



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 06:34 PM EDT

PDB ID : 3CIR
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

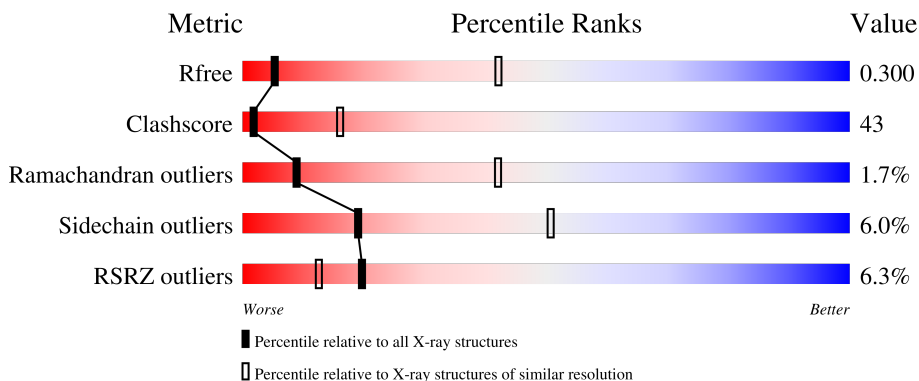
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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}	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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	
1	M	602	
2	B	243	
2	N	243	
3	C	130	

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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	-
8	SF4	B	246	-	-	X	-

2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	541	4140	2576	752	783	29	0	0	0
1	M	504	3718	2295	682	715	26	0	0	0

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
			Total	C	N	O	S			
2	B	243	1888	1189	323	357	19	0	0	0
2	N	243	1888	1189	323	357	19	0	0	0

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

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

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

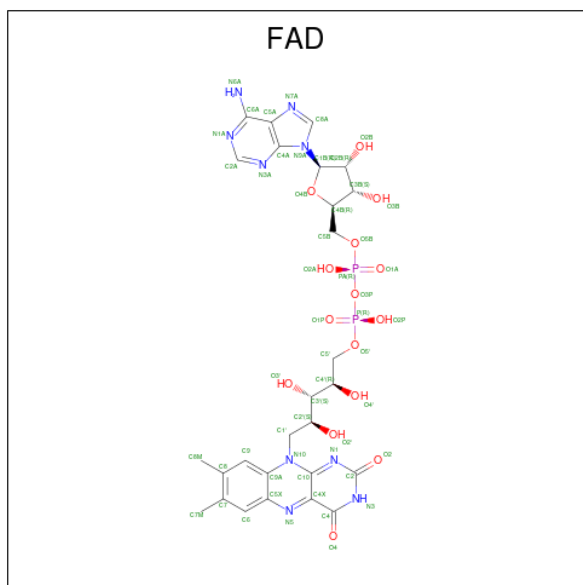
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	119	926	626	151	142	7	0	0	0

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

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



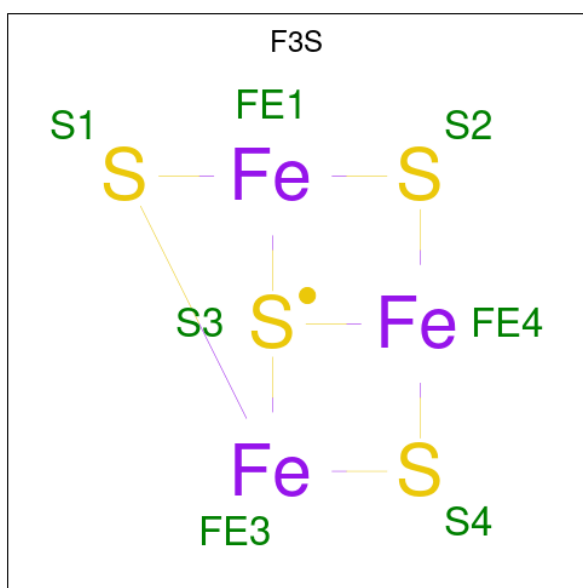
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	53	27	9	15	2	0	0
5	M	1	53	27	9	15	2	0	0

- Molecule 6 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



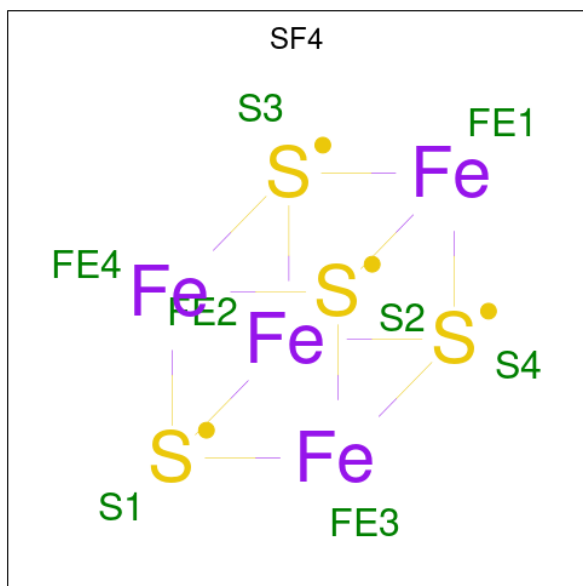
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	S	0	0
			4	2	2		
6	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 7 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



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 (three-letter code: SF4) (formula: Fe₄S₄).

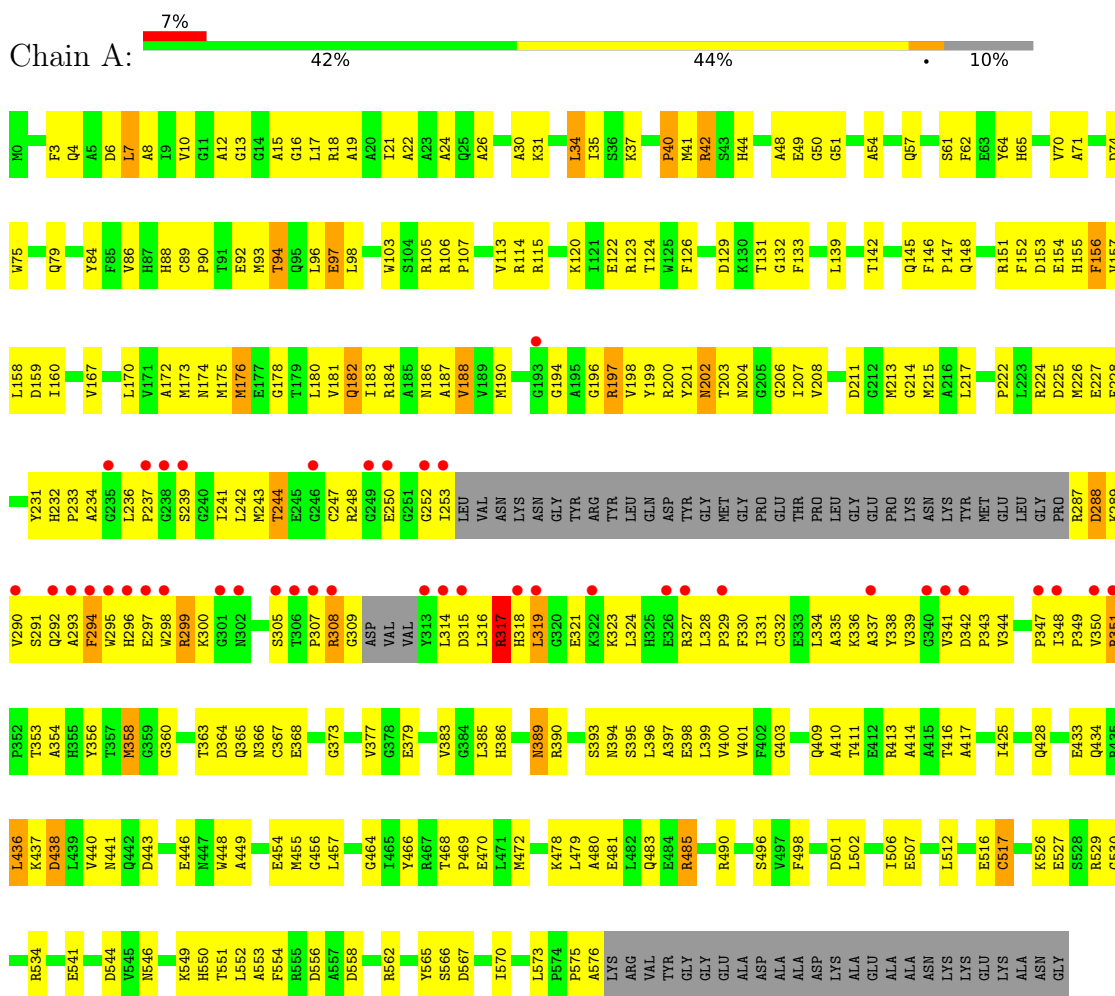


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			8	4	4		
8	N	1	Total	Fe	S	0	0
			8	4	4		

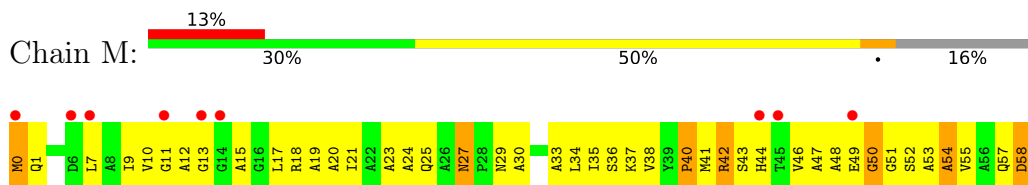
3 Residue-property plots

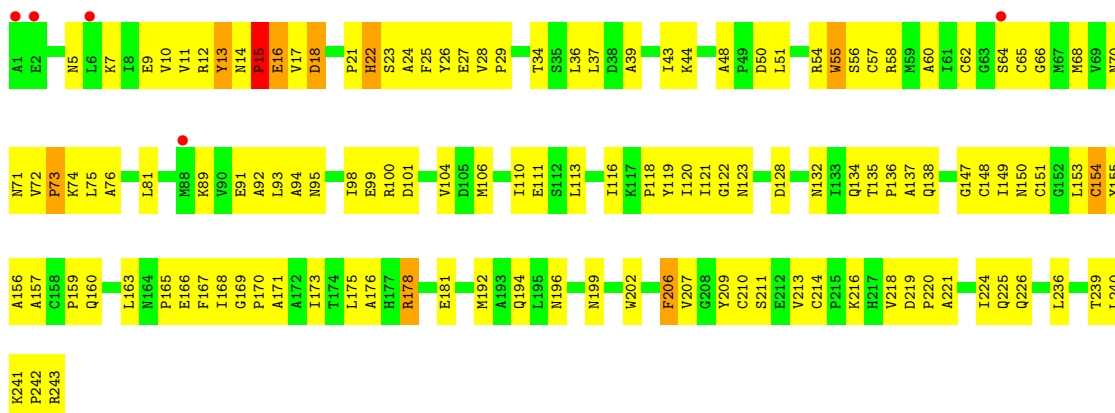
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



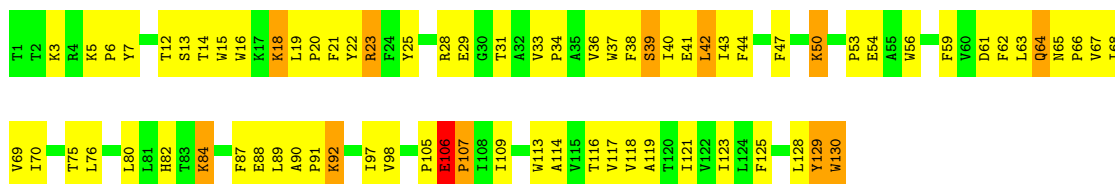
- Molecule 1: Fumarate reductase flavoprotein subunit





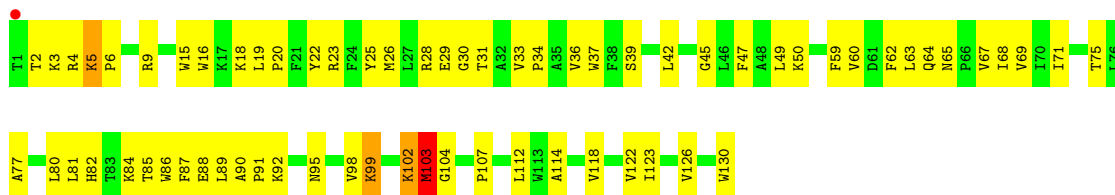
- Molecule 3: Fumarate reductase subunit C

Chain C: 42% 48% 8%



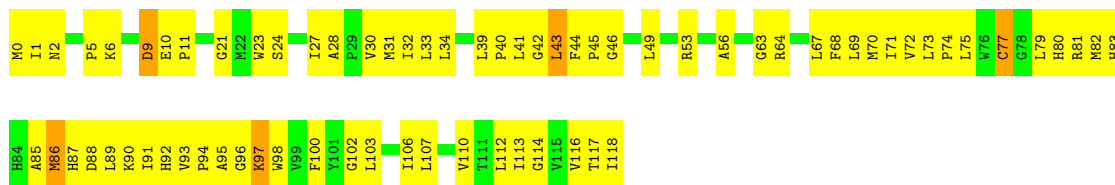
- Molecule 3: Fumarate reductase subunit C

Chain O: 48% 48%



- Molecule 4: Fumarate reductase subunit D

Chain D: 39% 56%



- Molecule 4: Fumarate reductase subunit D

Chain P: 45% 55%



C78	L79	H80	R81	M82
H82	V93	P94	A95	W98
Y99	F100	Y101	G102	L103
A104	A105	I106	V109	L112
I113	G114	V115	V116	T117
I118				

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 42.62 – 3.30	Depositor EDS
% Data completeness (in resolution range)	80.8 (266.00-3.65) 78.8 (42.62-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.39	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 3.32Å)	Xtrriage
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	Xtrriage
Anisotropy	0.269	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.56	4/4221 (0.1%)	0.79	1/5705 (0.0%)
1	M	0.52	0/3778	0.81	7/5107 (0.1%)
2	B	0.58	1/1931 (0.1%)	0.79	1/2617 (0.0%)
2	N	0.44	0/1931	0.70	3/2617 (0.1%)
3	C	0.57	1/1094 (0.1%)	0.70	2/1496 (0.1%)
3	O	0.52	0/1094	0.74	2/1496 (0.1%)
4	D	0.50	0/956	0.72	0/1303
4	P	0.43	0/956	0.68	0/1303
All	All	0.53	6/15961 (0.0%)	0.77	16/21644 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	LYS	N-CA	7.04	1.60	1.46
3	C	106	GLU	C-N	6.50	1.46	1.34
1	A	299	ARG	CA-C	6.22	1.69	1.52
1	A	182	GLN	CG-CD	5.40	1.63	1.51
2	B	215	PRO	N-CD	-5.33	1.40	1.47
1	A	307	PRO	CA-C	5.03	1.62	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	323	LYS	N-CA-C	8.75	134.62	111.00
1	M	114	ARG	NE-CZ-NH2	-6.90	116.85	120.30
3	C	107	PRO	CA-N-CD	-6.35	102.61	111.50
1	M	303	THR	N-CA-C	-6.26	94.09	111.00
2	B	93	LEU	CA-C-N	-6.24	103.47	117.20
1	M	418	GLY	N-CA-C	-6.05	97.97	113.10
1	M	554	PHE	CB-CG-CD2	-6.04	116.57	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	554	PHE	CB-CG-CD1	5.88	124.92	120.80
1	A	308	ARG	N-CA-C	5.72	126.46	111.00
2	N	154	CYS	CA-CB-SG	5.50	123.89	114.00
2	N	15	PRO	CA-N-CD	-5.45	103.87	111.50
2	N	148	CYS	CA-CB-SG	-5.23	104.58	114.00
1	M	7	LEU	CA-CB-CG	5.22	127.31	115.30
3	O	103	MET	C-N-CA	5.18	133.18	122.30
3	O	103	MET	CB-CA-C	5.16	120.71	110.40
3	C	129	TYR	CA-CB-CG	5.14	123.17	113.40

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	343	0
1	M	3718	0	3461	445	0
2	B	1888	0	1837	168	0
2	N	1888	0	1837	163	0
3	C	1058	0	1108	108	1
3	O	1058	0	1108	85	1
4	D	926	0	971	85	0
4	P	926	0	971	74	0
5	A	53	0	31	12	0
5	M	53	0	31	26	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	1323	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 43.

All (1323) 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
1:M:44:HIS:NE2	5:M:601:FAD:HM82	1.09	1.39
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:44:HIS:NE2	5:A:601:FAD:HM82	1.05	1.33
1:A:330:PHE:CE2	2:B:59:MET:CE	2.13	1.31
1:M:44:HIS:CE1	5:M:601:FAD:HM82	1.65	1.30
1:A:330:PHE:HE2	2:B:59:MET:CE	1.44	1.30
1:M:119:MET:SD	1:M:123:ARG:NH1	2.16	1.19
1:A:44:HIS:CE1	5:A:601:FAD:HM82	1.79	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
1:A:330:PHE:CE2	2:B:59:MET:HE3	1.83	1.11
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:M:497:VAL:HG21	2:N:15:PRO:HG3	1.18	1.09
1:A:358:MET:HE1	1:A:389:ASN:HA	1.35	1.07
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:M:358:MET:HE3	1:M:389:ASN:HA	1.37	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
1:A:330:PHE:CE2	2:B:59:MET:HE2	1.88	1.06
1:M:395:SER:OG	5:M:601:FAD:H2'	1.55	1.05
1:A:243:MET:SD	1:A:331:ILE:CG2	2.45	1.04
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	2.00	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: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
1:M:356:TYR:CE1	1:M:379:GLU:HG3	2.04	0.93
1:A:213:MET:HE3	1:A:360:GLY:HA2	1.50	0.93
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:203:THR:CG2	1:A:242:LEU:HD21	2.02	0.89
1:A:44:HIS:NE2	5:A:601:FAD:HM81	1.87	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
1:M:194:GLY:HA3	1:M:379:GLU:CD	1.93	0.88
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
1:A:358:MET:HE1	1:A:389:ASN:CA	2.04	0.87
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
2:B:68:MET:HE2	2:B:94:ALA:HB2	1.55	0.87
1:A:105:ARG:HH12	2:B:134:GLN:HB3	1.33	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:339:VAL:HA	2:B:33:THR:HG22	1.56	0.85
2:N:106:MET:HE2	2:N:106:MET:HA	1.56	0.85
1:A:350:VAL:O	1:A:351:ARG:HD2	1.76	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:0:MET:HE1	1:M:180:LEU:HD13	1.63	0.81
2:B:68:MET:SD	2:B:94:ALA:HB2	2.20	0.81
1:M:44:HIS:NE2	5:M:601:FAD:HM81	1.95	0.81
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
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
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: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
4:P:69:LEU:HD22	4:P:73:LEU:HD11	1.64	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
3:O:89:LEU:C	3:O:91:PRO:HD2	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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	1.50	0.74
2:N:168:ILE:HD11	2:N:173:ILE:HG12	1.69	0.74
4:D:9:ASP:C	4:D:11:PRO:HD2	2.08	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
2:N:106:MET:HA	2:N:106:MET:CE	2.17	0.74
1:A:103:TRP:O	2:B:139:MET:HE1	1.88	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
1:A:330:PHE:CZ	2:B:59:MET:HE3	2.15	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:448:TRP:CH2	1:M:504:TYR:HB3	2.23	0.73
1:A:287:ARG:C	1:A:289:LYS:H	1.91	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: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
1:A:241:ILE:HD13	1:A:334:LEU:HB3	1.71	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
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
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:0:MET:HE3	1:M:171:VAL:HG11	1.72	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:397:ALA:O	1:M:401:VAL:HG23	1.89	0.71
1:A:203:THR:OG1	5:A:601:FAD:HM83	1.91	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
1:M:0:MET:HE3	1:M:171:VAL:CG1	2.21	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
1:A:446:GLU:CD	1:A:485:ARG:HD3	2.13	0.68
3:C:130:TRP:N	3:C:130:TRP:CD1	2.59	0.68
1:M:58:ASP:C	1:M:60:ASP:H	1.97	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
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
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: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:0:MET:HE2	1:M:180:LEU:CD1	2.26	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
2:N:211:SER:HA	2:N:220:PRO:HD2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:0:MET:HE2	1:M:180:LEU:HD13	1.79	0.65
1:M:78:GLU:O	1:M:81:VAL:HG22	1.97	0.65
1:M:170:LEU:C	1:M:170:LEU:HD12	2.17	0.65
1:A:213:MET:CE	1:A:360:GLY:HA2	2.24	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: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
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
1:M:20:ALA:O	1:M:23:ALA:HB3	1.98	0.64
1:A:42:ARG:NH2	2:B:150:ASN:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:118:VAL:O	3:O:122:VAL:HG23	1.98	0.64
2:B:236:LEU:HD23	2:B:236:LEU:C	2.19	0.63
2:N:36:LEU:HD23	2:N:76:ALA:HA	1.81	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
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:287:ARG:C	1:A:289:LYS:N	2.52	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
1:M:465:ILE:O	1:M:465:ILE:CG2	2.48	0.62
4:P:79:LEU:HA	4:P:82:MET:HE3	1.82	0.62
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:126:VAL:HA	3:O:130:TRP:HB3	1.82	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
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:A:196:GLY:HA3	1:A:204:ASN:OD1	2.00	0.60
2:B:93:LEU:HD12	2:B:94:ALA:H	1.67	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:421:ASN:HD22	1:M:422:GLU:H	1.50	0.59
1:M:527:GLU:CD	1:M:529:ARG:NH1	2.56	0.59
2:N:120:ILE:C	2:N:121:ILE:HG13	2.21	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
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
1:M:126:PHE:CD1	1:M:126:PHE:C	2.74	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:194:GLY:CA	1:M:379:GLU:CD	2.71	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
1:A:200:ARG:HB2	1:A:456:GLY:C	2.23	0.59
2:B:134:GLN:HA	2:B:138:GLN:OE1	2.03	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
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: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:129:ASP:N	1:M:129:ASP:OD2	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:31:MET:HG3	4:D:70:MET:SD	2.44	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
2:N:175:LEU:O	2:N:178:ARG:HB3	2.03	0.57
1:A:454:GLU:CD	1:A:485:ARG:HH22	2.07	0.57
4:P:33:LEU:HA	4:P:37:ILE:HD12	1.86	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:12:ARG:HE	2:B:101:ASP:CG	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:467:ARG:HB3	1:M:472:MET:HE2	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: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:A:309:GLY:C	1:A:351:ARG:CD	2.72	0.56
1:M:231:TYR:CD2	1:M:352:PRO:HB2	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: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
2:N:135:THR:CG2	2:N:136:PRO:HD2	2.35	0.56
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:M:358:MET:HE3	1:M:389:ASN:CA	2.26	0.56
2:N:181:GLU:OE2	2:N:181:GLU:HA	2.05	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
3:C:125:PHE:CD1	3:C:129:TYR:CD1	2.94	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
1:M:232:HIS:C	1:M:234:ALA:H	2.07	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
1:A:242:LEU:HD12	5:A:601:FAD:HM73	1.88	0.55
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:358:MET:HE1	1:M:390:ARG:H	1.68	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
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
3:O:86:TRP:HE1	4:P:22:MET:HE2	1.70	0.55
1:M:41:MET:CE	2:N:150:ASN:HD22	2.19	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
4:D:24:SER:O	4:D:28:ALA:HB3	2.06	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
1:M:295:TRP:O	1:M:299:ARG:N	2.37	0.55
1:M:527:GLU:CD	1:M:529:ARG:HH11	2.09	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
2:B:142:TYR:CD1	2:B:142:TYR:C	2.80	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: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:183:ILE:HD12	1:M:183:ILE:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:193:GLY:C	1:M:379:GLU:HB3	2.28	0.54
1:M:356:TYR:CE1	1:M:379:GLU:CG	2.86	0.54
1:A:176:MET:HE3	2:B:99:GLU:HG3	1.90	0.54
2:B:206:PHE:O	3:C:28:ARG:NH2	2.41	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: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
1:M:204:ASN:N	1:M:204:ASN:HD22	2.05	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
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
2:B:206:PHE:C	2:B:206:PHE:CD2	2.80	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:316:LEU:O	1:A:317:ARG:C	2.47	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: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:106:MET:CE	2:N:106:MET:CA	2.85	0.53
2:N:157:ALA:HB2	2:N:213:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:CD2	5:A:601:FAD:C8M	2.80	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:A:7:LEU:C	1:A:7:LEU:HD12	2.29	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:437:LYS:C	1:A:441:ASN:ND2	2.62	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:232:HIS:C	1:M:234:ALA:N	2.62	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:104:SER:HG	1:M:127:ALA:HA	1.74	0.52
1:M:115:ARG:O	1:M:115:ARG:HG3	2.01	0.52
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: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:119:MET:HE2	1:M:391:LEU:HD23	1.90	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
1:M:34:LEU:O	1:M:151:ARG:HA	2.11	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
2:N:178:ARG:HD3	2:N:178:ARG:C	2.31	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:12:ARG:HH22	2:N:50:ASP:CG	2.14	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
2:N:239:THR:HG22	2:N:239:THR:O	2.11	0.51
1:A:156:PHE:C	1:A:156:PHE:CD2	2.84	0.51
4:D:0:MET:HG3	4:D:1:ILE:N	2.25	0.51
1:M:94:THR:HG1	1:M:125:TRP:HH2	1.57	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
3:O:89:LEU:C	3:O:91:PRO:CD	2.77	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:512:LEU:O	1:M:516:GLU:HG3	2.12	0.50
2:N:111:GLU:CD	4:P:1:ILE:HG13	2.32	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: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: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
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
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:44:HIS:C	1:M:46:VAL:N	2.65	0.50
1:M:159:ASP:OD1	1:M:219:HIS:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:PHE:HE2	2:B:59:MET:HE3	1.30	0.49
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
4:P:113:ILE:HA	4:P:116:VAL:CG2	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
1:M:496:SER:HB2	3:O:3:LYS:HD3	1.95	0.49
2:N:12:ARG:HH22	2:N:50:ASP:C	2.15	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:M:59:HIS:ND1	1:M:59:HIS:C	2.66	0.49
1:A:17:LEU:CD2	1:A:34:LEU:HD11	2.43	0.49
3:C:87:PHE:HE1	3:C:116:THR:HG1	1.59	0.49
1:M:53:ALA:HA	1:M:123:ARG:O	2.12	0.49
2:N:73:PRO:C	2:N:153:LEU:HD22	2.33	0.49
2:N:225:GLN:HA	2:N:225:GLN:NE2	2.28	0.49
3:O:29:GLU:C	3:O:31:THR:H	2.16	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: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
1:M:523:MET:HA	1:M:523:MET:HE3	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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:B:43:ILE:HG23	2:B:47:LEU:HB2	1.96	0.48
2:B:242:PRO:HG2	4:P:93:VAL:C	2.33	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
1:M:547:PHE:C	1:M:549:LYS:H	2.16	0.48
3:O:123:ILE:CD1	4:P:27:ILE:HG23	2.42	0.48
1:A:527:GLU:CD	1:A:529:ARG:HH11	2.16	0.48
3:C:56:TRP:O	3:C:59:PHE:HB3	2.12	0.48
1:M:154:GLU:O	1:M:175:MET:HG3	2.13	0.48
1:M:211:ASP:O	1:M:215:MET:HE2	2.12	0.48
1:M:363:THR:OG1	1:M:383:VAL:HA	2.14	0.48
1:A:98:LEU:CD2	2:B:132:ASN:HD21	2.19	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
2:N:120:ILE:O	2:N:121:ILE:HG13	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:528:SER:OG	1:M:539:CYS:O	2.23	0.48
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
2:N:13:TYR:O	2:N:100:ARG:HD2	2.13	0.48
1:M:58:ASP:C	1:M:60:ASP:N	2.67	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
2:N:68:MET:HE3	2:N:73:PRO:HD3	1.94	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:122:GLU:H	1:A:122:GLU:CD	2.16	0.47
2:B:206:PHE:O	2:B:206:PHE:CD2	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
1:M:378:GLY:C	1:M:380:CYS:H	2.16	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:M:192:THR:C	5:M:601:FAD:H51A	2.34	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:MET:CE	1:A:390:ARG:H	2.27	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
1:A:562:ARG:HG3	1:A:562:ARG:HH11	1.80	0.47
3:C:76:LEU:HD23	3:C:76:LEU:C	2.34	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:44:HIS:CD2	5:A:601:FAD:HM81	2.49	0.47
1:A:167:VAL:HG21	1:A:188:VAL:HG23	1.97	0.47
1:M:0:MET:HE1	1:M:171:VAL:HG13	1.97	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
3:O:29:GLU:C	3:O:31:THR:N	2.67	0.47
3:O:60:VAL:O	3:O:64:GLN:HG3	2.15	0.47
1:M:38:VAL:HA	1:M:154:GLU:HG2	1.96	0.47
1:M:54:ALA:C	1:M:123:ARG:HB2	2.35	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
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:M:60:ASP:CG	1:M:121:ILE:HG21	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ALA:O	2:B:227:GLY:N	2.48	0.46
1:M:0:MET:CE	1:M:171:VAL:HG11	2.41	0.46
1:M:0:MET:HE1	1:M:171:VAL:CG1	2.45	0.46
1:M:187:ALA:HB2	1:M:414:ALA:HB2	1.96	0.46
2:N:104:VAL:HG23	2:N:106:MET:HE3	1.97	0.46
1:A:291:SER:O	1:A:294:PHE:CD2	2.68	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
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:M:205:GLY:C	1:M:207:ILE:N	2.69	0.46
1:A:84:TYR:O	1:A:88:HIS:HD2	1.99	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:0:MET:HE2	1:M:180:LEU:HD12	1.97	0.46
1:M:48:ALA:HA	5:M:601:FAD:C6	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:309:GLY:C	1:A:351:ARG:HD2	2.34	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: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
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
1:M:472:MET:HE3	1:M:523:MET:HE1	1.99	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
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
3:O:63:LEU:HA	3:O:68:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:206:PHE:CD2	2:N:206:PHE:C	2.90	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
2:B:134:GLN:HE21	2:B:139:MET:CE	2.29	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
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:201:TYR:C	1:A:353:THR:HG1	2.20	0.44
1:A:314:LEU:HG	1:A:316:LEU:HD21	1.98	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:211:ASP:CG	1:M:510:HIS:CD2	2.90	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:40:LEU:HD11	2:B:67:MET:HE1	1.98	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:M:44:HIS:C	1:M:46:VAL:H	2.19	0.44
1:A:160:ILE:HG13	1:A:160:ILE:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:LEU:HB3	1:A:554:PHE:CE1	2.53	0.44
2:B:169:GLY:O	2:B:173:ILE:HG13	2.17	0.44
2:N:16:GLU:C	2:N:18:ASP:N	2.68	0.44
2:N:135:THR:HB	2:N:138:GLN:NE2	2.33	0.44
1:A:156:PHE:C	1:A:156:PHE:HD2	2.21	0.44
2:B:40:LEU:HD11	2:B:67:MET:CE	2.48	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: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
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:20:ALA:C	1:M:23:ALA:HB3	2.38	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
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:201:TYR:C	1:M:353:THR:HG23	2.38	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: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
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:0:MET:HE3	4:D:1:ILE:H	1.83	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:M:551:THR:C	1:M:552:LEU:HD23	2.39	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
3:C:23:ARG:NH1	3:C:23:ARG:HG2	2.32	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: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
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
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:195:ALA:C	1:M:197:ARG:N	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:119:MET:CE	1:M:391:LEU:HD23	2.49	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:68:PHE:CZ	4:P:72:VAL:HG21	2.54	0.43
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
1:M:34:LEU:O	1:M:152:PHE:N	2.50	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: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
3:C:65:ASN:HD22	3:C:68:ILE:HG12	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:212:GLY:HA2	1:M:215:MET:HE2	2.01	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
1:M:10:VAL:HG21	1:M:190:MET:HE1	2.02	0.42
1:M:194:GLY:HA3	1:M:379:GLU:OE1	2.18	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
1:A:358:MET:CE	1:A:390:ARG:N	2.82	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:444:GLY:HA3	1:M:488:ARG:C	2.40	0.42
2:N:135:THR:OG1	2:N:138:GLN:NE2	2.50	0.42
2:N:165:PRO:C	2:N:167:PHE:H	2.22	0.42
2:B:60:ALA:HA	6:B:244:FES:S1	2.60	0.42
3:C:106:GLU:CD	3:C:107:PRO:HD2	2.40	0.42
4:D:117:THR:C	4:D:118:ILE:HG12	2.40	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: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:228:PHE:HB2	1:M:358:MET:CB	2.50	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:201:TYR:C	1:A:353:THR:OG1	2.59	0.41
1:A:298:TRP:CD1	1:A:298:TRP:N	2.88	0.41
2:B:236:LEU:C	2:B:236:LEU:CD2	2.88	0.41
1:M:145:GLN:HB3	2:N:119:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:60:ALA:HA	6:N:244:FES:S1	2.60	0.41
1:M:27:ASN:C	1:M:27:ASN:HD22	2.23	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
1:A:213:MET:CE	1:A:226:MET:SD	3.09	0.41
1:A:358:MET:HE1	1:A:390:ARG:H	1.85	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:64:TYR:CD2	1:A:120:LYS:HE2	2.56	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:M:226:MET:HE2	1:M:514:VAL:HG13	2.02	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:236:LEU:HD23	2:N:236:LEU:C	2.40	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:37:LYS:NZ	1:A:507:GLU:OE2	2.40	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
4:D:97:LYS:HB2	4:D:97:LYS:HZ3	1.80	0.41
2:N:120:ILE:HD13	2:N:120:ILE:HA	1.88	0.41
2:N:209:TYR:HD2	3:O:22:TYR:HH	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLY:O	1:A:19:ALA:HB3	2.20	0.41
1:M:83:ASP:O	1:M:87:HIS:HD2	2.04	0.41
1:M:203:THR:C	1:M:204:ASN:HD22	2.24	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
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:225:ASP:C	1:M:227:GLU:H	2.23	0.41
2:N:73:PRO:CA	2:N:153:LEU:HD22	2.50	0.41
2:N:149:ILE:HD11	2:N:151:CYS:HB3	2.01	0.41
2:N:206:PHE:C	2:N:206:PHE:HD2	2.24	0.41
1:A:332:CYS:CA	1:A:343:PRO:HG2	2.16	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: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
1:M:0:MET:HE1	1:M:180:LEU:HB3	2.04	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
4:D:93:VAL:H	2:N:243:ARG:C	2.23	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
1:A:358:MET:HE1	1:A:390:ARG:N	2.36	0.40
2:B:94:ALA:O	2:B:95:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:TRP:CG	3:C:16:TRP:N	2.90	0.40
1:M:538:GLY:C	1:M:539:CYS:SG	2.99	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: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:358:MET:H	1:A:358:MET:HG2	1.31	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 [i](#)

5.3.1 Protein backbone [i](#)

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%)	12	47
1	M	494/602 (82%)	437 (88%)	44 (9%)	13 (3%)	5	34
2	B	241/243 (99%)	220 (91%)	19 (8%)	2 (1%)	19	56
2	N	241/243 (99%)	204 (85%)	30 (12%)	7 (3%)	4	32
3	C	128/130 (98%)	113 (88%)	13 (10%)	2 (2%)	9	43
3	O	128/130 (98%)	116 (91%)	9 (7%)	3 (2%)	6	36
4	D	117/119 (98%)	98 (84%)	19 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P	117/119 (98%)	100 (86%)	17 (14%)	0	100	100
All	All	2001/2188 (92%)	1775 (89%)	192 (10%)	34 (2%)	9	42

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
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 [i](#)

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%)	393 (93%)	31 (7%)	14	44
1	M	355/474 (75%)	331 (93%)	24 (7%)	16	47
2	B	205/205 (100%)	195 (95%)	10 (5%)	25	56
2	N	205/205 (100%)	197 (96%)	8 (4%)	32	60
3	C	111/111 (100%)	101 (91%)	10 (9%)	9	37
3	O	111/111 (100%)	104 (94%)	7 (6%)	18	49
4	D	97/97 (100%)	90 (93%)	7 (7%)	14	45
4	P	97/97 (100%)	97 (100%)	0	100	100
All	All	1605/1774 (90%)	1508 (94%)	97 (6%)	19	51

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	34	LEU
1	A	42	ARG
1	A	74	ASP
1	A	94	THR
1	A	96	LEU
1	A	97	GLU
1	A	156	PHE
1	A	159	ASP
1	A	176	MET
1	A	188	VAL
1	A	197	ARG
1	A	202	ASN
1	A	294	PHE
1	A	299	ARG
1	A	305	SER
1	A	317	ARG
1	A	319	LEU
1	A	327	ARG

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Mol	Chain	Res	Type
1	A	351	ARG
1	A	358	MET
1	A	394	ASN
1	A	413	ARG
1	A	436	LEU
1	A	438	ASP
1	A	457	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	128	ASP
2	B	154	CYS
2	B	178	ARG
2	B	206	PHE
2	B	212	GLU
2	B	230	GLU
3	C	23	ARG
3	C	39	SER
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	106	GLU
3	C	130	TRP
4	D	9	ASP
4	D	43	LEU
4	D	77	CYS
4	D	86	MET
4	D	87	HIS
4	D	88	ASP
4	D	97	LYS
1	M	0	MET
1	M	27	ASN
1	M	40	PRO

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Mol	Chain	Res	Type
1	M	42	ARG
1	M	58	ASP
1	M	59	HIS
1	M	75	TRP
1	M	89	CYS
1	M	93	MET
1	M	101	CYS
1	M	115	ARG
1	M	122	GLU
1	M	129	ASP
1	M	159	ASP
1	M	168	ARG
1	M	179	THR
1	M	367	CYS
1	M	395	SER
1	M	413	ARG
1	M	421	ASN
1	M	529	ARG
1	M	541	GLU
1	M	554	PHE
1	M	558	ASP
2	N	16	GLU
2	N	18	ASP
2	N	22	HIS
2	N	123	ASN
2	N	128	ASP
2	N	178	ARG
2	N	206	PHE
2	N	226	GLN
3	O	5	LYS
3	O	37	TRP
3	O	39	SER
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 (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	57	GLN

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Mol	Chain	Res	Type
1	A	88	HIS
1	A	137	HIS
1	A	141	GLN
1	A	219	HIS
1	A	389	ASN
1	A	409	GLN
1	A	434	GLN
1	A	441	ASN
2	B	95	ASN
2	B	132	ASN
2	B	134	GLN
2	B	150	ASN
3	C	51	ASN
3	C	65	ASN
3	C	72	ASN
4	D	4	ASN
4	D	59	GLN
1	M	27	ASN
1	M	87	HIS
1	M	95	GLN
1	M	137	HIS
1	M	148	GLN
1	M	174	ASN
1	M	204	ASN
1	M	409	GLN
1	M	421	ASN
1	M	434	GLN
1	M	510	HIS
1	M	520	HIS
2	N	5	ASN
2	N	22	HIS
2	N	95	ASN
2	N	138	GLN
2	N	150	ASN
2	N	177	HIS
2	N	196	ASN
2	N	226	GLN
3	O	72	ASN
3	O	95	ASN
4	P	4	ASN
4	P	59	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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
6	FES	N	244	2	0,4,4	-	-	-		
7	F3S	N	245	2	0,9,9	-	-	-		
5	FAD	M	601	-	53,58,58	3.68	29 (54%)	68,89,89	1.53	13 (19%)
5	FAD	A	601	-	53,58,58	3.21	24 (45%)	68,89,89	1.37	9 (13%)
7	F3S	B	245	2	0,9,9	-	-	-		
8	SF4	B	246	2	0,12,12	-	-	-		
6	FES	B	244	2	0,4,4	-	-	-		
8	SF4	N	246	2	0,12,12	-	-	-		

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
6	FES	N	244	2	-	-	0/1/1/1
7	F3S	N	245	2	-	-	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	M	601	-	-	8/30/50/50	0/6/6/6
5	FAD	A	601	-	-	4/30/50/50	0/6/6/6
7	F3S	B	245	2	-	-	0/3/3/3
8	SF4	B	246	2	-	-	0/6/5/5
6	FES	B	244	2	-	-	0/1/1/1
8	SF4	N	246	2	-	-	0/6/5/5

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	601	FAD	C9A-C5X	9.14	1.56	1.41
5	M	601	FAD	C4A-N3A	8.36	1.47	1.35
5	A	601	FAD	C4X-N5	8.32	1.46	1.30
5	M	601	FAD	C4X-N5	8.23	1.46	1.30
5	A	601	FAD	C9A-C5X	8.17	1.54	1.41
5	A	601	FAD	C4A-N3A	7.76	1.46	1.35
5	M	601	FAD	C2A-N3A	7.70	1.44	1.32
5	A	601	FAD	C2A-N3A	7.31	1.43	1.32
5	M	601	FAD	C8-C7	6.56	1.57	1.40
5	M	601	FAD	C10-N10	6.43	1.51	1.37
5	A	601	FAD	C6-C7	6.40	1.49	1.39
5	M	601	FAD	C10-N1	6.27	1.46	1.33
5	M	601	FAD	C6-C7	6.06	1.48	1.39
5	A	601	FAD	C10-N10	5.59	1.49	1.37
5	M	601	FAD	O4B-C1B	5.48	1.48	1.41
5	A	601	FAD	C10-N1	5.44	1.44	1.33
5	A	601	FAD	C8-C7	5.39	1.54	1.40
5	M	601	FAD	C5'-C4'	5.04	1.58	1.51
5	M	601	FAD	C2B-C3B	-4.95	1.39	1.53
5	A	601	FAD	C9A-N10	4.64	1.49	1.41
5	A	601	FAD	C9-C9A	4.42	1.46	1.39
5	M	601	FAD	C5B-C4B	-4.20	1.38	1.51
5	M	601	FAD	C4-N3	4.13	1.46	1.38
5	M	601	FAD	C9-C9A	4.06	1.46	1.39
5	M	601	FAD	C9A-N10	3.84	1.47	1.41
5	M	601	FAD	C9-C8	3.75	1.45	1.39
5	A	601	FAD	C9-C8	3.60	1.44	1.39
5	A	601	FAD	C4-N3	3.55	1.45	1.38
5	A	601	FAD	C5A-C4A	-3.28	1.32	1.40
5	M	601	FAD	C7M-C7	-3.23	1.44	1.51
5	A	601	FAD	C7M-C7	-3.14	1.44	1.51
5	M	601	FAD	C3B-C4B	3.10	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	601	FAD	C5A-C4A	-3.08	1.32	1.40
5	M	601	FAD	C8A-N7A	-3.06	1.29	1.34
5	A	601	FAD	C8A-N7A	-2.87	1.29	1.34
5	M	601	FAD	C4X-C10	2.82	1.52	1.44
5	A	601	FAD	C8M-C8	-2.78	1.45	1.51
5	M	601	FAD	C2A-N1A	2.66	1.38	1.33
5	M	601	FAD	P-O1P	2.66	1.60	1.50
5	M	601	FAD	C2-N3	2.65	1.45	1.39
5	M	601	FAD	C6-C5X	2.55	1.44	1.40
5	A	601	FAD	P-O5'	-2.47	1.49	1.59
5	A	601	FAD	C2A-N1A	2.43	1.38	1.33
5	M	601	FAD	O5B-C5B	2.39	1.54	1.44
5	M	601	FAD	C1'-N10	2.38	1.54	1.48
5	A	601	FAD	C6-C5X	2.34	1.43	1.40
5	A	601	FAD	C2-N3	2.29	1.44	1.39
5	M	601	FAD	O2B-C2B	2.26	1.48	1.43
5	A	601	FAD	C4X-C10	2.26	1.50	1.44
5	A	601	FAD	C2B-C1B	-2.21	1.50	1.53
5	M	601	FAD	C8M-C8	-2.11	1.46	1.51
5	A	601	FAD	C2B-C3B	-2.06	1.47	1.53
5	A	601	FAD	C1'-N10	2.05	1.53	1.48

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	FAD	O4B-C4B-C3B	4.23	113.49	105.11
5	A	601	FAD	N3A-C2A-N1A	-3.68	122.93	128.68
5	M	601	FAD	P-O3P-PA	3.14	143.62	132.83
5	A	601	FAD	O4'-C4'-C5'	-3.10	102.95	109.92
5	M	601	FAD	N3A-C2A-N1A	-3.06	123.89	128.68
5	M	601	FAD	O4B-C1B-C2B	2.70	110.88	106.93
5	M	601	FAD	O5B-C5B-C4B	-2.70	99.69	108.99
5	A	601	FAD	O4-C4-C4X	-2.68	119.48	126.60
5	A	601	FAD	C4-C4X-N5	2.65	122.00	118.23
5	M	601	FAD	O4-C4-C4X	-2.64	119.61	126.60
5	A	601	FAD	C4X-C4-N3	2.57	119.72	113.19
5	A	601	FAD	O4B-C1B-C2B	-2.55	103.19	106.93
5	M	601	FAD	O4'-C4'-C5'	-2.54	104.21	109.92
5	M	601	FAD	C4-C4X-N5	2.52	121.82	118.23
5	M	601	FAD	PA-O5B-C5B	2.47	136.14	121.68
5	M	601	FAD	C4X-C4-N3	2.44	119.39	113.19
5	M	601	FAD	C10-N1-C2	2.43	121.76	116.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	C10-N1-C2	2.38	121.67	116.90
5	A	601	FAD	C1'-C2'-C3'	2.33	116.31	109.79
5	A	601	FAD	C4-N3-C2	-2.33	121.34	125.64
5	M	601	FAD	O5B-PA-O1A	-2.32	100.00	109.07
5	M	601	FAD	O5'-C5'-C4'	2.16	115.11	109.36

There are no chirality outliers.

All (12) 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	C5'-O5'-P-O1P
5	M	601	FAD	O4B-C4B-C5B-O5B
5	A	601	FAD	O4B-C4B-C5B-O5B
5	M	601	FAD	PA-O3P-P-O1P
5	M	601	FAD	C5B-O5B-PA-O1A
5	M	601	FAD	O4'-C4'-C5'-O5'

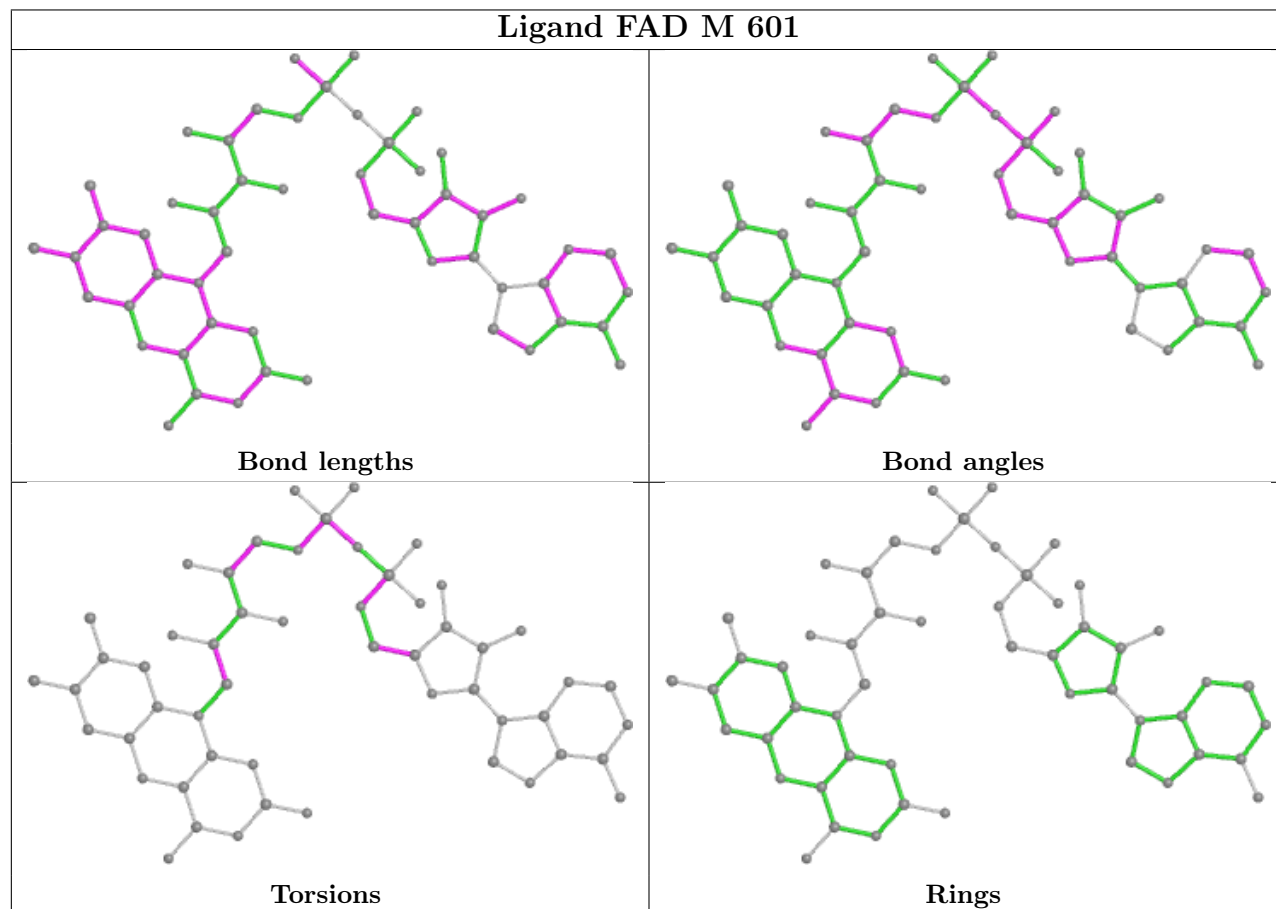
There are no ring outliers.

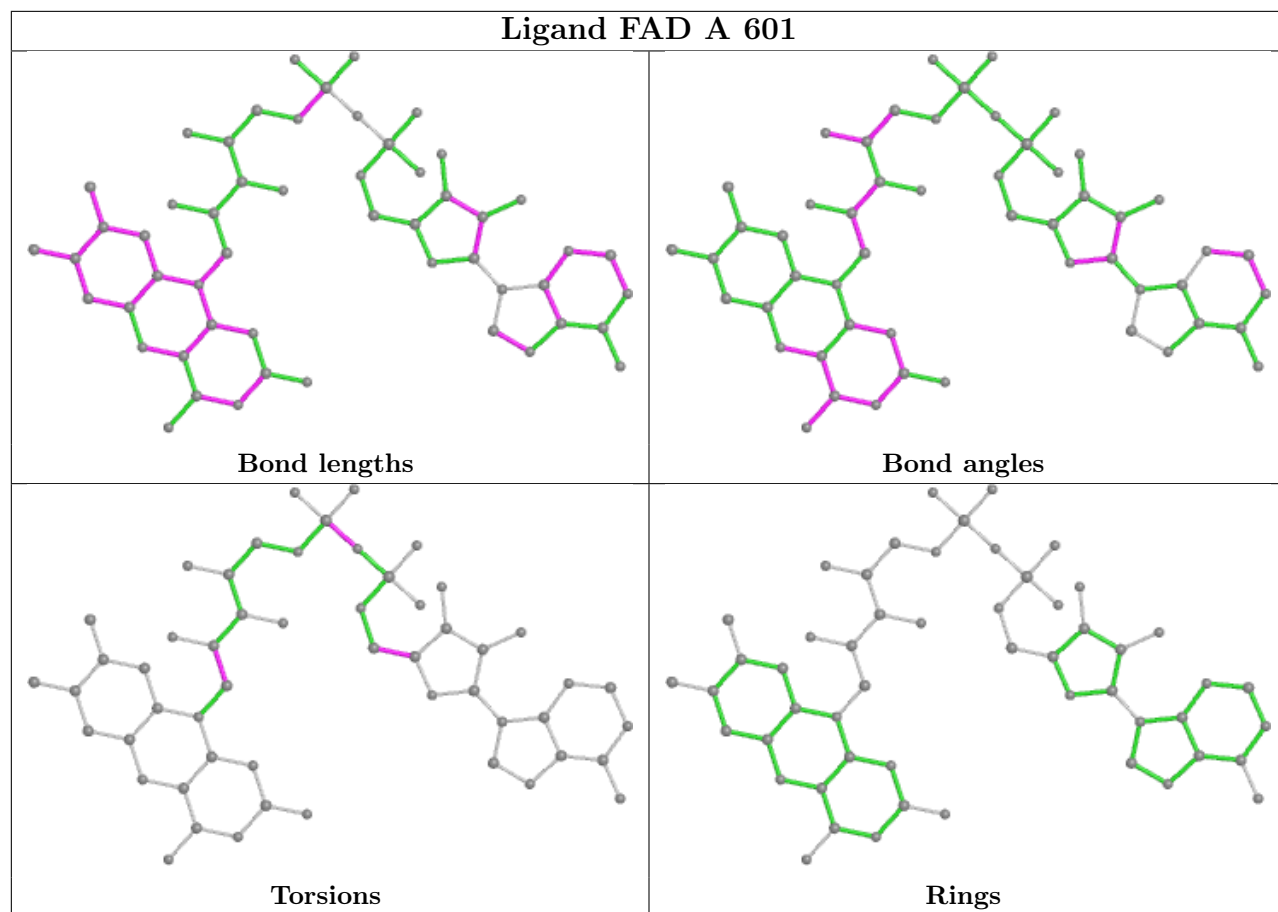
8 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	244	FES	1	0
7	N	245	F3S	1	0
5	M	601	FAD	26	0
5	A	601	FAD	12	0
7	B	245	F3S	1	0
8	B	246	SF4	2	0
6	B	244	FES	1	0
8	N	246	SF4	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%)	-0.23	41 (7%) 13 9	23, 82, 161, 206	0
1	M	504/602 (83%)	0.64	79 (15%) 2 1	117, 184, 208, 208	0
2	B	243/243 (100%)	-0.73	1 (0%) 92 88	19, 76, 126, 205	0
2	N	243/243 (100%)	-0.25	5 (2%) 63 50	100, 161, 195, 206	0
3	C	130/130 (100%)	-0.84	0 100 100	38, 87, 136, 196	0
3	O	130/130 (100%)	-0.55	1 (0%) 86 77	44, 105, 153, 182	0
4	D	119/119 (100%)	-0.94	0 100 100	24, 84, 143, 159	0
4	P	119/119 (100%)	-0.79	1 (0%) 86 77	47, 90, 131, 208	0
All	All	2029/2188 (92%)	-0.21	128 (6%) 20 12	19, 113, 201, 208	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	326	GLU	16.2
1	M	325	HIS	10.7
1	M	238	GLY	9.3
1	A	307	PRO	8.1
1	M	237	PRO	6.3
1	A	306	THR	5.9
1	M	334	LEU	5.9
1	M	287	ARG	5.8
1	M	335	ALA	5.6
1	M	291	SER	5.5
1	M	338	TYR	5.4
1	M	551	THR	5.2
1	M	117	GLY	5.2
1	A	348	ILE	5.2
1	A	302	ASN	5.0
1	A	237	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
1	M	336	LYS	4.9
1	M	465	ILE	4.8
1	A	293	ALA	4.7
1	M	349	PRO	4.6
1	A	326	GLU	4.6
1	A	305	SER	4.5
1	M	293	ALA	4.4
1	M	192	THR	4.4
1	M	330	PHE	4.4
1	M	337	ALA	4.4
1	M	491	ILE	4.3
1	M	461	GLU	4.3
1	A	341	VAL	4.2
1	M	292	GLN	4.2
1	M	193	GLY	4.0
1	M	544	ASP	4.0
1	A	238	GLY	4.0
1	M	548	LEU	3.9
1	A	350	VAL	3.8
1	M	490	ARG	3.8
1	A	347	PRO	3.7
1	M	75	TRP	3.7
1	A	327	ARG	3.7
1	A	340	GLY	3.7
1	M	247	CYS	3.6
1	M	187	ALA	3.6
1	M	378	GLY	3.6
1	M	246	GLY	3.5
1	M	234	ALA	3.5
1	A	315	ASP	3.5
1	A	337	ALA	3.5
1	A	314	LEU	3.4
1	M	324	LEU	3.4
1	A	329	PRO	3.4
1	A	351	ARG	3.4
1	A	253	ILE	3.3
1	M	243	MET	3.3
1	A	297	GLU	3.3
1	A	322	LYS	3.3
1	M	322	LYS	3.3
1	A	342	ASP	3.2
3	O	1	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	13	GLY	3.2
1	A	252	GLY	3.1
1	M	333	GLU	3.1
1	M	299	ARG	3.1
2	B	243	ARG	3.1
1	M	11	GLY	3.1
1	M	554	PHE	3.1
1	A	292	GLN	3.0
1	M	332	CYS	3.0
1	M	239	SER	3.0
1	A	290	VAL	3.0
1	M	45	THR	2.9
1	A	298	TRP	2.8
1	A	246	GLY	2.8
1	A	295	TRP	2.8
1	A	301	GLY	2.8
1	A	319	LEU	2.7
1	A	296	HIS	2.7
1	M	231	TYR	2.7
1	A	193	GLY	2.6
1	M	294	PHE	2.6
1	A	235	GLY	2.6
1	M	295	TRP	2.6
1	M	288	ASP	2.6
1	M	553	ALA	2.6
1	M	179	THR	2.5
1	M	63	GLU	2.5
4	P	0	MET	2.5
1	A	249	GLY	2.5
1	M	245	GLU	2.5
1	M	209	THR	2.5
1	M	0	MET	2.5
2	N	2	GLU	2.4
1	M	44	HIS	2.4
1	A	308	ARG	2.4
1	M	206	GLY	2.4
1	M	442	GLN	2.4
1	M	14	GLY	2.4
1	M	373	GLY	2.4
1	M	416	THR	2.4
1	M	183	ILE	2.3
1	A	318	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	227	GLU	2.3
2	N	6	LEU	2.3
1	M	72	GLY	2.3
1	M	538	GLY	2.3
1	A	239	SER	2.2
1	M	412	GLU	2.2
1	M	562	ARG	2.2
1	M	6	ASP	2.2
1	M	79	GLN	2.2
1	M	244	THR	2.2
1	M	296	HIS	2.2
1	A	250	GLU	2.2
1	M	305	SER	2.2
1	M	365	GLN	2.2
1	M	49	GLU	2.2
1	M	395	SER	2.2
1	A	313	TYR	2.2
1	M	191	ALA	2.1
1	M	522	ALA	2.1
1	M	290	VAL	2.1
1	M	379	GLU	2.1
1	M	7	LEU	2.1
1	A	294	PHE	2.1
2	N	88	MET	2.1
1	M	537	GLU	2.1
1	M	380	CYS	2.0
2	N	1	ALA	2.0
2	N	64	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

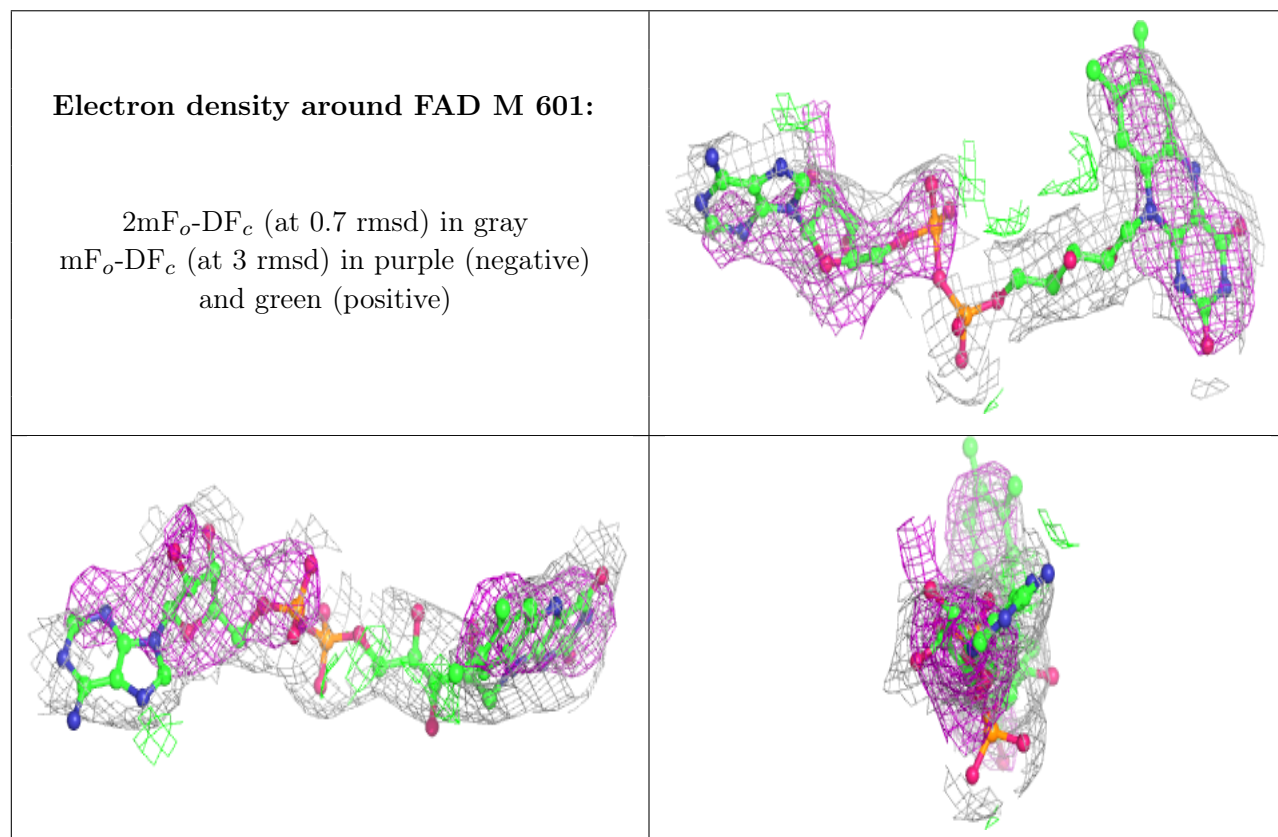
6.4 Ligands [i](#)

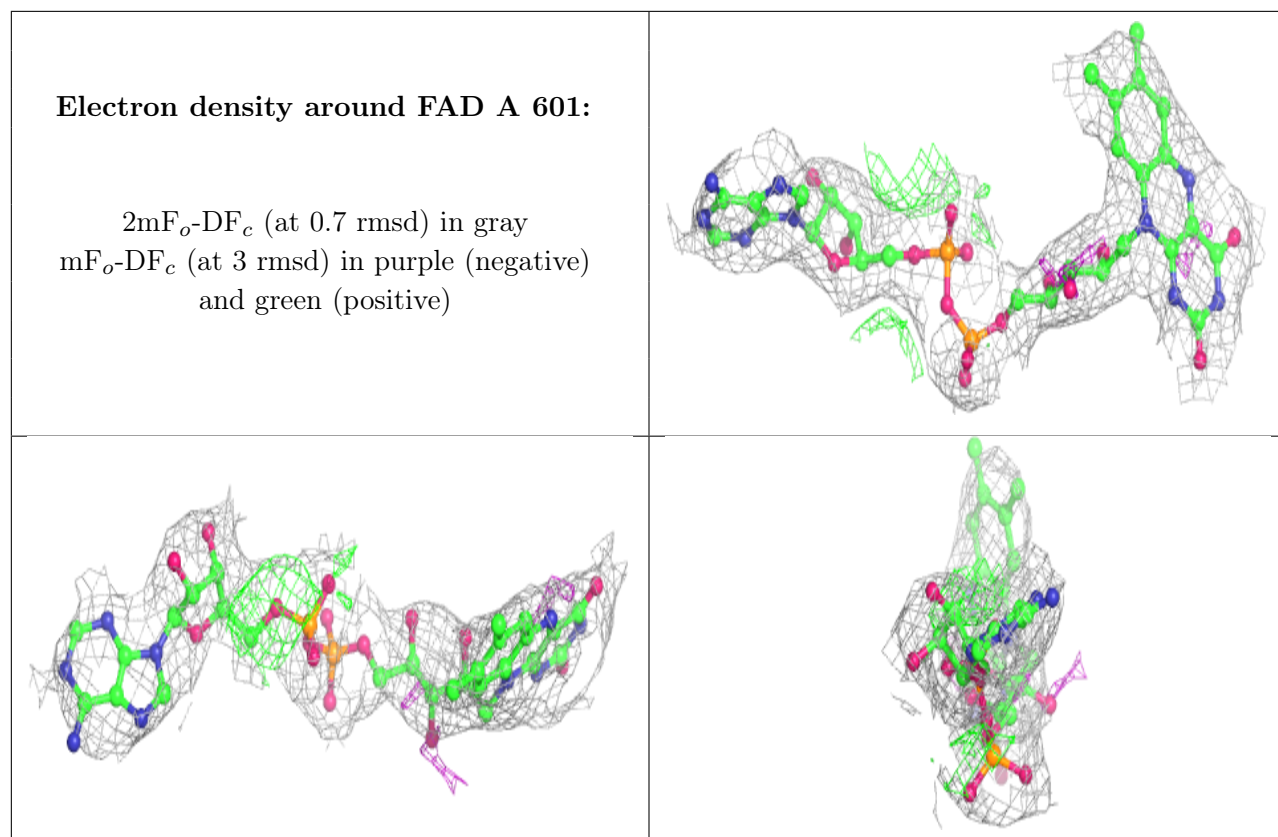
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	FAD	M	601	53/53	0.86	0.18	55,71,78,80	0
5	FAD	A	601	53/53	0.95	0.23	37,41,51,56	0
6	FES	N	244	4/4	0.98	0.21	123,126,146,154	0
6	FES	B	244	4/4	0.99	0.33	102,105,107,110	0
7	F3S	B	245	7/7	0.99	0.27	109,113,117,126	0
7	F3S	N	245	7/7	0.99	0.22	116,118,131,151	0
8	SF4	B	246	8/8	0.99	0.32	111,123,129,129	0
8	SF4	N	246	8/8	0.99	0.25	122,131,151,155	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.