



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 11:36 AM EDT

PDB ID : 3P4P / pdb_00003p4p
Title : Crystal structure of Menaquinol:fumarate oxidoreductase in complex with fumarate
Authors : Tomasiak, T.M.; Archuleta, T.L.; Andr ll, J.; Luna-Ch vez, C.; Davis, T.A.; Sarwar, M.; Ham, A.J.; McDonald, W.H.; Yankowskaya, V.; Stern, H.A.; Johnston, J.N.; Maklashina, E.; Cecchini, G.; Iverson, T.M.
Deposited on : 2010-10-06
Resolution : 2.80 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](#) ①) were used in the production of this report:

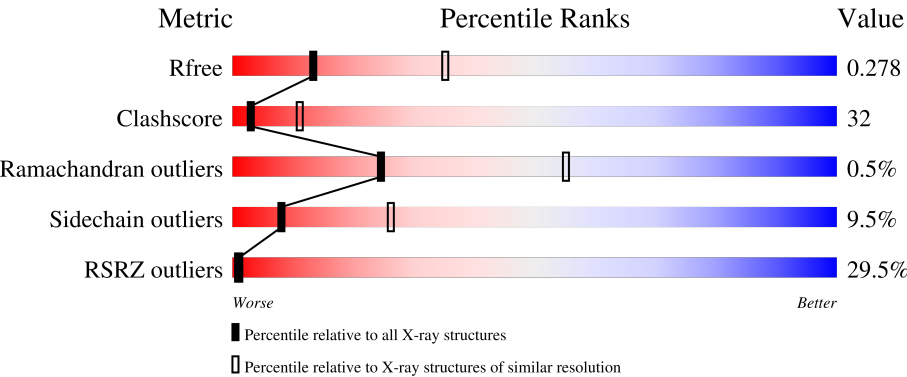
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	577	3% 63% 33% .
1	M	577	75% 45% 48% 7%
2	B	243	7% 63% 33% .
2	N	243	50% 40% 51% 9%
3	C	130	% 57% 37% 5% .

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	FAD	M	601	-	-	X	-
7	FES	B	244	-	-	X	-
8	F3S	B	245	-	-	X	-
9	SF4	B	246	-	-	X	-
9	SF4	N	246	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 16873 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4449	2775	802	841	31			
1	M	577	Total	C	N	O	S	0	0	0
			4449	2775	802	841	31			

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

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

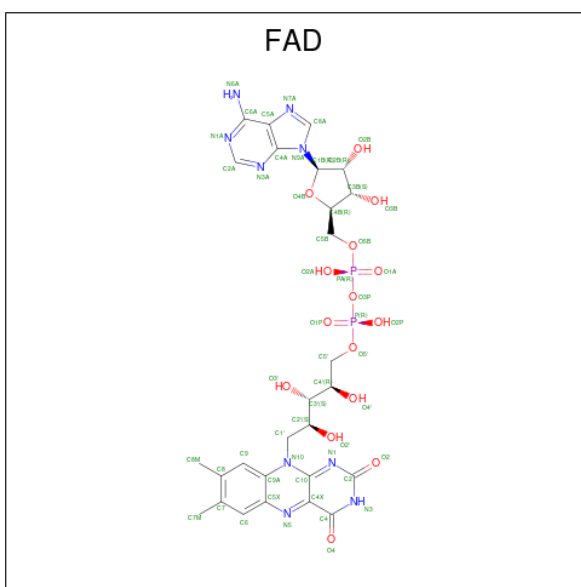
- Molecule 3 is a protein called Fumarate reductase subunit C.

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

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

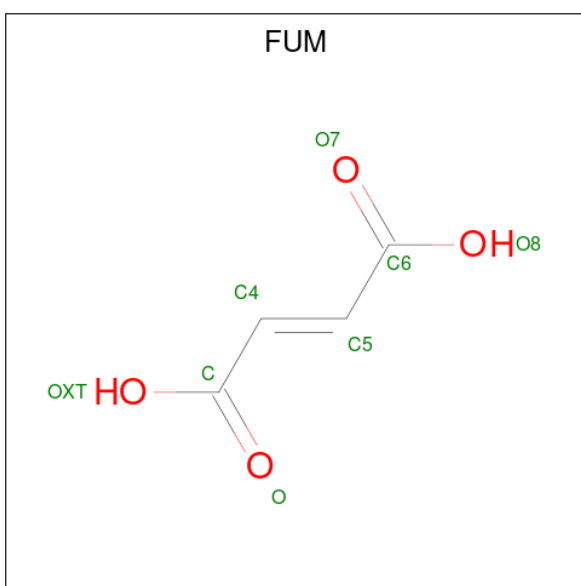
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



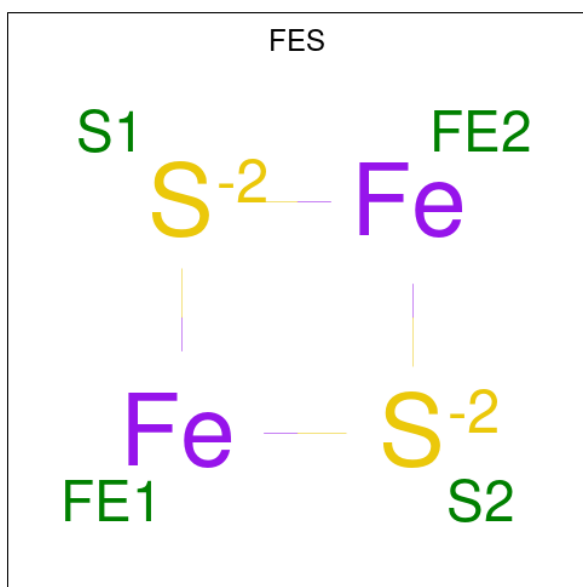
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	M	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is FUMARIC ACID (CCD ID: FUM) (formula: $C_4H_4O_4$).



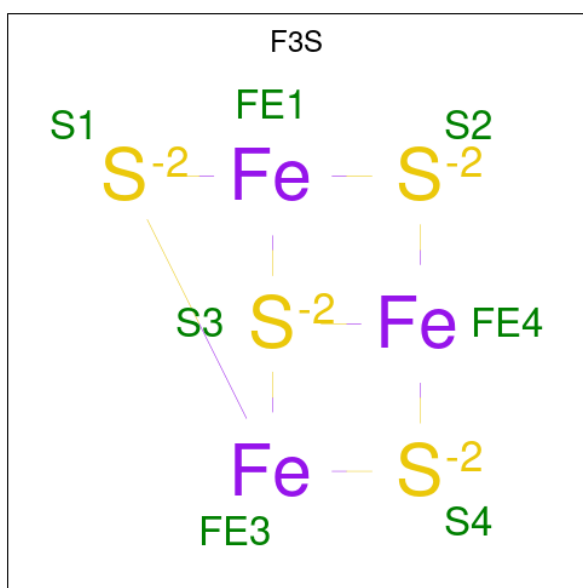
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	4	4		

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



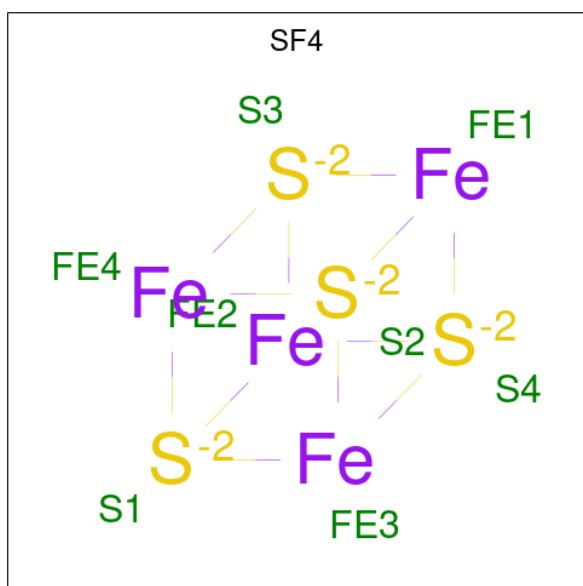
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



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

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	60	Total	O	0	0
			60	60		
10	B	10	Total	O	0	0
			10	10		
10	C	2	Total	O	0	0
			2	2		
10	D	4	Total	O	0	0
			4	4		
10	M	1	Total	O	0	0
			1	1		
10	N	2	Total	O	0	0
			2	2		

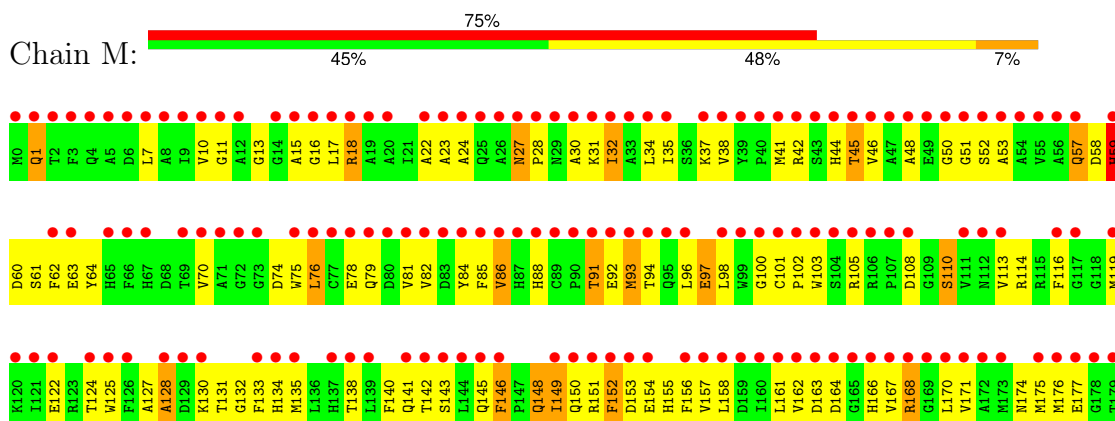
3 Residue-property plots

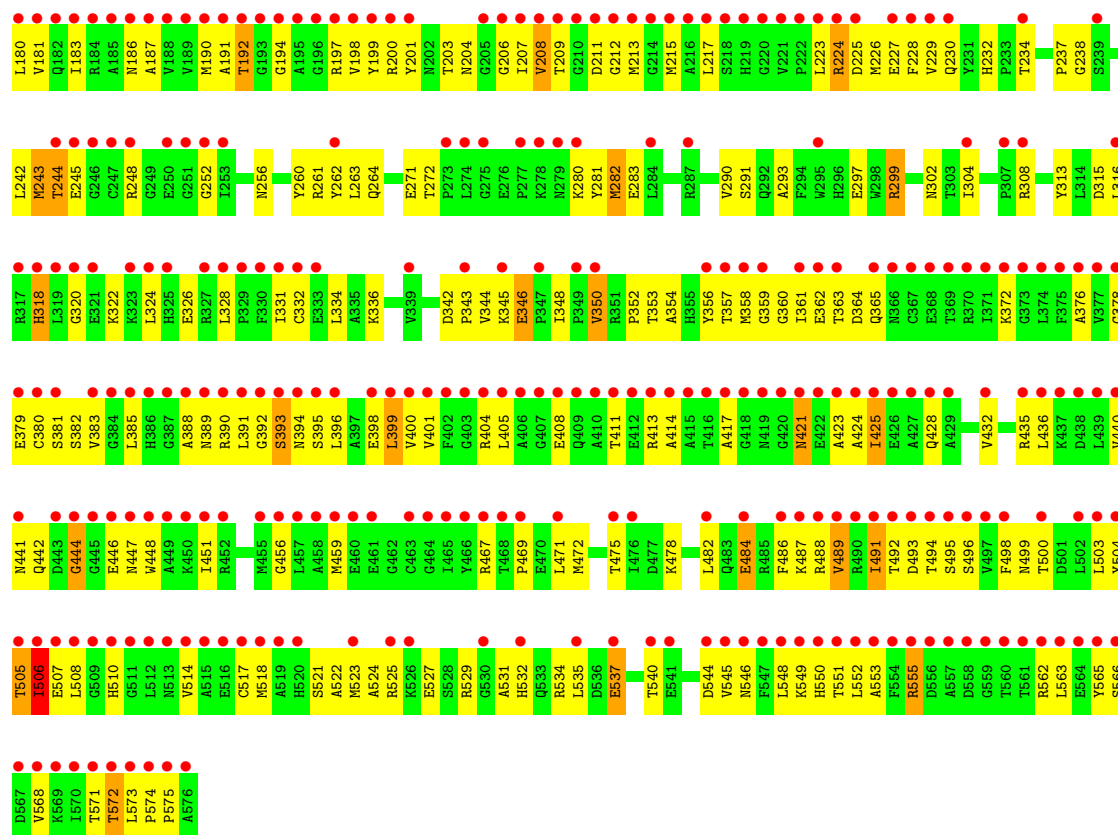
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Fumarate reductase flavoprotein subunit

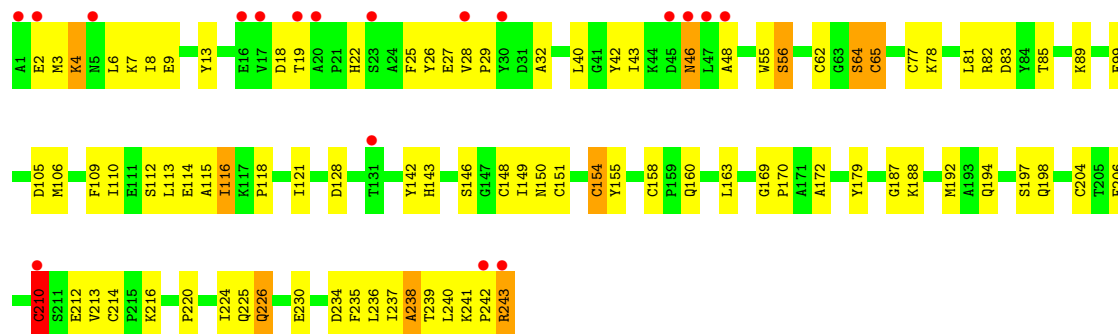


• Molecule 1: Fumarate reductase flavoprotein subunit

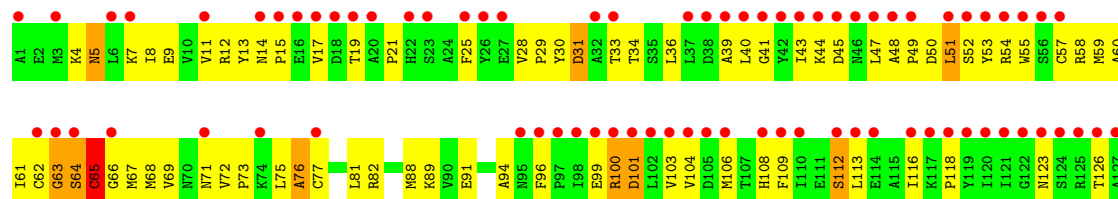
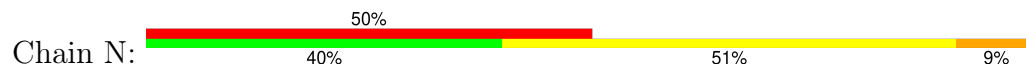


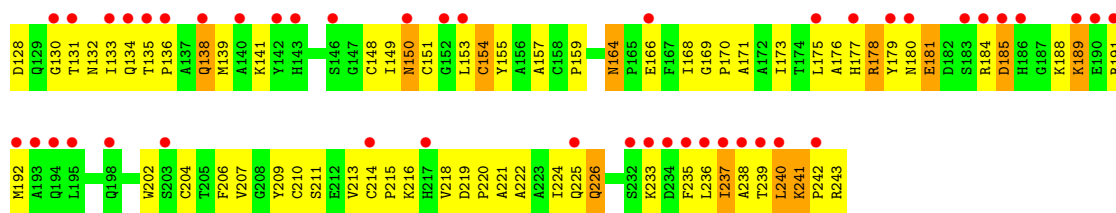


• Molecule 2: Fumarate reductase iron-sulfur protein

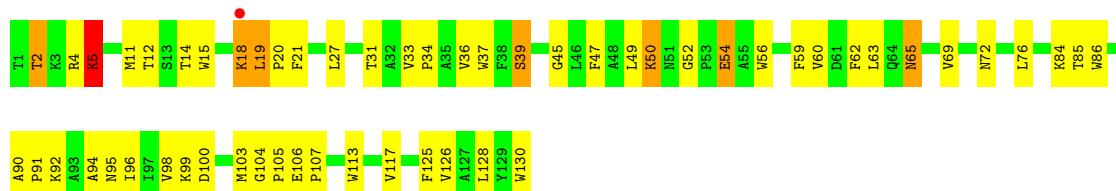


• Molecule 2: Fumarate reductase iron-sulfur protein

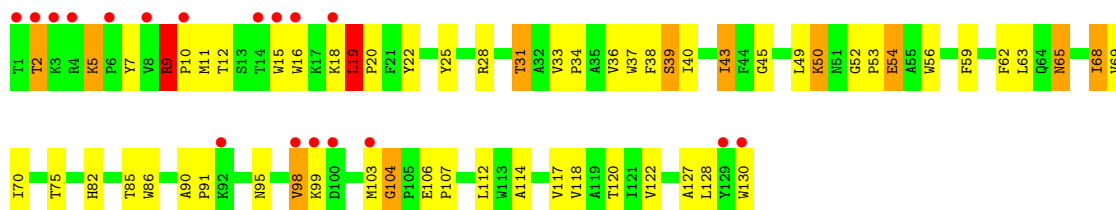




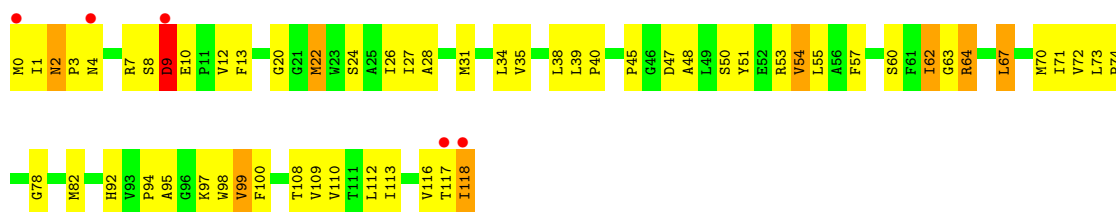
● Molecule 3: Fumarate reductase subunit C



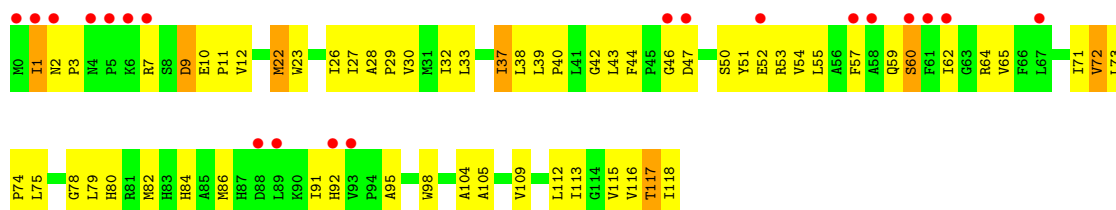
● Molecule 3: Fumarate reductase subunit C



● Molecule 4: Fumarate reductase subunit D



● Molecule 4: Fumarate reductase subunit D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.32Å 137.63Å 270.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.92 – 2.80 38.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.92-2.80) 94.8 (38.92-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.249 , 0.272 0.258 , 0.278	Depositor DCC
R_{free} test set	1408 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 89.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16873	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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, FUM, F3S, SF4, FAD

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	0.95	0/4541	1.11	16/6139 (0.3%)
1	M	0.67	3/4541 (0.1%)	1.02	10/6139 (0.2%)
2	B	1.00	1/1931 (0.1%)	1.15	12/2617 (0.5%)
2	N	0.70	1/1931 (0.1%)	1.07	9/2617 (0.3%)
3	C	0.72	0/1094	1.09	6/1496 (0.4%)
3	O	0.71	0/1094	1.16	13/1496 (0.9%)
4	D	0.80	0/956	1.05	6/1303 (0.5%)
4	P	0.69	0/956	1.02	1/1303 (0.1%)
All	All	0.81	5/17044 (0.0%)	1.08	73/23110 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	210	CYS	C-N	17.95	1.58	1.33
2	N	77	CYS	C-N	14.41	1.52	1.33
1	M	505	THR	C-N	12.30	1.49	1.33
1	M	506	ILE	CA-CB	6.59	1.63	1.54
1	M	59	HIS	N-CA	5.40	1.53	1.46

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	210	CYS	O-C-N	16.39	138.96	122.07
1	M	346	GLU	N-CA-C	15.71	122.06	108.07
1	M	344	VAL	N-CA-C	-10.62	101.58	111.67
2	B	210	CYS	CA-C-N	-10.21	103.66	120.72
2	B	210	CYS	C-N-CA	-10.21	103.66	120.72
3	O	52	GLY	CA-C-N	9.74	129.36	119.82
3	O	52	GLY	C-N-CA	9.74	129.36	119.82
1	M	45	THR	N-CA-C	-8.65	102.90	113.97
2	N	65	CYS	N-CA-CB	-8.09	96.83	110.49
4	P	72	VAL	N-CA-C	7.59	117.66	110.53
2	N	76	ALA	CA-C-N	7.38	130.91	120.28
2	N	76	ALA	C-N-CA	7.38	130.91	120.28
1	M	208	VAL	N-CA-C	6.77	113.46	106.21
1	A	545	VAL	N-CA-C	-6.56	104.09	110.72
2	B	48	ALA	CA-C-N	6.44	126.13	119.56
2	B	48	ALA	C-N-CA	6.44	126.13	119.56
2	N	65	CYS	O-C-N	-6.43	114.04	122.59
1	M	1	GLN	N-CA-C	-6.42	97.13	110.80
3	C	52	GLY	CA-C-N	6.40	126.90	119.47
3	C	52	GLY	C-N-CA	6.40	126.90	119.47
3	O	19	LEU	CA-C-N	6.35	126.56	119.32
3	O	19	LEU	C-N-CA	6.35	126.56	119.32
3	C	65	ASN	CA-C-N	6.30	126.78	119.47
3	C	65	ASN	C-N-CA	6.30	126.78	119.47
3	O	65	ASN	CA-C-N	6.20	126.39	119.32
3	O	65	ASN	C-N-CA	6.20	126.39	119.32
3	C	5	LYS	CA-C-N	6.18	127.56	119.84
3	C	5	LYS	C-N-CA	6.18	127.56	119.84
3	O	9	ARG	CA-C-N	6.10	127.47	119.84
3	O	9	ARG	C-N-CA	6.10	127.47	119.84
1	A	361	ILE	CB-CA-C	-6.05	101.73	111.59
2	N	192	MET	N-CA-C	6.04	117.86	111.28
2	N	63	GLY	N-CA-C	6.03	124.44	115.64
3	O	104	GLY	CA-C-N	5.99	125.38	118.85
3	O	104	GLY	C-N-CA	5.99	125.38	118.85
1	M	146	PHE	CA-C-N	5.85	125.39	119.19
1	M	146	PHE	C-N-CA	5.85	125.39	119.19
2	B	64	SER	N-CA-C	5.83	120.67	113.50
1	A	306	THR	CA-C-N	5.80	125.49	119.05
1	A	306	THR	C-N-CA	5.80	125.49	119.05
2	B	210	CYS	N-CA-C	-5.79	104.87	111.07
2	B	226	GLN	N-CA-C	-5.77	105.13	111.82
1	M	50	GLY	N-CA-C	5.73	119.42	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	GLY	CA-C-N	5.65	126.91	119.84
2	B	169	GLY	C-N-CA	5.65	126.91	119.84
1	A	282	MET	CB-CA-C	-5.65	110.08	116.63
4	D	4	ASN	CA-C-N	5.50	125.41	119.85
4	D	4	ASN	C-N-CA	5.50	125.41	119.85
1	A	547	PHE	N-CA-C	5.49	119.55	112.41
1	A	386	HIS	N-CA-C	5.48	120.12	113.38
1	A	221	VAL	CA-C-N	-5.47	113.62	120.51
1	A	221	VAL	C-N-CA	-5.47	113.62	120.51
4	D	2	ASN	CA-C-N	5.41	124.60	118.97
4	D	2	ASN	C-N-CA	5.41	124.60	118.97
1	A	312	VAL	N-CA-C	-5.41	101.61	109.29
1	M	1	GLN	N-CA-CB	5.39	119.61	110.49
3	O	5	LYS	CA-C-N	-5.39	113.79	120.79
3	O	5	LYS	C-N-CA	-5.39	113.79	120.79
2	B	192	MET	N-CA-C	5.35	117.11	111.28
2	B	238	ALA	N-CA-C	-5.29	105.59	111.36
1	M	282	MET	CB-CA-C	-5.28	110.47	116.54
4	D	54	VAL	CB-CA-C	-5.27	104.96	111.70
3	O	99	LYS	CB-CA-C	-5.25	110.09	117.23
4	D	9	ASP	N-CA-C	-5.23	106.85	113.18
1	A	263	LEU	N-CA-C	5.23	118.92	112.54
1	A	35	ILE	N-CA-C	5.22	116.10	108.53
2	N	72	VAL	CA-C-N	5.22	126.65	120.23
2	N	72	VAL	C-N-CA	5.22	126.65	120.23
2	N	31	ASP	N-CA-C	-5.20	103.17	110.35
1	A	226	MET	N-CA-C	5.02	117.48	111.71
1	A	573	LEU	N-CA-C	5.02	117.77	108.94
1	A	380	CYS	CA-C-N	-5.01	114.07	123.03
1	A	380	CYS	C-N-CA	-5.01	114.07	123.03

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	64	SER	Mainchain

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	4449	0	4335	176	0
1	M	4449	0	4335	420	0
2	B	1888	0	1844	94	0
2	N	1888	0	1839	209	0
3	C	1058	0	1108	66	0
3	O	1058	0	1108	75	0
4	D	926	0	971	81	0
4	P	926	0	970	71	0
5	A	53	0	30	13	0
5	M	53	0	30	24	0
6	A	8	0	1	0	0
7	B	4	0	0	3	0
7	N	4	0	0	1	0
8	B	7	0	0	4	0
8	N	7	0	0	1	0
9	B	8	0	0	11	0
9	N	8	0	0	5	0
10	A	60	0	0	2	0
10	B	10	0	0	0	0
10	C	2	0	0	0	0
10	D	4	0	0	0	0
10	M	1	0	0	5	0
10	N	2	0	0	0	0
All	All	16873	0	16571	1054	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1054) 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:M:44:HIS:NE2	5:M:601:FAD:HM82	1.24	1.52
1:A:44:HIS:CE1	5:A:601:FAD:HM82	1.43	1.48
1:A:44:HIS:NE2	5:A:601:FAD:C8M	1.77	1.45
2:N:31:ASP:OD2	2:N:33:THR:N	1.57	1.33
1:A:44:HIS:NE2	5:A:601:FAD:HM82	1.00	1.32
1:M:168:ARG:HD2	10:M:577:HOH:O	1.19	1.27
1:M:527:GLU:OE1	1:M:529:ARG:NH1	1.72	1.21
1:A:119:MET:HE2	1:A:391:LEU:HD23	1.24	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:116:ILE:HG21	2:N:176:ALA:HB2	1.17	1.09
2:N:189:LYS:H	2:N:189:LYS:HD2	0.99	1.08
3:C:86:TRP:HE1	4:D:22:MET:CE	1.67	1.07
1:M:100:GLY:C	2:N:184:ARG:NH2	2.12	1.07
1:A:346:GLU:HG3	1:A:347:PRO:HD2	1.31	1.06
4:P:1:ILE:HD12	4:P:1:ILE:H	1.16	1.06
1:M:44:HIS:NE2	5:M:601:FAD:C8M	2.20	1.04
2:N:71:ASN:HB3	3:O:18:LYS:HE3	1.33	1.04
1:M:155:HIS:CE1	1:M:174:ASN:HD22	1.76	1.02
2:B:204:CYS:SG	8:B:245:F3S:FE1	1.51	1.02
1:M:146:PHE:HB2	1:M:149:ILE:HD13	1.39	1.02
1:M:168:ARG:CD	10:M:577:HOH:O	1.81	1.01
2:N:178:ARG:HH11	2:N:178:ARG:HG2	1.22	1.01
3:C:86:TRP:NE1	4:D:22:MET:CE	2.24	1.01
3:C:86:TRP:HE1	4:D:22:MET:HE3	1.21	1.01
1:A:151:ARG:NH1	1:A:153:ASP:OD2	1.95	1.00
1:M:243:MET:HE2	1:M:331:ILE:HG23	1.43	1.00
1:M:192:THR:HG21	1:M:212:GLY:HA3	1.42	1.00
1:M:212:GLY:HA2	1:M:215:MET:HE2	1.44	1.00
3:C:50:LYS:HE2	3:C:50:LYS:HA	1.44	0.99
1:M:451:ILE:HG23	1:M:482:LEU:HD12	1.38	0.99
2:B:198:GLN:HE22	4:D:10:GLU:HG3	1.27	0.99
3:C:86:TRP:CD1	4:D:22:MET:HE2	1.97	0.99
2:N:13:TYR:HB2	2:N:21:PRO:HB3	1.45	0.99
2:N:159:PRO:HG2	2:N:207:VAL:HG21	1.45	0.99
1:M:549:LYS:HD2	1:M:565:TYR:HB3	1.45	0.98
1:M:537:GLU:H	1:M:537:GLU:CD	1.71	0.98
2:B:151:CYS:SG	9:B:246:SF4:FE1	1.55	0.98
1:A:57:GLN:HE22	1:A:122:GLU:HG2	1.25	0.97
1:M:100:GLY:CA	2:N:184:ARG:HH21	1.76	0.97
1:A:44:HIS:CE1	5:A:601:FAD:C8M	2.37	0.97
1:M:425:ILE:HD11	10:M:577:HOH:O	1.63	0.96
1:M:421:ASN:OD1	1:M:424:ALA:N	1.96	0.96
2:B:151:CYS:HG	9:B:246:SF4:FE1	0.78	0.95
1:M:243:MET:HE3	1:M:243:MET:HA	1.47	0.95
2:B:198:GLN:OE1	4:D:8:SER:OG	1.85	0.95
3:O:130:TRP:O	4:P:53:ARG:NH2	2.00	0.95
1:M:81:VAL:HG11	1:M:383:VAL:HG12	1.48	0.94
1:M:328:LEU:O	1:M:332:CYS:SG	2.26	0.93
2:N:189:LYS:HD2	2:N:189:LYS:N	1.84	0.92
2:B:148:CYS:HG	9:B:246:SF4:FE3	0.83	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:154:CYS:HB2	2:N:170:PRO:HG2	1.50	0.92
2:N:71:ASN:HB3	3:O:18:LYS:CE	1.98	0.92
1:A:328:LEU:O	1:A:332:CYS:SG	2.29	0.91
1:M:197:ARG:HD2	1:M:206:GLY:HA2	1.51	0.91
1:M:155:HIS:CE1	1:M:174:ASN:HA	2.04	0.91
2:N:189:LYS:H	2:N:189:LYS:CD	1.84	0.91
1:M:444:GLY:HA3	1:M:488:ARG:C	1.95	0.91
1:M:42:ARG:NH2	2:N:150:ASN:O	2.04	0.90
2:N:116:ILE:HG21	2:N:176:ALA:CB	2.00	0.90
1:M:119:MET:HE2	1:M:391:LEU:HD23	1.52	0.90
2:N:151:CYS:HG	9:N:246:SF4:FE1	0.76	0.90
1:M:192:THR:HG21	1:M:212:GLY:CA	2.02	0.90
2:B:154:CYS:SG	9:B:246:SF4:FE2	1.64	0.89
1:A:60:ASP:CG	1:A:123:ARG:HH21	1.80	0.89
1:M:149:ILE:HD12	1:M:149:ILE:H	1.36	0.89
1:M:11:GLY:HA2	5:M:601:FAD:O4B	1.72	0.89
1:M:100:GLY:HA2	2:N:184:ARG:HH21	1.36	0.89
3:C:86:TRP:CD1	4:D:22:MET:CE	2.55	0.88
1:M:525:ARG:O	1:M:534:ARG:NH1	2.07	0.88
3:C:50:LYS:HA	3:C:50:LYS:CE	2.05	0.87
2:B:242:PRO:HB2	4:P:92:HIS:HB3	1.55	0.87
1:M:42:ARG:HD2	2:N:64:SER:HB3	1.56	0.87
4:D:92:HIS:HB3	2:N:243:ARG:HB2	1.56	0.87
1:M:360:GLY:C	1:M:382:SER:OG	2.17	0.87
1:M:146:PHE:HB2	1:M:149:ILE:CD1	2.05	0.87
2:B:3:MET:HE2	2:B:29:PRO:HB2	1.57	0.86
4:D:0:MET:HG3	4:D:1:ILE:H	1.40	0.86
1:A:60:ASP:OD1	1:A:123:ARG:NH2	2.08	0.86
1:A:57:GLN:NE2	1:A:122:GLU:HG2	1.89	0.86
4:P:22:MET:HE3	4:P:22:MET:HA	1.56	0.85
2:N:222:ALA:O	2:N:226:GLN:NE2	2.10	0.85
2:N:149:ILE:HG23	2:N:216:LYS:HG3	1.58	0.85
1:M:93:MET:HE1	1:M:400:VAL:HG21	1.56	0.85
4:D:64:ARG:HG2	4:D:64:ARG:HH11	1.40	0.84
2:N:63:GLY:O	2:N:151:CYS:HA	1.77	0.84
1:M:93:MET:HE3	1:M:93:MET:HA	1.58	0.83
4:P:1:ILE:H	4:P:1:ILE:CD1	1.92	0.83
2:B:4:LYS:CE	2:B:4:LYS:H	1.90	0.83
1:M:24:ALA:HB2	1:M:32:ILE:HD11	1.59	0.83
1:M:155:HIS:CE1	1:M:174:ASN:ND2	2.47	0.82
2:N:148:CYS:SG	9:N:246:SF4:FE3	1.70	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:CYS:SG	9:B:246:SF4:FE4	1.70	0.82
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.61	0.82
2:B:46:ASN:N	2:B:46:ASN:HD22	1.78	0.82
1:M:425:ILE:CD1	10:M:577:HOH:O	2.22	0.82
2:N:116:ILE:CG2	2:N:176:ALA:HB2	2.07	0.82
1:M:157:VAL:HG22	5:M:601:FAD:N1A	1.95	0.81
2:N:71:ASN:CB	3:O:18:LYS:HE3	2.11	0.81
3:O:120:THR:HG23	4:P:30:VAL:HB	1.62	0.81
1:M:260:TYR:CE1	1:M:264:GLN:NE2	2.47	0.81
1:M:297:GLU:OE1	1:M:297:GLU:HA	1.81	0.81
1:M:97:GLU:OE2	2:N:132:ASN:N	2.14	0.81
1:M:100:GLY:CA	2:N:184:ARG:NH2	2.42	0.80
1:M:390:ARG:HD2	1:M:391:LEU:O	1.81	0.80
1:A:154:GLU:O	1:A:175:MET:HG3	1.81	0.80
1:M:62:PHE:HB3	1:M:86:VAL:CG1	2.11	0.80
2:B:46:ASN:HD22	2:B:46:ASN:H	1.27	0.80
1:M:7:LEU:HB2	1:M:32:ILE:HG22	1.63	0.80
1:M:155:HIS:NE2	1:M:174:ASN:ND2	2.28	0.80
1:M:155:HIS:ND1	1:M:174:ASN:HA	1.96	0.79
4:P:9:ASP:C	4:P:11:PRO:HD2	2.07	0.79
1:M:146:PHE:CB	1:M:149:ILE:HD13	2.11	0.79
1:M:176:MET:HE1	2:N:99:GLU:CG	2.12	0.79
1:M:152:PHE:HB3	1:M:155:HIS:CD2	2.17	0.79
1:M:158:LEU:HG	1:M:506:ILE:HD12	1.62	0.79
1:M:92:GLU:HB3	1:M:400:VAL:HB	1.63	0.78
3:C:86:TRP:NE1	4:D:22:MET:HE2	1.93	0.78
3:C:50:LYS:HE2	3:C:50:LYS:CA	2.14	0.78
4:D:92:HIS:HB3	2:N:243:ARG:CB	2.13	0.78
1:M:79:GLN:NE2	1:M:571:THR:H	1.81	0.78
1:M:527:GLU:CD	1:M:529:ARG:NH1	2.41	0.78
2:B:65:CYS:SG	2:B:77:CYS:SG	2.83	0.77
2:B:32:ALA:O	2:B:82:ARG:NH1	2.17	0.77
1:M:152:PHE:O	1:M:155:HIS:HB2	1.83	0.77
1:A:232:HIS:CE1	1:A:242:LEU:HD11	2.19	0.77
2:N:12:ARG:NH2	2:N:50:ASP:OD1	2.18	0.77
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.67	0.77
1:M:100:GLY:HA2	2:N:184:ARG:NH2	1.98	0.77
2:N:148:CYS:HG	9:N:246:SF4:FE3	1.02	0.77
1:A:321:GLU:HG2	1:A:344:VAL:HG11	1.67	0.77
2:B:9:GLU:HB2	2:B:25:PHE:CE2	2.20	0.76
2:N:116:ILE:O	2:N:191:ARG:HG2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:102:PRO:HG2	1:M:134:HIS:CD2	2.21	0.76
1:M:230:GLN:HB3	1:M:356:TYR:H	1.51	0.76
1:A:44:HIS:NE2	5:A:601:FAD:HM81	1.95	0.76
1:M:156:PHE:CE1	5:M:601:FAD:N6A	2.53	0.76
1:M:237:PRO:HB2	1:M:308:ARG:HB3	1.68	0.76
1:M:24:ALA:CA	1:M:32:ILE:HD11	2.16	0.75
1:M:146:PHE:CB	1:M:149:ILE:CD1	2.65	0.75
3:O:54:GLU:CD	3:O:54:GLU:H	1.94	0.75
1:M:62:PHE:HB3	1:M:86:VAL:HG13	1.67	0.75
2:B:163:LEU:HG	3:C:11:MET:HE2	1.68	0.75
1:M:81:VAL:HG11	1:M:383:VAL:CG1	2.17	0.75
4:D:34:LEU:HD23	4:D:38:LEU:HD12	1.68	0.75
4:D:26:ILE:HG22	4:D:27:ILE:HG13	1.69	0.74
1:M:93:MET:HE3	1:M:93:MET:CA	2.17	0.74
1:M:11:GLY:HA2	5:M:601:FAD:C1B	2.16	0.74
1:M:100:GLY:C	2:N:184:ARG:HH22	1.94	0.74
1:M:155:HIS:CE1	1:M:174:ASN:CA	2.70	0.74
1:M:24:ALA:CB	1:M:32:ILE:HD11	2.17	0.74
1:M:114:ARG:O	1:M:124:THR:HB	1.88	0.74
2:N:31:ASP:OD2	2:N:33:THR:CA	2.35	0.74
2:N:12:ARG:NH1	2:N:50:ASP:OD1	2.21	0.74
2:N:177:HIS:O	2:N:181:GLU:HB2	1.87	0.74
1:A:41:MET:HE2	2:B:150:ASN:HD22	1.52	0.74
2:N:96:PHE:O	3:O:9:ARG:NH1	2.20	0.74
3:C:54:GLU:OE1	3:C:54:GLU:HA	1.87	0.74
1:M:328:LEU:HD22	1:M:331:ILE:CD1	2.16	0.73
2:B:65:CYS:SG	7:B:244:FES:FE1	1.79	0.73
1:M:444:GLY:HA3	1:M:488:ARG:O	1.89	0.73
1:M:176:MET:HE1	2:N:99:GLU:HG3	1.71	0.73
1:M:421:ASN:OD1	1:M:421:ASN:C	2.30	0.73
1:A:45:THR:OG1	5:A:601:FAD:O2A	2.06	0.73
1:M:360:GLY:O	1:M:382:SER:OG	2.07	0.72
2:B:99:GLU:OE2	3:C:4:ARG:NH1	2.23	0.72
3:O:19:LEU:HD21	3:O:22:TYR:CE2	2.25	0.72
3:C:33:VAL:HA	4:D:82:MET:HE2	1.70	0.72
1:A:10:VAL:HG21	1:A:190:MET:HE3	1.72	0.72
2:B:154:CYS:HG	9:B:246:SF4:FE2	0.90	0.72
1:M:192:THR:HG21	1:M:212:GLY:N	2.03	0.72
1:A:49:GLU:HG2	1:A:129:ASP:O	1.89	0.72
1:M:224:ARG:HB2	1:M:552:LEU:HD23	1.72	0.72
1:M:546:ASN:O	1:M:549:LYS:NZ	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:13:GLY:H	5:M:601:FAD:H4B	1.54	0.72
1:M:549:LYS:HD2	1:M:565:TYR:CB	2.19	0.72
1:A:275:GLY:O	1:A:277:PRO:HD3	1.89	0.72
1:M:166:HIS:CD2	1:M:372:LYS:HB3	2.24	0.72
1:A:200:ARG:HD3	1:A:201:TYR:CZ	2.24	0.71
2:B:46:ASN:N	2:B:46:ASN:ND2	2.35	0.71
2:B:214:CYS:HG	9:B:246:SF4:FE4	1.03	0.71
1:M:93:MET:HA	1:M:93:MET:CE	2.20	0.71
3:O:54:GLU:CD	3:O:54:GLU:N	2.48	0.71
1:A:151:ARG:NH2	2:B:114:GLU:OE1	2.23	0.71
1:A:346:GLU:HG3	1:A:347:PRO:CD	2.14	0.71
1:A:18:ARG:NH1	1:A:92:GLU:OE2	2.23	0.71
2:B:241:LYS:CG	2:B:241:LYS:O	2.39	0.71
1:M:141:GLN:HB3	2:N:118:PRO:O	1.90	0.70
1:A:366:ASN:O	1:A:367:CYS:HB2	1.90	0.70
1:M:242:LEU:HG	1:M:244:THR:H	1.56	0.70
1:A:497:VAL:HG12	1:A:497:VAL:O	1.90	0.70
1:M:192:THR:HG21	1:M:212:GLY:H	1.56	0.70
1:A:197:ARG:HD2	1:A:206:GLY:HA2	1.72	0.70
3:C:19:LEU:HD13	3:C:20:PRO:HD2	1.73	0.70
1:M:217:LEU:HG	1:M:555:ARG:HB2	1.72	0.70
2:N:15:PRO:HB3	3:O:5:LYS:H	1.54	0.70
1:M:467:ARG:NH1	1:M:532:HIS:ND1	2.39	0.70
1:A:27:ASN:OD1	1:A:27:ASN:C	2.35	0.70
1:M:37:LYS:HE2	5:M:601:FAD:C8A	2.22	0.70
1:M:105:ARG:HD3	2:N:134:GLN:O	1.92	0.69
1:M:149:ILE:HD12	1:M:149:ILE:N	2.06	0.69
1:A:200:ARG:HD3	1:A:201:TYR:CE1	2.27	0.69
4:D:92:HIS:CB	2:N:243:ARG:HB2	2.22	0.69
2:N:164:ASN:OD1	2:N:164:ASN:C	2.36	0.69
3:O:75:THR:HG22	4:P:32:ILE:HD13	1.74	0.69
4:D:0:MET:HG3	4:D:1:ILE:N	2.08	0.69
1:M:213:MET:HB3	1:M:223:LEU:HD21	1.74	0.69
3:O:49:LEU:HD21	4:P:55:LEU:HA	1.73	0.69
4:P:33:LEU:HD12	4:P:37:ILE:HD12	1.73	0.69
1:A:342:ASP:OD2	1:A:344:VAL:HG23	1.93	0.68
1:M:357:THR:HG22	1:M:359:GLY:O	1.93	0.68
2:N:240:LEU:O	2:N:243:ARG:CZ	2.41	0.68
1:A:125:TRP:CD1	1:A:125:TRP:N	2.54	0.68
1:M:553:ALA:HA	1:M:562:ARG:O	1.93	0.68
4:P:79:LEU:HD12	4:P:104:ALA:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:9:ASP:OD2	4:D:97:LYS:NZ	2.24	0.68
1:M:360:GLY:C	1:M:382:SER:HG	1.99	0.68
2:N:109:PHE:CE2	2:N:113:LEU:HD11	2.28	0.68
3:C:59:PHE:HE2	3:C:63:LEU:HD11	1.59	0.68
1:M:84:TYR:CE2	1:M:405:LEU:HD22	2.29	0.68
1:M:342:ASP:HB3	1:M:345:LYS:CB	2.24	0.68
2:B:4:LYS:H	2:B:4:LYS:HE3	1.58	0.68
4:D:64:ARG:HH12	4:D:117:THR:HG23	1.58	0.68
1:M:176:MET:HE1	2:N:99:GLU:CD	2.19	0.68
1:M:227:GLU:HB2	1:M:522:ALA:HB2	1.76	0.68
1:M:260:TYR:OH	1:M:264:GLN:NE2	2.27	0.67
4:P:105:ALA:O	4:P:109:VAL:HG23	1.94	0.67
1:M:102:PRO:CB	2:N:139:MET:HE2	2.25	0.67
1:A:10:VAL:HB	1:A:190:MET:CE	2.24	0.67
1:M:244:THR:HG23	1:M:245:GLU:N	2.08	0.67
4:P:55:LEU:O	4:P:59:GLN:HG3	1.93	0.67
1:A:341:VAL:HG13	1:A:346:GLU:HB3	1.75	0.67
2:N:214:CYS:SG	2:N:218:VAL:HG23	2.35	0.67
2:N:41:GLY:HA2	2:N:53:TYR:OH	1.94	0.67
3:C:50:LYS:HD3	4:D:118:ILE:H	1.60	0.67
1:A:346:GLU:CG	1:A:347:PRO:HD2	2.17	0.67
1:A:10:VAL:HB	1:A:190:MET:HE2	1.77	0.66
4:D:95:ALA:HB1	4:D:98:TRP:HB2	1.76	0.66
2:N:31:ASP:OD1	2:N:33:THR:OG1	2.12	0.66
3:O:18:LYS:HE2	3:O:19:LEU:HD22	1.75	0.66
1:M:158:LEU:HD23	1:M:158:LEU:O	1.95	0.66
3:C:50:LYS:HB3	4:D:118:ILE:HG22	1.77	0.66
1:M:243:MET:HA	1:M:243:MET:CE	2.22	0.66
1:A:125:TRP:N	1:A:125:TRP:HD1	1.93	0.66
1:A:306:THR:HB	1:A:307:PRO:HD2	1.78	0.66
1:A:166:HIS:CD2	1:A:372:LYS:HB3	2.30	0.66
1:A:549:LYS:HB2	1:A:566:SER:O	1.96	0.66
2:N:210:CYS:SG	2:N:221:ALA:HB2	2.36	0.66
1:M:151:ARG:NH1	1:M:153:ASP:OD2	2.22	0.66
1:M:53:ALA:HB2	1:M:393:SER:OG	1.95	0.65
1:M:146:PHE:HB3	1:M:148:GLN:HE22	1.61	0.65
1:M:212:GLY:HA2	1:M:215:MET:CE	2.22	0.65
1:M:358:MET:SD	1:M:389:ASN:HA	2.37	0.65
1:A:37:LYS:HE2	5:A:601:FAD:N7A	2.11	0.65
1:M:299:ARG:HE	1:M:299:ARG:CA	2.06	0.65
1:M:332:CYS:HA	1:M:343:PRO:HG2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:HG2	1:A:344:VAL:CG1	2.27	0.65
1:M:37:LYS:HD3	1:M:156:PHE:CE1	2.31	0.65
1:A:322:LYS:HA	1:A:322:LYS:HE3	1.78	0.65
1:M:436:LEU:O	1:M:440:VAL:HG23	1.97	0.65
1:A:341:VAL:O	1:A:343:PRO:HD3	1.96	0.65
2:B:65:CYS:SG	7:B:244:FES:S1	2.94	0.65
1:M:51:GLY:O	1:M:396:LEU:HD12	1.97	0.65
1:M:151:ARG:HH12	1:M:153:ASP:CG	2.03	0.65
1:M:328:LEU:HB3	1:M:331:ILE:HD12	1.78	0.65
1:M:44:HIS:CD2	1:M:44:HIS:O	2.50	0.64
1:M:573:LEU:HD12	1:M:574:PRO:HD2	1.78	0.64
2:B:4:LYS:H	2:B:4:LYS:HE2	1.60	0.64
4:D:92:HIS:HA	2:N:243:ARG:O	1.97	0.64
2:N:108:HIS:O	2:N:112:SER:OG	2.13	0.64
1:M:478:LYS:O	1:M:482:LEU:HD23	1.97	0.64
4:P:95:ALA:HB1	4:P:98:TRP:HB2	1.79	0.64
1:A:361:ILE:HG13	1:A:380:CYS:O	1.97	0.64
4:D:92:HIS:HA	2:N:243:ARG:C	2.23	0.64
1:M:320:GLY:O	1:M:324:LEU:HB2	1.98	0.64
2:B:198:GLN:HE22	4:D:10:GLU:CG	2.06	0.64
4:D:64:ARG:HH11	4:D:64:ARG:CG	2.10	0.64
1:M:226:MET:O	1:M:518:MET:HG2	1.98	0.64
3:O:53:PRO:HG3	4:P:51:TYR:CE2	2.33	0.64
3:C:125:PHE:CE2	3:C:130:TRP:HH2	2.16	0.64
2:N:68:MET:HE1	2:N:73:PRO:HD3	1.78	0.64
1:M:41:MET:HE2	2:N:150:ASN:HD22	1.63	0.64
1:M:134:HIS:O	1:M:138:THR:OG1	2.15	0.63
2:N:54:ARG:HE	2:N:103:VAL:HG13	1.62	0.63
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.79	0.63
1:M:97:GLU:OE2	2:N:132:ASN:O	2.15	0.63
1:A:59:HIS:CD2	1:A:59:HIS:H	2.15	0.63
1:M:192:THR:CG2	1:M:212:GLY:HA3	2.22	0.63
1:M:11:GLY:CA	5:M:601:FAD:O4B	2.46	0.63
1:M:155:HIS:CE1	1:M:174:ASN:CB	2.82	0.63
1:A:37:LYS:HE2	5:A:601:FAD:C8A	2.29	0.63
1:A:425:ILE:O	1:A:428:GLN:HB2	1.98	0.63
1:M:342:ASP:HB3	1:M:345:LYS:HB3	1.81	0.63
1:A:443:ASP:OD1	1:A:444:GLY:N	2.32	0.63
1:A:527:GLU:CD	1:A:529:ARG:HH11	2.07	0.63
1:M:70:VAL:HG11	1:M:573:LEU:HD23	1.81	0.63
2:N:141:LYS:HB3	2:N:181:GLU:OE1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:VAL:CG2	2:B:43:ILE:HD11	2.29	0.63
1:M:156:PHE:HE1	5:M:601:FAD:N6A	1.96	0.63
1:A:358:MET:HE3	1:A:389:ASN:HA	1.80	0.62
1:A:119:MET:HE2	1:A:391:LEU:CD2	2.16	0.62
1:M:234:THR:HA	1:M:350:VAL:HG13	1.80	0.62
3:C:50:LYS:HD3	4:D:118:ILE:HG22	1.81	0.62
1:M:61:SER:N	1:M:64:TYR:HD1	1.97	0.62
2:N:73:PRO:HG2	2:N:213:VAL:HG11	1.79	0.62
1:M:93:MET:HE3	1:M:93:MET:N	2.14	0.62
1:M:102:PRO:CA	2:N:139:MET:HE2	2.29	0.62
1:M:280:LYS:C	1:M:281:TYR:HD2	2.08	0.62
4:P:1:ILE:HD12	4:P:1:ILE:N	2.00	0.62
1:A:529:ARG:CZ	1:A:542:ARG:HD2	2.29	0.62
2:N:12:ARG:CZ	2:N:50:ASP:OD1	2.47	0.62
1:A:542:ARG:NH1	1:A:544:ASP:OD2	2.32	0.61
1:A:556:ASP:HB2	1:A:558:ASP:OD2	2.00	0.61
3:C:90:ALA:N	3:C:91:PRO:HD2	2.15	0.61
1:M:149:ILE:H	1:M:149:ILE:CD1	2.11	0.61
2:N:235:PHE:C	2:N:235:PHE:CD2	2.78	0.61
1:A:213:MET:HE3	1:A:380:CYS:HA	1.82	0.61
1:M:102:PRO:CG	1:M:134:HIS:HD2	2.12	0.61
1:M:361:ILE:O	1:M:363:THR:HG23	2.00	0.61
3:C:12:THR:HG23	3:C:14:THR:H	1.66	0.61
1:M:38:VAL:HG11	1:M:207:ILE:HG21	1.82	0.61
1:M:299:ARG:HA	1:M:299:ARG:NE	2.14	0.61
1:A:202:ASN:HA	1:A:353:THR:HG22	1.80	0.61
4:D:48:ALA:O	4:D:53:ARG:HD3	2.01	0.61
1:M:113:VAL:HG12	1:M:125:TRP:HA	1.82	0.61
4:P:10:GLU:OE2	4:P:84:HIS:NE2	2.32	0.61
1:A:176:MET:HG3	3:C:4:ARG:HD3	1.83	0.61
4:D:13:PHE:HE2	4:D:97:LYS:HZ1	1.49	0.61
1:M:15:ALA:HB2	1:M:399:LEU:HD22	1.82	0.61
1:M:51:GLY:O	5:M:601:FAD:N3	2.33	0.61
1:M:304:ILE:HD12	1:M:304:ILE:H	1.65	0.61
3:C:15:TRP:O	3:C:18:LYS:HG2	2.01	0.60
2:N:31:ASP:OD2	2:N:31:ASP:C	2.42	0.60
2:N:34:THR:HG22	2:N:81:LEU:HD13	1.83	0.60
4:P:28:ALA:N	4:P:29:PRO:HD2	2.16	0.60
1:M:15:ALA:HB2	1:M:399:LEU:CD2	2.31	0.60
1:A:11:GLY:HA2	5:A:601:FAD:H1B	1.82	0.60
1:M:76:LEU:HG	1:M:529:ARG:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:176:MET:CE	2:N:99:GLU:HG3	2.30	0.60
3:O:75:THR:HG22	4:P:32:ILE:CD1	2.31	0.60
4:P:10:GLU:N	4:P:11:PRO:CD	2.64	0.60
4:P:22:MET:HA	4:P:22:MET:CE	2.31	0.60
2:B:240:LEU:O	2:B:242:PRO:HD3	2.00	0.60
2:B:28:VAL:HG22	2:B:43:ILE:HD11	1.84	0.60
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.37	0.60
2:N:12:ARG:NH2	2:N:101:ASP:OD1	2.31	0.60
2:B:9:GLU:HB2	2:B:25:PHE:CD2	2.37	0.60
3:O:86:TRP:CD1	4:P:22:MET:HE3	2.37	0.60
1:A:148:GLN:OE1	1:A:148:GLN:N	2.33	0.60
4:D:0:MET:CG	4:D:1:ILE:H	2.14	0.60
1:M:44:HIS:CE1	5:M:601:FAD:HM82	2.22	0.60
2:N:65:CYS:HB3	2:N:75:LEU:HD22	1.82	0.60
1:M:152:PHE:HB3	1:M:155:HIS:HD2	1.61	0.60
1:M:500:THR:HA	1:M:503:LEU:HB2	1.84	0.60
2:N:59:MET:HE2	2:N:61:ILE:HG21	1.84	0.60
4:D:51:TYR:C	4:D:51:TYR:CD2	2.80	0.59
1:M:232:HIS:O	1:M:352:PRO:HA	2.01	0.59
1:M:491:ILE:HD13	1:M:491:ILE:N	2.15	0.59
2:N:9:GLU:HG3	2:N:25:PHE:CZ	2.37	0.59
3:O:33:VAL:O	3:O:36:VAL:HG22	2.01	0.59
1:M:27:ASN:C	1:M:27:ASN:HD22	2.09	0.59
1:M:102:PRO:CG	1:M:134:HIS:CD2	2.84	0.59
1:A:250:GLU:O	1:A:319:LEU:HD11	2.01	0.59
1:A:546:ASN:O	1:A:549:LYS:HE2	2.02	0.59
1:M:42:ARG:HH22	2:N:150:ASN:C	2.10	0.59
1:M:208:VAL:O	1:M:208:VAL:HG12	2.01	0.59
3:O:103:MET:HG2	3:O:104:GLY:N	2.17	0.59
2:B:3:MET:CE	2:B:29:PRO:HB2	2.31	0.59
3:C:50:LYS:HB3	4:D:118:ILE:CG2	2.31	0.59
1:A:10:VAL:CG2	1:A:190:MET:HE3	2.31	0.59
2:N:5:ASN:N	2:N:5:ASN:HD22	2.00	0.59
1:M:234:THR:HG22	1:M:350:VAL:HG11	1.85	0.59
2:B:170:PRO:HA	2:B:224:ILE:HD11	1.85	0.59
1:M:97:GLU:C	1:M:97:GLU:OE1	2.46	0.59
1:A:27:ASN:OD1	1:A:29:ASN:N	2.36	0.58
1:M:151:ARG:NH1	1:M:153:ASP:CG	2.61	0.58
1:M:11:GLY:O	1:M:16:GLY:HA3	2.03	0.58
1:M:217:LEU:HD13	1:M:223:LEU:HG	1.84	0.58
2:N:157:ALA:HB1	2:N:209:TYR:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:118:VAL:O	3:O:122:VAL:HG23	2.03	0.58
1:A:493:ASP:OD1	1:A:495:SER:OG	2.20	0.58
1:M:223:LEU:HD13	1:M:226:MET:HE2	1.85	0.58
1:M:224:ARG:NH1	1:M:382:SER:O	2.36	0.58
2:N:31:ASP:CG	2:N:33:THR:OG1	2.46	0.58
2:N:238:ALA:O	2:N:242:PRO:HD3	2.02	0.58
1:M:34:LEU:O	1:M:151:ARG:HA	2.03	0.58
1:A:493:ASP:OD1	1:A:493:ASP:C	2.47	0.58
1:M:260:TYR:HE1	1:M:264:GLN:NE2	2.00	0.58
2:N:36:LEU:HD23	2:N:76:ALA:HA	1.85	0.58
2:N:236:LEU:HD23	2:N:236:LEU:C	2.28	0.58
2:B:206:PHE:CE1	2:B:225:GLN:HG3	2.38	0.58
1:M:360:GLY:CA	1:M:382:SER:OG	2.51	0.58
1:M:392:GLY:O	1:M:393:SER:HB3	2.03	0.58
1:M:155:HIS:HE1	1:M:174:ASN:HB2	1.69	0.58
3:C:59:PHE:CE2	3:C:63:LEU:HD11	2.39	0.57
1:M:245:GLU:O	1:M:245:GLU:HG2	2.04	0.57
1:A:213:MET:HE1	1:A:357:THR:HG21	1.85	0.57
1:A:28:PRO:HA	1:A:148:GLN:HE21	1.70	0.57
1:A:306:THR:HB	1:A:307:PRO:CD	2.34	0.57
1:M:198:VAL:CG1	1:M:459:MET:HG3	2.33	0.57
2:N:36:LEU:HD13	2:N:88:MET:HE2	1.87	0.57
2:N:206:PHE:CE1	2:N:225:GLN:HG3	2.39	0.57
4:P:60:SER:O	4:P:64:ARG:HG3	2.04	0.57
1:A:336:LYS:O	1:A:340:GLY:HA2	2.04	0.57
1:A:442:GLN:NE2	1:A:487:LYS:C	2.63	0.57
1:A:228:PHE:O	1:A:358:MET:HB2	2.05	0.57
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.87	0.57
1:M:74:ASP:O	1:M:75:TRP:HB2	2.02	0.57
2:N:178:ARG:HG2	2:N:178:ARG:NH1	2.00	0.57
1:A:142:THR:O	1:A:145:GLN:HG2	2.04	0.57
3:C:50:LYS:CG	4:D:118:ILE:HG22	2.35	0.57
1:A:286:PRO:O	1:A:290:VAL:HG23	2.04	0.57
1:M:444:GLY:CA	1:M:488:ARG:O	2.53	0.57
1:M:552:LEU:HD11	1:M:566:SER:HB2	1.86	0.57
3:O:68:ILE:N	3:O:68:ILE:HD12	2.18	0.57
4:P:78:GLY:O	4:P:82:MET:HG3	2.05	0.57
1:A:154:GLU:C	1:A:175:MET:HG3	2.30	0.57
1:A:10:VAL:CB	1:A:190:MET:CE	2.82	0.56
3:O:15:TRP:CD2	3:O:16:TRP:N	2.73	0.56
1:A:178:GLY:HA3	1:A:496:SER:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:ALA:HB1	3:C:96:ILE:HD11	1.86	0.56
4:D:92:HIS:HB3	2:N:243:ARG:CG	2.34	0.56
4:D:112:LEU:O	4:D:116:VAL:HG22	2.04	0.56
1:M:27:ASN:C	1:M:27:ASN:ND2	2.60	0.56
1:M:342:ASP:HB3	1:M:345:LYS:HB2	1.86	0.56
2:B:241:LYS:O	2:B:241:LYS:HG2	2.05	0.56
1:M:24:ALA:HA	1:M:32:ILE:HD11	1.86	0.56
1:M:146:PHE:HB3	1:M:148:GLN:NE2	2.19	0.56
1:M:151:ARG:NH1	1:M:153:ASP:OD1	2.37	0.56
1:M:213:MET:HE2	1:M:360:GLY:HA2	1.87	0.56
3:C:54:GLU:OE1	3:C:54:GLU:CA	2.54	0.56
1:M:85:PHE:HE1	1:M:398:GLU:HA	1.71	0.56
4:P:113:ILE:O	4:P:117:THR:OG1	2.24	0.56
2:N:14:ASN:HD22	2:N:15:PRO:HD2	1.69	0.56
1:A:44:HIS:NE2	5:A:601:FAD:C8	2.65	0.56
2:N:180:ASN:ND2	2:N:188:LYS:HG3	2.20	0.56
2:N:202:TRP:CZ2	4:P:11:PRO:HG3	2.41	0.56
3:O:86:TRP:CD1	4:P:22:MET:CE	2.89	0.56
4:P:9:ASP:C	4:P:11:PRO:CD	2.79	0.56
2:B:210:CYS:O	2:B:213:VAL:HG22	2.04	0.56
1:M:13:GLY:N	5:M:601:FAD:H4B	2.19	0.56
1:M:61:SER:H	1:M:64:TYR:HD1	1.51	0.56
1:M:527:GLU:CD	1:M:529:ARG:HH12	2.09	0.56
3:O:15:TRP:CE3	3:O:16:TRP:HA	2.41	0.56
1:A:141:GLN:HB3	2:B:118:PRO:O	2.05	0.56
1:M:100:GLY:C	2:N:184:ARG:HH21	1.92	0.56
2:N:21:PRO:HD3	3:O:7:TYR:CE2	2.41	0.56
4:P:112:LEU:O	4:P:116:VAL:HG22	2.07	0.55
1:M:225:ASP:HB3	1:M:228:PHE:CD2	2.41	0.55
1:A:529:ARG:HG3	1:A:542:ARG:HD3	1.87	0.55
4:P:51:TYR:CZ	4:P:55:LEU:HD22	2.41	0.55
2:B:194:GLN:O	2:B:197:SER:HB3	2.05	0.55
1:M:469:PRO:HG3	1:M:534:ARG:HH21	1.70	0.55
1:M:24:ALA:N	1:M:32:ILE:CD1	2.69	0.55
1:M:243:MET:O	1:M:244:THR:HG22	2.06	0.55
4:P:62:ILE:O	4:P:65:VAL:HG22	2.06	0.55
3:C:130:TRP:HB2	4:D:53:ARG:NH2	2.22	0.55
3:O:33:VAL:CB	3:O:34:PRO:HD3	2.36	0.55
2:N:71:ASN:HD22	3:O:18:LYS:NZ	2.04	0.55
3:O:39:SER:OG	4:P:71:ILE:O	2.25	0.55
1:A:127:ALA:HB3	1:A:131:THR:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:92:HIS:C	2:N:243:ARG:HB2	2.32	0.55
1:M:10:VAL:HG13	5:M:601:FAD:C2A	2.36	0.55
1:M:389:ASN:OD1	1:M:531:ALA:HB2	2.07	0.55
4:P:50:SER:O	4:P:51:TYR:C	2.50	0.55
1:M:18:ARG:NH1	1:M:92:GLU:OE2	2.40	0.55
1:M:62:PHE:HB3	1:M:86:VAL:HG11	1.89	0.55
2:N:13:TYR:HB2	2:N:21:PRO:CB	2.29	0.55
2:B:154:CYS:HB2	2:B:170:PRO:HG2	1.88	0.54
1:M:93:MET:HE2	1:M:96:LEU:HD12	1.88	0.54
1:M:322:LYS:O	1:M:326:GLU:HB3	2.06	0.54
1:M:467:ARG:HB3	1:M:472:MET:HE3	1.89	0.54
1:M:225:ASP:HB3	1:M:228:PHE:HD2	1.72	0.54
1:M:24:ALA:HB2	1:M:32:ILE:CD1	2.35	0.54
1:M:52:SER:O	1:M:125:TRP:N	2.39	0.54
1:M:299:ARG:HE	1:M:299:ARG:HA	1.69	0.54
2:N:241:LYS:O	2:N:243:ARG:HG2	2.06	0.54
1:A:42:ARG:HG2	2:B:64:SER:HB3	1.88	0.54
2:B:188:LYS:HZ3	2:B:230:GLU:HG3	1.72	0.54
2:B:154:CYS:SG	9:B:246:SF4:S4	3.04	0.54
1:M:30:ALA:O	1:M:148:GLN:HB3	2.08	0.54
4:P:27:ILE:C	4:P:29:PRO:HD2	2.33	0.54
1:A:440:VAL:HG13	10:A:606:HOH:O	2.08	0.54
1:M:7:LEU:HD11	1:M:411:THR:CG2	2.37	0.54
1:M:299:ARG:CA	1:M:299:ARG:NE	2.71	0.54
2:N:8:ILE:HD11	2:N:81:LEU:HD21	1.89	0.54
2:N:135:THR:HB	2:N:138:GLN:HB2	1.90	0.54
1:A:273:PRO:HG2	1:A:276:GLU:HB2	1.89	0.54
1:A:493:ASP:CG	1:A:495:SER:OG	2.51	0.54
3:C:33:VAL:HA	4:D:82:MET:CE	2.35	0.54
1:M:308:ARG:NH2	2:N:33:THR:HB	2.22	0.54
1:M:472:MET:SD	1:M:523:MET:HA	2.48	0.54
1:A:59:HIS:H	1:A:59:HIS:HD2	1.56	0.54
3:O:50:LYS:HD2	4:P:117:THR:HB	1.89	0.54
1:M:448:TRP:CH2	1:M:504:TYR:HB3	2.43	0.54
1:M:88:HIS:CB	1:M:401:VAL:HG13	2.38	0.53
1:M:94:THR:HA	2:N:131:THR:CG2	2.38	0.53
1:A:15:ALA:HB2	1:A:399:LEU:HD22	1.90	0.53
1:M:365:GLN:H	1:M:365:GLN:CD	2.16	0.53
2:N:73:PRO:HB2	2:N:153:LEU:HD22	1.90	0.53
3:O:68:ILE:N	3:O:68:ILE:CD1	2.70	0.53
4:D:92:HIS:HD2	2:N:243:ARG:OXT	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:152:PHE:N	1:M:152:PHE:CD2	2.77	0.53
1:M:194:GLY:O	1:M:208:VAL:HG13	2.09	0.53
2:N:51:LEU:HD23	2:N:52:SER:N	2.23	0.53
2:N:185:ASP:OD2	2:N:185:ASP:C	2.52	0.53
3:O:19:LEU:CD2	3:O:22:TYR:CD2	2.91	0.53
1:M:94:THR:O	1:M:98:LEU:HG	2.08	0.53
2:N:153:LEU:HD12	2:N:215:PRO:HD3	1.89	0.53
3:O:33:VAL:HB	3:O:34:PRO:CD	2.37	0.53
4:P:42:GLY:C	4:P:44:PHE:H	2.16	0.53
2:N:54:ARG:NH2	2:N:104:VAL:O	2.42	0.53
1:A:542:ARG:HG3	1:A:543:ASP:N	2.24	0.53
1:M:81:VAL:CG1	1:M:383:VAL:CG1	2.87	0.53
1:M:207:ILE:HG13	1:M:208:VAL:HG23	1.91	0.53
2:B:151:CYS:SG	9:B:246:SF4:S3	3.07	0.53
1:M:11:GLY:HA2	5:M:601:FAD:H1B	1.91	0.53
1:M:198:VAL:HG12	1:M:459:MET:HG3	1.89	0.53
3:O:38:PHE:HB2	3:O:75:THR:HG21	1.90	0.53
3:C:50:LYS:CB	4:D:118:ILE:HG22	2.39	0.53
1:M:396:LEU:HG	5:M:601:FAD:C2	2.38	0.53
2:N:60:ALA:HA	7:N:244:FES:S1	2.49	0.53
1:M:421:ASN:OD1	1:M:423:ALA:N	2.42	0.53
1:M:451:ILE:HG22	1:M:508:LEU:HD11	1.91	0.53
2:N:116:ILE:CG2	2:N:176:ALA:CB	2.78	0.53
1:A:527:GLU:OE1	1:A:529:ARG:HD2	2.10	0.52
2:N:135:THR:CG2	2:N:136:PRO:HD2	2.39	0.52
2:N:240:LEU:O	2:N:243:ARG:NH2	2.42	0.52
1:A:200:ARG:NH1	1:A:201:TYR:OH	2.42	0.52
1:M:37:LYS:HE2	5:M:601:FAD:N7A	2.24	0.52
1:M:97:GLU:OE1	1:M:98:LEU:HD23	2.10	0.52
4:P:22:MET:HE2	4:P:26:ILE:CD1	2.38	0.52
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.91	0.52
1:A:442:GLN:HE21	1:A:489:VAL:H	1.57	0.52
1:M:211:ASP:OD2	1:M:507:GLU:HG2	2.09	0.52
1:M:486:PHE:O	1:M:489:VAL:HB	2.10	0.52
1:M:524:ALA:HB2	1:M:563:LEU:CD1	2.39	0.52
2:B:42:TYR:C	2:B:42:TYR:CD2	2.87	0.52
2:N:175:LEU:O	2:N:178:ARG:HB3	2.10	0.52
4:P:50:SER:O	4:P:53:ARG:N	2.43	0.52
1:M:146:PHE:HB3	1:M:149:ILE:CD1	2.38	0.52
2:N:123:ASN:ND2	2:N:184:ARG:O	2.43	0.52
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:101:CYS:N	2:N:184:ARG:NH2	2.57	0.52
1:M:103:TRP:O	1:M:105:ARG:HG3	2.10	0.52
1:A:462:GLY:HA3	1:A:475:THR:OG1	2.10	0.52
3:C:2:THR:HG1	3:C:4:ARG:H	1.57	0.52
2:N:178:ARG:HH11	2:N:178:ARG:CG	2.07	0.52
1:A:43:SER:O	1:A:46:VAL:HG12	2.10	0.51
1:A:317:ARG:HD3	1:A:345:LYS:O	2.10	0.51
3:C:59:PHE:O	3:C:62:PHE:HB3	2.11	0.51
1:M:23:ALA:CB	1:M:32:ILE:HG21	2.40	0.51
1:M:225:ASP:OD2	1:M:550:HIS:HD2	1.93	0.51
4:P:33:LEU:HA	4:P:37:ILE:HG13	1.91	0.51
1:A:125:TRP:CD1	1:A:125:TRP:H	2.26	0.51
3:C:63:LEU:HB3	4:D:40:PRO:HG3	1.93	0.51
4:D:62:ILE:CG2	4:D:63:GLY:N	2.74	0.51
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.46	0.51
1:M:525:ARG:NH2	1:M:549:LYS:O	2.36	0.51
4:D:92:HIS:CD2	2:N:243:ARG:OXT	2.64	0.51
1:M:24:ALA:CA	1:M:32:ILE:CD1	2.87	0.51
3:O:9:ARG:HB3	3:O:10:PRO:HD2	1.91	0.51
1:A:448:TRP:CG	1:A:449:ALA:N	2.78	0.51
1:A:356:TYR:HE1	5:A:601:FAD:O3'	1.93	0.51
1:M:510:HIS:O	1:M:514:VAL:HG23	2.11	0.51
1:A:50:GLY:HA3	1:A:116:PHE:CZ	2.46	0.51
1:A:257:LYS:NZ	1:A:301:GLY:O	2.39	0.51
2:N:151:CYS:SG	9:N:246:SF4:S3	3.09	0.51
2:B:188:LYS:NZ	2:B:230:GLU:HG3	2.25	0.51
1:M:34:LEU:N	1:M:150:GLN:O	2.36	0.51
1:M:51:GLY:N	5:M:601:FAD:O4	2.44	0.51
1:M:211:ASP:OD1	1:M:507:GLU:HA	2.11	0.51
1:M:414:ALA:HA	1:M:417:ALA:HB2	1.93	0.51
1:M:447:ASN:ND2	2:N:45:ASP:O	2.44	0.51
2:N:155:TYR:CE1	2:N:170:PRO:HD2	2.46	0.51
1:M:101:CYS:C	2:N:184:ARG:HH22	2.18	0.51
1:M:190:MET:SD	1:M:215:MET:HE3	2.51	0.51
2:N:206:PHE:HA	8:N:245:F3S:S1	2.51	0.51
1:A:525:ARG:NH2	1:A:549:LYS:O	2.39	0.51
1:M:524:ALA:CB	1:M:563:LEU:CD1	2.89	0.51
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.93	0.50
3:C:96:ILE:HB	3:C:103:MET:HE2	1.93	0.50
3:C:130:TRP:HB2	4:D:53:ARG:HH21	1.75	0.50
1:M:42:ARG:NH1	2:N:62:CYS:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:112:SER:O	2:N:116:ILE:HG12	2.11	0.50
3:O:59:PHE:O	3:O:62:PHE:HB3	2.11	0.50
4:P:64:ARG:HH21	4:P:116:VAL:HA	1.77	0.50
1:A:493:ASP:OD2	1:A:495:SER:OG	2.29	0.50
1:M:61:SER:HB3	1:M:64:TYR:CD1	2.47	0.50
1:M:263:LEU:CD1	1:M:283:GLU:HA	2.41	0.50
1:M:535:LEU:O	1:M:540:THR:HG22	2.11	0.50
1:A:527:GLU:OE1	1:A:529:ARG:NH1	2.41	0.50
2:B:99:GLU:CD	3:C:4:ARG:HH11	2.20	0.50
1:M:93:MET:CE	1:M:400:VAL:HG21	2.37	0.50
2:N:64:SER:O	2:N:66:GLY:N	2.45	0.50
1:A:279:ASN:O	1:A:280:LYS:HB2	2.12	0.50
1:A:442:GLN:HG2	1:A:489:VAL:O	2.11	0.50
2:B:204:CYS:SG	8:B:245:F3S:S2	2.90	0.50
4:D:92:HIS:HB3	2:N:243:ARG:HG3	1.94	0.50
1:M:48:ALA:HA	5:M:601:FAD:C6	2.42	0.50
1:M:155:HIS:HE1	1:M:174:ASN:CB	2.20	0.50
1:M:232:HIS:HE1	1:M:244:THR:O	1.93	0.50
1:M:342:ASP:O	1:M:346:GLU:N	2.44	0.50
1:M:388:ALA:HB2	1:M:529:ARG:HD3	1.93	0.50
3:O:28:ARG:O	3:O:31:THR:HB	2.11	0.50
1:A:84:TYR:CE1	1:A:88:HIS:CE1	2.99	0.50
2:B:13:TYR:OH	3:C:5:LYS:O	2.25	0.50
2:B:115:ALA:HB2	4:D:1:ILE:HD12	1.94	0.50
2:B:234:ASP:OD1	4:D:7:ARG:NH2	2.45	0.50
1:M:158:LEU:HD13	1:M:436:LEU:HD23	1.94	0.50
1:M:168:ARG:HD3	10:M:577:HOH:O	1.78	0.50
1:A:97:GLU:OE1	1:A:105:ARG:NH2	2.45	0.50
1:M:224:ARG:CB	1:M:552:LEU:HD23	2.41	0.50
2:N:28:VAL:CG1	2:N:29:PRO:HD2	2.42	0.50
2:N:159:PRO:O	3:O:11:MET:HE1	2.11	0.50
1:M:521:SER:HA	1:M:551:THR:HG21	1.94	0.50
1:M:7:LEU:HD22	1:M:187:ALA:HB3	1.93	0.50
1:M:256:ASN:HB2	1:M:302:ASN:O	2.12	0.50
1:A:454:GLU:CD	1:A:485:ARG:HH22	2.19	0.49
2:B:2:GLU:N	2:B:2:GLU:CD	2.70	0.49
1:M:70:VAL:CG1	1:M:573:LEU:HD23	2.41	0.49
1:M:113:VAL:HB	1:M:124:THR:O	2.11	0.49
1:M:243:MET:O	1:M:244:THR:C	2.54	0.49
2:B:149:ILE:HG23	2:B:216:LYS:HG3	1.93	0.49
2:B:241:LYS:O	2:B:241:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:105:ARG:NH1	2:N:134:GLN:H	2.10	0.49
2:N:44:LYS:HA	2:N:48:ALA:O	2.12	0.49
2:N:51:LEU:HA	2:N:101:ASP:OD1	2.13	0.49
1:A:262:TYR:OH	1:A:312:VAL:HG11	2.13	0.49
1:A:317:ARG:HD3	1:A:345:LYS:C	2.37	0.49
1:A:556:ASP:CB	1:A:558:ASP:OD2	2.59	0.49
2:B:154:CYS:SG	9:B:246:SF4:S3	2.95	0.49
1:M:48:ALA:O	1:M:132:GLY:N	2.43	0.49
1:M:114:ARG:NE	1:M:116:PHE:HE1	2.11	0.49
1:M:177:GLU:OE1	1:M:177:GLU:HA	2.11	0.49
1:M:331:ILE:HA	1:M:334:LEU:HD12	1.95	0.49
1:M:444:GLY:CA	1:M:488:ARG:C	2.78	0.49
2:N:135:THR:HG22	2:N:136:PRO:HD2	1.95	0.49
2:N:155:TYR:HE1	2:N:171:ALA:CB	2.25	0.49
3:O:56:TRP:CD1	4:P:51:TYR:HB2	2.47	0.49
3:C:98:VAL:HG23	3:C:98:VAL:O	2.12	0.49
1:M:85:PHE:CD2	1:M:385:LEU:HD11	2.48	0.49
2:N:57:CYS:O	2:N:58:ARG:HB2	2.11	0.49
4:P:10:GLU:N	4:P:11:PRO:HD2	2.28	0.49
1:A:27:ASN:OD1	1:A:30:ALA:N	2.42	0.49
4:D:73:LEU:HB2	4:D:74:PRO:HD3	1.94	0.49
1:M:17:LEU:HD22	1:M:140:PHE:HA	1.94	0.49
1:M:245:GLU:HG3	1:M:248:ARG:NH2	2.28	0.49
1:M:395:SER:OG	5:M:601:FAD:H2'	2.12	0.49
4:P:2:ASN:HB2	4:P:3:PRO:CD	2.42	0.49
1:M:102:PRO:HB2	2:N:139:MET:HE2	1.93	0.49
1:M:158:LEU:CD1	1:M:436:LEU:HD23	2.42	0.49
2:N:5:ASN:N	2:N:5:ASN:ND2	2.60	0.49
2:N:5:ASN:C	2:N:30:TYR:HE2	2.21	0.49
3:O:127:ALA:C	3:O:128:LEU:HD23	2.37	0.49
1:M:378:GLY:HA2	1:M:399:LEU:HD23	1.94	0.49
2:N:28:VAL:HG13	2:N:29:PRO:HD2	1.94	0.49
3:O:28:ARG:HG3	3:O:85:THR:HG21	1.95	0.49
1:A:536:ASP:OD1	1:A:536:ASP:N	2.40	0.49
4:D:39:LEU:HB3	4:D:40:PRO:HD3	1.95	0.49
1:M:7:LEU:HD21	1:M:411:THR:HA	1.94	0.49
3:O:19:LEU:HD23	3:O:22:TYR:CD2	2.48	0.49
4:P:22:MET:HE2	4:P:26:ILE:HD12	1.95	0.49
1:M:78:GLU:OE1	1:M:550:HIS:HE1	1.96	0.49
1:M:161:LEU:HD21	1:M:171:VAL:HG23	1.95	0.49
1:M:186:ASN:HB3	1:M:417:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASN:HB2	1:A:302:ASN:O	2.12	0.48
1:M:499:ASN:O	1:M:503:LEU:HG	2.12	0.48
4:P:86:MET:CE	4:P:91:ILE:HG21	2.42	0.48
2:B:188:LYS:NZ	2:B:230:GLU:CG	2.77	0.48
1:M:92:GLU:C	1:M:93:MET:HE3	2.38	0.48
1:A:44:HIS:CE1	1:A:204:ASN:HA	2.48	0.48
1:M:28:PRO:O	1:M:148:GLN:HG2	2.12	0.48
1:M:225:ASP:OD1	1:M:550:HIS:HB3	2.13	0.48
1:M:442:GLN:NE2	1:M:487:LYS:HA	2.29	0.48
4:P:30:VAL:O	4:P:33:LEU:HB3	2.13	0.48
3:C:50:LYS:CD	4:D:118:ILE:HG22	2.43	0.48
1:M:85:PHE:CE1	1:M:398:GLU:HA	2.49	0.48
2:N:109:PHE:CZ	2:N:113:LEU:HD11	2.48	0.48
1:M:31:LYS:O	1:M:31:LYS:HD3	2.14	0.48
1:M:75:TRP:O	1:M:568:VAL:HG11	2.14	0.48
1:M:232:HIS:CE1	1:M:242:LEU:CD1	2.97	0.48
2:N:134:GLN:NE2	2:N:184:ARG:HH11	2.11	0.48
1:A:10:VAL:HG11	1:A:190:MET:HE1	1.94	0.48
1:A:292:GLN:HG2	1:A:466:TYR:CZ	2.48	0.48
3:C:50:LYS:CD	4:D:118:ILE:H	2.26	0.48
1:M:363:THR:HG21	1:M:376:ALA:HB3	1.94	0.48
2:N:54:ARG:HH21	2:N:103:VAL:HG12	1.78	0.48
3:O:63:LEU:O	3:O:69:VAL:HG22	2.13	0.48
3:O:114:ALA:O	3:O:118:VAL:HG23	2.14	0.48
1:A:40:PRO:HG2	1:A:140:PHE:CE1	2.48	0.48
1:M:82:VAL:HG22	1:M:385:LEU:HD12	1.96	0.48
1:M:441:ASN:O	1:M:442:GLN:C	2.57	0.48
4:P:50:SER:C	4:P:52:GLU:N	2.72	0.48
2:B:28:VAL:HG22	2:B:43:ILE:CD1	2.42	0.48
1:A:62:PHE:CZ	1:A:90:PRO:HG2	2.49	0.47
3:O:18:LYS:HG2	3:O:19:LEU:HD22	1.94	0.47
3:O:65:ASN:O	3:O:69:VAL:HG23	2.14	0.47
1:M:102:PRO:CD	1:M:134:HIS:HD2	2.27	0.47
2:N:5:ASN:HA	2:N:28:VAL:O	2.14	0.47
2:N:57:CYS:HB3	2:N:62:CYS:HB3	1.96	0.47
2:N:7:LYS:HE2	2:N:25:PHE:CD1	2.49	0.47
3:O:68:ILE:CD1	3:O:68:ILE:H	2.26	0.47
4:D:50:SER:O	4:D:51:TYR:C	2.56	0.47
1:M:88:HIS:HB3	1:M:401:VAL:HG13	1.95	0.47
1:M:194:GLY:HA2	1:M:379:GLU:HG2	1.95	0.47
2:N:64:SER:C	2:N:66:GLY:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:43:ILE:HG13	4:P:71:ILE:HD13	1.96	0.47
1:A:529:ARG:NH2	1:A:542:ARG:HD2	2.28	0.47
3:C:45:GLY:N	3:C:59:PHE:CE1	2.82	0.47
1:M:37:LYS:HD3	1:M:156:PHE:CD1	2.49	0.47
1:M:58:ASP:C	1:M:60:ASP:H	2.22	0.47
1:M:290:VAL:O	1:M:293:ALA:HB3	2.14	0.47
2:N:14:ASN:HD22	2:N:15:PRO:CD	2.27	0.47
2:B:235:PHE:C	2:B:235:PHE:CD2	2.93	0.47
3:C:56:TRP:O	3:C:59:PHE:HB3	2.15	0.47
1:M:76:LEU:HD12	1:M:228:PHE:CZ	2.50	0.47
1:M:252:GLY:HA3	1:M:316:LEU:CD2	2.44	0.47
1:M:332:CYS:O	1:M:336:LYS:HG3	2.15	0.47
2:N:30:TYR:HA	2:N:34:THR:OG1	2.14	0.47
1:A:396:LEU:HG	5:A:601:FAD:C2	2.45	0.47
3:C:105:PRO:HD2	3:C:106:GLU:CD	2.39	0.47
3:C:113:TRP:O	3:C:117:VAL:HG23	2.15	0.47
1:M:146:PHE:CB	1:M:149:ILE:HD11	2.44	0.47
1:M:194:GLY:CA	1:M:379:GLU:HG2	2.44	0.47
1:M:432:VAL:HA	1:M:435:ARG:HH11	1.79	0.47
4:P:38:LEU:HD22	4:P:43:LEU:HB2	1.96	0.47
4:P:86:MET:HE3	4:P:91:ILE:HB	1.95	0.47
2:B:116:ILE:HD12	2:B:172:ALA:O	2.15	0.47
3:C:125:PHE:CE2	3:C:130:TRP:CH2	3.01	0.47
4:D:109:VAL:O	4:D:112:LEU:HB3	2.15	0.47
1:M:102:PRO:C	2:N:139:MET:HE1	2.40	0.47
2:N:226:GLN:HE21	2:N:226:GLN:HB2	1.57	0.47
1:M:38:VAL:HG11	1:M:207:ILE:CG2	2.44	0.47
1:M:261:ARG:HD3	1:M:271:GLU:OE1	2.15	0.47
2:N:11:VAL:HG21	2:N:91:GLU:HG2	1.95	0.47
3:O:15:TRP:HZ3	3:O:22:TYR:CG	2.33	0.47
1:M:114:ARG:NE	1:M:116:PHE:CE1	2.83	0.47
3:O:53:PRO:HG3	4:P:51:TYR:CD2	2.49	0.47
1:A:398:GLU:HG3	1:A:402:PHE:CD1	2.50	0.46
1:M:101:CYS:N	2:N:184:ARG:HH22	2.14	0.46
2:N:36:LEU:HD21	2:N:67:MET:SD	2.55	0.46
1:M:7:LEU:HD12	1:M:23:ALA:HB1	1.96	0.46
1:M:224:ARG:HG2	1:M:362:GLU:HA	1.97	0.46
2:N:65:CYS:O	2:N:66:GLY:C	2.57	0.46
1:A:159:ASP:OD1	1:A:160:ILE:N	2.48	0.46
1:M:57:GLN:HB2	1:M:59:HIS:CD2	2.51	0.46
1:A:232:HIS:O	1:A:352:PRO:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:LEU:HG	4:D:55:LEU:HD12	1.96	0.46
4:D:92:HIS:CA	2:N:243:ARG:HB2	2.44	0.46
1:M:94:THR:HA	2:N:131:THR:HG22	1.97	0.46
1:M:177:GLU:OE1	3:O:2:THR:HB	2.16	0.46
4:D:64:ARG:HH22	4:D:117:THR:CG2	2.28	0.46
1:M:103:TRP:O	2:N:139:MET:HE1	2.15	0.46
2:N:96:PHE:HB3	2:N:104:VAL:HB	1.97	0.46
2:B:62:CYS:HG	7:B:244:FES:FE2	1.31	0.46
3:C:36:VAL:HG23	4:D:78:GLY:HA3	1.96	0.46
2:N:15:PRO:HG3	2:N:99:GLU:O	2.15	0.46
1:M:203:THR:CG2	1:M:353:THR:HG23	2.46	0.46
1:M:358:MET:HE1	1:M:531:ALA:HB2	1.98	0.46
4:P:72:VAL:O	4:P:75:LEU:HB2	2.16	0.46
1:A:236:LEU:HD21	1:A:243:MET:HE3	1.98	0.46
1:M:130:LYS:NZ	2:N:216:LYS:HD2	2.31	0.46
1:M:154:GLU:O	1:M:175:MET:HB2	2.16	0.46
1:M:203:THR:HG22	1:M:353:THR:HG23	1.98	0.46
2:B:204:CYS:SG	8:B:245:F3S:S3	3.14	0.46
1:M:122:GLU:O	1:M:122:GLU:HG2	2.15	0.46
1:M:158:LEU:HG	1:M:506:ILE:CD1	2.40	0.46
1:A:542:ARG:HH11	1:A:544:ASP:CG	2.23	0.45
2:B:6:LEU:HD23	2:B:8:ILE:HG12	1.99	0.45
1:M:227:GLU:HB3	1:M:521:SER:HB2	1.98	0.45
1:M:320:GLY:O	1:M:324:LEU:CB	2.63	0.45
1:M:358:MET:SD	1:M:390:ARG:N	2.89	0.45
1:M:537:GLU:CD	1:M:537:GLU:N	2.51	0.45
2:N:36:LEU:HB3	2:N:76:ALA:O	2.17	0.45
1:A:395:SER:O	1:A:399:LEU:HG	2.15	0.45
1:A:398:GLU:HG3	1:A:402:PHE:HD1	1.80	0.45
1:M:51:GLY:HA2	1:M:131:THR:HG21	1.97	0.45
1:M:98:LEU:CD2	2:N:132:ASN:ND2	2.79	0.45
3:O:7:TYR:CD1	3:O:7:TYR:C	2.94	0.45
4:D:31:MET:HG3	4:D:70:MET:SD	2.57	0.45
1:M:113:VAL:HG23	1:M:122:GLU:O	2.16	0.45
2:N:100:ARG:O	2:N:101:ASP:C	2.59	0.45
2:B:26:TYR:HB3	2:B:43:ILE:HD12	1.97	0.45
4:D:35:VAL:O	4:D:40:PRO:HD3	2.16	0.45
1:M:93:MET:CA	1:M:93:MET:CE	2.87	0.45
1:A:7:LEU:HD21	1:A:410:ALA:HB1	1.99	0.45
2:B:105:ASP:OD1	2:B:105:ASP:C	2.60	0.45
2:B:112:SER:HA	4:D:1:ILE:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:219:ASP:N	2:N:220:PRO:CD	2.79	0.45
4:P:2:ASN:HB2	4:P:3:PRO:HD2	1.99	0.45
1:A:549:LYS:HA	1:A:568:VAL:HG23	1.98	0.45
2:B:226:GLN:OE1	3:C:95:ASN:ND2	2.49	0.45
2:N:155:TYR:HE1	2:N:171:ALA:HB3	1.81	0.45
1:A:93:MET:HB3	1:A:125:TRP:CZ3	2.52	0.45
2:N:17:VAL:HG12	2:N:17:VAL:O	2.16	0.45
2:N:204:CYS:CB	2:N:224:ILE:HG21	2.47	0.45
1:A:74:ASP:O	1:A:75:TRP:HB2	2.16	0.45
4:D:63:GLY:O	4:D:67:LEU:HD22	2.17	0.45
4:D:94:PRO:HG3	2:N:243:ARG:HE	1.82	0.45
1:M:27:ASN:O	1:M:30:ALA:HB3	2.17	0.45
1:M:102:PRO:C	2:N:139:MET:CE	2.90	0.45
2:N:65:CYS:HB3	2:N:75:LEU:CD2	2.46	0.45
2:N:149:ILE:HD11	2:N:151:CYS:HB3	1.99	0.45
3:O:15:TRP:CE3	3:O:16:TRP:CA	3.00	0.45
4:P:42:GLY:O	4:P:44:PHE:N	2.38	0.45
1:A:227:GLU:HB2	1:A:522:ALA:HB2	1.98	0.45
4:D:110:VAL:O	4:D:113:ILE:HB	2.17	0.45
1:M:242:LEU:CG	1:M:244:THR:H	2.25	0.45
3:O:53:PRO:HA	3:O:56:TRP:HB3	1.98	0.45
1:A:251:GLY:HA2	10:A:617:HOH:O	2.17	0.45
2:B:18:ASP:OD1	2:B:22:HIS:NE2	2.50	0.45
1:M:38:VAL:HB	1:M:42:ARG:HB2	1.98	0.45
1:M:206:GLY:HA3	2:N:55:TRP:CZ3	2.52	0.45
1:M:245:GLU:HG3	1:M:248:ARG:CZ	2.47	0.45
2:N:164:ASN:OD1	2:N:166:GLU:N	2.50	0.45
1:A:253:ILE:HG13	1:A:315:ASP:HB3	1.99	0.44
1:M:163:ASP:CG	1:M:424:ALA:HB1	2.42	0.44
2:B:238:ALA:HA	2:B:241:LYS:HD3	1.99	0.44
1:M:446:GLU:O	1:M:489:VAL:HG22	2.18	0.44
2:N:226:GLN:OE1	3:O:95:ASN:HB2	2.17	0.44
3:O:90:ALA:N	3:O:91:PRO:CD	2.79	0.44
2:B:82:ARG:HG3	2:B:83:ASP:N	2.32	0.44
2:B:109:PHE:HE1	2:B:155:TYR:CE1	2.35	0.44
3:C:103:MET:HG2	3:C:104:GLY:O	2.17	0.44
1:M:44:HIS:O	1:M:44:HIS:HD2	1.98	0.44
1:M:223:LEU:HB3	1:M:226:MET:CG	2.47	0.44
1:M:472:MET:CE	1:M:532:HIS:HE1	2.30	0.44
1:M:44:HIS:CE1	1:M:204:ASN:HA	2.53	0.44
1:M:98:LEU:HD21	2:N:130:GLY:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:304:ILE:HG12	1:M:313:TYR:CE1	2.53	0.44
1:M:364:ASP:C	1:M:364:ASP:OD1	2.60	0.44
1:A:162:VAL:HA	1:A:166:HIS:O	2.17	0.44
3:C:99:LYS:O	3:C:100:ASP:HB2	2.17	0.44
3:C:106:GLU:CD	3:C:106:GLU:H	2.25	0.44
1:M:237:PRO:HB2	1:M:308:ARG:CB	2.44	0.44
2:N:154:CYS:HB2	2:N:170:PRO:CG	2.36	0.44
3:O:112:LEU:HD23	3:O:112:LEU:HA	1.85	0.44
2:B:204:CYS:SG	8:B:245:F3S:S1	3.16	0.44
1:M:35:ILE:CD1	1:M:170:LEU:HD21	2.47	0.44
1:M:161:LEU:HA	1:M:428:GLN:OE1	2.17	0.44
1:M:484:GLU:OE2	1:M:484:GLU:C	2.61	0.44
2:N:155:TYR:CE1	2:N:171:ALA:HB3	2.52	0.44
4:D:95:ALA:HB2	2:N:240:LEU:HD23	2.00	0.44
1:M:135:MET:CE	1:M:396:LEU:HD22	2.48	0.44
1:M:18:ARG:HH21	1:M:22:ALA:HB2	1.81	0.44
1:M:322:LYS:O	1:M:326:GLU:N	2.40	0.44
1:M:478:LYS:HD2	1:M:478:LYS:HA	1.80	0.44
1:A:46:VAL:HB	1:A:136:LEU:CD2	2.48	0.43
2:N:178:ARG:NH1	2:N:178:ARG:CG	2.71	0.43
3:C:45:GLY:O	3:C:49:LEU:HB2	2.17	0.43
1:M:150:GLN:HG3	1:M:152:PHE:CE2	2.54	0.43
2:N:89:LYS:NZ	2:N:91:GLU:OE2	2.38	0.43
3:O:15:TRP:CE3	3:O:16:TRP:N	2.86	0.43
4:P:9:ASP:O	4:P:12:VAL:HG23	2.17	0.43
1:A:256:ASN:OD1	1:A:258:ASN:N	2.48	0.43
1:A:525:ARG:NH1	1:A:527:GLU:OE1	2.51	0.43
1:A:527:GLU:OE2	1:A:529:ARG:NH1	2.51	0.43
1:M:27:ASN:O	1:M:30:ALA:CB	2.66	0.43
1:M:113:VAL:HG11	1:M:125:TRP:CD1	2.54	0.43
1:M:162:VAL:HG22	1:M:167:VAL:HA	2.00	0.43
1:M:322:LYS:O	1:M:326:GLU:CB	2.66	0.43
1:M:11:GLY:HA3	1:M:191:ALA:O	2.18	0.43
1:M:262:TYR:CD1	1:M:262:TYR:C	2.96	0.43
2:N:51:LEU:HD22	2:N:53:TYR:HD2	1.82	0.43
1:A:442:GLN:HE22	1:A:487:LYS:HA	1.82	0.43
1:M:88:HIS:HB2	1:M:401:VAL:HG13	1.99	0.43
1:M:261:ARG:O	1:M:282:MET:HE1	2.19	0.43
2:N:106:MET:HE3	2:N:109:PHE:CD2	2.53	0.43
2:N:214:CYS:SG	2:N:218:VAL:CG2	3.06	0.43
4:D:2:ASN:HA	4:D:3:PRO:HD2	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:10:VAL:HG22	1:M:157:VAL:HG11	1.99	0.43
1:M:203:THR:HG22	1:M:353:THR:CG2	2.48	0.43
1:M:203:THR:HG23	1:M:354:ALA:O	2.18	0.43
1:A:275:GLY:C	1:A:277:PRO:HD3	2.43	0.43
2:B:18:ASP:OD1	2:B:22:HIS:CD2	2.71	0.43
2:B:121:ILE:HB	2:B:187:GLY:HA3	2.01	0.43
4:D:72:VAL:HG22	4:D:108:THR:HA	2.01	0.43
1:M:10:VAL:CG2	1:M:157:VAL:HG11	2.49	0.43
1:M:76:LEU:CD1	1:M:228:PHE:CZ	3.02	0.43
1:A:206:GLY:HA3	2:B:55:TRP:CH2	2.54	0.43
2:B:4:LYS:HE3	2:B:4:LYS:N	2.28	0.43
1:M:408:GLU:O	1:M:411:THR:OG1	2.31	0.43
4:P:28:ALA:N	4:P:29:PRO:CD	2.81	0.43
1:A:369:THR:HG23	1:A:374:LEU:O	2.19	0.43
3:C:86:TRP:CD1	4:D:22:MET:HE1	2.47	0.43
1:M:7:LEU:CD2	1:M:187:ALA:HB3	2.49	0.43
2:N:179:TYR:C	2:N:181:GLU:N	2.74	0.43
2:N:211:SER:OG	2:N:219:ASP:HA	2.19	0.43
3:O:86:TRP:HD1	4:P:22:MET:HE1	1.83	0.43
2:B:158:CYS:SG	2:B:160:GLN:HB2	2.59	0.43
1:M:7:LEU:HD11	1:M:411:THR:HG23	2.01	0.43
1:M:127:ALA:C	1:M:128:ALA:O	2.60	0.43
2:N:12:ARG:NH2	2:N:51:LEU:HA	2.34	0.43
2:N:39:ALA:O	2:N:43:ILE:HG12	2.19	0.43
1:A:7:LEU:HD12	1:A:23:ALA:HB1	2.01	0.42
1:A:308:ARG:HE	1:A:308:ARG:HB2	1.68	0.42
1:M:200:ARG:HB2	1:M:456:GLY:C	2.43	0.42
1:M:399:LEU:CD2	5:M:601:FAD:O2P	2.67	0.42
1:M:471:LEU:HD23	1:M:471:LEU:HA	1.93	0.42
2:N:241:LYS:HG3	2:N:242:PRO:N	2.34	0.42
1:A:76:LEU:HD22	1:A:568:VAL:HG21	2.01	0.42
1:A:96:LEU:HD11	1:A:135:MET:HE3	2.01	0.42
1:A:245:GLU:O	1:A:248:ARG:N	2.40	0.42
2:B:7:LYS:HE3	2:B:25:PHE:HB3	2.00	0.42
4:D:13:PHE:HE2	4:D:97:LYS:NZ	2.15	0.42
1:M:200:ARG:NH1	1:M:201:TYR:OH	2.52	0.42
2:N:153:LEU:HB2	9:N:246:SF4:S3	2.59	0.42
4:P:54:VAL:O	4:P:57:PHE:HB3	2.19	0.42
4:P:79:LEU:O	4:P:80:HIS:C	2.62	0.42
2:B:106:MET:O	2:B:109:PHE:HB3	2.19	0.42
3:C:31:THR:O	3:C:34:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:113:ILE:HG12	4:P:113:ILE:HG12	2.01	0.42
1:M:498:PHE:CD2	2:N:103:VAL:HG21	2.54	0.42
3:O:36:VAL:HG23	3:O:37:TRP:N	2.34	0.42
2:B:220:PRO:HG3	9:B:246:SF4:S1	2.58	0.42
1:M:495:SER:O	1:M:499:ASN:HB2	2.20	0.42
3:C:91:PRO:HB2	3:C:105:PRO:HB3	2.01	0.42
1:M:98:LEU:HD22	2:N:132:ASN:ND2	2.35	0.42
2:N:43:ILE:HD13	2:N:47:LEU:HD13	2.00	0.42
1:A:239:SER:OG	1:A:241:ILE:HG13	2.19	0.42
4:D:22:MET:HE2	4:D:22:MET:HA	2.01	0.42
1:M:232:HIS:CE1	1:M:242:LEU:HD11	2.55	0.42
1:M:421:ASN:O	1:M:425:ILE:HG12	2.19	0.42
1:M:493:ASP:OD1	2:N:50:ASP:CB	2.68	0.42
2:N:150:ASN:OD1	2:N:150:ASN:N	2.53	0.42
1:M:45:THR:OG1	5:M:601:FAD:O2A	2.33	0.42
1:M:52:SER:O	1:M:125:TRP:HB2	2.20	0.42
1:M:108:ASP:CG	1:M:110:SER:HG	2.26	0.42
1:M:200:ARG:HD3	1:M:201:TYR:CE1	2.54	0.42
1:M:213:MET:HE3	1:M:380:CYS:HA	2.02	0.42
1:M:360:GLY:HA3	1:M:381:SER:C	2.44	0.42
1:M:544:ASP:O	1:M:548:LEU:HB2	2.20	0.42
1:M:572:THR:O	1:M:574:PRO:HD3	2.19	0.42
2:N:40:LEU:HB3	2:N:53:TYR:CE2	2.55	0.42
1:A:48:ALA:HA	5:A:601:FAD:C6	2.50	0.42
1:M:78:GLU:OE1	1:M:568:VAL:HA	2.19	0.42
1:M:135:MET:HE1	1:M:396:LEU:HB3	2.01	0.42
1:M:223:LEU:HB3	1:M:226:MET:HG3	2.01	0.42
2:N:185:ASP:OD1	2:N:191:ARG:NH2	2.45	0.42
3:O:86:TRP:NE1	4:P:22:MET:HE3	2.34	0.42
1:A:332:CYS:HA	1:A:343:PRO:HG2	2.01	0.42
1:A:442:GLN:NE2	1:A:486:PHE:O	2.53	0.42
1:A:446:GLU:HB2	1:A:488:ARG:O	2.20	0.42
1:M:23:ALA:HB3	1:M:32:ILE:HG21	2.02	0.42
4:P:23:TRP:CD2	4:P:27:ILE:HD13	2.55	0.42
1:A:161:LEU:HD21	1:A:171:VAL:HG23	2.02	0.42
1:A:446:GLU:HB2	1:A:489:VAL:HA	2.02	0.42
4:D:24:SER:O	4:D:28:ALA:HB3	2.20	0.42
2:N:48:ALA:HA	2:N:49:PRO:HD3	1.80	0.42
2:N:204:CYS:HB2	2:N:224:ILE:HG21	2.01	0.42
2:N:235:PHE:HA	4:P:7:ARG:NH2	2.34	0.42
4:P:26:ILE:HG22	4:P:27:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:C	1:A:364:ASP:OD1	2.63	0.41
3:C:63:LEU:CD1	4:D:39:LEU:HD23	2.50	0.41
1:M:38:VAL:HG22	5:M:601:FAD:O2B	2.20	0.41
1:M:260:TYR:CZ	1:M:264:GLN:NE2	2.62	0.41
1:A:205:GLY:HA2	2:B:56:SER:O	2.20	0.41
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.55	0.41
2:B:143:HIS:O	2:B:146:SER:OG	2.33	0.41
1:M:23:ALA:HB1	1:M:32:ILE:HG21	2.02	0.41
1:M:46:VAL:HG23	1:M:133:PHE:HA	2.02	0.41
2:N:151:CYS:SG	2:N:153:LEU:HB2	2.60	0.41
3:O:106:GLU:N	3:O:107:PRO:CD	2.83	0.41
4:P:39:LEU:N	4:P:40:PRO:HD2	2.34	0.41
1:M:238:GLY:HA3	1:M:308:ARG:HD2	2.02	0.41
2:N:61:ILE:O	2:N:61:ILE:HG13	2.19	0.41
4:P:42:GLY:HA2	4:P:44:PHE:CE2	2.54	0.41
1:A:306:THR:CB	1:A:307:PRO:CD	2.95	0.41
1:M:213:MET:CB	1:M:223:LEU:HD21	2.48	0.41
2:N:71:ASN:CG	3:O:18:LYS:HE3	2.46	0.41
2:N:242:PRO:O	2:N:243:ARG:OXT	2.38	0.41
4:P:73:LEU:HB2	4:P:74:PRO:HD3	2.02	0.41
2:B:110:ILE:O	2:B:114:GLU:HG3	2.21	0.41
3:C:65:ASN:O	3:C:69:VAL:HG23	2.20	0.41
1:M:404:ARG:HG2	1:M:408:GLU:OE1	2.21	0.41
2:N:94:ALA:HA	3:O:9:ARG:NH2	2.36	0.41
2:N:216:LYS:HA	2:N:216:LYS:HD3	1.78	0.41
3:O:15:TRP:CZ3	3:O:16:TRP:HA	2.55	0.41
3:O:33:VAL:CB	3:O:34:PRO:CD	2.97	0.41
3:O:49:LEU:HD21	4:P:55:LEU:CA	2.48	0.41
1:A:232:HIS:ND1	1:A:242:LEU:HD11	2.34	0.41
1:A:421:ASN:OD1	1:A:421:ASN:C	2.64	0.41
1:M:170:LEU:HG	1:M:183:ILE:HB	2.02	0.41
1:M:232:HIS:CE1	1:M:244:THR:O	2.73	0.41
1:M:392:GLY:O	1:M:393:SER:CB	2.67	0.41
2:N:68:MET:HE3	2:N:68:MET:HB3	1.96	0.41
3:O:98:VAL:HG23	3:O:103:MET:HB2	2.02	0.41
3:C:72:ASN:HD22	3:C:72:ASN:HA	1.62	0.41
1:M:18:ARG:NH2	1:M:404:ARG:HG3	2.36	0.41
1:M:79:GLN:NE2	1:M:571:THR:N	2.60	0.41
1:M:91:THR:HG22	1:M:92:GLU:OE1	2.21	0.41
1:M:174:ASN:HB3	1:M:177:GLU:HB2	2.01	0.41
1:M:261:ARG:NH1	1:M:272:THR:O	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:4:LYS:HB3	2:N:30:TYR:CE2	2.56	0.41
2:N:149:ILE:CG2	2:N:216:LYS:HG3	2.39	0.41
2:N:235:PHE:C	2:N:235:PHE:HD2	2.26	0.41
1:A:213:MET:HE2	1:A:360:GLY:HA2	2.02	0.41
1:A:442:GLN:NE2	1:A:487:LYS:HA	2.36	0.41
4:D:50:SER:O	4:D:54:VAL:HG23	2.20	0.41
1:M:142:THR:O	1:M:145:GLN:HB3	2.20	0.41
1:M:206:GLY:HA3	2:N:55:TRP:CH2	2.56	0.41
1:M:328:LEU:CB	1:M:331:ILE:HD12	2.49	0.41
3:O:18:LYS:CE	3:O:19:LEU:HD22	2.47	0.41
1:A:10:VAL:CB	1:A:190:MET:HE3	2.51	0.41
1:A:13:GLY:O	1:A:14:GLY:C	2.63	0.41
1:A:147:PRO:HD2	1:A:148:GLN:OE1	2.21	0.41
1:A:322:LYS:HE3	1:A:322:LYS:CA	2.48	0.41
2:B:216:LYS:HA	2:B:216:LYS:HD3	1.91	0.41
3:C:47:PHE:HA	3:C:50:LYS:HB2	2.03	0.41
3:C:56:TRP:O	3:C:60:VAL:HG23	2.20	0.41
3:C:106:GLU:HB2	3:C:107:PRO:HD3	2.02	0.41
4:D:57:PHE:O	4:D:60:SER:OG	2.32	0.41
1:M:57:GLN:NE2	1:M:122:GLU:O	2.47	0.41
1:M:243:MET:O	1:M:244:THR:CG2	2.68	0.41
1:M:315:ASP:CG	1:M:318:HIS:HE1	2.28	0.41
1:M:324:LEU:O	1:M:328:LEU:N	2.50	0.41
1:M:492:THR:HG21	2:N:49:PRO:HG2	2.03	0.41
2:N:116:ILE:HD11	2:N:168:ILE:HD12	2.03	0.41
2:N:159:PRO:CG	2:N:207:VAL:HG21	2.31	0.41
4:P:23:TRP:CD1	4:P:23:TRP:C	2.99	0.41
1:A:141:GLN:NE2	2:B:179:TYR:OH	2.54	0.41
1:A:445:GLY:H	1:A:490:ARG:HB2	1.86	0.41
2:B:40:LEU:HA	2:B:40:LEU:HD23	1.82	0.41
1:M:44:HIS:H	1:M:207:ILE:HD11	1.86	0.41
3:O:50:LYS:CG	4:P:118:ILE:HA	2.51	0.41
2:B:6:LEU:HD23	2:B:8:ILE:CG1	2.51	0.40
1:M:574:PRO:HA	1:M:575:PRO:HD2	1.99	0.40
2:N:236:LEU:HD22	2:N:237:ILE:HD12	2.01	0.40
3:O:16:TRP:HA	3:O:22:TYR:HB3	2.03	0.40
3:O:25:TYR:HD1	3:O:28:ARG:NH2	2.19	0.40
1:A:15:ALA:HB2	1:A:399:LEU:CD2	2.50	0.40
1:A:92:GLU:OE1	1:A:404:ARG:HD2	2.22	0.40
1:A:319:LEU:O	1:A:323:LYS:HB2	2.21	0.40
1:A:431:GLY:O	1:A:435:ARG:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:TYR:CD1	2:B:142:TYR:C	2.98	0.40
2:B:198:GLN:NE2	4:D:10:GLU:HG3	2.11	0.40
3:C:56:TRP:CD1	4:D:51:TYR:HB2	2.57	0.40
4:D:99:VAL:HG12	4:D:100:PHE:N	2.36	0.40
1:M:224:ARG:HG3	1:M:382:SER:CB	2.51	0.40
3:O:50:LYS:HG2	4:P:118:ILE:HA	2.03	0.40
2:B:9:GLU:CD	2:B:89:LYS:HG3	2.47	0.40
3:C:39:SER:OG	4:D:71:ILE:O	2.32	0.40
1:M:503:LEU:O	1:M:507:GLU:HG3	2.21	0.40
3:O:19:LEU:HA	3:O:20:PRO:HD3	1.90	0.40
2:B:112:SER:HA	4:D:1:ILE:HD11	2.03	0.40
1:M:522:ALA:HB1	1:M:532:HIS:CE1	2.56	0.40
2:N:113:LEU:HD22	2:N:175:LEU:HD22	2.03	0.40
3:O:45:GLY:HA3	3:O:59:PHE:CZ	2.57	0.40
2:B:116:ILE:CD1	2:B:172:ALA:O	2.69	0.40
2:B:242:PRO:HD2	2:B:243:ARG:HG2	2.03	0.40
3:C:128:LEU:HD22	4:D:45:PRO:HD2	2.02	0.40
1:M:88:HIS:HB2	1:M:401:VAL:CG1	2.51	0.40
1:M:192:THR:OG1	5:M:601:FAD:N7A	2.55	0.40
1:M:328:LEU:HD22	1:M:331:ILE:HD11	1.99	0.40
2:N:180:ASN:OD1	2:N:191:ARG:NH1	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	575/577 (100%)	551 (96%)	23 (4%)	1 (0%)	43	72
1	M	575/577 (100%)	546 (95%)	24 (4%)	5 (1%)	14	41
2	B	241/243 (99%)	225 (93%)	15 (6%)	1 (0%)	30	60
2	N	241/243 (99%)	227 (94%)	12 (5%)	2 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	128/130 (98%)	124 (97%)	3 (2%)	1 (1%)	16	44
3	O	128/130 (98%)	118 (92%)	10 (8%)	0	100	100
4	D	117/119 (98%)	113 (97%)	4 (3%)	0	100	100
4	P	117/119 (98%)	104 (89%)	12 (10%)	1 (1%)	14	41
All	All	2122/2138 (99%)	2008 (95%)	103 (5%)	11 (0%)	24	55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	65	CYS
1	M	1	GLN
1	M	244	THR
4	P	46	GLY
1	M	128	ALA
3	C	18	LYS
1	M	59	HIS
2	N	101	ASP
2	B	56	SER
1	M	444	GLY
1	A	320	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	460/460 (100%)	429 (93%)	31 (7%)	15	42
1	M	460/460 (100%)	413 (90%)	47 (10%)	7	23
2	B	205/205 (100%)	188 (92%)	17 (8%)	10	32
2	N	205/205 (100%)	179 (87%)	26 (13%)	4	15
3	C	111/111 (100%)	98 (88%)	13 (12%)	5	18
3	O	111/111 (100%)	97 (87%)	14 (13%)	4	15
4	D	97/97 (100%)	88 (91%)	9 (9%)	8	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	P	97/97 (100%)	89 (92%)	8 (8%)	10	33
All	All	1746/1746 (100%)	1581 (90%)	165 (10%)	8	26

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	18	ARG
1	A	27	ASN
1	A	42	ARG
1	A	59	HIS
1	A	74	ASP
1	A	76	LEU
1	A	91	THR
1	A	116	PHE
1	A	120	LYS
1	A	122	GLU
1	A	129	ASP
1	A	170	LEU
1	A	175	MET
1	A	182	GLN
1	A	190	MET
1	A	209	THR
1	A	253	ILE
1	A	287	ARG
1	A	310	ASP
1	A	322	LYS
1	A	325	HIS
1	A	391	LEU
1	A	411	THR
1	A	489	VAL
1	A	490	ARG
1	A	495	SER
1	A	497	VAL
1	A	536	ASP
1	A	541	GLU
1	A	560	THR
2	B	4	LYS
2	B	19	THR
2	B	27	GLU
2	B	46	ASN
2	B	65	CYS

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Mol	Chain	Res	Type
2	B	78	LYS
2	B	81	LEU
2	B	85	THR
2	B	113	LEU
2	B	116	ILE
2	B	128	ASP
2	B	154	CYS
2	B	210	CYS
2	B	236	LEU
2	B	237	ILE
2	B	239	THR
2	B	243	ARG
3	C	2	THR
3	C	5	LYS
3	C	19	LEU
3	C	27	LEU
3	C	37	TRP
3	C	39	SER
3	C	50	LYS
3	C	54	GLU
3	C	76	LEU
3	C	84	LYS
3	C	85	THR
3	C	92	LYS
3	C	126	VAL
4	D	9	ASP
4	D	12	VAL
4	D	22	MET
4	D	47	ASP
4	D	62	ILE
4	D	64	ARG
4	D	67	LEU
4	D	99	VAL
4	D	118	ILE
1	M	18	ARG
1	M	27	ASN
1	M	32	ILE
1	M	57	GLN
1	M	63	GLU
1	M	76	LEU
1	M	86	VAL
1	M	91	THR

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Mol	Chain	Res	Type
1	M	93	MET
1	M	97	GLU
1	M	110	SER
1	M	143	SER
1	M	148	GLN
1	M	149	ILE
1	M	152	PHE
1	M	164	ASP
1	M	168	ARG
1	M	180	LEU
1	M	181	VAL
1	M	192	THR
1	M	209	THR
1	M	224	ARG
1	M	243	MET
1	M	291	SER
1	M	299	ARG
1	M	318	HIS
1	M	348	ILE
1	M	350	VAL
1	M	393	SER
1	M	394	ASN
1	M	399	LEU
1	M	413	ARG
1	M	421	ASN
1	M	425	ILE
1	M	475	THR
1	M	484	GLU
1	M	489	VAL
1	M	491	ILE
1	M	494	THR
1	M	496	SER
1	M	505	THR
1	M	506	ILE
1	M	517	CYS
1	M	537	GLU
1	M	545	VAL
1	M	555	ARG
1	M	572	THR
2	N	5	ASN
2	N	19	THR
2	N	51	LEU

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Mol	Chain	Res	Type
2	N	65	CYS
2	N	69	VAL
2	N	82	ARG
2	N	100	ARG
2	N	112	SER
2	N	126	THR
2	N	128	ASP
2	N	133	ILE
2	N	138	GLN
2	N	150	ASN
2	N	154	CYS
2	N	164	ASN
2	N	173	ILE
2	N	178	ARG
2	N	181	GLU
2	N	185	ASP
2	N	189	LYS
2	N	226	GLN
2	N	233	LYS
2	N	237	ILE
2	N	239	THR
2	N	240	LEU
2	N	241	LYS
3	O	2	THR
3	O	9	ARG
3	O	12	THR
3	O	19	LEU
3	O	31	THR
3	O	39	SER
3	O	40	ILE
3	O	43	ILE
3	O	50	LYS
3	O	54	GLU
3	O	68	ILE
3	O	70	ILE
3	O	98	VAL
3	O	117	VAL
4	P	1	ILE
4	P	9	ASP
4	P	22	MET
4	P	37	ILE
4	P	47	ASP

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Mol	Chain	Res	Type
4	P	60	SER
4	P	115	VAL
4	P	117	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	88	HIS
1	A	141	GLN
1	A	166	HIS
1	A	204	ASN
1	A	230	GLN
1	A	279	ASN
1	A	292	GLN
1	A	428	GLN
1	A	442	GLN
2	B	5	ASN
2	B	46	ASN
2	B	150	ASN
2	B	225	GLN
3	C	51	ASN
3	C	72	ASN
4	D	59	GLN
4	D	92	HIS
1	M	27	ASN
1	M	59	HIS
1	M	79	GLN
1	M	134	HIS
1	M	137	HIS
1	M	145	GLN
1	M	148	GLN
1	M	166	HIS
1	M	204	ASN
1	M	264	GLN
1	M	442	GLN
1	M	447	ASN
1	M	473	GLN
1	M	546	ASN
1	M	550	HIS
2	N	5	ASN
2	N	14	ASN

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Mol	Chain	Res	Type
2	N	22	HIS
2	N	71	ASN
2	N	95	ASN
2	N	108	HIS
2	N	132	ASN
2	N	160	GLN
4	P	4	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	$\# Z > 2$
9	SF4	N	246	2	0,12,12	-	-	-		
8	F3S	B	245	2	0,9,9	-	-	-		
5	FAD	A	601	-	58,58,58	1.86	12 (20%)	85,89,89	1.87	28 (32%)
5	FAD	M	601	-	58,58,58	2.32	11 (18%)	85,89,89	1.78	23 (27%)
9	SF4	B	246	2	0,12,12	-	-	-		
8	F3S	N	245	2	0,9,9	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	FES	B	244	2	0,4,4	-	-	-		
7	FES	N	244	2	0,4,4	-	-	-		
6	FUM	A	577	-	7,7,7	3.38	4 (57%)	8,8,8	1.50	1 (12%)

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
9	SF4	N	246	2	-	-	0/6/5/5
8	F3S	B	245	2	-	-	0/3/3/3
5	FAD	A	601	-	-	5/34/50/50	0/6/6/6
5	FAD	M	601	-	-	6/34/50/50	0/6/6/6
9	SF4	B	246	2	-	-	0/6/5/5
8	F3S	N	245	2	-	-	0/3/3/3
7	FES	B	244	2	-	-	0/1/1/1
7	FES	N	244	2	-	-	0/1/1/1
6	FUM	A	577	-	-	2/5/5/5	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	601	FAD	P-O3P	9.60	1.69	1.59
5	A	601	FAD	O2B-C2B	-9.56	1.19	1.43
5	M	601	FAD	O2B-C2B	-8.82	1.21	1.43
5	M	601	FAD	PA-O3P	6.48	1.66	1.59
6	A	577	FUM	C5-C4	6.40	1.52	1.33
6	A	577	FUM	C4-C	-5.11	1.35	1.48
5	M	601	FAD	C4X-N5	3.72	1.38	1.30
5	A	601	FAD	C4X-N5	3.60	1.38	1.30
5	M	601	FAD	C2B-C3B	3.38	1.62	1.53
5	A	601	FAD	C2B-C1B	3.20	1.63	1.53
5	A	601	FAD	C10-N10	3.10	1.44	1.37
5	M	601	FAD	C10-N10	3.01	1.43	1.37
5	A	601	FAD	C8A-N7A	2.89	1.37	1.31
5	M	601	FAD	C2B-C1B	2.66	1.61	1.53
5	M	601	FAD	C8A-N7A	2.56	1.36	1.31
5	A	601	FAD	C10-N1	2.52	1.38	1.33
5	A	601	FAD	C2B-C3B	2.51	1.60	1.53
5	M	601	FAD	O2-C2	2.48	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	FAD	P-O3P	2.31	1.62	1.59
5	A	601	FAD	O3B-C3B	2.27	1.48	1.43
5	A	601	FAD	C8A-N9A	-2.25	1.33	1.37
5	A	601	FAD	C9A-N10	2.19	1.45	1.41
6	A	577	FUM	OXT-C	-2.19	1.24	1.30
6	A	577	FUM	O8-C6	-2.10	1.25	1.30
5	M	601	FAD	C9A-N10	2.07	1.44	1.41
5	A	601	FAD	PA-O2A	-2.02	1.46	1.55
5	M	601	FAD	C4A-N9A	-2.01	1.33	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	FAD	N3A-C2A-N1A	-5.19	120.72	128.58
5	M	601	FAD	C2B-C1B-N9A	-4.39	102.39	113.30
5	A	601	FAD	O3'-C3'-C2'	-4.25	99.28	108.93
5	A	601	FAD	N3A-C2A-N1A	-4.22	122.20	128.58
5	A	601	FAD	C5A-C4A-N3A	-3.81	121.47	126.72
5	M	601	FAD	N9A-C8A-N7A	-3.68	108.71	113.94
5	A	601	FAD	C5X-N5-C4X	3.56	123.85	118.09
5	M	601	FAD	C3B-C2B-C1B	-3.55	94.75	101.46
5	A	601	FAD	C3B-C2B-C1B	-3.41	95.01	101.46
5	M	601	FAD	C5A-C4A-N3A	-3.41	122.02	126.72
5	A	601	FAD	C4-N3-C2	-3.33	119.72	125.64
5	A	601	FAD	C4X-C4-N3	3.30	121.66	113.25
5	M	601	FAD	C4X-C4-N3	3.30	121.64	113.25
5	M	601	FAD	C4-C4X-N5	3.18	122.60	118.21
5	M	601	FAD	C9A-C5X-N5	-3.16	119.10	122.45
5	A	601	FAD	C9A-C5X-N5	-3.16	119.11	122.45
5	A	601	FAD	O4'-C4'-C5'	-3.15	103.03	109.99
5	M	601	FAD	C4-N3-C2	-3.15	120.06	125.64
5	A	601	FAD	C4A-N9A-C8A	3.10	108.99	105.74
5	M	601	FAD	C4A-N9A-C8A	3.09	108.98	105.74
5	M	601	FAD	C2A-N3A-C4A	3.04	119.26	111.83
5	A	601	FAD	N9A-C8A-N7A	-3.00	109.68	113.94
5	A	601	FAD	C10-N1-C2	2.98	123.30	116.85
5	A	601	FAD	C4X-C10-N1	-2.96	117.33	124.59
6	A	577	FUM	C4-C5-C6	-2.89	112.36	127.05
5	A	601	FAD	O2'-C2'-C3'	-2.87	102.54	109.25
5	M	601	FAD	C5X-N5-C4X	2.78	122.58	118.09
5	A	601	FAD	C4A-C5A-N7A	-2.72	107.47	110.58
5	M	601	FAD	C10-N1-C2	2.70	122.70	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	C2A-N3A-C4A	2.69	118.40	111.83
5	A	601	FAD	O4-C4-C4X	-2.63	119.59	126.53
5	M	601	FAD	O2B-C2B-C3B	2.61	120.17	111.82
5	A	601	FAD	C4-C4X-N5	2.55	121.73	118.21
5	A	601	FAD	C1'-C2'-C3'	2.53	116.52	109.66
5	A	601	FAD	C10-C4X-N5	-2.48	119.75	124.81
5	M	601	FAD	O2B-C2B-C1B	-2.41	101.79	110.10
5	M	601	FAD	O4-C4-N3	-2.39	115.61	120.11
5	M	601	FAD	C4A-N9A-C1B	-2.36	121.10	126.63
5	A	601	FAD	C2B-C1B-N9A	-2.35	107.46	113.30
5	A	601	FAD	N3A-C4A-N9A	2.34	131.14	127.17
5	A	601	FAD	C6-C5X-C9A	2.32	122.23	119.05
5	A	601	FAD	C9-C8-C7	2.26	123.01	119.69
5	A	601	FAD	O4B-C4B-C3B	2.25	109.62	105.15
5	M	601	FAD	C10-C4X-N5	-2.25	120.22	124.81
5	M	601	FAD	C5A-N7A-C8A	2.21	106.92	103.45
5	M	601	FAD	C4A-C5A-N7A	-2.20	108.06	110.58
5	A	601	FAD	C4A-N9A-C1B	-2.17	121.55	126.63
5	M	601	FAD	O3P-PA-O1A	2.14	117.15	110.70
5	A	601	FAD	O3P-P-O1P	-2.13	104.30	110.70
5	A	601	FAD	O3B-C3B-C4B	2.10	117.12	111.08
5	M	601	FAD	N3A-C4A-N9A	2.05	130.66	127.17
5	M	601	FAD	C4X-C10-N1	-2.05	119.57	124.59

There are no chirality outliers.

All (13) torsion outliers are listed below:

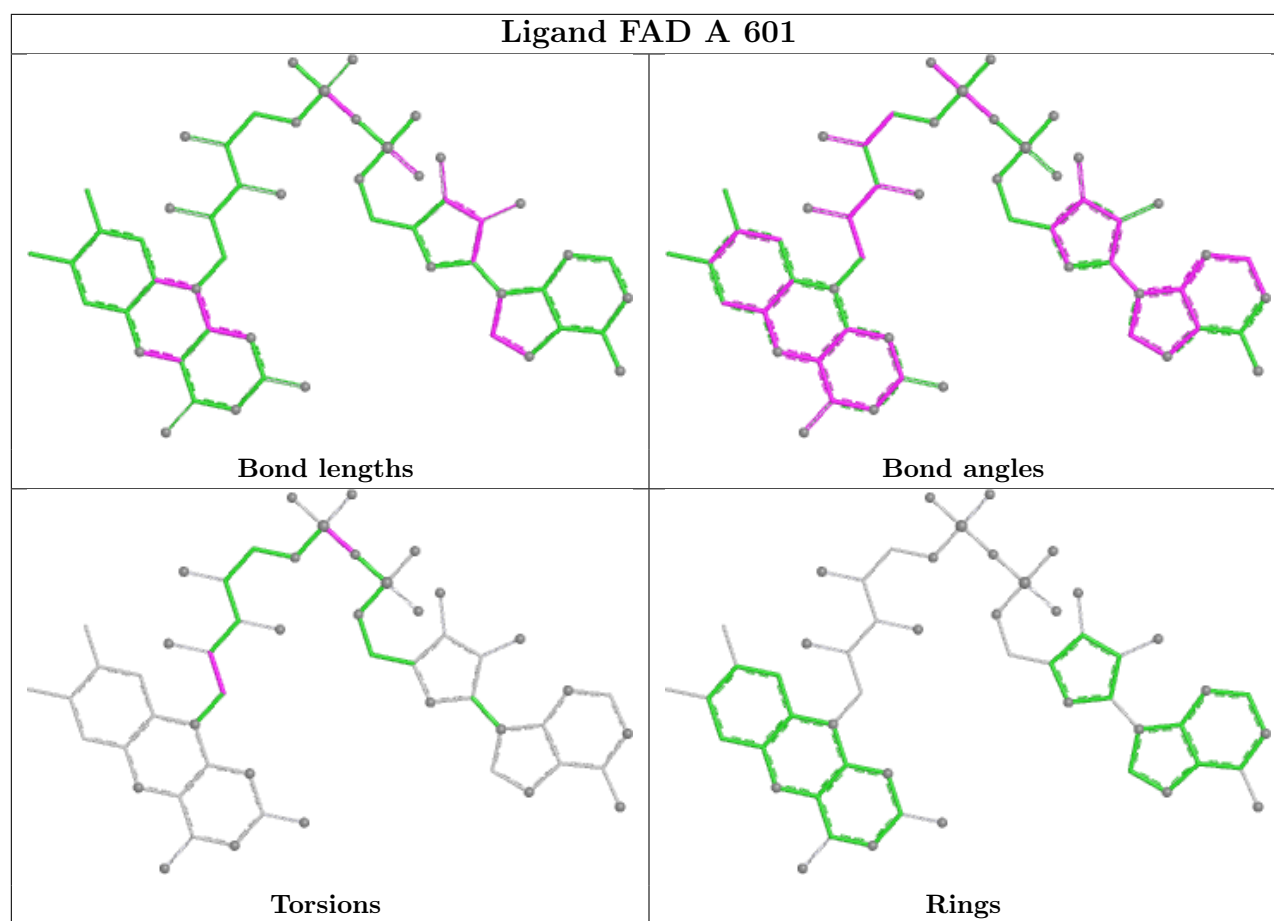
Mol	Chain	Res	Type	Atoms
5	A	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	N10-C1'-C2'-C3'
6	A	577	FUM	C4-C5-C6-O7
6	A	577	FUM	C4-C5-C6-O8
5	M	601	FAD	P-O3P-PA-O1A
5	A	601	FAD	PA-O3P-P-O5'
5	M	601	FAD	PA-O3P-P-O5'
5	M	601	FAD	P-O3P-PA-O2A
5	M	601	FAD	O4'-C4'-C5'-O5'
5	A	601	FAD	N10-C1'-C2'-C3'
5	A	601	FAD	PA-O3P-P-O1P
5	A	601	FAD	PA-O3P-P-O2P

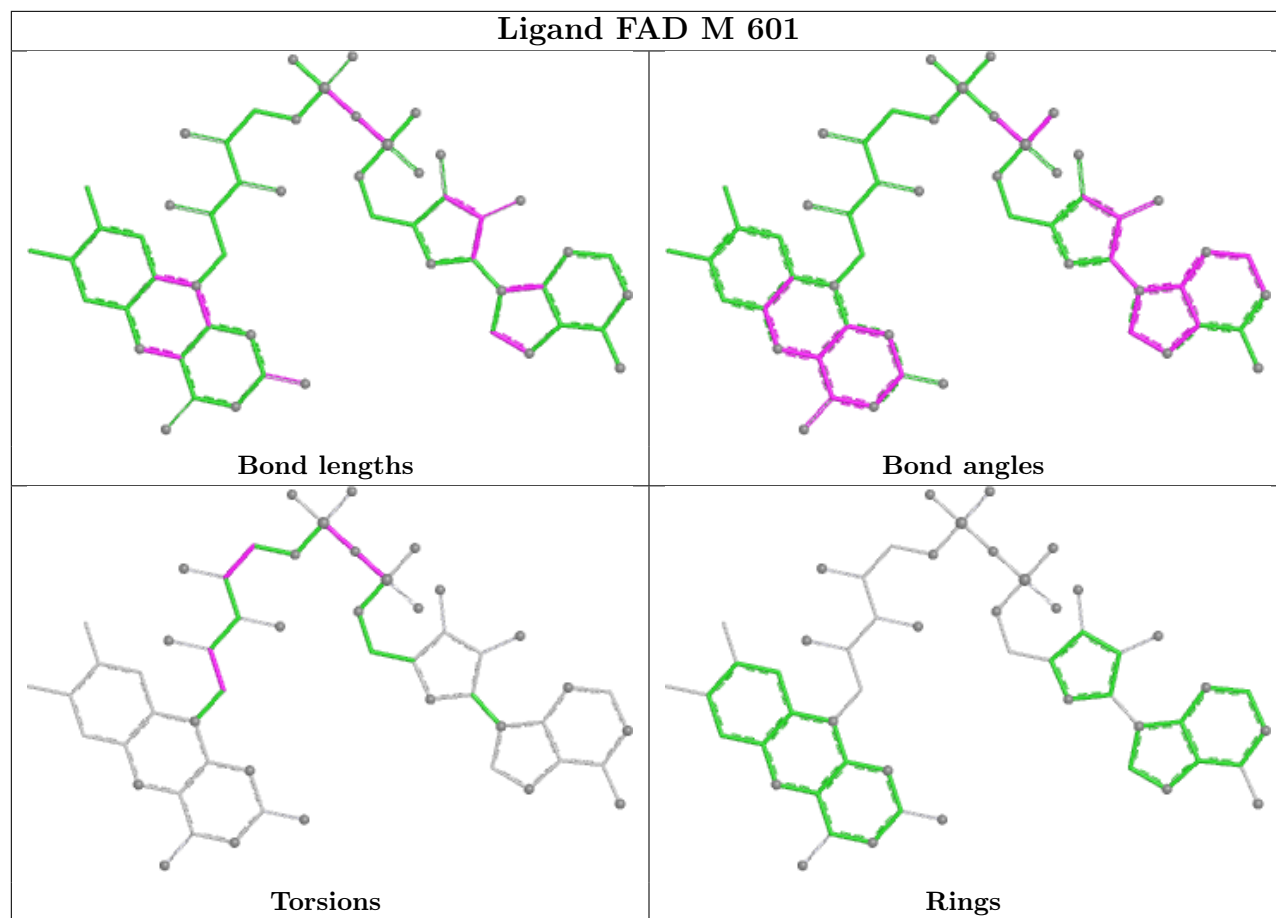
There are no ring outliers.

8 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	246	SF4	5	0
8	B	245	F3S	4	0
5	A	601	FAD	13	0
5	M	601	FAD	24	0
9	B	246	SF4	11	0
8	N	245	F3S	1	0
7	B	244	FES	3	0
7	N	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	577/577 (100%)	0.16	16 (2%) 55 45	38, 56, 93, 138	0
1	M	577/577 (100%)	2.90	431 (74%) 0 0	68, 160, 235, 266	0
2	B	243/243 (100%)	0.64	18 (7%) 20 15	39, 71, 104, 151	0
2	N	243/243 (100%)	2.03	121 (49%) 0 0	64, 131, 202, 235	0
3	C	130/130 (100%)	0.37	1 (0%) 82 75	51, 74, 110, 136	0
3	O	130/130 (100%)	0.88	18 (13%) 6 5	60, 93, 154, 215	0
4	D	119/119 (100%)	0.43	5 (4%) 40 32	55, 76, 107, 144	0
4	P	119/119 (100%)	1.00	20 (16%) 4 3	64, 86, 144, 224	0
All	All	2138/2138 (100%)	1.28	630 (29%) 1 1	38, 88, 208, 266	0

All (630) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	407	GLY	9.1
1	M	8	ALA	7.2
1	M	188	VAL	7.0
1	M	411	THR	6.5
1	M	17	LEU	6.5
1	M	189	VAL	6.4
1	M	565	TYR	6.3
1	M	209	THR	6.2
1	M	165	GLY	6.0
1	M	186	ASN	6.0
1	M	167	VAL	6.0
1	M	386	HIS	5.9
1	M	375	PHE	5.7
1	M	180	LEU	5.7
1	M	172	ALA	5.7
1	M	377	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	M	396	LEU	5.5
1	M	373	GLY	5.4
1	M	125	TRP	5.4
1	M	492	THR	5.4
1	M	220	GLY	5.3
1	M	362	GLU	5.3
1	M	170	LEU	5.3
1	M	497	VAL	5.3
1	M	89	CYS	5.3
1	M	207	ILE	5.2
1	M	551	THR	5.2
1	M	129	ASP	5.2
1	M	295	TRP	5.2
1	M	80	ASP	5.1
2	N	133	ILE	5.1
1	M	548	LEU	5.1
1	M	424	ALA	5.1
1	M	10	VAL	5.1
1	M	116	PHE	5.1
1	M	158	LEU	5.1
1	M	219	HIS	5.1
1	M	491	ILE	5.1
1	M	14	GLY	5.1
1	M	169	GLY	5.1
1	M	486	PHE	5.0
4	P	1	ILE	5.0
1	M	162	VAL	5.0
1	M	385	LEU	5.0
1	M	552	LEU	5.0
1	M	99	TRP	5.0
1	M	187	ALA	4.9
2	N	56	SER	4.9
2	N	124	SER	4.9
1	M	221	VAL	4.9
1	M	402	PHE	4.9
1	M	183	ILE	4.9
1	M	361	ILE	4.9
1	M	214	GLY	4.8
2	N	98	ILE	4.8
1	M	33	ALA	4.8
1	M	39	TYR	4.7
1	M	192	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	M	76	LEU	4.7
1	M	376	ALA	4.7
1	M	400	VAL	4.7
1	M	374	LEU	4.6
1	M	436	LEU	4.6
1	M	405	LEU	4.6
1	M	210	GLY	4.6
1	M	287	ARG	4.6
1	M	330	PHE	4.5
1	M	32	ILE	4.5
1	M	228	PHE	4.5
1	M	134	HIS	4.5
1	M	211	ASP	4.5
1	M	383	VAL	4.5
1	M	31	LYS	4.5
1	M	117	GLY	4.5
1	M	356	TYR	4.5
2	N	119	TYR	4.5
1	M	191	ALA	4.5
2	N	114	GLU	4.4
1	M	144	LEU	4.4
1	M	494	THR	4.4
1	M	553	ALA	4.4
1	M	498	PHE	4.4
2	N	46	ASN	4.4
1	M	224	ARG	4.4
1	M	137	HIS	4.4
2	N	237	ILE	4.4
1	M	439	LEU	4.3
2	N	63	GLY	4.3
1	M	42	ARG	4.3
1	M	378	GLY	4.3
1	M	27	ASN	4.3
2	N	123	ASN	4.3
1	M	9	ILE	4.3
1	M	506	ILE	4.3
1	M	90	PRO	4.3
1	M	440	VAL	4.3
1	M	95	GLN	4.3
1	M	215	MET	4.3
1	M	489	VAL	4.3
1	M	425	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	M	161	LEU	4.2
1	M	145	GLN	4.2
1	M	85	PHE	4.2
1	M	38	VAL	4.2
1	M	6	ASP	4.2
1	M	390	ARG	4.2
1	M	171	VAL	4.2
1	M	557	ALA	4.2
1	M	484	GLU	4.2
1	M	93	MET	4.2
1	M	409	GLN	4.1
1	M	447	ASN	4.1
1	M	448	TRP	4.1
1	M	504	TYR	4.1
1	M	26	ALA	4.1
1	M	445	GLY	4.1
1	M	564	GLU	4.1
1	M	86	VAL	4.1
2	N	26	TYR	4.1
1	M	395	SER	4.1
1	M	414	ALA	4.1
1	M	496	SER	4.1
1	M	66	PHE	4.1
1	M	370	ARG	4.1
1	M	413	ARG	4.1
1	M	15	ALA	4.1
1	M	199	TYR	4.1
1	M	34	LEU	4.0
1	M	108	ASP	4.0
1	M	81	VAL	4.0
1	M	12	ALA	4.0
1	M	3	PHE	4.0
1	M	410	ALA	4.0
2	N	48	ALA	4.0
1	M	173	MET	4.0
1	M	503	LEU	4.0
1	M	575	PRO	4.0
2	N	184	ARG	4.0
1	M	367	CYS	4.0
1	M	40	PRO	4.0
1	M	222	PRO	4.0
1	M	429	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
4	D	118	ILE	4.0
1	M	205	GLY	4.0
1	M	406	ALA	3.9
1	M	563	LEU	3.9
1	M	198	VAL	3.9
1	M	487	LYS	3.9
4	P	5	PRO	3.9
1	M	561	THR	3.9
1	M	559	GLY	3.9
1	M	88	HIS	3.9
1	M	20	ALA	3.9
2	N	19	THR	3.9
1	M	135	MET	3.9
1	M	102	PRO	3.9
2	B	243	ARG	3.9
1	M	323	LYS	3.8
1	M	245	GLU	3.8
1	M	566	SER	3.8
1	M	182	GLN	3.8
1	M	184	ARG	3.8
2	N	108	HIS	3.8
1	M	388	ALA	3.8
1	M	554	PHE	3.8
3	O	6	PRO	3.8
1	M	252	GLY	3.8
1	M	371	ILE	3.8
2	N	240	LEU	3.8
4	D	117	THR	3.8
1	M	218	SER	3.7
1	M	65	HIS	3.7
1	M	164	ASP	3.7
1	M	510	HIS	3.7
1	M	212	GLY	3.7
1	M	359	GLY	3.7
1	M	403	GLY	3.7
1	M	154	GLU	3.7
3	O	8	VAL	3.7
2	N	117	LYS	3.7
2	N	1	ALA	3.7
2	N	55	TRP	3.7
2	N	198	GLN	3.7
1	M	96	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	M	482	LEU	3.7
1	M	544	ASP	3.7
2	N	101	ASP	3.7
1	M	206	GLY	3.7
1	M	44	HIS	3.7
1	M	274	LEU	3.7
1	M	502	LEU	3.7
1	M	508	LEU	3.7
1	M	567	ASP	3.7
1	M	366	ASN	3.7
1	M	444	GLY	3.7
1	M	63	GLU	3.7
1	M	568	VAL	3.7
2	N	110	ILE	3.7
1	M	550	HIS	3.6
1	A	129	ASP	3.6
1	M	51	GLY	3.6
2	N	43	ILE	3.6
1	M	69	THR	3.6
1	M	107	PRO	3.6
1	M	223	LEU	3.6
1	M	41	MET	3.6
1	M	495	SER	3.6
2	N	127	ALA	3.6
1	M	149	ILE	3.6
1	M	7	LEU	3.6
1	M	427	ALA	3.6
1	M	384	GLY	3.6
1	M	49	GLU	3.6
1	A	324	LEU	3.6
4	P	0	MET	3.6
1	M	77	CYS	3.5
1	M	52	SER	3.5
2	N	130	GLY	3.5
1	M	82	VAL	3.5
1	M	0	MET	3.5
2	N	225	GLN	3.5
1	M	399	LEU	3.5
1	M	394	ASN	3.5
3	O	14	THR	3.5
2	N	54	ARG	3.5
1	M	152	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
2	N	23	SER	3.5
2	N	53	TYR	3.5
2	N	11	VAL	3.5
1	M	91	THR	3.5
1	M	419	ASN	3.5
1	M	421	ASN	3.5
1	M	55	VAL	3.4
1	M	101	CYS	3.4
1	M	573	LEU	3.4
2	N	16	GLU	3.4
1	M	185	ALA	3.4
1	M	4	GLN	3.4
1	M	35	ILE	3.4
2	N	120	ILE	3.4
2	N	109	PHE	3.4
1	M	213	MET	3.4
1	M	569	LYS	3.4
1	M	181	VAL	3.4
1	M	138	THR	3.4
2	B	46	ASN	3.4
1	M	570	ILE	3.4
4	P	47	ASP	3.4
1	M	156	PHE	3.4
1	M	176	MET	3.4
1	M	446	GLU	3.4
1	M	87	HIS	3.4
2	N	192	MET	3.4
1	M	547	PHE	3.4
2	N	121	ILE	3.3
2	N	51	LEU	3.3
1	M	84	TYR	3.3
1	M	193	GLY	3.3
1	M	372	LYS	3.3
2	N	238	ALA	3.3
1	M	457	LEU	3.3
1	M	452	ARG	3.3
2	N	150	ASN	3.3
1	M	398	GLU	3.3
1	M	549	LYS	3.3
1	M	415	ALA	3.3
1	M	519	ALA	3.3
4	P	62	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	2	THR	3.3
1	M	157	VAL	3.3
1	M	572	THR	3.3
1	M	251	GLY	3.3
1	M	78	GLU	3.3
1	M	278	LYS	3.3
1	M	160	ILE	3.3
1	M	166	HIS	3.3
2	N	113	LEU	3.3
2	N	134	GLN	3.3
1	M	37	LYS	3.2
1	M	490	ARG	3.2
2	B	19	THR	3.2
2	N	41	GLY	3.2
3	O	16	TRP	3.2
1	M	417	ALA	3.2
1	M	428	GLN	3.2
1	M	505	THR	3.2
1	M	333	GLU	3.2
1	M	347	PRO	3.2
2	N	64	SER	3.2
1	M	53	ALA	3.2
1	M	328	LEU	3.2
2	N	102	LEU	3.2
2	N	112	SER	3.2
2	N	39	ALA	3.2
1	A	325	HIS	3.2
1	M	141	GLN	3.2
1	M	11	GLY	3.2
1	M	178	GLY	3.2
1	M	511	GLY	3.2
1	M	363	THR	3.2
1	M	460	GLU	3.2
2	N	27	GLU	3.2
2	B	210	CYS	3.1
2	N	100	ARG	3.1
1	M	111	VAL	3.1
1	M	545	VAL	3.1
1	M	79	GLN	3.1
1	M	175	MET	3.1
2	N	236	LEU	3.1
2	N	146	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	229	VAL	3.1
1	M	25	GLN	3.1
1	M	387	GLY	3.1
1	M	451	ILE	3.1
1	M	247	CYS	3.1
2	N	105	ASP	3.1
4	D	9	ASP	3.1
1	M	75	TRP	3.1
2	N	106	MET	3.1
1	M	420	GLY	3.1
1	M	438	ASP	3.0
1	M	196	GLY	3.0
1	M	422	GLU	3.0
1	M	535	LEU	3.0
1	M	159	ASP	3.0
1	A	320	GLY	3.0
1	A	490	ARG	3.0
1	M	50	GLY	3.0
1	M	332	CYS	3.0
1	M	392	GLY	3.0
1	M	275	GLY	3.0
1	M	526	LYS	3.0
1	M	279	ASN	3.0
1	M	408	GLU	3.0
1	M	45	THR	3.0
1	M	19	ALA	3.0
1	M	133	PHE	3.0
2	N	47	LEU	3.0
1	M	389	ASN	3.0
2	N	232	SER	3.0
4	P	60	SER	3.0
4	P	93	VAL	3.0
4	P	46	GLY	2.9
1	M	23	ALA	2.9
1	M	71	ALA	2.9
2	N	193	ALA	2.9
1	M	514	VAL	2.9
1	M	130	LYS	2.9
1	M	476	ILE	2.9
2	N	40	LEU	2.9
1	M	190	MET	2.9
1	M	146	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	380	CYS	2.9
3	O	1	THR	2.9
1	M	248	ARG	2.9
1	M	1	GLN	2.9
2	N	42	TYR	2.9
1	M	507	GLU	2.9
1	M	345	LYS	2.9
2	N	52	SER	2.9
1	M	200	ARG	2.9
1	M	416	THR	2.9
1	M	525	ARG	2.9
1	M	391	LEU	2.9
1	M	16	GLY	2.9
1	M	103	TRP	2.9
2	N	194	GLN	2.9
2	N	142	TYR	2.9
1	M	450	LYS	2.9
1	A	576	ALA	2.9
1	M	48	ALA	2.9
1	M	163	ASP	2.9
1	M	195	ALA	2.9
2	N	103	VAL	2.9
2	N	234	ASP	2.9
1	M	168	ARG	2.9
4	P	7	ARG	2.9
4	D	0	MET	2.8
1	M	393	SER	2.8
1	M	324	LEU	2.8
1	M	471	LEU	2.8
1	M	463	CYS	2.8
1	M	459	MET	2.8
1	M	56	ALA	2.8
1	M	488	ARG	2.8
1	A	319	LEU	2.8
1	M	104	SER	2.8
4	P	6	LYS	2.8
2	N	97	PRO	2.8
2	N	190	GLU	2.8
1	M	316	LEU	2.8
1	M	465	ILE	2.8
2	N	131	THR	2.8
1	M	28	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	574	PRO	2.8
1	M	250	GLU	2.8
1	M	426	GLU	2.8
2	B	16	GLU	2.8
1	M	555	ARG	2.8
2	N	6	LEU	2.8
2	N	37	LEU	2.8
1	M	325	HIS	2.8
1	M	120	LYS	2.8
1	M	437	LYS	2.8
1	M	562	ARG	2.7
2	N	22	HIS	2.7
1	M	560	THR	2.7
1	M	456	GLY	2.7
1	M	62	PHE	2.7
1	M	515	ALA	2.7
2	N	96	PHE	2.7
3	O	129	TYR	2.7
1	M	179	THR	2.7
2	N	203	SER	2.7
1	M	379	GLU	2.7
1	M	30	ALA	2.7
1	M	139	LEU	2.7
1	M	449	ALA	2.7
1	M	318	HIS	2.7
2	N	177	HIS	2.7
1	M	509	GLY	2.7
2	N	126	THR	2.7
1	M	307	PRO	2.7
2	N	183	SER	2.7
2	N	153	LEU	2.7
1	M	18	ARG	2.7
1	M	441	ASN	2.7
3	O	10	PRO	2.7
4	P	4	ASN	2.7
1	M	150	GLN	2.7
1	M	43	SER	2.7
1	M	475	THR	2.6
1	M	319	LEU	2.6
2	N	195	LEU	2.6
4	P	89	LEU	2.6
1	M	253	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	235	PHE	2.6
2	N	95	ASN	2.6
1	M	537	GLU	2.6
1	M	216	ALA	2.6
2	N	32	ALA	2.6
1	M	100	GLY	2.6
2	N	118	PRO	2.6
1	A	323	LYS	2.6
1	M	234	THR	2.6
2	N	17	VAL	2.6
2	N	239	THR	2.6
1	M	576	ALA	2.6
2	N	186	HIS	2.6
1	M	72	GLY	2.6
1	M	369	THR	2.6
1	M	468	THR	2.6
1	M	517	CYS	2.6
2	N	99	GLU	2.6
1	A	330	PHE	2.6
1	M	83	ASP	2.6
1	M	67	HIS	2.5
1	M	308	ARG	2.5
1	M	239	SER	2.5
1	M	121	ILE	2.5
1	M	412	GLU	2.5
1	M	24	ALA	2.5
1	M	105	ARG	2.5
1	A	130	LYS	2.5
1	M	217	LEU	2.5
1	M	46	VAL	2.5
2	N	179	TYR	2.5
1	M	57	GLN	2.5
4	P	58	ALA	2.5
2	N	77	CYS	2.5
1	M	432	VAL	2.5
2	N	104	VAL	2.5
2	B	30	TYR	2.5
1	M	122	GLU	2.5
1	M	47	ALA	2.5
4	P	2	ASN	2.5
1	M	556	ASP	2.5
2	B	242	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	401	VAL	2.5
1	M	92	GLU	2.5
1	M	368	GLU	2.5
2	N	166	GLU	2.5
1	M	435	ARG	2.5
1	M	523	MET	2.4
2	B	45	ASP	2.4
2	N	175	LEU	2.4
3	O	103	MET	2.4
1	M	343	PRO	2.4
3	O	130	TRP	2.4
3	O	3	LYS	2.4
1	M	571	THR	2.4
1	M	455	MET	2.4
1	M	512	LEU	2.4
1	M	225	ASP	2.4
2	B	23	SER	2.4
1	M	98	LEU	2.4
1	M	513	ASN	2.4
2	N	136	PRO	2.4
2	B	17	VAL	2.4
1	A	299	ARG	2.4
1	M	151	ARG	2.4
3	O	99	LYS	2.4
1	M	230	GLN	2.4
2	N	3	MET	2.4
1	M	73	GLY	2.4
1	M	153	ASP	2.4
1	M	467	ARG	2.4
4	P	52	GLU	2.4
1	M	128	ALA	2.4
1	M	358	MET	2.4
1	M	540	THR	2.4
1	M	546	ASN	2.3
2	N	180	ASN	2.3
2	N	122	GLY	2.3
1	M	493	ASP	2.3
2	N	38	ASP	2.3
2	N	62	CYS	2.3
1	M	201	TYR	2.3
1	M	284	LEU	2.3
1	M	273	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	N	242	PRO	2.3
3	O	92	LYS	2.3
1	A	445	GLY	2.3
1	M	177	GLU	2.3
2	B	1	ALA	2.3
1	M	381	SER	2.3
2	B	131	THR	2.3
1	M	280	LYS	2.3
2	N	44	LYS	2.3
1	M	404	ARG	2.3
1	M	469	PRO	2.3
1	M	208	VAL	2.3
2	N	66	GLY	2.3
1	M	520	HIS	2.3
1	M	244	THR	2.3
1	A	28	PRO	2.3
1	M	277	PRO	2.3
1	M	112	ASN	2.3
2	N	71	ASN	2.3
1	A	250	GLU	2.3
1	M	321	GLU	2.3
1	M	558	ASP	2.3
2	N	138	GLN	2.3
4	P	67	LEU	2.3
2	N	116	ILE	2.3
1	M	143	SER	2.3
1	M	357	THR	2.3
1	M	113	VAL	2.3
1	M	194	GLY	2.3
2	N	25	PHE	2.2
1	M	119	MET	2.2
1	M	54	ALA	2.2
1	M	461	GLU	2.2
2	B	20	ALA	2.2
3	O	100	ASP	2.2
2	N	214	CYS	2.2
1	M	500	THR	2.2
2	N	135	THR	2.2
1	M	464	GLY	2.2
4	P	57	PHE	2.2
4	D	4	ASN	2.2
3	O	4	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	124	THR	2.2
3	O	2	THR	2.2
1	M	518	MET	2.2
2	N	233	LYS	2.2
1	M	541	GLU	2.2
1	M	331	ILE	2.2
3	C	18	LYS	2.2
1	M	516	GLU	2.2
1	M	106	ARG	2.2
1	M	365	GLN	2.2
2	N	14	ASN	2.2
1	A	343	PRO	2.2
2	N	15	PRO	2.2
2	N	33	THR	2.2
3	O	15	TRP	2.2
2	N	125	ARG	2.1
1	M	70	VAL	2.1
1	M	339	VAL	2.1
2	N	18	ASP	2.1
1	M	142	THR	2.1
2	N	189	LYS	2.1
1	M	530	GLY	2.1
2	N	57	CYS	2.1
1	M	5	ALA	2.1
1	M	458	ALA	2.1
2	N	20	ALA	2.1
1	M	317	ARG	2.1
2	N	191	ARG	2.1
1	M	29	ASN	2.1
3	O	18	LYS	2.1
2	N	152	GLY	2.1
1	M	59	HIS	2.1
2	N	217	HIS	2.1
4	P	92	HIS	2.1
2	B	28	VAL	2.1
1	M	329	PRO	2.1
2	N	7	LYS	2.1
1	M	418	GLY	2.1
2	N	45	ASP	2.1
2	N	185	ASP	2.1
4	P	61	PHE	2.1
4	P	88	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	48	ALA	2.1
2	N	140	ALA	2.1
1	M	532	HIS	2.1
2	N	143	HIS	2.1
3	O	98	VAL	2.1
2	N	49	PRO	2.1
1	M	197	ARG	2.1
1	M	304	ILE	2.1
1	M	423	ALA	2.1
1	A	49	GLU	2.1
2	B	5	ASN	2.0
2	B	47	LEU	2.0
1	M	320	GLY	2.0
1	M	327	ARG	2.0
1	M	22	ALA	2.0
1	M	227	GLU	2.0
1	M	262	TYR	2.0
1	M	466	TYR	2.0
1	M	350	VAL	2.0
1	M	349	PRO	2.0
1	M	126	PHE	2.0
1	M	246	GLY	2.0
1	M	94	THR	2.0
1	M	443	ASP	2.0
2	B	2	GLU	2.0
2	N	74	LYS	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](#)

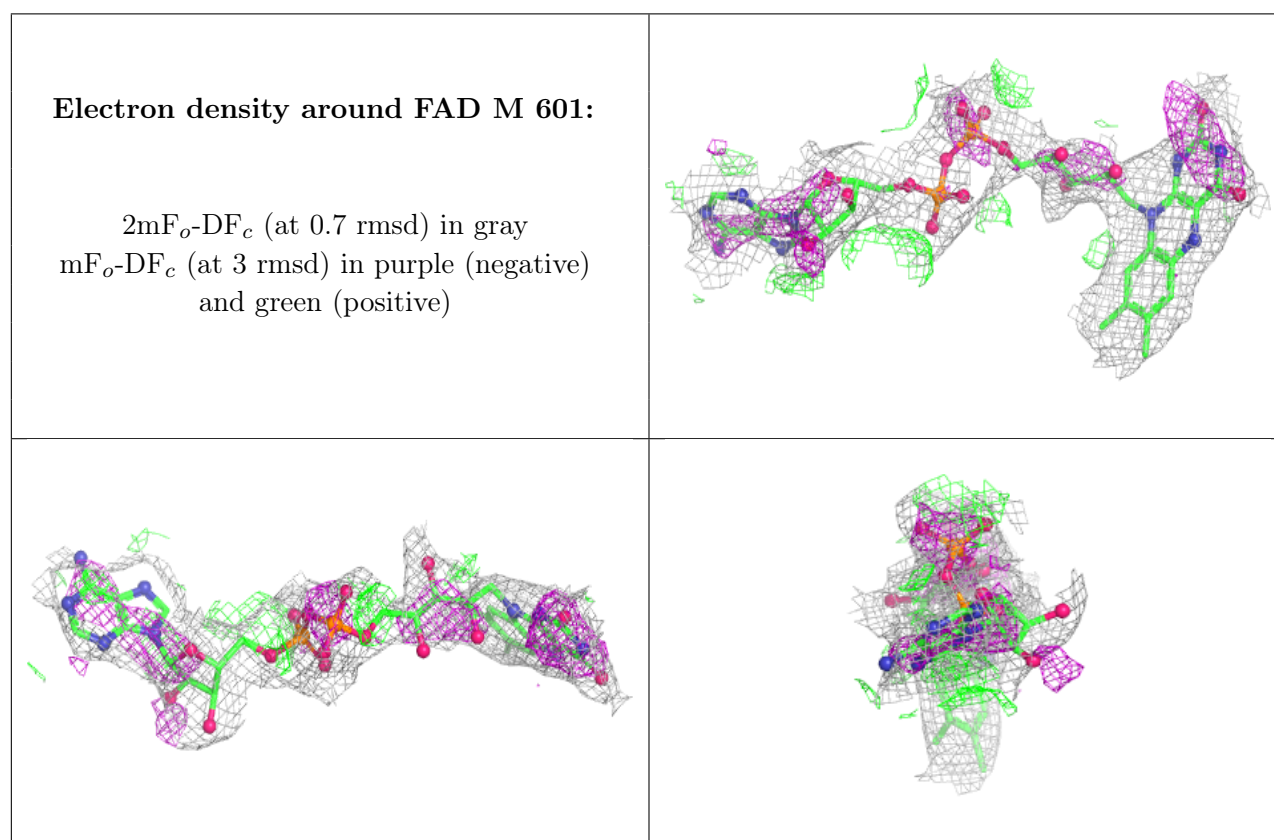
There are no oligosaccharides in this entry.

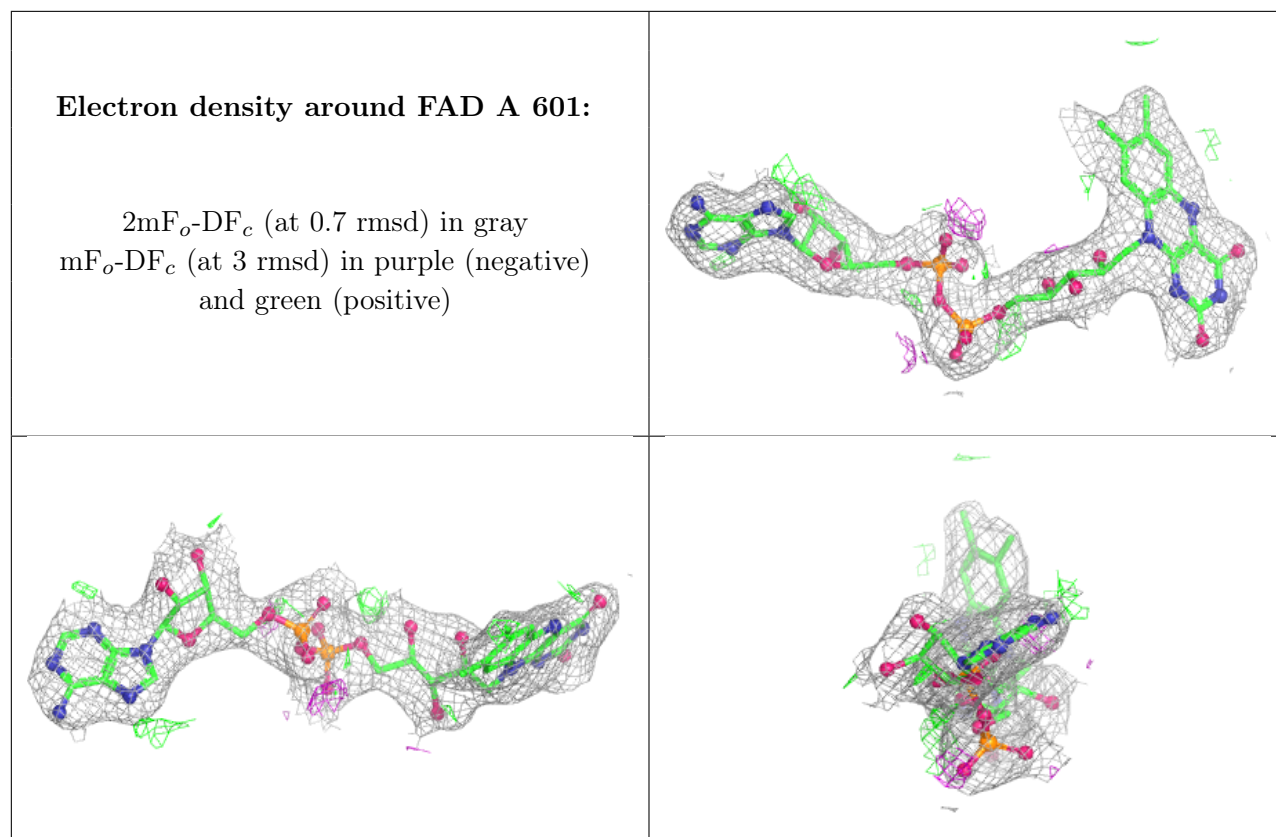
6.4 Ligands [i](#)

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	0.80	0.14	49,74,85,86	0
9	SF4	B	246	8/8	0.89	0.22	86,104,134,134	0
6	FUM	A	577	8/8	0.90	0.19	66,67,70,103	0
7	FES	B	244	4/4	0.94	0.18	98,107,110,114	0
9	SF4	N	246	8/8	0.94	0.12	103,112,131,134	0
7	FES	N	244	4/4	0.95	0.09	76,90,94,104	0
8	F3S	N	245	7/7	0.95	0.12	86,90,101,134	0
5	FAD	A	601	53/53	0.96	0.09	34,41,78,78	0
8	F3S	B	245	7/7	0.99	0.06	60,64,70,93	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.