE	2.42	0.49
4:P:79:LEU:HD23	4:P:82:MET:CE	2.43	0.49
1:A:113:VAL:HG23	1:A:124:THR:N	2.28	0.49
1:A:175:MET:HE2	1:A:498:PHE:CE1	2.48	0.49
3:C:39:SER:OG	4:D:71:ILE:O	2.31	0.49
1:M:78:GLU:O	1:M:80:ASP:N	2.45	0.49
1:M:84:TYR:OH	1:M:405:LEU:HD13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:157:VAL:HA	1:M:172:ALA:HA	1.95	0.49
1:M:228:PHE:HB2	1:M:358:MET:HB3	1.95	0.49
1:M:231:TYR:HD2	1:M:352:PRO:HB2	1.76	0.49
2:N:135:THR:HB	2:N:138:GLN:HE21	1.78	0.49
4:P:57:PHE:CZ	4:P:63:GLY:HA2	2.47	0.49
1:M:44:HIS:C	1:M:46:VAL:H	2.19	0.48
1:M:513:ASN:HA	1:M:516:GLU:OE1	2.13	0.48
1:M:549:LYS:HE3	1:M:565:TYR:CE2	2.48	0.48
2:N:11:VAL:CG2	2:N:91:GLU:HG2	2.43	0.48
2:N:16:GLU:C	2:N:18:ASP:N	2.68	0.48
2:B:43:ILE:HG23	2:B:47:LEU:HB2	1.96	0.48
2:B:242:PRO:HB2	4:P:92:HIS:HB3	1.95	0.48
1:M:504:TYR:N	1:M:504:TYR:CD2	2.79	0.48
2:N:225:GLN:HA	2:N:225:GLN:NE2	2.28	0.48
3:O:123:ILE:CD1	4:P:27:ILE:HG23	2.42	0.48
3:C:56:TRP:O	3:C:59:PHE:HB3	2.12	0.48
1:M:20:ALA:C	1:M:23:ALA:HB3	2.38	0.48
1:M:154:GLU:O	1:M:175:MET:HG3	2.13	0.48
1:M:363:THR:OG1	1:M:383:VAL:HA	2.14	0.48
2:N:69:VAL:HG11	2:N:88:MET:HE3	1.94	0.48
2:N:206:PHE:CD2	2:N:206:PHE:C	2.90	0.48
1:A:98:LEU:CD2	2:B:132:ASN:HD21	2.19	0.48
1:A:330:PHE:HE2	2:B:59:MET:HE3	1.30	0.48
4:D:86:MET:SD	4:D:86:MET:N	2.86	0.48
1:M:448:TRP:HE3	1:M:508:LEU:HD22	1.78	0.48
1:M:549:LYS:HD2	1:M:565:TYR:CG	2.48	0.48
1:A:6:ASP:OD2	1:A:31:LYS:N	2.36	0.48
1:A:248:ARG:HB3	1:A:248:ARG:NH1	2.29	0.48
1:A:294:PHE:CE1	1:A:351:ARG:CG	2.64	0.48
1:M:27:ASN:ND2	1:M:29:ASN:H	2.11	0.48
1:M:49:GLU:HG2	1:M:129:ASP:O	2.14	0.48
1:M:358:MET:CE	1:M:390:ARG:N	2.70	0.48
1:M:370:ARG:NH2	1:M:554:PHE:CE2	2.71	0.48
4:P:26:ILE:HG22	4:P:27:ILE:HG13	1.95	0.48
2:B:206:PHE:HA	7:B:245:F3S:S2	2.54	0.48
3:C:33:VAL:HA	4:D:82:MET:HE3	1.94	0.48
3:C:33:VAL:CB	3:C:34:PRO:HD3	2.30	0.48
3:C:65:ASN:O	3:C:69:VAL:HG23	2.13	0.48
1:M:167:VAL:HG22	1:M:168:ARG:N	2.28	0.48
1:M:204:ASN:N	1:M:204:ASN:ND2	2.61	0.48
1:M:297:GLU:O	1:M:302:ASN:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:135:THR:HG22	2:N:137:ALA:N	2.29	0.48
1:A:321:GLU:OE1	1:A:344:VAL:HG11	2.14	0.48
1:A:356:TYR:CE1	1:A:379:GLU:HG3	2.49	0.48
1:M:198:VAL:HA	1:M:455:MET:HE3	1.94	0.48
2:N:13:TYR:O	2:N:100:ARG:HD2	2.13	0.48
2:N:163:LEU:HD23	3:O:11:MET:HE2	1.96	0.48
1:M:551:THR:C	1:M:552:LEU:HD23	2.39	0.48
1:A:247:CYS:SG	1:A:328:LEU:HD21	2.54	0.48
3:C:15:TRP:CD2	3:C:16:TRP:N	2.82	0.48
1:M:92:GLU:HB3	1:M:400:VAL:HG23	1.96	0.48
4:P:68:PHE:O	4:P:72:VAL:HG23	2.14	0.48
1:A:115:ARG:HG3	1:A:115:ARG:HH11	1.78	0.48
3:C:61:ASP:HA	3:C:64:GLN:HB2	1.95	0.48
1:M:102:PRO:O	1:M:127:ALA:HB2	2.12	0.48
2:N:65:CYS:CB	2:N:75:LEU:HD22	2.41	0.48
1:A:358:MET:CE	1:A:389:ASN:CA	2.90	0.47
2:B:206:PHE:CD2	2:B:206:PHE:O	2.67	0.47
1:M:534:ARG:HB3	1:M:536:ASP:OD1	2.13	0.47
4:P:2:ASN:O	4:P:5:PRO:HD3	2.13	0.47
1:A:469:PRO:CD	1:A:470:GLU:N	2.77	0.47
1:A:549:LYS:HD2	1:A:565:TYR:HB3	1.96	0.47
3:C:39:SER:HB3	4:D:75:LEU:HD21	1.97	0.47
3:C:123:ILE:N	3:C:123:ILE:CD1	2.77	0.47
1:M:114:ARG:HG3	1:M:116:PHE:HE1	1.78	0.47
1:M:356:TYR:HE1	1:M:379:GLU:CG	2.27	0.47
3:O:49:LEU:HG	4:P:55:LEU:CD1	2.43	0.47
1:M:19:ALA:O	1:M:23:ALA:HB2	2.15	0.47
1:A:12:ALA:HB2	1:A:34:LEU:HD21	1.97	0.47
2:B:135:THR:OG1	2:B:138:GLN:HG3	2.13	0.47
2:B:173:ILE:HD13	2:B:201:VAL:HG12	1.97	0.47
1:M:27:ASN:C	1:M:27:ASN:HD22	2.23	0.47
1:M:82:VAL:HG22	1:M:385:LEU:HD12	1.95	0.47
1:M:495:SER:CB	2:N:14:ASN:HD21	2.27	0.47
2:N:7:LYS:HE2	2:N:25:PHE:CD2	2.50	0.47
2:N:44:LYS:HA	2:N:48:ALA:O	2.14	0.47
2:B:6:LEU:HB2	2:B:30:TYR:CE2	2.48	0.47
3:C:37:TRP:HA	3:C:40:ILE:HD12	1.97	0.47
1:M:60:ASP:OD2	1:M:61:SER:N	2.45	0.47
1:A:3:PHE:CD2	1:A:152:PHE:HZ	2.33	0.47
1:A:97:GLU:HG2	2:B:131:THR:HG22	1.95	0.47
1:A:434:GLN:NE2	1:A:434:GLN:CA	2.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ARG:HG3	1:A:562:ARG:HH11	1.80	0.47
1:M:76:LEU:HD12	1:M:388:ALA:HB2	1.96	0.47
1:M:115:ARG:HG2	1:M:115:ARG:NH1	2.08	0.47
1:M:474:LYS:O	1:M:478:LYS:HB2	2.13	0.47
2:N:14:ASN:HA	2:N:100:ARG:CD	2.44	0.47
1:A:89:CYS:HB2	1:A:90:PRO:CD	2.40	0.47
1:A:113:VAL:HG21	1:A:123:ARG:CA	2.45	0.47
3:C:61:ASP:HA	3:C:64:GLN:OE1	2.15	0.47
4:D:0:MET:HG3	4:D:1:ILE:H	1.79	0.47
1:M:194:GLY:HA3	1:M:379:GLU:CG	2.43	0.47
2:N:221:ALA:O	2:N:224:ILE:HB	2.15	0.47
3:O:33:VAL:O	3:O:36:VAL:HG22	2.14	0.47
1:A:167:VAL:HG21	1:A:188:VAL:HG23	1.97	0.47
1:M:444:GLY:HA3	1:M:488:ARG:C	2.40	0.47
1:M:528:SER:OG	1:M:540:THR:HA	2.14	0.47
2:N:14:ASN:O	2:N:16:GLU:N	2.48	0.47
2:N:65:CYS:HB3	2:N:75:LEU:HA	1.97	0.47
2:N:165:PRO:C	2:N:167:PHE:H	2.22	0.47
3:O:60:VAL:O	3:O:64:GLN:HG3	2.15	0.47
3:C:106:GLU:CD	3:C:107:PRO:HD2	2.40	0.47
4:D:117:THR:C	4:D:118:ILE:HG12	2.40	0.47
1:M:38:VAL:HA	1:M:154:GLU:HG2	1.96	0.47
1:M:129:ASP:OD2	1:M:129:ASP:N	2.23	0.47
2:N:106:MET:CE	2:N:106:MET:CA	2.85	0.47
1:A:173:MET:HG2	1:A:180:LEU:HD23	1.96	0.46
1:A:225:ASP:O	1:A:228:PHE:HD1	1.98	0.46
1:A:410:ALA:O	1:A:414:ALA:HB2	2.15	0.46
2:B:6:LEU:HD12	2:B:7:LYS:H	1.80	0.46
2:B:19:THR:HA	3:C:5:LYS:HZ3	1.79	0.46
3:C:50:LYS:HZ2	4:D:118:ILE:HD12	1.80	0.46
3:C:123:ILE:N	3:C:123:ILE:HD12	2.31	0.46
1:A:201:TYR:C	1:A:353:THR:OG1	2.59	0.46
1:M:209:THR:HG21	1:M:507:GLU:HB3	1.97	0.46
1:A:70:VAL:HG23	1:A:71:ALA:N	2.30	0.46
1:A:341:VAL:O	1:A:343:PRO:HD3	2.15	0.46
2:B:125:ARG:HG3	2:B:125:ARG:NH1	2.29	0.46
2:B:223:ALA:O	2:B:227:GLY:N	2.48	0.46
2:B:236:LEU:C	2:B:236:LEU:CD2	2.88	0.46
1:M:0:MET:CE	1:M:171:VAL:HG11	2.41	0.46
1:M:187:ALA:HB2	1:M:414:ALA:HB2	1.96	0.46
1:A:291:SER:O	1:A:294:PHE:CD2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:MET:HE1	1:A:389:ASN:C	2.40	0.46
1:A:443:ASP:HA	1:A:490:ARG:HG3	1.96	0.46
1:M:18:ARG:HD2	1:M:18:ARG:O	2.15	0.46
1:M:168:ARG:NH2	1:M:419:ASN:HA	2.27	0.46
1:M:198:VAL:HG23	1:M:199:TYR:CD1	2.51	0.46
1:M:459:MET:SD	1:M:479:LEU:HD11	2.54	0.46
1:M:483:GLN:NE2	1:M:516:GLU:OE2	2.41	0.46
2:N:12:ARG:NH1	2:N:50:ASP:OD1	2.46	0.46
2:N:120:ILE:O	2:N:121:ILE:HG13	2.13	0.46
1:A:253:ILE:HG12	1:A:318:HIS:CE1	2.51	0.46
2:B:6:LEU:HD12	2:B:7:LYS:N	2.31	0.46
3:C:15:TRP:HZ3	3:C:22:TYR:CD1	2.33	0.46
1:A:84:TYR:O	1:A:88:HIS:HD2	1.99	0.46
1:A:93:MET:HE2	1:A:93:MET:HA	1.97	0.46
1:A:187:ALA:HA	1:A:373:GLY:O	2.16	0.46
4:D:41:LEU:HB2	4:D:43:LEU:HD11	1.95	0.46
4:D:53:ARG:O	4:D:56:ALA:HB3	2.16	0.46
1:M:62:PHE:CB	1:M:87:HIS:CE1	2.99	0.46
1:M:96:LEU:HD21	1:M:139:LEU:CD2	2.44	0.46
1:A:44:HIS:CE1	1:A:204:ASN:HA	2.51	0.46
1:A:174:ASN:O	1:A:178:GLY:N	2.48	0.46
1:A:232:HIS:CG	1:A:233:PRO:HD2	2.50	0.46
1:A:291:SER:O	1:A:294:PHE:HD2	1.99	0.46
1:A:294:PHE:O	1:A:298:TRP:CD1	2.69	0.46
1:M:44:HIS:CE1	1:M:47:ALA:HB3	2.50	0.46
3:O:19:LEU:HD21	3:O:22:TYR:HE2	1.69	0.46
3:O:33:VAL:HB	3:O:34:PRO:CD	2.38	0.46
1:A:208:VAL:O	1:A:208:VAL:CG1	2.61	0.46
3:C:59:PHE:CE2	3:C:63:LEU:HD11	2.51	0.46
3:C:76:LEU:HB2	4:D:32:ILE:HG21	1.97	0.46
3:C:84:LYS:O	3:C:88:GLU:HG3	2.16	0.46
1:M:48:ALA:HA	5:M:601:FAD:C6	2.45	0.46
2:N:236:LEU:HD23	2:N:236:LEU:C	2.40	0.46
3:O:19:LEU:H	3:O:19:LEU:CD2	2.23	0.46
3:O:77:ALA:O	3:O:80:LEU:HB2	2.16	0.46
4:P:33:LEU:O	4:P:37:ILE:HB	2.15	0.46
3:C:47:PHE:HE1	4:D:114:GLY:CA	2.29	0.46
4:D:41:LEU:HD12	4:D:43:LEU:HD11	1.98	0.46
1:M:12:ALA:N	5:M:601:FAD:H4B	2.31	0.46
1:M:66:PHE:CD1	1:M:82:VAL:HG12	2.51	0.46
1:M:225:ASP:C	1:M:227:GLU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:396:LEU:HG	5:M:601:FAD:C2	2.46	0.46
2:N:11:VAL:HA	2:N:22:HIS:O	2.15	0.46
4:P:69:LEU:HB3	4:P:73:LEU:HD12	1.98	0.46
1:A:12:ALA:CB	1:A:40:PRO:HG3	2.46	0.46
1:M:203:THR:C	1:M:204:ASN:HD22	2.24	0.46
2:N:16:GLU:CG	3:O:5:LYS:NZ	2.77	0.46
2:N:111:GLU:OE2	4:P:1:ILE:HG13	2.16	0.46
1:A:70:VAL:CG2	1:A:573:LEU:HD23	2.34	0.45
1:A:204:ASN:O	2:B:58:ARG:NH2	2.45	0.45
1:A:334:LEU:O	1:A:338:TYR:HD1	1.99	0.45
1:M:217:LEU:HD13	1:M:223:LEU:HG	1.98	0.45
1:M:377:VAL:N	1:M:381:SER:HB3	2.30	0.45
1:A:211:ASP:HB3	1:A:215:MET:HE3	1.98	0.45
1:A:292:GLN:CG	1:A:466:TYR:HE1	2.29	0.45
1:M:64:TYR:CD2	1:M:121:ILE:CG1	2.99	0.45
1:M:94:THR:HG1	1:M:125:TRP:HH2	1.63	0.45
2:N:221:ALA:O	2:N:225:GLN:HG2	2.17	0.45
1:A:232:HIS:ND1	1:A:233:PRO:CD	2.79	0.45
1:A:529:ARG:NH2	1:A:544:ASP:OD1	2.49	0.45
3:C:121:ILE:HD12	3:C:121:ILE:N	2.31	0.45
1:M:17:LEU:N	1:M:17:LEU:CD1	2.79	0.45
1:M:89:CYS:CB	1:M:90:PRO:HD3	2.46	0.45
1:M:93:MET:HB3	1:M:125:TRP:CE3	2.51	0.45
1:M:167:VAL:CG2	1:M:168:ARG:N	2.79	0.45
1:M:513:ASN:O	1:M:516:GLU:HB2	2.16	0.45
1:A:365:GLN:N	1:A:365:GLN:OE1	2.49	0.45
1:M:448:TRP:O	1:M:451:ILE:HB	2.16	0.45
2:N:9:GLU:HG3	2:N:25:PHE:CZ	2.51	0.45
4:P:52:GLU:OE2	4:P:52:GLU:N	2.41	0.45
1:A:170:LEU:HD23	1:A:170:LEU:N	2.32	0.45
3:C:23:ARG:CG	3:C:23:ARG:HH11	2.29	0.45
1:A:231:TYR:OH	1:A:464:GLY:HA2	2.17	0.45
4:D:93:VAL:H	2:N:243:ARG:C	2.23	0.45
1:M:538:GLY:C	1:M:539:CYS:SG	2.99	0.45
3:O:98:VAL:CG2	3:O:103:MET:CB	2.93	0.45
1:A:182:GLN:CG	1:A:184:ARG:HH12	2.29	0.45
4:D:0:MET:CG	4:D:1:ILE:H	2.28	0.45
1:M:59:HIS:ND1	1:M:59:HIS:O	2.50	0.45
2:N:206:PHE:C	2:N:206:PHE:HD2	2.24	0.45
3:O:47:PHE:HE2	4:P:114:GLY:HA3	1.81	0.45
3:O:59:PHE:O	3:O:62:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:63:LEU:HA	3:O:68:ILE:HG21	1.97	0.45
1:A:203:THR:HG23	1:A:354:ALA:O	2.17	0.45
3:C:65:ASN:HD21	3:C:67:VAL:HB	1.77	0.45
1:M:174:ASN:HD22	1:M:177:GLU:H	1.62	0.45
4:P:113:ILE:HA	4:P:116:VAL:HG22	1.98	0.45
1:A:236:LEU:HD21	1:A:339:VAL:CG1	2.47	0.45
1:A:377:VAL:HG21	1:A:403:GLY:HA2	1.99	0.45
1:M:467:ARG:NH1	1:M:531:ALA:O	2.50	0.45
2:N:220:PRO:HG2	2:N:221:ALA:H	1.82	0.45
4:P:79:LEU:HD13	4:P:100:PHE:O	2.16	0.45
4:P:112:LEU:HA	4:P:115:VAL:HG12	1.98	0.45
1:M:472:MET:HE3	1:M:523:MET:HE3	1.98	0.45
3:O:19:LEU:HA	3:O:20:PRO:HD3	1.64	0.45
3:O:20:PRO:O	3:O:23:ARG:HB2	2.16	0.45
3:O:130:TRP:O	4:P:53:ARG:NH2	2.50	0.45
4:P:50:SER:O	4:P:54:VAL:HG23	2.16	0.45
1:A:502:LEU:HD12	1:A:502:LEU:O	2.17	0.44
3:C:84:LYS:HE2	3:C:88:GLU:OE2	2.17	0.44
1:M:167:VAL:C	1:M:168:ARG:HG2	2.41	0.44
2:N:11:VAL:HG21	2:N:91:GLU:HG2	1.98	0.44
2:N:207:VAL:HB	7:N:245:F3S:S4	2.56	0.44
1:A:172:ALA:O	1:A:181:VAL:HG22	2.17	0.44
1:A:314:LEU:HG	1:A:316:LEU:HD21	1.98	0.44
2:B:3:MET:C	2:B:4:LYS:HZ2	2.08	0.44
2:B:57:CYS:O	2:B:59:MET:HG2	2.17	0.44
4:D:21:GLY:N	4:D:77:CYS:HB2	2.32	0.44
1:M:379:GLU:CG	1:M:379:GLU:O	2.66	0.44
1:M:502:LEU:O	1:M:502:LEU:HD12	2.18	0.44
1:M:549:LYS:CD	1:M:565:TYR:CD2	3.00	0.44
2:N:12:ARG:NH2	2:N:51:LEU:HA	2.31	0.44
2:N:206:PHE:CZ	3:O:89:LEU:HD22	2.52	0.44
1:M:421:ASN:ND2	1:M:423:ALA:H	2.15	0.44
1:M:552:LEU:HB2	1:M:554:PHE:HE1	1.82	0.44
4:P:34:LEU:HD23	4:P:38:LEU:HD12	2.00	0.44
1:A:70:VAL:HG23	1:A:71:ALA:H	1.83	0.44
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.99	0.44
2:B:206:PHE:C	2:B:206:PHE:HD2	2.23	0.44
4:D:28:ALA:O	4:D:32:ILE:HG13	2.17	0.44
1:M:20:ALA:HA	1:M:23:ALA:HB3	1.99	0.44
1:A:160:ILE:HG13	1:A:160:ILE:O	2.17	0.44
1:A:552:LEU:HB3	1:A:554:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:GLY:O	2:B:173:ILE:HG13	2.17	0.44
2:N:135:THR:HB	2:N:138:GLN:NE2	2.33	0.44
2:N:139:MET:C	2:N:141:LYS:N	2.76	0.44
1:A:41:MET:C	1:A:42:ARG:HD2	2.42	0.44
3:C:66:PRO:O	3:C:70:ILE:HG13	2.17	0.44
4:D:92:HIS:HA	2:N:243:ARG:OXT	2.17	0.44
1:A:294:PHE:CZ	1:A:295:TRP:HE3	2.35	0.44
2:B:242:PRO:CG	4:P:93:VAL:C	2.89	0.44
2:N:160:GLN:O	2:N:163:LEU:HB2	2.18	0.44
3:O:98:VAL:CG2	3:O:103:MET:CG	2.95	0.44
4:P:39:LEU:N	4:P:40:PRO:HD2	2.33	0.44
1:A:154:GLU:O	1:A:175:MET:HB2	2.17	0.44
2:B:140:ALA:HB3	3:C:97:ILE:HD12	1.99	0.44
2:B:230:GLU:O	2:B:233:LYS:HB3	2.18	0.44
4:D:64:ARG:HH22	4:D:118:ILE:HG22	1.83	0.44
1:M:48:ALA:CB	1:M:396:LEU:HD21	2.48	0.44
1:M:97:GLU:OE2	1:M:98:LEU:HD23	2.18	0.44
1:M:377:VAL:HA	1:M:381:SER:OG	2.17	0.44
2:N:104:VAL:CG2	2:N:106:MET:HE3	2.45	0.44
2:N:163:LEU:CD2	3:O:11:MET:HE2	2.48	0.44
1:A:62:PHE:CD1	1:A:86:VAL:HG12	2.53	0.44
1:A:241:ILE:HG21	1:A:334:LEU:CB	2.48	0.44
3:C:25:TYR:CE1	3:C:29:GLU:HG3	2.52	0.44
4:D:96:GLY:O	4:D:100:PHE:HD1	2.01	0.44
1:M:174:ASN:ND2	1:M:177:GLU:HG2	2.32	0.44
1:M:491:ILE:HD13	1:M:502:LEU:HD13	1.98	0.44
3:O:22:TYR:O	3:O:25:TYR:HB3	2.18	0.44
4:P:23:TRP:CD1	4:P:23:TRP:C	2.96	0.44
1:A:364:ASP:OD1	1:A:368:GLU:HB3	2.17	0.43
1:A:395:SER:O	1:A:398:GLU:HB3	2.18	0.43
2:B:25:PHE:CD1	2:B:25:PHE:N	2.85	0.43
4:D:71:ILE:O	4:D:74:PRO:HD2	2.17	0.43
2:N:11:VAL:CG1	2:N:21:PRO:HB2	2.48	0.43
2:N:210:CYS:SG	2:N:220:PRO:HG2	2.58	0.43
1:A:51:GLY:O	1:A:393:SER:HB2	2.18	0.43
2:B:210:CYS:SG	2:B:220:PRO:HG2	2.58	0.43
4:D:103:LEU:O	4:D:103:LEU:HD23	2.18	0.43
1:M:34:LEU:HB3	1:M:151:ARG:HG2	1.99	0.43
1:M:35:ILE:HG22	1:M:36:SER:N	2.33	0.43
1:M:472:MET:HB3	1:M:523:MET:SD	2.58	0.43
1:M:497:VAL:HG13	3:O:4:ARG:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:89:LYS:HE2	2:N:91:GLU:OE1	2.18	0.43
1:A:239:SER:O	2:B:58:ARG:NH1	2.48	0.43
3:C:80:LEU:O	3:C:84:LYS:HB2	2.18	0.43
1:M:97:GLU:CG	1:M:105:ARG:HH22	2.31	0.43
1:M:114:ARG:HH22	1:M:128:ALA:C	2.26	0.43
1:M:363:THR:HG21	1:M:376:ALA:O	2.18	0.43
4:P:112:LEU:O	4:P:115:VAL:HG12	2.17	0.43
2:B:194:GLN:HA	4:D:5:PRO:HG3	2.01	0.43
4:D:75:LEU:O	4:D:79:LEU:HB2	2.19	0.43
1:M:59:HIS:O	1:M:59:HIS:CG	2.71	0.43
1:M:167:VAL:HG11	1:M:373:GLY:C	2.42	0.43
1:M:195:ALA:C	1:M:197:ARG:N	2.71	0.43
2:N:214:CYS:SG	2:N:218:VAL:HG23	2.58	0.43
1:A:41:MET:HG3	1:A:42:ARG:NE	2.33	0.43
1:A:41:MET:CE	2:B:150:ASN:HD22	2.31	0.43
4:D:89:LEU:HB3	4:D:91:ILE:HG13	2.00	0.43
1:M:12:ALA:HA	1:M:17:LEU:CD1	2.37	0.43
1:M:169:GLY:HA2	1:M:183:ILE:O	2.17	0.43
1:M:496:SER:CB	3:O:3:LYS:HD3	2.48	0.43
1:A:13:GLY:O	1:A:17:LEU:HG	2.18	0.43
1:A:315:ASP:O	1:A:318:HIS:HE1	2.02	0.43
2:B:178:ARG:C	2:B:178:ARG:HD2	2.43	0.43
3:C:23:ARG:NH1	3:C:23:ARG:HG2	2.32	0.43
1:M:24:ALA:C	1:M:26:ALA:N	2.76	0.43
1:M:167:VAL:HG12	1:M:373:GLY:HA3	1.99	0.43
1:M:191:ALA:O	5:M:601:FAD:C5B	2.65	0.43
1:M:213:MET:CB	1:M:223:LEU:HD21	2.48	0.43
1:M:433:GLU:HG2	1:M:437:LYS:HZ2	1.83	0.43
1:M:434:GLN:HA	1:M:434:GLN:NE2	2.34	0.43
1:M:547:PHE:C	1:M:549:LYS:N	2.75	0.43
1:A:48:ALA:HB3	1:A:132:GLY:CA	2.49	0.43
1:M:116:PHE:CD2	1:M:245:GLU:CB	3.02	0.43
2:N:68:MET:HG2	2:N:92:ALA:O	2.19	0.43
2:N:170:PRO:HB2	2:N:220:PRO:HB2	2.01	0.43
2:B:163:LEU:HD23	2:B:163:LEU:HA	1.79	0.43
1:M:131:THR:HG22	1:M:396:LEU:CD1	2.49	0.43
2:N:14:ASN:HB3	2:N:17:VAL:HB	2.01	0.43
2:N:81:LEU:N	2:N:81:LEU:HD12	2.34	0.43
2:N:180:ASN:C	2:N:182:ASP:H	2.27	0.43
1:A:145:GLN:HB3	2:B:119:TYR:CZ	2.54	0.43
2:B:21:PRO:HD3	3:C:7:TYR:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:PRO:HG2	3:C:54:GLU:H	1.84	0.43
4:D:10:GLU:N	4:D:11:PRO:CD	2.80	0.43
1:M:140:PHE:O	1:M:143:SER:OG	2.22	0.43
1:M:194:GLY:C	1:M:208:VAL:CG1	2.92	0.43
1:A:42:ARG:HG2	1:A:42:ARG:HH11	1.84	0.43
1:A:289:LYS:HG3	1:A:290:VAL:N	2.34	0.43
2:B:24:ALA:C	2:B:25:PHE:CD1	2.96	0.43
3:C:63:LEU:HA	3:C:68:ILE:HG21	2.00	0.43
3:C:123:ILE:CD1	3:C:123:ILE:H	2.31	0.43
1:M:64:TYR:CD2	1:M:121:ILE:HG13	2.54	0.43
1:M:223:LEU:HB3	1:M:226:MET:HG3	2.01	0.43
1:M:448:TRP:CG	1:M:449:ALA:N	2.87	0.43
4:P:48:ALA:C	4:P:49:LEU:HD23	2.44	0.43
4:P:68:PHE:CZ	4:P:72:VAL:HG21	2.54	0.43
1:A:176:MET:HE3	2:B:99:GLU:CB	2.49	0.42
2:B:69:VAL:O	2:B:72:VAL:HG23	2.18	0.42
2:B:151:CYS:SG	2:B:153:LEU:HD12	2.59	0.42
4:D:93:VAL:N	2:N:243:ARG:C	2.77	0.42
1:M:34:LEU:O	1:M:152:PHE:N	2.50	0.42
1:M:358:MET:HE1	1:M:390:ARG:H	1.81	0.42
1:M:469:PRO:O	1:M:473:GLN:HB2	2.19	0.42
4:P:105:ALA:O	4:P:109:VAL:HG23	2.18	0.42
1:A:65:HIS:ND1	1:A:86:VAL:HG13	2.34	0.42
1:A:75:TRP:NE1	1:A:575:PRO:HA	2.34	0.42
1:A:448:TRP:CG	1:A:449:ALA:N	2.86	0.42
3:C:62:PHE:HD1	3:C:63:LEU:HG	1.83	0.42
1:M:194:GLY:C	1:M:208:VAL:HG13	2.44	0.42
1:M:205:GLY:C	1:M:207:ILE:H	2.27	0.42
1:M:224:ARG:N	1:M:360:GLY:O	2.44	0.42
1:M:528:SER:CB	1:M:539:CYS:O	2.67	0.42
3:O:45:GLY:HA3	3:O:59:PHE:CE1	2.54	0.42
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.87	0.42
1:A:292:GLN:CB	1:A:466:TYR:HE1	2.32	0.42
1:A:356:TYR:CD2	1:A:390:ARG:HD3	2.53	0.42
2:B:95:ASN:HD22	2:B:156:ALA:HA	1.83	0.42
2:B:108:HIS:HA	2:B:111:GLU:OE2	2.19	0.42
2:B:212:GLU:OE2	2:B:212:GLU:O	2.38	0.42
3:C:28:ARG:O	3:C:31:THR:HG22	2.19	0.42
2:N:68:MET:HB2	2:N:91:GLU:O	2.19	0.42
1:A:15:ALA:HB2	1:A:399:LEU:CD2	2.36	0.42
1:A:106:ARG:C	1:A:108:ASP:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:ASN:HD22	3:C:68:ILE:HG12	1.84	0.42
1:M:378:GLY:C	1:M:380:CYS:N	2.77	0.42
1:M:453:ASP:O	1:M:457:LEU:HG	2.18	0.42
2:N:93:LEU:HD11	2:N:153:LEU:HD23	1.99	0.42
2:N:135:THR:CB	2:N:138:GLN:NE2	2.82	0.42
4:P:72:VAL:O	4:P:75:LEU:HB2	2.20	0.42
1:A:12:ALA:CB	1:A:17:LEU:HD21	2.36	0.42
1:A:97:GLU:OE2	2:B:131:THR:HB	2.19	0.42
1:A:146:PHE:HA	1:A:147:PRO:HD2	1.86	0.42
1:A:250:GLU:HB3	1:A:323:LYS:HZ3	1.75	0.42
2:B:8:ILE:HD11	2:B:81:LEU:CD1	2.48	0.42
4:D:71:ILE:HG22	4:D:75:LEU:HD11	2.01	0.42
4:D:117:THR:O	4:D:118:ILE:HG12	2.20	0.42
1:M:54:ALA:H	1:M:123:ARG:HG3	1.83	0.42
1:M:83:ASP:O	1:M:87:HIS:CD2	2.72	0.42
1:M:105:ARG:NH1	2:N:132:ASN:O	2.52	0.42
1:M:211:ASP:OD1	1:M:510:HIS:CD2	2.73	0.42
1:M:223:LEU:HB3	1:M:226:MET:SD	2.60	0.42
3:O:31:THR:O	3:O:34:PRO:HD2	2.19	0.42
1:A:480:ALA:O	1:A:483:GLN:HB2	2.20	0.42
2:N:154:CYS:SG	2:N:171:ALA:HB2	2.60	0.42
1:A:236:LEU:CD1	1:A:339:VAL:HG11	2.47	0.42
2:B:169:GLY:O	2:B:172:ALA:HB3	2.18	0.42
3:C:33:VAL:CB	3:C:34:PRO:CD	2.97	0.42
3:C:125:PHE:CE1	3:C:129:TYR:CG	3.08	0.42
3:C:128:LEU:O	4:D:45:PRO:HG2	2.19	0.42
1:M:201:TYR:CE2	1:M:238:GLY:CA	3.03	0.42
1:M:361:ILE:HG21	1:M:369:THR:HG21	2.02	0.42
1:M:443:ASP:CG	1:M:444:GLY:N	2.78	0.42
2:N:135:THR:OG1	2:N:138:GLN:NE2	2.50	0.42
2:N:210:CYS:C	2:N:212:GLU:N	2.77	0.42
2:B:60:ALA:HA	6:B:244:FES:S1	2.60	0.42
1:M:386:HIS:CE1	1:M:390:ARG:HG3	2.55	0.42
1:M:497:VAL:HG21	2:N:15:PRO:HG2	1.93	0.42
1:A:448:TRP:CD2	1:A:449:ALA:N	2.88	0.42
2:B:13:TYR:HH	3:C:5:LYS:HG2	1.83	0.42
2:B:92:ALA:CB	2:B:98:ILE:CD1	2.96	0.42
4:D:73:LEU:HD23	4:D:73:LEU:HA	1.72	0.42
1:M:226:MET:HE2	1:M:514:VAL:HG13	2.02	0.42
1:M:228:PHE:HB2	1:M:358:MET:CB	2.50	0.42
2:N:82:ARG:HG3	2:N:83:ASP:CG	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HG2	2:B:139:MET:HE1	2.02	0.42
1:A:194:GLY:O	1:A:208:VAL:CG1	2.67	0.42
1:A:204:ASN:HB3	1:A:208:VAL:HB	2.01	0.42
1:A:248:ARG:HG3	1:A:252:GLY:O	2.19	0.42
2:B:3:MET:HA	2:B:4:LYS:NZ	2.34	0.42
2:N:24:ALA:CB	2:N:26:TYR:OH	2.68	0.42
1:A:37:LYS:HE3	1:A:207:ILE:CG2	2.48	0.41
1:A:167:VAL:HG11	1:A:373:GLY:O	2.20	0.41
1:A:298:TRP:CD1	1:A:298:TRP:N	2.88	0.41
1:A:446:GLU:CD	1:A:485:ARG:CD	2.90	0.41
1:M:145:GLN:HB3	2:N:119:TYR:CE2	2.55	0.41
2:N:60:ALA:HA	6:N:244:FES:S1	2.60	0.41
1:M:367:CYS:O	1:M:375:PHE:HD2	2.03	0.41
2:N:9:GLU:OE2	2:N:89:LYS:HE3	2.20	0.41
2:N:210:CYS:C	2:N:212:GLU:H	2.28	0.41
1:A:213:MET:CE	1:A:226:MET:SD	3.09	0.41
4:D:44:PHE:CD1	4:D:44:PHE:C	2.98	0.41
1:M:413:ARG:HH11	1:M:413:ARG:CA	2.33	0.41
1:M:519:ALA:O	1:M:523:MET:HB2	2.20	0.41
2:N:110:ILE:O	2:N:113:LEU:N	2.53	0.41
1:A:41:MET:HE2	1:A:41:MET:HB3	1.92	0.41
1:A:64:TYR:CD2	1:A:120:LYS:HE2	2.56	0.41
1:A:192:THR:C	5:A:601:FAD:H52A	2.45	0.41
1:A:228:PHE:HB2	1:A:358:MET:HG3	2.02	0.41
1:M:84:TYR:CZ	1:M:405:LEU:HD22	2.56	0.41
1:M:111:VAL:HG23	1:M:111:VAL:O	2.21	0.41
1:A:90:PRO:O	1:A:94:THR:OG1	2.36	0.41
1:A:199:TYR:HB2	1:A:202:ASN:HD22	1.85	0.41
1:A:211:ASP:O	1:A:214:GLY:N	2.54	0.41
2:B:92:ALA:HB3	2:B:98:ILE:HG12	2.03	0.41
3:C:36:VAL:O	3:C:39:SER:N	2.53	0.41
3:C:43:ILE:CG1	4:D:71:ILE:HG21	2.50	0.41
3:C:130:TRP:O	4:D:53:ARG:NE	2.54	0.41
1:M:11:GLY:HA2	5:M:601:FAD:C1B	2.51	0.41
1:M:59:HIS:CE1	1:M:121:ILE:HD12	2.56	0.41
1:M:484:GLU:HA	1:M:484:GLU:OE1	2.19	0.41
2:N:25:PHE:C	2:N:26:TYR:CG	2.98	0.41
3:O:81:LEU:HD12	3:O:85:THR:CG2	2.48	0.41
4:P:48:ALA:O	4:P:49:LEU:HD23	2.21	0.41
1:A:57:GLN:NE2	1:A:122:GLU:CG	2.80	0.41
1:A:502:LEU:O	1:A:506:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:120:ILE:HD13	2:N:120:ILE:HA	1.88	0.41
4:P:51:TYR:CE2	4:P:55:LEU:HD22	2.52	0.41
4:P:109:VAL:O	4:P:112:LEU:HB3	2.20	0.41
1:A:328:LEU:HB3	1:A:331:ILE:CB	2.47	0.41
2:B:173:ILE:HG23	2:B:195:LEU:CD2	2.51	0.41
1:M:9:ILE:HG22	1:M:10:VAL:N	2.36	0.41
1:M:41:MET:HG2	1:M:42:ARG:HD2	2.02	0.41
1:M:69:THR:HA	1:M:391:LEU:HD22	2.02	0.41
1:M:109:GLY:HA2	2:N:134:GLN:O	2.20	0.41
1:M:194:GLY:HA3	1:M:379:GLU:OE1	2.18	0.41
1:A:16:GLY:O	1:A:19:ALA:HB3	2.20	0.41
1:A:309:GLY:C	1:A:351:ARG:HG2	2.46	0.41
4:D:33:LEU:HD12	4:D:33:LEU:C	2.46	0.41
1:M:83:ASP:O	1:M:87:HIS:HD2	2.04	0.41
1:M:375:PHE:CD1	1:M:375:PHE:N	2.88	0.41
1:M:468:THR:O	1:M:472:MET:CB	2.68	0.41
2:N:28:VAL:HA	2:N:29:PRO:HD3	1.83	0.41
2:N:95:ASN:ND2	2:N:156:ALA:HA	2.32	0.41
2:N:121:ILE:HG22	2:N:122:GLY:N	2.35	0.41
1:A:4:GLN:OE1	1:A:4:GLN:HA	2.20	0.41
1:A:157:VAL:HG12	1:A:215:MET:SD	2.60	0.41
1:A:215:MET:HE1	5:A:601:FAD:N6A	2.36	0.41
3:C:125:PHE:CE1	3:C:129:TYR:CZ	3.09	0.41
1:M:12:ALA:HB3	1:M:43:SER:OG	2.21	0.41
1:M:244:THR:C	1:M:246:GLY:N	2.78	0.41
2:N:73:PRO:CA	2:N:153:LEU:HD22	2.50	0.41
2:N:128:ASP:C	2:N:130:GLY:H	2.29	0.41
2:N:149:ILE:HD11	2:N:151:CYS:HB3	2.01	0.41
1:A:332:CYS:CA	1:A:343:PRO:HG2	2.16	0.41
1:A:437:LYS:C	1:A:441:ASN:HD21	2.28	0.41
1:A:526:LYS:HA	1:A:534:ARG:HH11	1.85	0.41
1:M:10:VAL:HG12	1:M:10:VAL:O	2.20	0.41
1:M:85:PHE:HB2	1:M:402:PHE:CE1	2.56	0.41
1:M:97:GLU:OE2	1:M:97:GLU:C	2.64	0.41
1:M:361:ILE:HG21	1:M:369:THR:CG2	2.51	0.41
2:N:16:GLU:CG	3:O:5:LYS:HZ3	2.25	0.41
2:N:202:TRP:CZ2	4:P:11:PRO:HG3	2.55	0.41
3:O:42:LEU:HD23	3:O:42:LEU:HA	1.85	0.41
2:B:155:TYR:HE1	2:B:171:ALA:HB3	1.86	0.40
3:C:121:ILE:HD12	3:C:121:ILE:H	1.86	0.40
4:D:42:GLY:HA2	4:D:44:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:170:LEU:C	1:M:170:LEU:CD1	2.89	0.40
1:M:227:GLU:OE2	1:M:525:ARG:NE	2.39	0.40
1:M:372:LYS:HE3	1:M:413:ARG:NE	2.36	0.40
1:A:147:PRO:CD	1:A:148:GLN:OE1	2.69	0.40
1:A:204:ASN:HB3	1:A:208:VAL:CB	2.52	0.40
1:A:526:LYS:HG2	1:A:534:ARG:HH12	1.87	0.40
3:C:28:ARG:NH1	3:C:89:LEU:HD11	2.37	0.40
4:D:9:ASP:OD1	4:D:9:ASP:N	2.53	0.40
4:D:73:LEU:HB2	4:D:74:PRO:HD3	2.03	0.40
1:M:244:THR:C	1:M:246:GLY:H	2.29	0.40
1:M:434:GLN:HA	1:M:434:GLN:HE21	1.85	0.40
3:O:5:LYS:HB3	3:O:5:LYS:HZ2	1.87	0.40
2:B:94:ALA:O	2:B:95:ASN:HB2	2.21	0.40
3:C:15:TRP:CG	3:C:16:TRP:N	2.90	0.40
3:O:64:GLN:HG2	4:P:40:PRO:O	2.20	0.40
1:A:54:ALA:CB	1:A:93:MET:HG3	2.50	0.40
1:A:182:GLN:CD	1:A:184:ARG:HH12	2.28	0.40
1:A:383:VAL:HG23	1:A:385:LEU:HB2	2.04	0.40
1:A:438:ASP:HA	1:A:441:ASN:HD22	1.87	0.40
1:M:12:ALA:HB3	5:M:601:FAD:O3B	2.22	0.40
1:M:53:ALA:N	1:M:393:SER:O	2.54	0.40
3:O:16:TRP:CE3	3:O:26:MET:HG3	2.56	0.40
1:A:223:LEU:HD23	1:A:360:GLY:C	2.46	0.40
1:A:358:MET:H	1:A:358:MET:HG2	1.31	0.40
1:A:499:ASN:C	1:A:499:ASN:OD1	2.64	0.40
2:B:195:LEU:HD23	2:B:195:LEU:HA	1.94	0.40
4:D:44:PHE:HE1	4:D:46:GLY:O	2.05	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:129:TYR:OH	3:O:80:LEU:CB[3_654]	2.13	0.07

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	535/602 (89%)	487 (91%)	41 (8%)	7 (1%)	9	36
1	M	494/602 (82%)	437 (88%)	44 (9%)	13 (3%)	4	24
2	B	241/243 (99%)	220 (91%)	19 (8%)	2 (1%)	16	45
2	N	241/243 (99%)	204 (85%)	30 (12%)	7 (3%)	3	22
3	C	128/130 (98%)	113 (88%)	13 (10%)	2 (2%)	7	32
3	O	128/130 (98%)	116 (91%)	9 (7%)	3 (2%)	5	26
4	D	117/119 (98%)	98 (84%)	19 (16%)	0	100	100
4	P	117/119 (98%)	100 (86%)	17 (14%)	0	100	100
All	All	2001/2188 (92%)	1775 (89%)	192 (10%)	34 (2%)	7	31

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	18	LYS
2	N	15	PRO
1	A	244	THR
1	A	530	GLY
2	B	56	SER
1	M	50	GLY
1	M	79	GLN
1	M	382	SER
2	N	66	GLY
3	O	18	LYS
3	O	30	GLY
1	A	40	PRO
1	A	288	ASP
1	M	54	ALA
1	M	233	PRO
2	N	55	TRP
2	N	56	SER
1	A	317	ARG
1	A	389	ASN
1	M	59	HIS
1	M	107	PRO
1	M	185	ALA
1	M	226	MET

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Mol	Chain	Res	Type
1	M	465	ILE
2	N	13	TYR
2	N	101	ASP
3	O	99	LYS
3	C	6	PRO
1	M	469	PRO
2	N	73	PRO
1	A	50	GLY
1	M	240	GLY
2	B	170	PRO
1	M	40	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	424/474 (90%)	396 (93%)	28 (7%)	15	40
1	M	355/474 (75%)	333 (94%)	22 (6%)	16	41
2	B	205/205 (100%)	195 (95%)	10 (5%)	22	47
2	N	205/205 (100%)	197 (96%)	8 (4%)	28	51
3	C	111/111 (100%)	101 (91%)	10 (9%)	9	31
3	O	111/111 (100%)	103 (93%)	8 (7%)	13	38
4	D	97/97 (100%)	88 (91%)	9 (9%)	8	30
4	P	97/97 (100%)	97 (100%)	0	100	100
All	All	1605/1774 (90%)	1510 (94%)	95 (6%)	18	43

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	34	LEU
1	A	45	THR
1	A	70	VAL

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Mol	Chain	Res	Type
1	A	74	ASP
1	A	94	THR
1	A	96	LEU
1	A	97	GLU
1	A	159	ASP
1	A	176	MET
1	A	188	VAL
1	A	202	ASN
1	A	203	THR
1	A	207	ILE
1	A	294	PHE
1	A	299	ARG
1	A	319	LEU
1	A	321	GLU
1	A	351	ARG
1	A	358	MET
1	A	436	LEU
1	A	457	LEU
1	A	479	LEU
1	A	485	ARG
1	A	496	SER
1	A	517	CYS
1	A	541	GLU
1	A	567	ASP
2	B	4	LYS
2	B	5	ASN
2	B	59	MET
2	B	61	ILE
2	B	72	VAL
2	B	154	CYS
2	B	178	ARG
2	B	212	GLU
2	B	230	GLU
2	B	240	LEU
3	C	23	ARG
3	C	42	LEU
3	C	44	PHE
3	C	50	LYS
3	C	64	GLN
3	C	84	LYS
3	C	92	LYS
3	C	103	MET

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Mol	Chain	Res	Type
3	C	106	GLU
3	C	130	TRP
4	D	9	ASP
4	D	39	LEU
4	D	43	LEU
4	D	77	CYS
4	D	87	HIS
4	D	88	ASP
4	D	97	LYS
4	D	113	ILE
4	D	118	ILE
1	M	0	MET
1	M	40	PRO
1	M	58	ASP
1	M	59	HIS
1	M	77	CYS
1	M	89	CYS
1	M	101	CYS
1	M	107	PRO
1	M	115	ARG
1	M	119	MET
1	M	122	GLU
1	M	129	ASP
1	M	157	VAL
1	M	179	THR
1	M	207	ILE
1	M	367	CYS
1	M	394	ASN
1	M	395	SER
1	M	413	ARG
1	M	541	GLU
1	M	554	PHE
1	M	558	ASP
2	N	16	GLU
2	N	17	VAL
2	N	18	ASP
2	N	106	MET
2	N	116	ILE
2	N	128	ASP
2	N	150	ASN
2	N	226	GLN
3	O	5	LYS

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Mol	Chain	Res	Type
3	O	37	TRP
3	O	39	SER
3	O	54	GLU
3	O	92	LYS
3	O	99	LYS
3	O	102	LYS
3	O	103	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	25	GLN
1	A	57	GLN
1	A	88	HIS
1	A	137	HIS
1	A	141	GLN
1	A	219	HIS
1	A	409	GLN
1	A	434	GLN
1	A	441	ASN
2	B	5	ASN
2	B	95	ASN
2	B	129	GLN
2	B	132	ASN
2	B	134	GLN
2	B	150	ASN
2	B	217	HIS
3	C	51	ASN
3	C	65	ASN
3	C	72	ASN
3	C	95	ASN
4	D	4	ASN
4	D	59	GLN
4	D	92	HIS
1	M	27	ASN
1	M	87	HIS
1	M	95	GLN
1	M	112	ASN
1	M	134	HIS
1	M	137	HIS
1	M	148	GLN

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Mol	Chain	Res	Type
1	M	166	HIS
1	M	174	ASN
1	M	204	ASN
1	M	409	GLN
1	M	421	ASN
1	M	434	GLN
2	N	5	ASN
2	N	95	ASN
2	N	138	GLN
2	N	144	GLN
2	N	150	ASN
2	N	177	HIS
2	N	180	ASN
2	N	196	ASN
2	N	199	ASN
2	N	225	GLN
2	N	226	GLN
3	O	72	ASN
3	O	95	ASN
4	P	4	ASN
4	P	59	GLN
4	P	92	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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
5	FAD	M	601	-	58,58,58	3.87	33 (56%)	85,89,89	1.85	20 (23%)
7	F3S	N	245	2	0,9,9	-	-	-		
5	FAD	A	601	-	58,58,58	3.13	25 (43%)	85,89,89	1.62	15 (17%)
8	SF4	N	246	2	0,12,12	-	-	-		
7	F3S	B	245	2	0,9,9	-	-	-		
8	SF4	B	246	2	0,12,12	-	-	-		
6	FES	N	244	2	0,4,4	-	-	-		
6	FES	B	244	2	0,4,4	-	-	-		

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
5	FAD	M	601	-	-	7/34/50/50	0/6/6/6
7	F3S	N	245	2	-	-	0/3/3/3
5	FAD	A	601	-	-	6/34/50/50	0/6/6/6
8	SF4	N	246	2	-	-	0/6/5/5
7	F3S	B	245	2	-	-	0/3/3/3
8	SF4	B	246	2	-	-	0/6/5/5
6	FES	N	244	2	-	-	0/1/1/1
6	FES	B	244	2	-	-	0/1/1/1

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	601	FAD	PA-O3P	10.64	1.71	1.59
5	M	601	FAD	C9A-C5X	9.55	1.56	1.41
5	A	601	FAD	C9A-C5X	8.53	1.54	1.41
5	A	601	FAD	C4X-N5	7.50	1.46	1.30
5	M	601	FAD	C4X-N5	7.42	1.46	1.30
5	A	601	FAD	C6-C7	6.86	1.49	1.39
5	M	601	FAD	C4A-N3A	6.83	1.47	1.34
5	M	601	FAD	P-O3P	6.81	1.66	1.59
5	M	601	FAD	C8-C7	6.76	1.57	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	FAD	PA-O3P	6.74	1.66	1.59
5	M	601	FAD	C10-N10	6.52	1.51	1.37
5	M	601	FAD	C6-C7	6.49	1.48	1.39
5	A	601	FAD	C4A-N3A	6.38	1.46	1.34
5	M	601	FAD	C10-N1	6.35	1.46	1.33
5	M	601	FAD	C2A-N3A	5.96	1.44	1.33
5	A	601	FAD	C10-N10	5.66	1.49	1.37
5	A	601	FAD	C2A-N3A	5.61	1.43	1.33
5	A	601	FAD	C8-C7	5.55	1.54	1.40
5	A	601	FAD	C10-N1	5.51	1.44	1.33
5	M	601	FAD	C5'-C4'	5.24	1.58	1.51
5	M	601	FAD	C1B-N9A	-5.12	1.32	1.46
5	M	601	FAD	C2B-C3B	-5.01	1.39	1.53
5	A	601	FAD	C9A-N10	4.70	1.49	1.41
5	A	601	FAD	C9-C9A	4.45	1.46	1.39
5	M	601	FAD	C5B-C4B	-4.34	1.38	1.51
5	M	601	FAD	C9-C9A	4.09	1.46	1.39
5	M	601	FAD	C4-N3	4.09	1.46	1.38
5	M	601	FAD	C9-C8	4.00	1.45	1.39
5	M	601	FAD	C9A-N10	3.89	1.47	1.41
5	A	601	FAD	C9-C8	3.85	1.44	1.39
5	A	601	FAD	C5A-C4A	-3.84	1.32	1.39
5	M	601	FAD	C5A-C4A	-3.53	1.32	1.39
5	A	601	FAD	C4-N3	3.51	1.45	1.38
5	M	601	FAD	C7M-C7	-3.45	1.44	1.51
5	M	601	FAD	C6A-N1A	3.44	1.45	1.35
5	A	601	FAD	C7M-C7	-3.35	1.44	1.51
5	M	601	FAD	C3B-C4B	3.13	1.60	1.53
5	A	601	FAD	C8M-C8	-2.97	1.45	1.51
5	M	601	FAD	O4B-C1B	2.91	1.48	1.42
5	M	601	FAD	C4X-C10	2.83	1.52	1.44
5	M	601	FAD	C2-N3	2.83	1.45	1.39
5	A	601	FAD	C6A-N1A	2.77	1.43	1.35
5	M	601	FAD	C2A-N1A	2.77	1.38	1.33
5	M	601	FAD	P-O1P	2.74	1.60	1.50
5	M	601	FAD	C6-C5X	2.63	1.44	1.40
5	M	601	FAD	C1'-N10	2.62	1.54	1.47
5	A	601	FAD	P-O5'	-2.58	1.49	1.59
5	A	601	FAD	C8A-N9A	2.53	1.41	1.37
5	A	601	FAD	C2A-N1A	2.53	1.38	1.33
5	M	601	FAD	O5B-C5B	2.47	1.54	1.44
5	M	601	FAD	C8A-N9A	2.45	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	FAD	C2-N3	2.45	1.44	1.39
5	A	601	FAD	C6-C5X	2.41	1.43	1.40
5	A	601	FAD	C1'-N10	2.27	1.53	1.47
5	A	601	FAD	C4X-C10	2.26	1.50	1.44
5	M	601	FAD	C8M-C8	-2.25	1.46	1.51
5	M	601	FAD	O2B-C2B	2.16	1.48	1.43
5	A	601	FAD	C2B-C3B	-2.09	1.47	1.53

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	FAD	O3P-PA-O1A	7.29	132.63	110.70
5	A	601	FAD	C4A-N9A-C8A	-4.94	100.55	105.74
5	A	601	FAD	C5A-C4A-N9A	4.57	110.80	105.81
5	M	601	FAD	N3A-C4A-N9A	-4.49	119.54	127.17
5	A	601	FAD	N3A-C4A-N9A	-4.48	119.55	127.17
5	M	601	FAD	C4B-O4B-C1B	-4.33	99.91	109.47
5	M	601	FAD	O2A-PA-O3P	4.22	118.68	107.27
5	M	601	FAD	O4B-C4B-C3B	4.20	113.49	105.15
5	A	601	FAD	O3P-PA-O1A	3.76	122.02	110.70
5	A	601	FAD	N3A-C2A-N1A	-3.73	122.93	128.58
5	M	601	FAD	C5A-C4A-N9A	3.54	109.67	105.81
5	A	601	FAD	O4'-C4'-C5'	-3.19	102.95	109.99
5	M	601	FAD	N3A-C2A-N1A	-3.10	123.89	128.58
5	A	601	FAD	C4-C4X-N5	2.74	122.00	118.21
5	M	601	FAD	O5B-C5B-C4B	-2.73	99.69	108.99
5	M	601	FAD	C5A-C4A-N3A	2.68	130.41	126.72
5	A	601	FAD	O4-C4-C4X	-2.67	119.48	126.53
5	A	601	FAD	O3P-P-O1P	-2.66	102.71	110.70
5	M	601	FAD	O4-C4-C4X	-2.62	119.61	126.53
5	M	601	FAD	O4'-C4'-C5'	-2.62	104.21	109.99
5	M	601	FAD	C4-C4X-N5	2.62	121.82	118.21
5	M	601	FAD	PA-O5B-C5B	2.58	136.14	121.35
5	A	601	FAD	C4X-C4-N3	2.54	119.72	113.25
5	A	601	FAD	C1'-C2'-C3'	2.45	116.31	109.66
5	A	601	FAD	C4-N3-C2	-2.42	121.34	125.64
5	M	601	FAD	C4X-C4-N3	2.41	119.39	113.25
5	M	601	FAD	C10-N1-C2	2.27	121.76	116.85
5	M	601	FAD	O5B-PA-O1A	-2.25	100.00	108.94
5	A	601	FAD	C10-N1-C2	2.23	121.67	116.85
5	M	601	FAD	O5'-C5'-C4'	2.16	115.11	109.36
5	A	601	FAD	O3'-C3'-C2'	-2.06	104.25	108.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	FAD	O3'-C3'-C2'	-2.06	104.25	108.93
5	M	601	FAD	C1'-C2'-C3'	2.03	115.17	109.66
5	M	601	FAD	C5X-N5-C4X	2.03	121.38	118.09
5	A	601	FAD	C5X-N5-C4X	2.03	121.37	118.09

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	FAD	N10-C1'-C2'-O2'
5	A	601	FAD	N10-C1'-C2'-C3'
5	A	601	FAD	PA-O3P-P-O5'
5	M	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	N10-C1'-C2'-C3'
5	M	601	FAD	PA-O3P-P-O5'
5	M	601	FAD	C5B-O5B-PA-O1A
5	M	601	FAD	C5'-O5'-P-O1P
5	M	601	FAD	O4B-C4B-C5B-O5B
5	M	601	FAD	PA-O3P-P-O1P
5	A	601	FAD	O4B-C4B-C5B-O5B
5	A	601	FAD	PA-O3P-P-O1P
5	A	601	FAD	PA-O3P-P-O2P

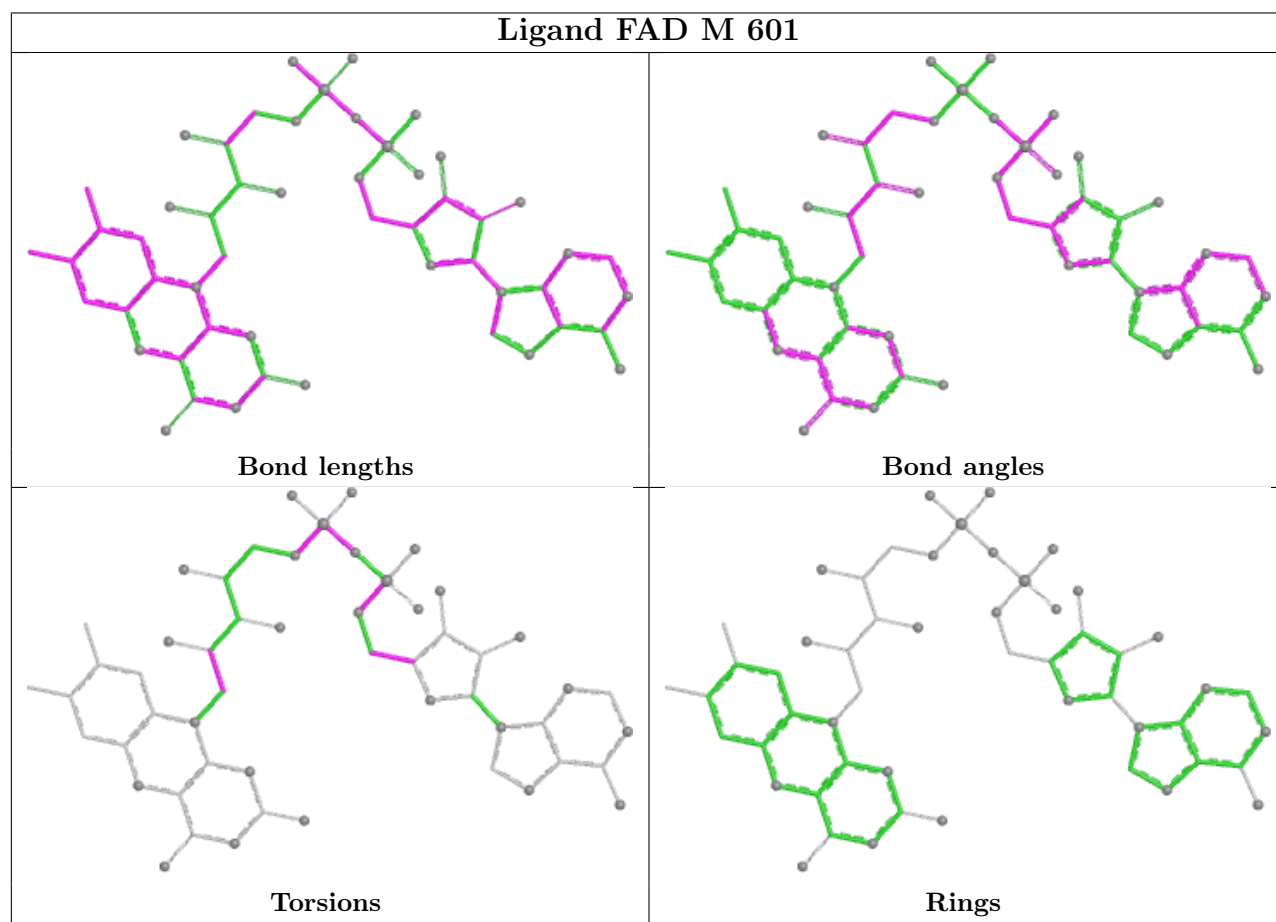
There are no ring outliers.

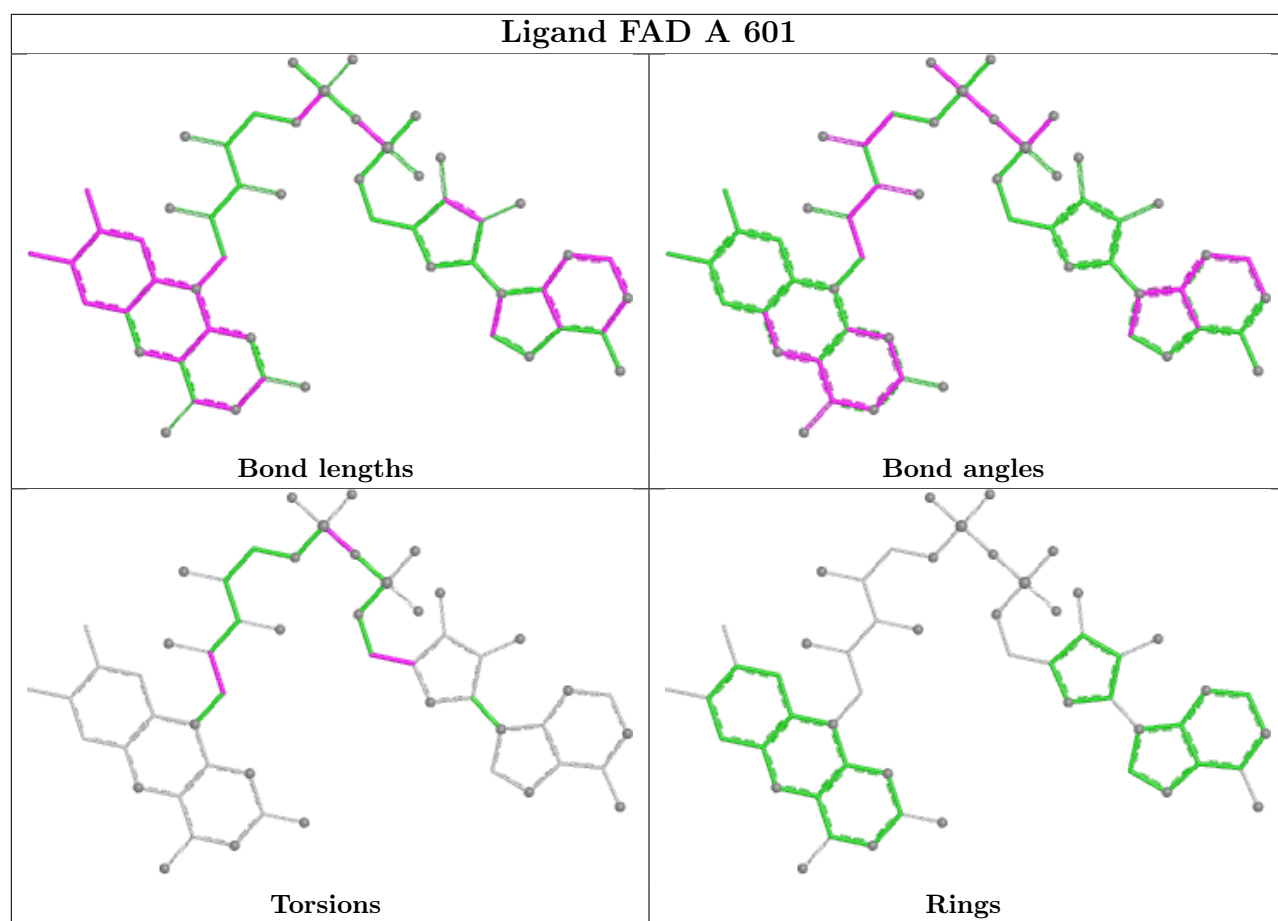
8 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	601	FAD	27	0
7	N	245	F3S	1	0
5	A	601	FAD	11	0
8	N	246	SF4	1	0
7	B	245	F3S	1	0
8	B	246	SF4	2	0
6	N	244	FES	1	0
6	B	244	FES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	541/602 (89%)	0.21	28 (5%) 33 21	23, 82, 161, 206	0
1	M	504/602 (83%)	0.72	40 (7%) 18 13	117, 184, 208, 208	0
2	B	243/243 (100%)	-0.06	3 (1%) 76 50	19, 76, 126, 205	0
2	N	243/243 (100%)	0.56	8 (3%) 49 29	100, 161, 195, 206	0
3	C	130/130 (100%)	-0.07	2 (1%) 72 44	38, 87, 136, 196	0
3	O	130/130 (100%)	-0.00	1 (0%) 82 59	44, 105, 153, 182	0
4	D	119/119 (100%)	-0.16	0 100 100	24, 84, 143, 159	0
4	P	119/119 (100%)	-0.10	0 100 100	47, 90, 131, 208	0
All	All	2029/2188 (92%)	0.28	82 (4%) 42 25	19, 113, 201, 208	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	351	ARG	4.9
1	A	306	THR	4.8
1	M	238	GLY	4.6
1	M	551	THR	4.6
1	M	44	HIS	4.4
1	M	237	PRO	4.3
1	A	316	LEU	4.3
1	A	193	GLY	4.0
1	M	325	HIS	4.0
1	M	337	ALA	3.9
1	M	335	ALA	3.8
1	M	291	SER	3.7
2	N	166	GLU	3.7
1	M	111	VAL	3.4
1	A	293	ALA	3.3
1	A	329	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	307	PRO	3.2
1	A	350	VAL	3.2
1	A	295	TRP	3.2
1	M	334	LEU	3.1
1	A	337	ALA	3.1
2	B	208	GLY	3.1
1	M	338	TYR	3.1
1	M	521	SER	3.1
1	M	376	ALA	3.1
1	A	348	ILE	3.0
1	A	242	LEU	3.0
1	M	189	VAL	3.0
1	M	563	LEU	2.9
1	M	326	GLU	2.9
1	M	367	CYS	2.9
1	A	239	SER	2.8
2	N	115	ALA	2.8
2	N	145	PHE	2.8
1	A	305	SER	2.7
1	A	330	PHE	2.7
2	N	106	MET	2.7
1	M	239	SER	2.7
1	M	192	THR	2.6
1	M	385	LEU	2.6
1	A	290	VAL	2.6
1	M	206	GLY	2.6
1	M	193	GLY	2.5
1	M	191	ALA	2.5
1	A	238	GLY	2.4
1	M	209	THR	2.4
1	M	211	ASP	2.4
1	A	314	LEU	2.4
1	M	553	ALA	2.4
1	M	11	GLY	2.4
2	N	146	SER	2.4
1	M	56	ALA	2.4
2	N	143	HIS	2.4
1	A	234	ALA	2.3
1	M	225	ASP	2.3
1	M	377	VAL	2.3
1	M	207	ILE	2.3
1	A	315	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	116	PHE	2.2
1	A	294	PHE	2.2
1	M	230	GLN	2.2
1	A	341	VAL	2.2
1	A	331	ILE	2.2
3	C	21	PHE	2.2
1	M	188	VAL	2.2
1	A	470	GLU	2.2
1	M	183	ILE	2.1
2	B	145	PHE	2.1
3	C	130	TRP	2.1
1	M	330	PHE	2.1
1	A	302	ASN	2.1
1	M	46	VAL	2.1
2	N	88	MET	2.1
1	M	386	HIS	2.0
1	M	379	GLU	2.0
1	A	241	ILE	2.0
1	M	75	TRP	2.0
1	M	361	ILE	2.0
2	B	57	CYS	2.0
1	A	237	PRO	2.0
3	O	108	ILE	2.0
2	N	113	LEU	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](#)

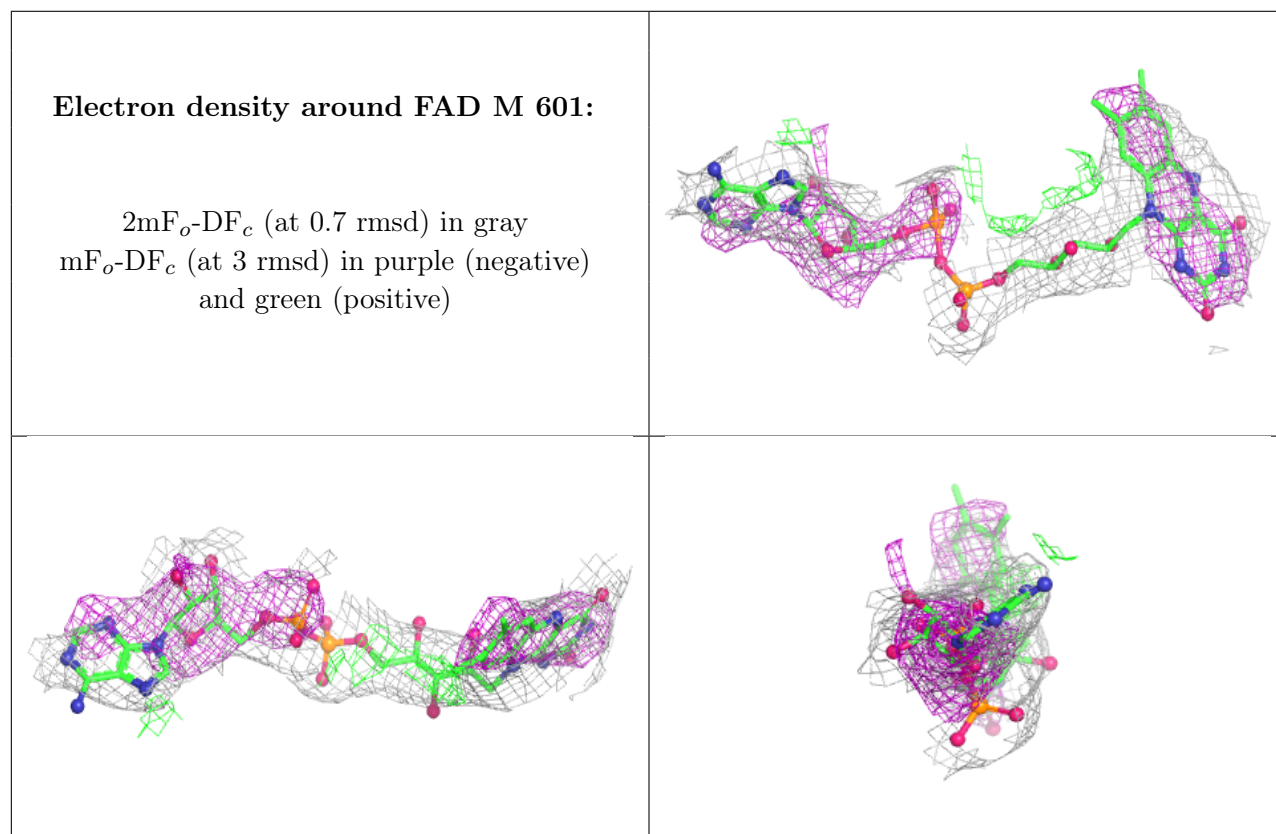
There are no oligosaccharides in this entry.

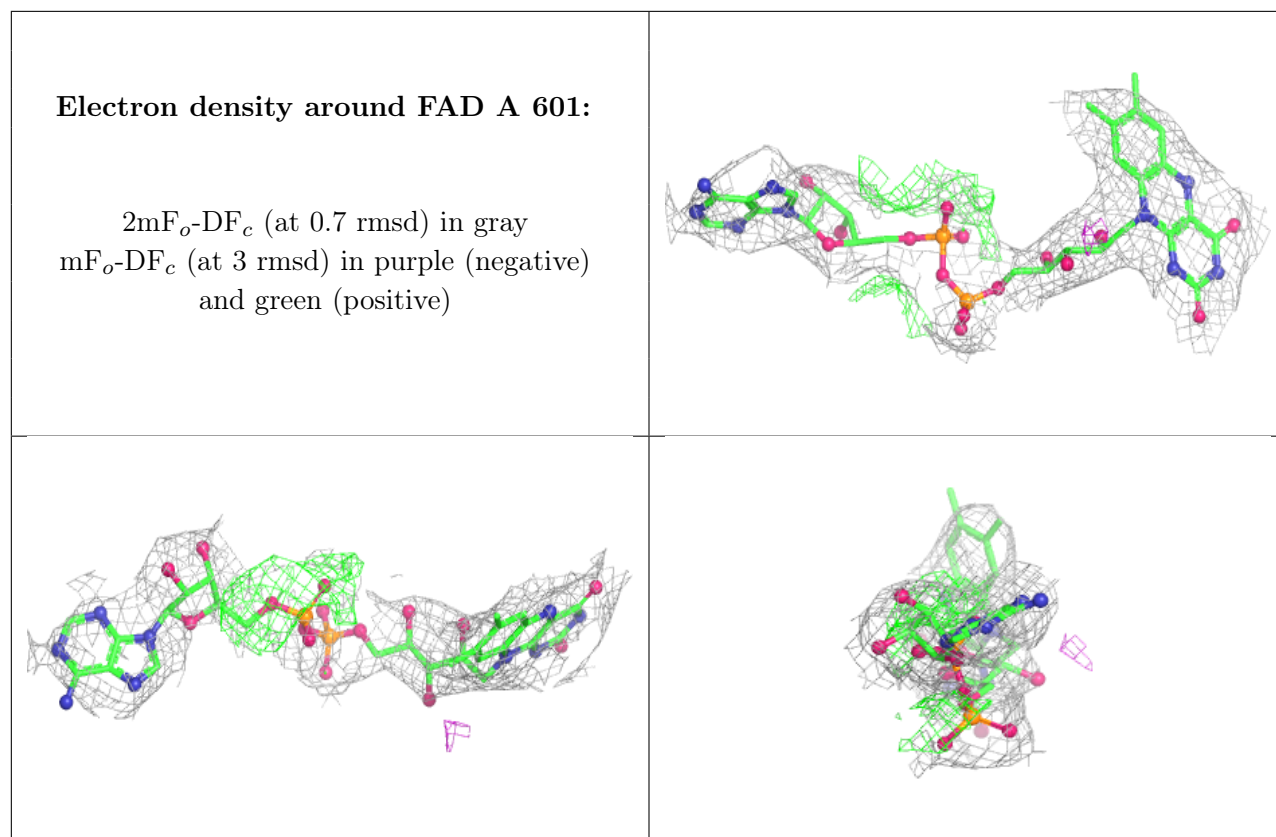
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
5	FAD	M	601	53/53	0.78	0.13	55,71,78,80	0
5	FAD	A	601	53/53	0.94	0.09	37,41,51,56	0
6	FES	N	244	4/4	0.97	0.06	123,126,146,154	0
7	F3S	B	245	7/7	0.98	0.13	109,113,117,126	0
8	SF4	N	246	8/8	0.98	0.09	122,131,151,155	0
7	F3S	N	245	7/7	0.99	0.08	116,118,131,151	0
8	SF4	B	246	8/8	0.99	0.13	111,123,129,129	0
6	FES	B	244	4/4	0.99	0.10	102,105,107,110	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.