Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:54 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

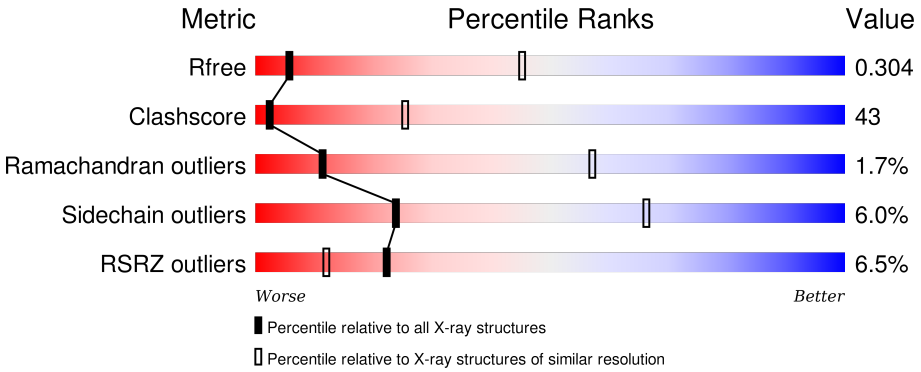
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1010 (3.82-3.50)
Clashscore	102246	1125 (3.82-3.50)
Ramachandran outliers	100387	1079 (3.82-3.50)
Sidechain outliers	100360	1078 (3.82-3.50)
RSRZ outliers	91569	1017 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	7% 42% 44% • 10%
1	M	602	14% 30% 50% • 16%
2	B	243	50% 47% •
2	N	243	2% 47% 49% •
3	C	130	42% 48% 8% •

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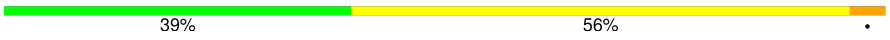
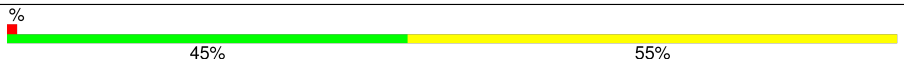
Mol	Chain	Length	Quality of chain
3	O	130	
4	D	119	
4	P	119	

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
6	F3S	B	245	-	-	-	X
7	SF4	B	246	-	-	X	X
8	FAD	M	601	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15746 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4140	2576	752	783	29			
1	M	504	Total	C	N	O	S	0	0	0
			3718	2295	682	715	26			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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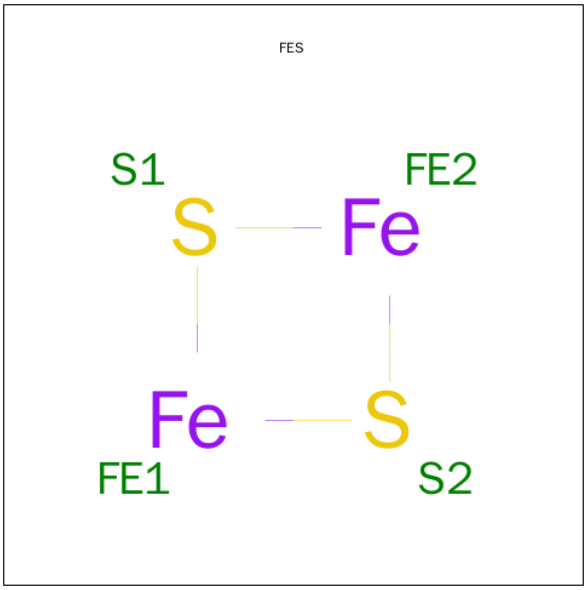
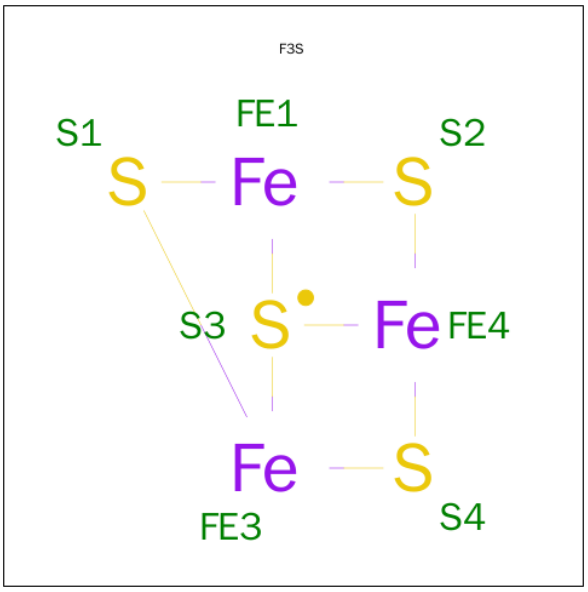
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



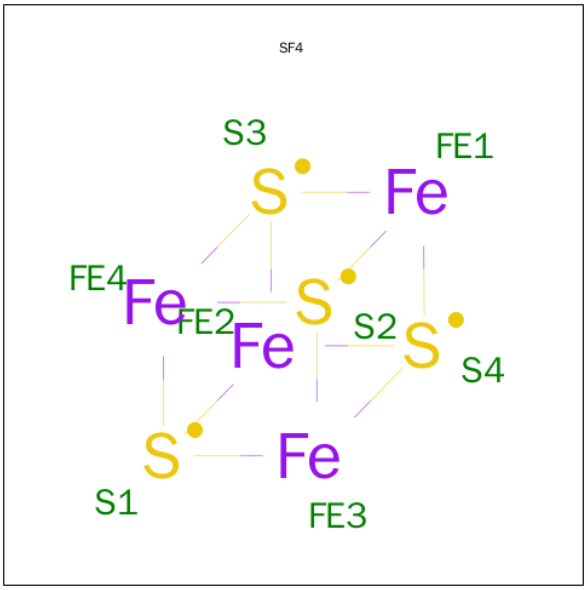
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	Fe	S		0	0
			4	2	2			
5	N	1	Total	Fe	S		0	0
			4	2	2			

- Molecule 6 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



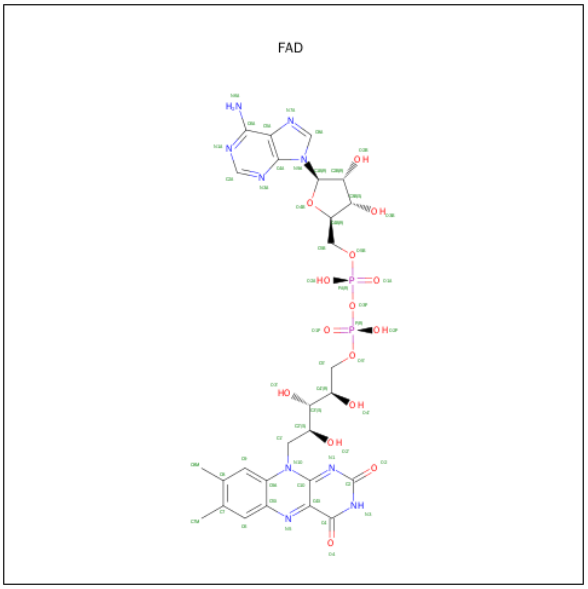
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Fe S 7 3 4	0	0
6	N	1	Total Fe S 7 3 4	0	0

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



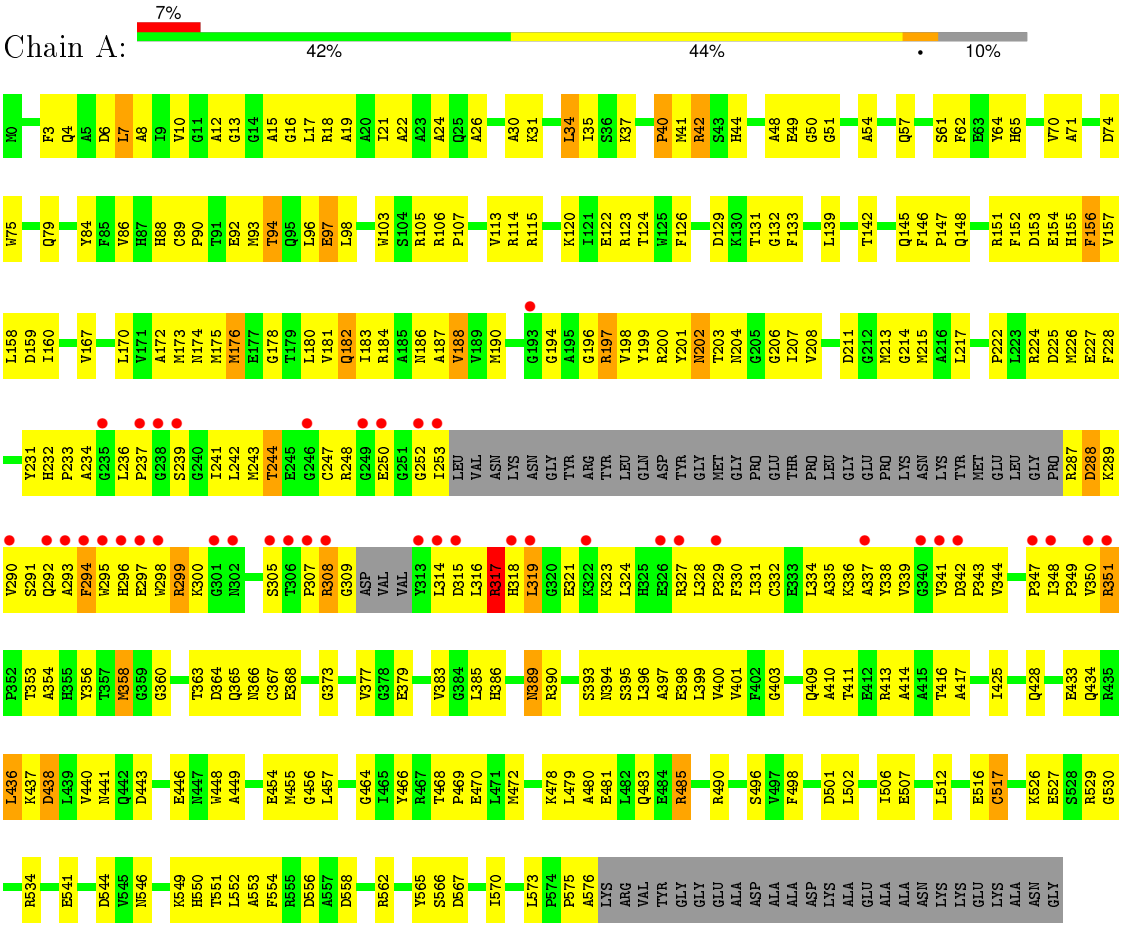
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
8	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

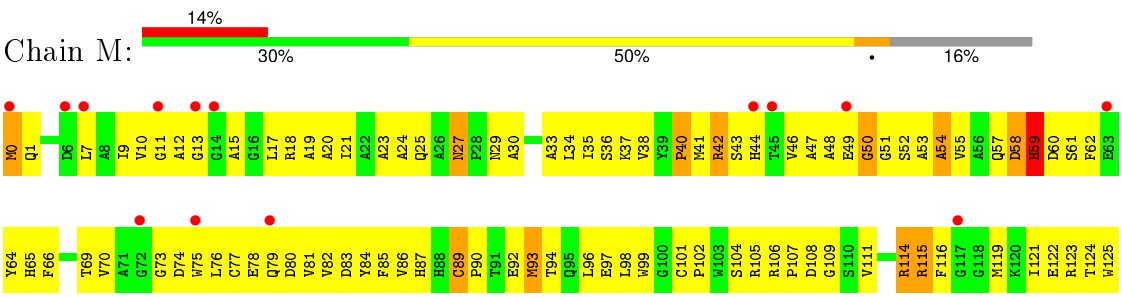
- Molecule 1: Fumarate reductase flavoprotein subunit

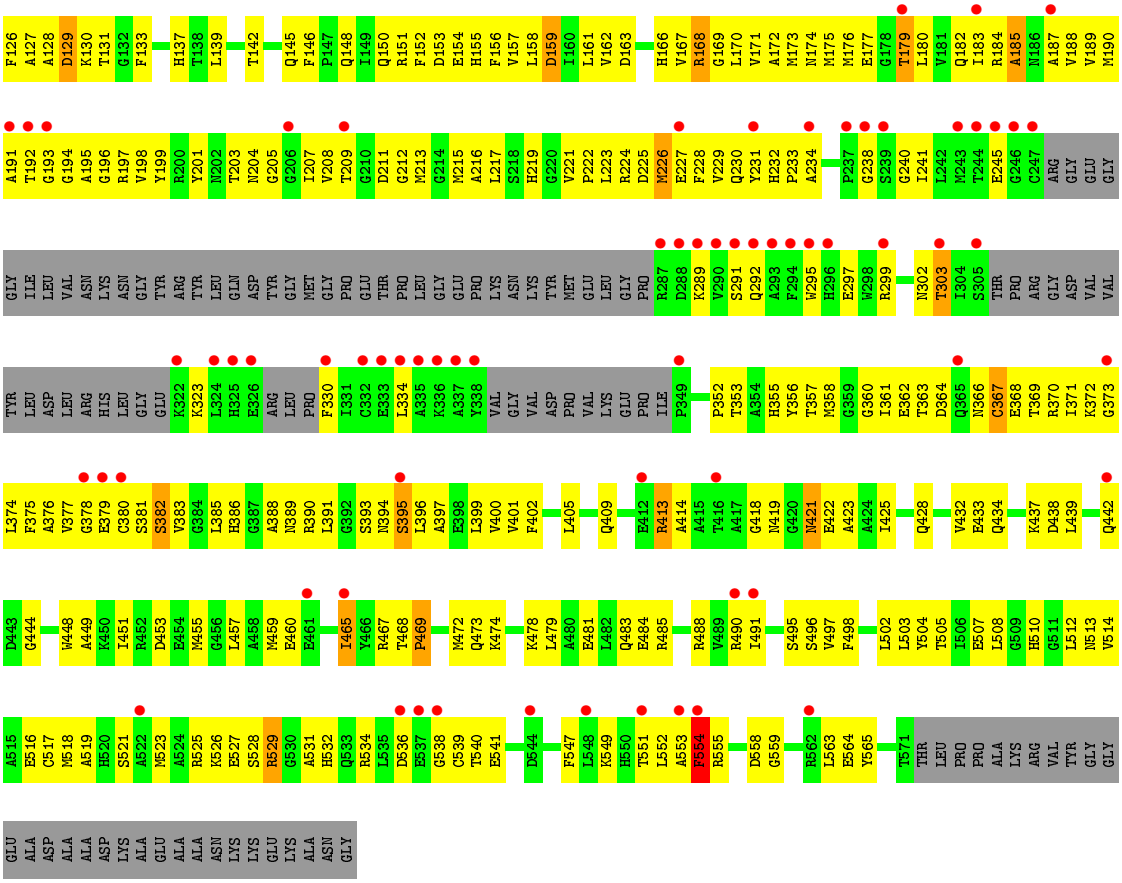
Chain A:



- Molecule 1: Fumarate reductase flavoprotein subunit

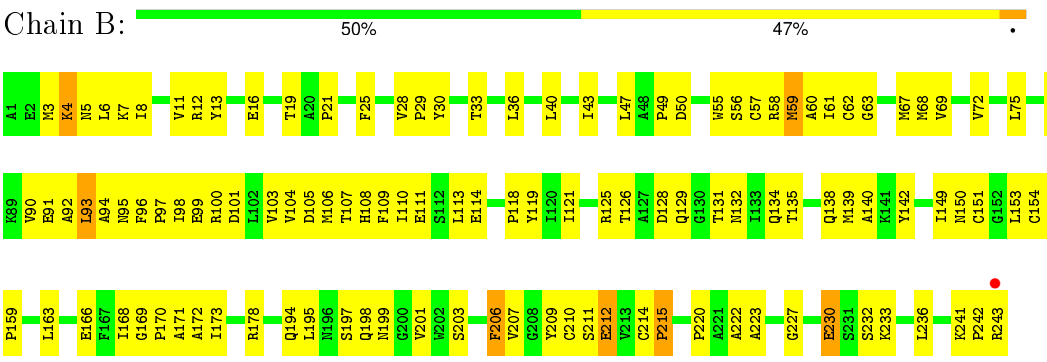
Chain M:





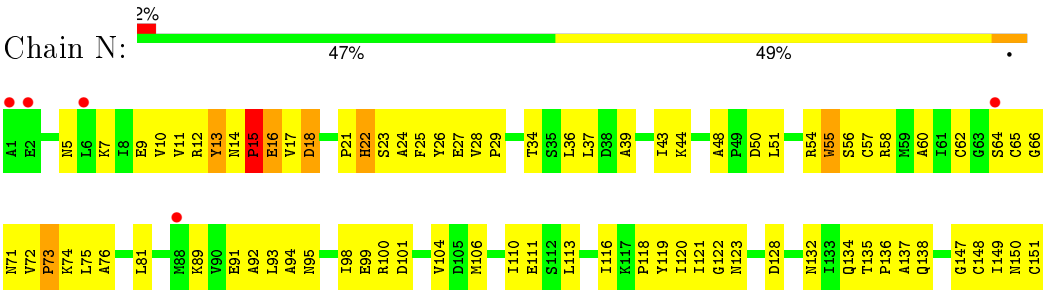
• Molecule 2: Fumarate reductase iron-sulfur subunit

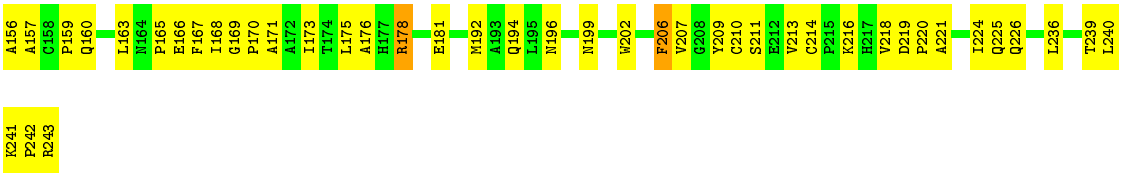
Chain B:



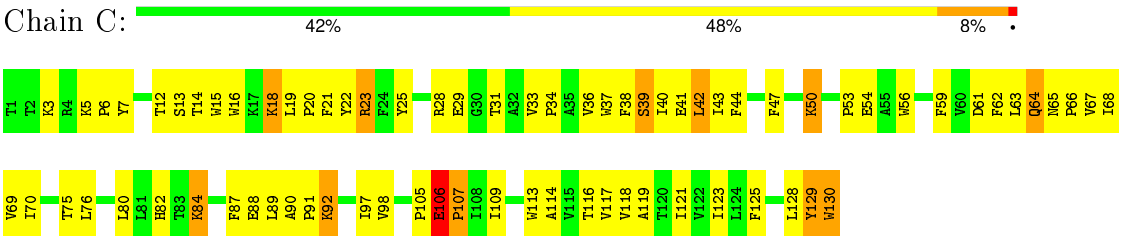
• Molecule 2: Fumarate reductase iron-sulfur subunit

Chain N:

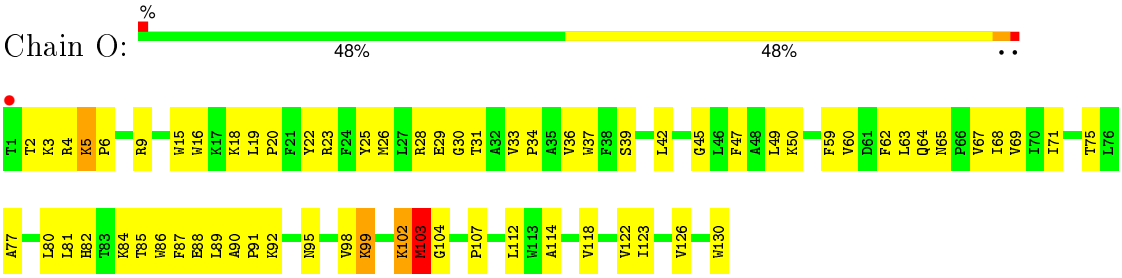




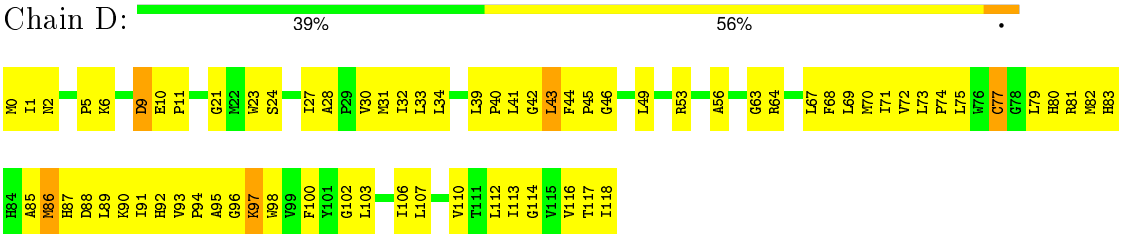
- Molecule 3: Fumarate reductase subunit C



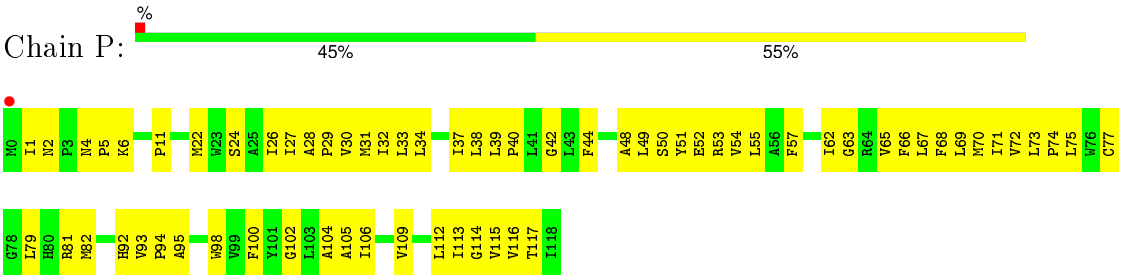
- Molecule 3: Fumarate reductase subunit C



- Molecule 4: Fumarate reductase subunit D



- Molecule 4: Fumarate reductase subunit D



4 Data and refinement statistics (i)

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)	2.0 (266.00-3.65) 78.8 (42.62-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.39	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.296 0.260 , 0.304	Depositor DCC
R_{free} test set	761 reflections (2.41%)	DCC
Wilson B-factor (Å^2)	79.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 78.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 53063 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	15746	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SF4, F3S, FES, 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	0.56	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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	B	4	0	0	1	0
5	N	4	0	0	1	0
6	B	7	0	0	1	0
6	N	7	0	0	1	0
7	B	8	0	0	2	0
7	N	8	0	0	1	0
8	A	53	0	31	12	0
8	M	53	0	31	26	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	8:A:601:FAD:C8M	1.77	1.48
1:M:44:HIS:NE2	8: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	8:M:601:FAD:HM82	1.09	1.39
2:B:4:LYS:NZ	2:B:4:LYS:H	1.17	1.38
2:B:4:LYS:HZ2	2:B:4:LYS:N	1.20	1.35
1:A:44:HIS:NE2	8: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	8: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	8: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	8: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:HH11	1:M:115:ARG:CG	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:CE	2.48	0.96
1:A:330:PHE:CZ	2:B:59:MET:HE2	2.00	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
2:N:15:PRO:O	3:O:5:LYS:NZ	1.99	0.94
1:A:12:ALA:HB1	1:A:17:LEU:HD21	1.49	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
1:M:115:ARG:CB	1:M:115:ARG:NH1	2.35	0.89
2:B:206:PHE:CZ	3:C:89:LEU:HD22	2.08	0.89
1:M:13:GLY:HA3	8: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:332:CYS:SG	1:A:343:PRO:HB2	2.12	0.89
1:A:44:HIS:NE2	8:A:601:FAD:HM81	1.87	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
2:N:192:MET:HB3	2:N:196:ASN:HD21	1.36	0.88
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.55	0.88
3:O:19:LEU:HD21	3:O:22:TYR:CD2	2.09	0.88
1:M:527:GLU:OE2	1:M:529:ARG:NH1	2.07	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
2:B:68:MET:HE2	2:B:94:ALA:HB2	1.55	0.87
1:A:288:ASP:O	1:A:292:GLN:HB2	1.72	0.87
1:A:105:ARG:HH12	2:B:134:GLN:HB3	1.33	0.87

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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
1:M:12:ALA:HA	1:M:17:LEU:HD11	1.58	0.86
3:C:5:LYS:O	3:C:5:LYS:HG3	1.73	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:HA	2:N:106:MET:HE2	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	8: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:330:PHE:CZ	2:B:59:MET:HB2	2.15	0.81
1:A:244:THR:HG22	1:A:328:LEU:HD22	1.63	0.81
1:M:366:ASN:HB3	1:M:409:GLN:HE21	1.44	0.81
1:M:465:ILE:O	1:M:465:ILE:HG22	1.77	0.81
1:M:166:HIS:HB3	1:M:168:ARG:NH1	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:ARG:NE	2:B:101:ASP:OD2	2.13	0.81
1:A:89:CYS:HB2	1:A:90:PRO:HD3	1.61	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
1:M:44:HIS:NE2	8:M:601:FAD:HM81	1.95	0.81
2:B:68:MET:SD	2:B:94:ALA:HB2	2.20	0.81
1:A:244:THR:CG2	1:A:328:LEU:HD22	2.11	0.80
1:M:114:ARG:NH2	1:M:128:ALA:O	2.15	0.80
1:A:437:LYS:O	1:A:441:ASN:ND2	2.14	0.80
2:N:16:GLU:HG2	3:O:5:LYS:HZ3	1.45	0.80
1:M:44:HIS:N	8: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
1:M:363:THR:HA	1:M:368:GLU:O	1.83	0.79
3:C:113:TRP:O	3:C:117:VAL:HG23	1.82	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
2:N:17:VAL:HG12	2:N:18:ASP:OD2	1.84	0.77
2:B:109:PHE:CE2	2:B:113:LEU:HD11	2.19	0.77
1:A:316:LEU:O	1:A:319:LEU:N	2.16	0.77
1:A:250:GLU:HB3	1:A:323:LYS:NZ	1.98	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
1:M:11:GLY:HA2	8:M:601:FAD:O4B	1.85	0.77
2:B:4:LYS:CE	2:B:4:LYS:N	2.48	0.77
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.20	0.77
1:M:199:TYR:OH	1:M:229:VAL:HG21	1.85	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	8:M:601:FAD:C8	2.48	0.76
1:M:54:ALA:HB3	1:M:125:TRP:CD1	2.19	0.76
1:M:50:GLY:HA2	1:M:131:THR:CB	2.16	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
3:O:50:LYS:HD2	4:P:117:THR:HG22	1.68	0.76
2:N:216:LYS:HE2	2:N:216:LYS:HA	1.66	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: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:337:ALA:HB1	2:B:80:PHE:CZ	2.21	0.75
1:M:370:ARG:HH22	1:M:554:PHE:HE2	1.34	0.75
1:A:170:LEU:CD2	1:A:183:ILE:HB	2.17	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
1:M:391:LEU:O	1:M:394:ASN:HB2	1.87	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
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:CZ	1:M:115:ARG:HB2	2.17	0.74
2:B:207:VAL:HG22	3:C:25:TYR:CE1	2.21	0.74
1:A:330:PHE:CZ	2:B:59:MET:HE3	2.15	0.74
1:A:244:THR:CG2	1:A:328:LEU:CD2	2.66	0.74
1:M:52:SER:O	1:M:125:TRP:N	2.19	0.74
4:D:112:LEU:HG	4:D:116:VAL:HG11	1.69	0.74
4:D:71:ILE:O	4:D:75:LEU:HG	1.87	0.74
1:M:177:GLU:CB	1:M:179:THR:HG23	2.17	0.73
2:B:212:GLU:HG3	3:C:21:PHE:HE2	1.53	0.73
1:A:151:ARG:NH1	1:A:153:ASP:OD1	2.19	0.73
3:C:50:LYS:HE3	3:C:50:LYS:HA	1.68	0.73
1:A:324:LEU:CD1	1:A:344:VAL:HG22	2.19	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:M:364:ASP:OD2	1:M:368:GLU:HB3	1.87	0.73
1:A:316:LEU:O	1:A:319:LEU:HB2	1.87	0.73
1:A:241:ILE:HD13	1:A:334:LEU:HB3	1.71	0.73
1:A:335:ALA:O	1:A:339:VAL:HG22	1.89	0.72
1:A:292:GLN:HG3	1:A:466:TYR:CE1	2.24	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
1:M:194:GLY:HA2	1:M:379:GLU:HG2	1.71	0.72
3:C:63:LEU:HD23	3:C:68:ILE:HG21	1.72	0.72
1:A:208:VAL:O	1:A:208:VAL:HG12	1.89	0.72
1:A:105:ARG:HH12	2:B:134:GLN:CB	2.02	0.72
2:N:169:GLY:O	2:N:173:ILE:HG13	1.90	0.72
1:M:455:MET:SD	1:M:512:LEU:HD23	2.29	0.72
1:M:24:ALA:HA	1:M:148:GLN:HE22	1.54	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:M:191:ALA:O	8:M:601:FAD:H52A	1.90	0.71
1:A:42:ARG:HD2	1:A:42:ARG:N	2.05	0.71
1:M:397:ALA:O	1:M:401:VAL:HG23	1.89	0.71
1:A:203:THR:OG1	8: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:526:LYS:HA	1:A:534:ARG:NH1	2.07	0.70
1:A:200:ARG:HD3	1:A:201:TYR:CE1	2.26	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:360:GLY:H	1:M:382:SER:HB2	1.56	0.70
1:M:33:ALA:HA	1:M:150:GLN:O	1.92	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:M:50:GLY:HA2	1:M:131:THR:OG1	1.92	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:15:ALA:HA	1:M:399:LEU:O	1.93	0.69
1:A:234:ALA:CB	1:A:243:MET:HB2	2.23	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:467:ARG:HH11	1:M:532:HIS:HA	1.56	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:96:LEU:HD21	1:M:139:LEU:HD21	1.74	0.69
2:B:215:PRO:HD2	7:B:246:SF4:S3	2.32	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:68:MET:CE	2:B:94:ALA:CB	2.70	0.69
1:M:57:GLN:O	1:M:60:ASP:HB3	1.94	0.68
2:B:168:ILE:HD11	2:B:173:ILE:HG12	1.74	0.68
1:M:1:GLN:O	1:M:182:GLN:N	2.21	0.68
1:M:58:ASP:C	1:M:60:ASP:H	1.97	0.68
3:C:130:TRP:N	3:C:130:TRP:CD1	2.59	0.68
1:A:446:GLU:CD	1:A:485:ARG:HD3	2.13	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:M:163:ASP:HB3	1:M:168:ARG:HD2	1.75	0.68
1:A:250:GLU:HB3	1:A:323:LYS:HZ1	1.56	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:M:13:GLY:CA	8:M:601:FAD:O1P	2.41	0.68
1:M:177:GLU:HB3	1:M:179:THR:CG2	2.24	0.68
1:A:436:LEU:O	1:A:440:VAL:HG23	1.94	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
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
2:B:157:ALA:HB1	2:B:209:TYR:CD2	2.29	0.67
2:B:57:CYS:O	2:B:58:ARG:HB2	1.94	0.66
1:M:485:ARG:HG2	1:M:488:ARG:NH2	2.10	0.66
4:D:10:GLU:N	4:D:11:PRO:HD2	2.10	0.66
4:P:102:GLY:O	4:P:106:ILE:HG13	1.95	0.66
1:A:434:GLN:NE2	1:A:434:GLN:HA	2.10	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
1:M:27:ASN:HB3	1:M:30:ALA:HB2	1.77	0.66
4:D:41:LEU:HB2	4:D:43:LEU:CD1	2.25	0.66
1:M:116:PHE:CE2	1:M:245:GLU:CB	2.79	0.66
1:M:0:MET:HE2	1:M:180:LEU:CD1	2.26	0.66
3:O:50:LYS:NZ	4:P:117:THR:HG21	2.11	0.66
2:N:68:MET:CE	2:N:73:PRO:HD3	2.25	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
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
1:M:116:PHE:HE2	1:M:245:GLU:CB	2.09	0.65
1:M:413:ARG:NH1	1:M:413:ARG:HB2	2.11	0.65
1:M:168:ARG:HD3	1:M:425:ILE:CG1	2.24	0.65
2:N:211:SER:HA	2:N:220:PRO:HD2	1.78	0.65
4:D:39:LEU:HB2	4:D:49:LEU:HD13	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:115:ARG:HB2	1:M:115:ARG:NH1	2.11	0.65
1:M:508:LEU:O	1:M:512:LEU:HG	1.97	0.65
2:B:211:SER:HA	2:B:220:PRO:HD2	1.76	0.65
1:A:351:ARG:HA	1:A:351:ARG:NE	2.09	0.65
1:A:97:GLU:HG3	1:A:98:LEU:N	2.11	0.65
1:M:54:ALA:HB3	1:M:125:TRP:NE1	2.11	0.65
1:A:206:GLY:HA3	2:B:55:TRP:CH2	2.31	0.65
3:O:50:LYS:HD2	4:P:117:THR:CG2	2.26	0.65
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.30	0.65
1:M:53:ALA:HA	1:M:124:THR:HA	1.79	0.65
1:M:0:MET:CE	1:M:171:VAL:CG1	2.74	0.65
4:D:93:VAL:O	2:N:243:ARG:O	2.15	0.65
1:M:133:PHE:CE2	2:N:147:GLY:HA2	2.32	0.65
4:D:106:ILE:O	4:D:110:VAL:HG23	1.96	0.65
1:A:469:PRO:HD2	1:A:470:GLU:H	1.60	0.65
1:M:0:MET:HE2	1:M:180:LEU:HD13	1.79	0.65
3:C:125:PHE:CE1	3:C:129:TYR:CE2	2.81	0.65
1:M:78:GLU:O	1:M:81:VAL:HG22	1.97	0.65
1:M:170:LEU:HD12	1:M:170:LEU:C	2.17	0.65
2:B:57:CYS:SG	2:B:59:MET:N	2.64	0.65
1:A:213:MET:CE	1:A:360:GLY:HA2	2.24	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
2:N:211:SER:OG	2:N:220:PRO:HD2	1.97	0.64
2:B:214:CYS:HA	7:B:246:SF4:S3	2.37	0.64
1:A:133:PHE:CE1	2:B:149:ILE:HG22	2.32	0.64
3:O:28:ARG:HD2	4:P:81:ARG:NH2	2.13	0.64
1:M:241:ILE:CB	1:M:334:LEU:CB	2.75	0.64
1:A:386:HIS:ND1	1:A:390:ARG:HG3	2.12	0.64
1:M:176:MET:HG3	3:O:4:ARG:HD3	1.79	0.64
1:M:497:VAL:CG2	2:N:15:PRO:HG3	2.11	0.64
1:M:361:ILE:HG22	1:M:362:GLU:N	2.13	0.64
1:M:145:GLN:HG3	1:M:146:PHE:CE1	2.31	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
1:M:0:MET:CE	1:M:171:VAL:HG13	2.27	0.64
3:C:125:PHE:HD1	3:C:129:TYR:CE1	2.16	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:N:36:LEU:HD23	2:N:76:ALA:HA	1.81	0.63
2:B:236:LEU:HD23	2:B:236:LEU:C	2.19	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
4:P:31:MET:HG3	4:P:70:MET:SD	2.39	0.63
1:M:297:GLU:O	1:M:303:THR:N	2.31	0.63
3:O:123:ILE:HD12	4:P:30:VAL:HG11	1.81	0.63
1:A:351:ARG:HE	1:A:351:ARG:HA	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:295:TRP:O	1:M:299:ARG:CB	2.47	0.63
1:M:106:ARG:HB3	1:M:108:ASP:OD2	1.99	0.63
1:A:324:LEU:HD13	1:A:344:VAL:HG22	1.81	0.62
1:A:287:ARG:C	1:A:289:LYS:N	2.52	0.62
1:A:10:VAL:HG11	1:A:190:MET:SD	2.39	0.62
1:M:92:GLU:HG3	1:M:401:VAL:HA	1.80	0.62
2:B:157:ALA:O	2:B:159:PRO:HD3	1.99	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
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:37:LYS:HE3	1:A:207:ILE:HG22	1.80	0.62
1:M:24:ALA:HA	1:M:148:GLN:NE2	2.15	0.62
1:A:364:ASP:OD1	1:A:368:GLU:N	2.33	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:HE3	2:B:4:LYS:N	2.15	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:168:ARG:HD3	1:M:425:ILE:CD1	2.29	0.61
1:M:42:ARG:N	1:M:42:ARG:HD2	2.15	0.61
1:A:293:ALA:O	1:A:297:GLU:HG3	2.00	0.61
2:N:211:SER:HB3	2:N:219:ASP:HA	1.83	0.61
3:O:126:VAL:HA	3:O:130:TRP:HB3	1.82	0.61
1:A:446:GLU:OE1	1:A:485:ARG:HD3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:LEU:O	2:B:36:LEU:HD12	2.00	0.61
1:M:213:MET:O	1:M:217:LEU:HB2	2.00	0.61
1:M:421:ASN:O	1:M:425:ILE:HG13	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
3:O:29:GLU:O	3:O:31:THR:N	2.33	0.61
2:B:125:ARG:HD2	2:B:132:ASN:OD1	2.00	0.61
4:P:63:GLY:O	4:P:67:LEU:HG	2.00	0.61
3:C:37:TRP:O	3:C:41:GLU:HG3	2.00	0.61
2:B:57:CYS:HB3	2:B:62:CYS:CB	2.24	0.61
4:P:70:MET:O	4:P:74:PRO:HG2	2.00	0.61
3:C:98:VAL:O	3:C:98:VAL:HG23	1.99	0.61
1:M:232:HIS:O	1:M:234:ALA:N	2.34	0.61
3:O:49:LEU:HG	4:P:55:LEU:HD13	1.81	0.61
1:M:504:TYR:HA	1:M:507:GLU:OE1	2.01	0.61
1:M:70:VAL:HA	1:M:77:CYS:SG	2.40	0.61
1:A:411:THR:O	1:A:414:ALA:HB3	2.00	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:416:THR:O	1:A:416:THR:HG22	2.01	0.60
1:A:105:ARG:NH1	2:B:134:GLN:CB	2.54	0.60
1:M:115:ARG:CZ	1:M:115:ARG:CB	2.79	0.60
1:A:363:THR:OG1	1:A:383:VAL:HA	2.00	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
2:N:211:SER:CA	2:N:220:PRO:HD2	2.31	0.60
1:M:377:VAL:CA	1:M:381:SER:HB3	2.32	0.60
2:N:54:ARG:O	2:N:55:TRP:HB3	2.01	0.60
1:A:199:TYR:O	1:A:202:ASN:ND2	2.35	0.60
1:M:421:ASN:HD22	1:M:422:GLU:N	1.99	0.60
1:M:208:VAL:HG12	1:M:208:VAL:O	2.01	0.60
1:M:35:ILE:CG2	1:M:155:HIS:HB2	2.32	0.60
3:C:90:ALA:HB3	3:C:91:PRO:HD3	1.81	0.60
1:M:157:VAL:HG12	1:M:158:LEU:N	2.17	0.60
1:M:413:ARG:HH11	1:M:413:ARG:HB2	1.66	0.60
1:A:92:GLU:HB3	1:A:400:VAL:CG1	2.32	0.60
1:M:377:VAL:HG22	1:M:378:GLY:H	1.67	0.60
1:A:468:THR:O	1:A:472:MET:HG3	2.02	0.60
1:M:209:THR:HG21	1:M:507:GLU:CA	2.32	0.60
1:M:395:SER:HG	8:M:601:FAD:H2'	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:168:ARG:HD3	1:M:425:ILE:HD11	1.83	0.60
1:M:9:ILE:HG23	1:M:189:VAL:HB	1.84	0.59
1:M:421:ASN:HD22	1:M:422:GLU:H	1.50	0.59
1:M:194:GLY:CA	1:M:379:GLU:CG	2.79	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
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
3:C:38:PHE:HA	3:C:41:GLU:OE1	2.01	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:M:157:VAL:HG13	1:M:171:VAL:O	2.02	0.59
2:B:241:LYS:HG2	2:B:243:ARG:HB2	1.84	0.59
1:A:455:MET:SD	1:A:512:LEU:HD23	2.43	0.59
1:M:176:MET:O	1:M:497:VAL:HA	2.02	0.59
3:C:13:SER:HA	4:D:90:LYS:HD3	1.85	0.59
1:A:293:ALA:HA	1:A:296:HIS:CE1	2.38	0.59
1:M:175:MET:O	1:M:498:PHE:HA	2.03	0.59
1:A:395:SER:OG	8: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
2:B:134:GLN:HA	2:B:138:GLN:OE1	2.03	0.59
1:A:200:ARG:HB2	1:A:456:GLY:C	2.23	0.59
1:M:230:GLN:O	1:M:355:HIS:HB3	2.02	0.59
1:M:48:ALA:HA	8: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
2:B:8:ILE:HD11	2:B:81:LEU:HD13	1.85	0.58
4:D:117:THR:O	4:D:118:ILE:HG23	2.04	0.58
1:M:503:LEU:O	1:M:507:GLU:HG3	2.02	0.58
1:A:366:ASN:HB3	1:A:409:GLN:HG3	1.86	0.58
1:M:74:ASP:HB2	1:M:388:ALA:HB3	1.85	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:OD2	1:M:129:ASP:N	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
3:O:84:LYS:HG3	3:O:85:THR:N	2.19	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
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
2:B:104:VAL:HG22	2:B:105:ASP:N	2.18	0.58
1:M:413:ARG:CB	1:M:413:ARG:HH11	2.17	0.58
1:A:433:GLU:HG2	1:A:437:LYS:HE3	1.85	0.58
1:M:201:TYR:CE2	1:M:238:GLY:HA2	2.39	0.58
4:D:2:ASN:HD21	4:P:4:ASN:HD22	1.51	0.58
1:A:236:LEU:HD12	1:A:349:PRO:O	2.03	0.57
2:N:167:PHE:CE2	2:N:169:GLY:HA2	2.39	0.57
1:M:223:LEU:HB3	1:M:226:MET:CG	2.34	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
2:B:57:CYS:SG	2:B:60:ALA:N	2.77	0.57
1:M:43:SER:HB3	8:M:601:FAD:O2A	2.05	0.57
2:B:68:MET:O	2:B:90:VAL:HA	2.04	0.57
1:A:469:PRO:CD	1:A:470:GLU:H	2.17	0.57
2:N:175:LEU:O	2:N:178:ARG:HB3	2.03	0.57
1:A:550:HIS:HB2	1:A:566:SER:OG	2.05	0.57
2:B:197:SER:HB3	4:D:5:PRO:HB2	1.87	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
1:M:157:VAL:HG22	1:M:172:ALA:HB2	1.87	0.57
2:B:166:GLU:O	2:B:199:ASN:HB3	2.03	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
2:B:104:VAL:CG2	2:B:105:ASP:N	2.67	0.57
2:B:12:ARG:HE	2:B:101:ASP:CG	2.05	0.57
3:C:117:VAL:O	3:C:121:ILE:HD13	2.04	0.57
4:P:28:ALA:HB3	4:P:29:PRO:HD3	1.86	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:M:433:GLU:HG2	1:M:437:LYS:NZ	2.20	0.57
1:M:467:ARG:HB3	1:M:472:MET:HE2	1.87	0.57
4:D:95:ALA:HB2	2:N:239:THR:HG22	1.87	0.57
4:D:33:LEU:HG	4:D:34:LEU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:HIS:ND1	1:A:233:PRO:HD2	2.20	0.57
1:A:92:GLU:HB3	1:A:400:VAL:HG12	1.87	0.57
2:N:206:PHE:O	2:N:206:PHE:CD2	2.57	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
1:M:13:GLY:HA3	8:M:601:FAD:P	2.44	0.56
1:M:168:ARG:HA	1:M:185:ALA:O	2.05	0.56
3:C:114:ALA:O	3:C:118:VAL:HG23	2.06	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
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: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
2:N:16:GLU:HA	2:N:18:ASP:O	2.05	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:241:LYS:HG3	2:N:242:PRO:N	2.19	0.56
1:A:114:ARG:HG2	1:A:126:PHE:CD2	2.41	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
1:M:201:TYR:HE2	1:M:238:GLY:HA2	1.70	0.56
1:M:358:MET:HE3	1:M:389:ASN:CA	2.26	0.56
4:D:112:LEU:HG	4:D:116:VAL:CG1	2.35	0.56
2:N:181:GLU:OE2	2:N:181:GLU:HA	2.05	0.56
1:M:478:LYS:O	1:M:481:GLU:HB3	2.06	0.56
1:A:30:ALA:O	1:A:148:GLN: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:M:176:MET:CG	3:O:4:ARG:HD3	2.35	0.56
1:A:35:ILE:HG23	1:A:155:HIS:HB2	1.88	0.56
1:M:232:HIS:C	1:M:234:ALA:H	2.07	0.56
2:N:14:ASN:HA	2:N:100:ARG:HD3	1.87	0.56
4:D:113:ILE:HA	4:D:116:VAL:HG22	1.87	0.56
3:C:12:THR:CG2	3:C:13:SER:N	2.68	0.56
2:N:73:PRO:HB3	2:N:153:LEU:HD22	1.88	0.56
1:A:242:LEU:HD12	8: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:M:497:VAL:O	2:N:100:ARG:NH1	2.40	0.55
1:M:358:MET:HE1	1:M:390:ARG:H	1.68	0.55
1:M:356:TYR:CG	1:M:357:THR:N	2.74	0.55
2:B:50:ASP:O	2:B:100:ARG:NH2	2.33	0.55
1:M:532:HIS:HE2	1:M:534:ARG:HD2	1.72	0.55
1:M:41:MET:HG3	2:N:150:ASN:HD22	1.69	0.55
1:A:133:PHE:HE1	2:B:149:ILE:HG22	1.70	0.55
1:M:502:LEU:O	1:M:505:THR:HB	2.06	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:M:66:PHE:HD1	1:M:82:VAL:HG12	1.71	0.55
1:A:309:GLY:HA3	1:A:351:ARG:HB2	1.88	0.55
1:M:373:GLY:HA2	1:M:413:ARG:HG2	1.89	0.55
3:C:50:LYS:HD3	4:D:118:ILE:CD1	2.36	0.55
1:M:29:ASN:O	1:M:29:ASN:OD1	2.24	0.55
3:O:86:TRP:HE1	4:P:22:MET:HE2	1.70	0.55
1:A:158:LEU:HD11	1:A:173:MET:HG3	1.86	0.55
1:M:84:TYR:CE2	1:M:405:LEU:HD22	2.41	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	8:A:601:FAD:N1	2.21	0.55
1:M:364:ASP:H	1:M:368:GLU:H	1.55	0.55
2:N:155:TYR:CZ	2:N:169:GLY:HA3	2.42	0.55
2:N:37:LEU:CD2	2:N:58:ARG:HG2	2.37	0.55
4:D:24:SER:O	4:D:28:ALA:HB3	2.06	0.55
2:N:99:GLU:OE2	3:O:6:PRO:HB3	2.07	0.55
1:A:366:ASN:O	1:A:367:CYS:HB2	2.06	0.55
1:M:527:GLU:CD	1:M:529:ARG:HH11	2.09	0.55
1:M:295:TRP:O	1:M:299:ARG:N	2.37	0.55
1:M:192:THR:HA	8:M:601:FAD:O4B	2.07	0.55
3:C:5:LYS:HG2	3:C:5:LYS:O	2.05	0.55
2:B:75:LEU:HD21	2:B:153:LEU:HD11	1.88	0.55
1:M:162:VAL:HG21	1:M:371:ILE:HD13	1.89	0.55
1:A:478:LYS:O	1:A:481:GLU:HB3	2.06	0.55
2:B:142:TYR:CD1	2:B:142:TYR:C	2.80	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
1:M:10:VAL:HG12	1:M:192:THR:HG22	1.89	0.54
1:M:213:MET:HB3	1:M:223:LEU:HD21	1.88	0.54
2:B:157:ALA:HB1	2:B:209:TYR:HD2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:183:ILE:N	1:M:183:ILE:HD12	2.23	0.54
1:A:204:ASN:N	1:A:204:ASN:ND2	2.54	0.54
1:A:48:ALA:HB3	1:A:132:GLY:HA3	1.89	0.54
1:A:198:VAL:HG13	1:A:199:TYR:CD1	2.42	0.54
1:M:358:MET:SD	1:M:390:ARG:N	2.81	0.54
1:M:490:ARG:HG2	1:M:491:ILE:N	2.21	0.54
1:M: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:M:106:ARG:O	1:M:108:ASP:N	2.41	0.54
1:A:575:PRO:O	1:A:576:ALA:HB2	2.07	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
1:A:176:MET:HE3	2:B:99:GLU:HG3	1.90	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: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
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.90	0.54
2:B:93:LEU:HD12	2:B:94:ALA:N	2.23	0.54
2:B:11:VAL:CG2	2:B:91:GLU:HG2	2.38	0.54
1:M:188:VAL:O	1:M:374:LEU:HD12	2.08	0.54
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:324:LEU:HD12	1:A:344:VAL:HG22	1.91	0.53
4:D:63:GLY:O	4:D:67:LEU:HD23	2.09	0.53
2:B:126:THR:H	2:B:129:GLN:HG3	1.73	0.53
1:M:358:MET:SD	1:M:390:ARG:HB2	2.48	0.53
2:B:206:PHE:CD2	2:B:206:PHE:C	2.80	0.53
2:B:81:LEU:HD22	2:B:88:MET:SD	2.49	0.53
1:A:167:VAL:HG21	1:A:188:VAL:CG2	2.38	0.53
2:N:70:ASN:O	2:N:71:ASN:HB2	2.08	0.53
1:M:11:GLY:HA3	1:M:191:ALA:O	2.08	0.53
1:M:379:GLU:HG2	1:M:379:GLU:O	2.08	0.53
1:A: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: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
2:N:106:MET:CE	2:N:106:MET:CA	2.85	0.53
1:M:555:ARG:HE	1:M:559:GLY:HA2	1.73	0.53
2:N:157:ALA:HB2	2:N:213:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:CD2	8:A:601:FAD:C8M	2.80	0.53
3:O:2:THR:OG1	3:O:4:ARG:HG2	2.09	0.53
1:M:55:VAL:HG13	1:M:60:ASP:OD1	2.08	0.53
1:A:89:CYS:O	1:A:93:MET:HG2	2.08	0.53
2:N:44:LYS:HD3	2:N:51:LEU:O	2.09	0.53
1:A:186:ASN:HB3	1:A:417:ALA:CB	2.39	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:7:LEU:C	1:A:7:LEU:HD12	2.29	0.53
1:M:194:GLY:N	1:M:379:GLU:HB3	2.23	0.52
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:209:THR:HG21	1:M:507:GLU:HA	1.91	0.52
1:M:361:ILE:CG2	1:M:362:GLU:N	2.72	0.52
1:M:232:HIS:C	1:M:234:ALA:N	2.62	0.52
1:A:241:ILE:HG21	1:A:334:LEU:HB3	1.90	0.52
1:M:115:ARG:O	1:M:115:ARG:HG3	2.01	0.52
1:M:104:SER:HG	1:M:127:ALA:HA	1.74	0.52
2:N:211:SER:CB	2:N:219:ASP:HA	2.39	0.52
1:M:145:GLN:HB3	2:N:119:TYR:CZ	2.45	0.52
1:A:35:ILE:HD12	1:A:35:ILE:N	2.25	0.52
2:N:55:TRP:HA	2:N:64:SER:OG	2.10	0.52
1:M:201:TYR:HB2	1:M:460:GLU:OE2	2.09	0.52
1:A:396:LEU:HG	8:A:601:FAD:C2	2.40	0.52
2:N:173:ILE:O	2:N:176:ALA:HB3	2.09	0.52
2:B:207:VAL:HG22	3:C:25:TYR:CZ	2.44	0.52
4:P:27:ILE:HG22	4:P:31:MET:HG2	1.91	0.52
2:B:11:VAL:HG21	2:B:91:GLU:HG2	1.91	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:434:GLN:HE21	1:A:434:GLN:HA	1.74	0.52
4:D:30:VAL:O	4:D:33:LEU:HB3	2.09	0.52
1:A:319:LEU:HG	1:A:324:LEU:HD21	1.91	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
4:D:95:ALA:CB	2:N:239:THR:HG22	2.40	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:22:ALA:O	1:A:26:ALA:N	2.36	0.52
4:D:70:MET:O	4:D:74:PRO:HG2	2.09	0.52
2:B:110:ILE:N	2:B:110:ILE:HD13	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:216:ALA:O	1:M:221:VAL:HB	2.10	0.52
1:A:61:SER:HB3	1:A:64:TYR:HD1	1.75	0.52
2:N:12:ARG:NH2	2:N:50:ASP:OD1	2.42	0.52
1:M:226:MET:HB2	1:M:517:CYS:O	2.09	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
3:C:130:TRP:HD1	3:C:130:TRP:N	2.08	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
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:8:ALA:O	1:A:188:VAL:HA	2.09	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
2:N:178:ARG:C	2:N:178:ARG:HD3	2.31	0.51
1:M:563:LEU:O	1:M:564:GLU:HG3	2.10	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:142:THR:O	1:M:145:GLN:HG2	2.11	0.51
1:M:377:VAL:HG22	1:M:378:GLY:N	2.24	0.51
2:N:239:THR:O	2:N:239:THR:HG22	2.11	0.51
1:M:94:THR:HG1	1:M:125:TRP:HH2	1.57	0.51
4:D:0:MET:HG3	4:D:1:ILE:N	2.25	0.51
1:A:156:PHE:CD2	1:A:156:PHE:C	2.84	0.51
4:P:51:TYR:OH	4:P:55:LEU:HD22	2.10	0.51
3:O:89:LEU:C	3:O:91:PRO:CD	2.77	0.51
2:B:232:SER:HA	4:D:11:PRO:HB3	1.92	0.51
3:C:105:PRO:O	3:C:109:ILE:HG13	2.10	0.51
1:A:44:HIS:NE2	8:A:601:FAD:C8	2.67	0.51
1:M:55:VAL:HG22	1:M:123:ARG:HE	1.76	0.51
1:M:35:ILE:HG23	1:M:155:HIS:HB2	1.93	0.51
1:A:54:ALA:HB2	1:A:93:MET:HG3	1.93	0.51
1:M:85:PHE:HB2	1:M:402:PHE:CZ	2.46	0.51
1:A:114:ARG:O	1:A:122:GLU:HB2	2.11	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:M:130:LYS:O	1:M:133:PHE:HB3	2.12	0.50
1:A:79:GLN:NE2	1:A:570:ILE:HD13	2.26	0.50
1:A:225:ASP:HA	1:A:227:GLU:OE2	2.11	0.50
1:M:395:SER:HB3	8:M:601:FAD:N1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:THR:CG2	4:D:81:ARG:HH12	2.25	0.50
1:M:526:LYS:HA	1:M:534:ARG:NH1	2.26	0.50
1:M:156:PHE:O	1:M:173:MET:N	2.40	0.50
1:A:217:LEU:HD11	1:A:517:CYS:SG	2.52	0.50
2:B:28:VAL:HG12	2:B:29:PRO:O	2.10	0.50
1:A:194:GLY:O	1:A:208:VAL:HG13	2.11	0.50
3:C:18:LYS:N	3:C:18:LYS:HD3	2.26	0.50
1:M:512:LEU:O	1:M:516:GLU:HG3	2.12	0.50
3:O:98:VAL:HG23	3:O:103:MET:CB	2.42	0.50
2:B:75:LEU:HD11	2:B:215:PRO:HG3	1.94	0.50
4:P:62:ILE:O	4:P:65:VAL:HG22	2.10	0.50
1:A:425:ILE:O	1:A:428:GLN:HB3	2.12	0.50
2:N:111:GLU:CD	4:P:1:ILE:HG13	2.32	0.50
4:D:98:TRP:O	4:D:102:GLY:N	2.43	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
2:B:110:ILE:O	2:B:114:GLU:HG3	2.12	0.50
1:M:115:ARG:HB3	1:M:115:ARG:NH1	2.23	0.50
1:M:199:TYR:CZ	1:M:229:VAL:HG21	2.46	0.50
1:M:197:ARG:HG2	1:M:208:VAL:HB	1.94	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
3:O:47:PHE:HE2	4:P:114:GLY:CA	2.24	0.50
1:M:17:LEU:N	1:M:17:LEU:HD12	2.26	0.50
1:M:73:GLY:O	1:M:388:ALA:HB3	2.12	0.50
2:N:111:GLU:OE2	4:P:1:ILE:N	2.45	0.50
2:N:10:VAL:O	2:N:23:SER:HA	2.12	0.50
1:M:114:ARG:O	1:M:124:THR:HB	2.11	0.50
2:B:106:MET:O	2:B:110:ILE:HG12	2.12	0.50
3:O:28:ARG:HD2	4:P:81:ARG:HH22	1.75	0.50
1:M:65:HIS:CE1	1:M:86:VAL:HG22	2.47	0.50
4:P:24:SER:O	4:P:28:ALA:HB3	2.12	0.50
2:N:151:CYS:N	7:N:246:SF4:S4	2.85	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:240:LEU:O	2:N:243:ARG:HG2	2.12	0.50
2:N:94:ALA:HA	3:O:9:ARG:CZ	2.42	0.50
1:A:61:SER:HB3	1:A:64:TYR:CD1	2.46	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
3:C:38:PHE:HB2	3:C:75:THR:HG21	1.93	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
1:M:11:GLY:HA2	8:M:601:FAD:C4B	2.42	0.49
1:M:228:PHE:O	1:M:358:MET:HB2	2.12	0.49
4:D:80:HIS:O	4:D:83:HIS:HB3	2.12	0.49
2:B:16:GLU:OE2	3:C:3:LYS:HD2	2.12	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
1:A:92:GLU:HG3	1:A:401:VAL:HA	1.94	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
3:O:88:GLU:O	3:O:91:PRO:HD2	2.13	0.49
1:M:479:LEU:O	1:M:483:GLN:HG2	2.12	0.49
1:M:213:MET:SD	1:M:223:LEU:HD22	2.52	0.49
3:O:75:THR:HG22	4:P:32:ILE:HD13	1.94	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
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
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
2:N:12:ARG:HH22	2:N:50:ASP:C	2.15	0.49
1:M:496:SER:HB2	3:O:3:LYS:HD3	1.95	0.49
1:M:59:HIS:ND1	1:M:59:HIS:C	2.66	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
1:A:21:ILE:O	1:A:24:ALA:HB3	2.12	0.49
4:D:23:TRP:CE2	4:D:27:ILE:HD12	2.46	0.49
1:M:53:ALA:HA	1:M:123:ARG:O	2.12	0.49
1:A:17:LEU:CD2	1:A:34:LEU:HD11	2.43	0.49
3:O:29:GLU:C	3:O:31:THR:H	2.16	0.49
2:N:225:GLN:HA	2:N:225:GLN:NE2	2.28	0.49
2:N:73:PRO:C	2:N:153:LEU:HD22	2.33	0.49
3:C:87:PHE:HE1	3:C:116:THR:HG1	1.59	0.49
3:O:95:ASN:ND2	3:O:102:LYS:HD2	2.27	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
1:A:145:GLN:HB3	2:B:119:TYR:CE2	2.47	0.49
2:N:34:THR:HG22	2:N:81:LEU:HD13	1.95	0.49
1:M:289:LYS:HA	1:M:292:GLN:CB	2.42	0.49
1:A:234:ALA:HB1	1:A:243:MET:HB2	1.93	0.49
3:C:50:LYS:HZ3	4:D:118:ILE:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:104:VAL:HG23	2:N:106:MET:CE	2.42	0.49
1:A:434:GLN:HE21	1:A:434:GLN:CA	2.26	0.49
4:P:79:LEU:HD23	4:P:82:MET:CE	2.43	0.49
1:A:517:CYS:HB3	1:A:553:ALA:CB	2.43	0.49
1:M:228:PHE:HB2	1:M:358:MET:HB3	1.95	0.49
3:C:39:SER:OG	4:D:71:ILE:O	2.31	0.49
1:M:157:VAL:HA	1:M:172:ALA:HA	1.95	0.49
2:N:135:THR:HB	2:N:138:GLN:HE21	1.78	0.49
1:M:78:GLU:O	1:M:80:ASP:N	2.45	0.49
4:P:57:PHE:CZ	4:P:63:GLY:HA2	2.47	0.49
1:M:231:TYR:HD2	1:M:352:PRO:HB2	1.76	0.49
1:A:113:VAL:HG23	1:A:124:THR:N	2.28	0.49
1:M:84:TYR:OH	1:M:405:LEU:HD13	2.13	0.49
1:M:513:ASN:HA	1:M:516:GLU:OE1	2.13	0.48
2:N:11:VAL:CG2	2:N:91:GLU:HG2	2.43	0.48
1:M:549:LYS:HE3	1:M:565:TYR:CE2	2.48	0.48
1:M:504:TYR:CD2	1:M:504:TYR:N	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
2:B:242:PRO:HB2	4:P:92:HIS:HB3	1.95	0.48
2:B:242:PRO:HG2	4:P:93:VAL:C	2.33	0.48
2:B:43:ILE:HG23	2:B:47:LEU:HB2	1.96	0.48
1:M:363:THR:OG1	1:M:383:VAL:HA	2.14	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:A:527:GLU:CD	1:A:529:ARG:HH11	2.16	0.48
1:M:211:ASP:O	1:M:215:MET:HE2	2.12	0.48
1:A:98:LEU:CD2	2:B:132:ASN:HD21	2.19	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
4:D:86:MET:SD	4:D:86:MET:N	2.86	0.48
1:A:294:PHE:CE1	1:A:351:ARG:CG	2.64	0.48
1:M:358:MET:CE	1:M:390:ARG:N	2.70	0.48
1:M:49:GLU:HG2	1:M:129:ASP:O	2.14	0.48
1:M:370:ARG:NH2	1:M:554:PHE:CE2	2.71	0.48
1:M:27:ASN:ND2	1:M:29:ASN:H	2.11	0.48
4:P:26:ILE:HG22	4:P:27:ILE:HG13	1.95	0.48
2:N:120:ILE:O	2:N:121:ILE:HG13	2.13	0.48
1:A:248:ARG:HB3	1:A:248:ARG:NH1	2.29	0.48
1:A:6:ASP:OD2	1:A:31:LYS:N	2.36	0.48
1:M:167:VAL:HG22	1:M:168:ARG:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:PHE:HA	6:B:245:F3S:S2	2.54	0.48
2:N:135:THR:HG22	2:N:137:ALA:N	2.29	0.48
3:C:33:VAL:CB	3:C:34:PRO:HD3	2.30	0.48
1:M:528:SER:OG	1:M:539:CYS:O	2.23	0.48
1:M:204:ASN:ND2	1:M:204:ASN:N	2.61	0.48
3:C:65:ASN:O	3:C:69:VAL:HG23	2.13	0.48
1:M:297:GLU:O	1:M:302:ASN:CB	2.62	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:A:321:GLU:OE1	1:A:344:VAL:HG11	2.14	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
4:P:68:PHE:O	4:P:72:VAL:HG23	2.14	0.48
2:N:68:MET:HE3	2:N:73:PRO:HD3	1.94	0.48
1:M:92:GLU:HB3	1:M:400:VAL:HG23	1.96	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: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
2:B:206:PHE:CD2	2:B:206:PHE:O	2.67	0.47
1:M:534:ARG:HB3	1:M:536:ASP:OD1	2.13	0.47
1:A:122:GLU:CD	1:A:122:GLU:H	2.16	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:M:114:ARG:HG3	1:M:116:PHE:HE1	1.78	0.47
3:C:39:SER:HB3	4:D:75:LEU:HD21	1.97	0.47
1:M:356:TYR:HE1	1:M:379:GLU:CG	2.27	0.47
3:O:49:LEU:HG	4:P:55:LEU:CD1	2.43	0.47
1:A:549:LYS:HD2	1:A:565:TYR:HB3	1.96	0.47
1:M:378:GLY:C	1:M:380:CYS:H	2.16	0.47
3:C:123:ILE:N	3:C:123:ILE:CD1	2.77	0.47
1:M:192:THR:C	8:M:601:FAD:H51A	2.34	0.47
1:M:19:ALA:O	1:M:23:ALA:HB2	2.15	0.47
1:M:82:VAL:HG22	1:M:385:LEU:HD12	1.95	0.47
2:B:135:THR:OG1	2:B:138:GLN:HG3	2.13	0.47
1:M:495:SER:CB	2:N:14:ASN:HD21	2.27	0.47
1:A:12:ALA:HB2	1:A:34:LEU:HD21	1.97	0.47
2:N:44:LYS:HA	2:N:48:ALA:O	2.14	0.47
2:N:7:LYS:HE2	2:N:25:PHE:CD2	2.50	0.47
2:B:173:ILE:HD13	2:B:201:VAL:HG12	1.97	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
1:M:60:ASP:OD2	1:M:61:SER:N	2.45	0.47
3:C:37:TRP:HA	3:C:40:ILE:HD12	1.97	0.47
2:B:6:LEU:HB2	2:B:30:TYR:CE2	2.48	0.47
2:N:14:ASN:HA	2:N:100:ARG:CD	2.44	0.47
1:M:115:ARG:HG2	1:M:115:ARG:NH1	2.08	0.47
1:A:97:GLU:HG2	2:B:131:THR:HG22	1.95	0.47
1:A:3:PHE:CD2	1:A:152:PHE:HZ	2.33	0.47
1:A:434:GLN:NE2	1:A:434:GLN:CA	2.74	0.47
1:M:76:LEU:HD12	1:M:388:ALA:HB2	1.96	0.47
1:M:474:LYS:O	1:M:478:LYS:HB2	2.13	0.47
3:C:76:LEU:HD23	3:C:76:LEU:C	2.34	0.47
1:A:562:ARG:HG3	1:A:562:ARG:HH11	1.80	0.47
1:M:194:GLY:HA3	1:M:379:GLU:CG	2.43	0.47
3:O:33:VAL:O	3:O:36:VAL:HG22	2.14	0.47
1:A:89:CYS:HB2	1:A:90:PRO:CD	2.40	0.47
2:N:221:ALA:O	2:N:224:ILE:HB	2.15	0.47
1:A:113:VAL:HG21	1:A:123:ARG:CA	2.45	0.47
4:D:0:MET:HG3	4:D:1:ILE:H	1.79	0.47
3:C:61:ASP:HA	3:C:64:GLN:OE1	2.15	0.47
1:A:44:HIS:CD2	8:A:601:FAD:HM81	2.49	0.47
2:N:14:ASN:O	2:N:16:GLU:N	2.48	0.47
1:M:0:MET:HE1	1:M:171:VAL:HG13	1.97	0.47
3:O:29:GLU:C	3:O:31:THR:N	2.67	0.47
1:M:528:SER:OG	1:M:540:THR:HA	2.14	0.47
2:N:65:CYS:HB3	2:N:75:LEU:HA	1.97	0.47
1:A:167:VAL:HG21	1:A:188:VAL:HG23	1.97	0.47
3:O:60:VAL:O	3:O:64:GLN:HG3	2.15	0.47
1:M:54:ALA:C	1:M:123:ARG:HB2	2.35	0.47
1:M:38:VAL:HA	1:M:154:GLU:HG2	1.96	0.47
1:A:225:ASP:O	1:A:228:PHE:HD1	1.98	0.46
1:M:60:ASP:CG	1:M:121:ILE:HG21	2.36	0.46
3:C:50:LYS:HZ2	4:D:118:ILE:HD12	1.80	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
1:A:173:MET:HG2	1:A:180:LEU:HD23	1.96	0.46
3:C:123:ILE:N	3:C:123:ILE:HD12	2.31	0.46
1:M:209:THR:HG21	1:M:507:GLU:HB3	1.97	0.46
1:A:341:VAL:O	1:A:343:PRO:HD3	2.15	0.46
1:M:0:MET:HE1	1:M:171:VAL:CG1	2.45	0.46
1:M:0:MET:CE	1:M:171:VAL:HG11	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HG23	1:A:71:ALA:N	2.30	0.46
2:N:104:VAL:HG23	2:N:106:MET:HE3	1.97	0.46
2:B:125:ARG:NH1	2:B:125:ARG:HG3	2.29	0.46
2:B:223:ALA:O	2:B:227:GLY:N	2.48	0.46
1:M:187:ALA:HB2	1:M:414:ALA:HB2	1.96	0.46
1:A:291:SER:O	1:A:294:PHE:CD2	2.68	0.46
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:M:18:ARG:HD2	1:M:18:ARG:O	2.15	0.46
1:A:443:ASP:HA	1:A:490:ARG:HG3	1.96	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
2:B:6:LEU:HD12	2:B:7:LYS:N	2.31	0.46
1:A:253:ILE:HG12	1:A:318:HIS:CE1	2.51	0.46
1:M:96:LEU:HD21	1:M:139:LEU:CD2	2.44	0.46
4:D:53:ARG:O	4:D:56:ALA:HB3	2.16	0.46
4:D:41:LEU:HB2	4:D:43:LEU:HD11	1.95	0.46
1:A:187:ALA:HA	1:A:373:GLY:O	2.16	0.46
1:M:62:PHE:CB	1:M:87:HIS:CE1	2.99	0.46
1:A:84:TYR:O	1:A:88:HIS:HD2	1.99	0.46
1:A:44:HIS:CE1	1:A:204:ASN:HA	2.51	0.46
1:M:44:HIS:CE1	1:M:47:ALA:HB3	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
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:232:HIS:CG	1:A:233:PRO:HD2	2.50	0.46
1:A:174:ASN:O	1:A:178:GLY:N	2.48	0.46
1:A:208:VAL:O	1:A:208:VAL:CG1	2.61	0.46
1:M:48:ALA:HA	8:M:601:FAD:C6	2.45	0.46
3:O:19:LEU:CD2	3:O:19:LEU:H	2.23	0.46
1:M:0:MET:HE2	1:M:180:LEU:HD12	1.97	0.46
3:C:59:PHE:CE2	3:C:63:LEU:HD11	2.51	0.46
4:P:33:LEU:O	4:P:37:ILE:HB	2.15	0.46
3:C:76:LEU:HB2	4:D:32:ILE:HG21	1.97	0.46
3:O:77:ALA:O	3:O:80:LEU:HB2	2.16	0.46
3:C:84:LYS:O	3:C:88:GLU:HG3	2.16	0.46
1:M:396:LEU:HG	8:M:601:FAD:C2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:12:ALA:N	8:M:601:FAD:H4B	2.31	0.46
1:M:66:PHE:CD1	1:M:82:VAL:HG12	2.51	0.46
4:P:69:LEU:HB3	4:P:73:LEU:HD12	1.98	0.46
2:N:11:VAL:HA	2:N:22:HIS:O	2.15	0.46
4:D:41:LEU:HD12	4:D:43:LEU:HD11	1.98	0.46
3:C:47:PHE:HE1	4:D:114:GLY:CA	2.29	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
1:A:12:ALA:CB	1:A:40:PRO:HG3	2.46	0.46
2:N:111:GLU:OE2	4:P:1:ILE:HG13	2.16	0.46
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:A:70:VAL:CG2	1:A:573:LEU:HD23	2.34	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:M:64:TYR:CD2	1:M:121:ILE:CG1	2.99	0.45
1:A:292:GLN:CG	1:A:466:TYR:HE1	2.29	0.45
2:N:221:ALA:O	2:N:225:GLN:HG2	2.17	0.45
1:M:17:LEU:CD1	1:M:17:LEU:N	2.79	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
3:C:121:ILE:N	3:C:121:ILE:HD12	2.31	0.45
1:M:513:ASN:O	1:M:516:GLU:HB2	2.16	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
1:M:89:CYS:CB	1:M:90:PRO:HD3	2.46	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:N	4:P:52:GLU:OE2	2.41	0.45
1:A:365:GLN:OE1	1:A:365:GLN:N	2.49	0.45
1:A:170:LEU:HD23	1:A:170:LEU:N	2.32	0.45
3:C:23:ARG:HH11	3:C:23:ARG:CG	2.29	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:231:TYR:OH	1:A:464:GLY:HA2	2.17	0.45
1:M:59:HIS:O	1:M:59:HIS:ND1	2.50	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
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
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
3:C:65:ASN:HD21	3:C:67:VAL:HB	1.77	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: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:112:LEU:HA	4:P:115:VAL:HG12	1.98	0.45
4:P:79:LEU:HD13	4:P:100:PHE:O	2.16	0.45
1:A:377:VAL:HG21	1:A:403:GLY:HA2	1.99	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
2:N:11:VAL:HG21	2:N:91:GLU:HG2	1.98	0.44
3:C:84:LYS:HE2	3:C:88:GLU:OE2	2.17	0.44
2:N:207:VAL:HB	6:N:245:F3S:S4	2.56	0.44
1:A:502:LEU:HD12	1:A:502:LEU:O	2.17	0.44
2:B:57:CYS:O	2:B:59:MET:HG2	2.17	0.44
1:M:379:GLU:CG	1:M:379:GLU:O	2.66	0.44
1:A:314:LEU:HG	1:A:316:LEU:HD21	1.98	0.44
2:N:206:PHE:CZ	3:O:89:LEU:HD22	2.52	0.44
2:N:12:ARG:NH2	2:N:51:LEU:HA	2.31	0.44
1:M:549:LYS:CD	1:M:565:TYR:CD2	3.00	0.44
1:A:201:TYR:C	1:A:353:THR:HG1	2.20	0.44
1:M:502:LEU:O	1:M:502:LEU:HD12	2.18	0.44
1:A:172:ALA:O	1:A:181:VAL:HG22	2.17	0.44
4:D:21:GLY:N	4:D:77:CYS:HB2	2.32	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
1:M:211:ASP:CG	1:M:510:HIS:CD2	2.90	0.44
4:P:34:LEU:HD23	4:P:38:LEU:HD12	2.00	0.44
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.99	0.44
1:M:44:HIS:C	1:M:46:VAL:H	2.19	0.44
1:A:70:VAL:HG23	1:A:71:ALA:H	1.83	0.44
1:M:20:ALA:HA	1:M:23:ALA:HB3	1.99	0.44
4:D:28:ALA:O	4:D:32:ILE:HG13	2.17	0.44
2:B:40:LEU:HD11	2:B:67:MET:HE1	1.98	0.44
2:N:16:GLU:C	2:N:18:ASP:N	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:135:THR:HB	2:N:138:GLN:NE2	2.33	0.44
2:B:169:GLY:O	2:B:173:ILE:HG13	2.17	0.44
1:A:552:LEU:HB3	1:A:554:PHE:CE1	2.53	0.44
1:A:160:ILE:O	1:A:160:ILE:HG13	2.17	0.44
4:D:92:HIS:HA	2:N:243:ARG:OXT	2.17	0.44
3:C:66:PRO:O	3:C:70:ILE:HG13	2.17	0.44
1:A:156:PHE:HD2	1:A:156:PHE:C	2.21	0.44
2:B:40:LEU:HD11	2:B:67:MET:CE	2.48	0.44
1:A:294:PHE:CZ	1:A:295:TRP:HE3	2.35	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
2:N:160:GLN:O	2:N:163:LEU:HB2	2.18	0.44
1:M:48:ALA:CB	1:M:396:LEU:HD21	2.48	0.44
4:D:64:ARG:HH22	4:D:118:ILE:HG22	1.83	0.44
1:M:97:GLU:OE2	1:M:98:LEU:HD23	2.18	0.44
1:M:377:VAL:HA	1:M:381:SER:OG	2.17	0.44
2:B:230:GLU:O	2:B:233:LYS:HB3	2.18	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
1:A:241:ILE:HG21	1:A:334:LEU:CB	2.48	0.44
3:O:22:TYR:O	3:O:25:TYR:HB3	2.18	0.44
1:M:174:ASN:ND2	1:M:177:GLU:HG2	2.32	0.44
3:C:25:TYR:CE1	3:C:29:GLU:HG3	2.52	0.44
1:M:20:ALA:C	1:M:23:ALA:HB3	2.38	0.44
1:M:491:ILE:HD13	1:M:502:LEU:HD13	1.98	0.44
4:D:96:GLY:O	4:D:100:PHE:HD1	2.01	0.44
1:A:62:PHE:CD1	1:A:86:VAL:HG12	2.53	0.44
1:A:395:SER:O	1:A:398:GLU:HB3	2.18	0.43
4:D:71:ILE:O	4:D:74:PRO:HD2	2.17	0.43
2:N:210:CYS:SG	2:N:220:PRO:HG2	2.58	0.43
2:N:11:VAL:CG1	2:N:21:PRO:HB2	2.48	0.43
1:A:364:ASP:OD1	1:A:368:GLU:HB3	2.17	0.43
2:B:25:PHE:CD1	2:B:25:PHE:N	2.85	0.43
1:M:497:VAL:HG13	3:O:4:ARG:HB3	2.00	0.43
1:M:34:LEU:HB3	1:M:151:ARG:HG2	1.99	0.43
1:M:35:ILE:HG22	1:M:36:SER:N	2.33	0.43
1:M:472:MET:HB3	1:M:523:MET:SD	2.58	0.43
2:N:89:LYS:HE2	2:N:91:GLU:OE1	2.18	0.43
2:B:210:CYS:SG	2:B:220:PRO:HG2	2.58	0.43
4:D:103:LEU:HD23	4:D:103:LEU:O	2.18	0.43
1:M:201:TYR:C	1:M:353:THR:HG23	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:O	1:A:393:SER:HB2	2.18	0.43
1:A:239:SER:O	2:B:58:ARG:NH1	2.48	0.43
1:M:363:THR:HG21	1:M:376:ALA:O	2.18	0.43
1:M:97:GLU:CG	1:M:105:ARG:HH22	2.31	0.43
4:P:112:LEU:O	4:P:115:VAL:HG12	2.17	0.43
3:C:80:LEU:O	3:C:84:LYS:HB2	2.18	0.43
1:M:59:HIS:O	1:M:59:HIS:CG	2.71	0.43
4:D:75:LEU:O	4:D:79:LEU:HB2	2.19	0.43
2:B:194:GLN:HA	4:D:5:PRO:HG3	2.01	0.43
2:N:214:CYS:SG	2:N:218:VAL:HG23	2.58	0.43
1:M:12:ALA:HA	1:M:17:LEU:CD1	2.37	0.43
1:M:551:THR:C	1:M:552:LEU:HD23	2.39	0.43
1:A:41:MET:CE	2:B:150:ASN:HD22	2.31	0.43
1:A:41:MET:HG3	1:A:42:ARG:NE	2.33	0.43
1:M:169:GLY:HA2	1:M:183:ILE:O	2.17	0.43
4:D:0:MET:HE3	4:D:1:ILE:H	1.83	0.43
1:M:496:SER:CB	3:O:3:LYS:HD3	2.48	0.43
4:D:89:LEU:HB3	4:D:91:ILE:HG13	2.00	0.43
1:M:191:ALA:O	8:M:601:FAD:C5B	2.65	0.43
1:M:167:VAL:HG12	1:M:373:GLY:HA3	1.99	0.43
1:A:13:GLY:O	1:A:17:LEU:HG	2.18	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:A:315:ASP:O	1:A:318:HIS:HE1	2.02	0.43
3:C:23:ARG:HG2	3:C:23:ARG:NH1	2.32	0.43
1:M:434:GLN:HA	1:M:434:GLN:NE2	2.34	0.43
1:M:116:PHE:CD2	1:M:245:GLU:CB	3.02	0.43
2:N:170:PRO:HB2	2:N:220:PRO:HB2	2.01	0.43
2:N:68:MET:HG2	2:N:92:ALA:O	2.19	0.43
1:A:48:ALA:HB3	1:A:132:GLY:CA	2.49	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:HD12	2:N:81:LEU:N	2.34	0.43
2:B:163:LEU:HD23	2:B:163:LEU:HA	1.79	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:145:GLN:HB3	2:B:119:TYR:CZ	2.54	0.43
3:C:53:PRO:HG2	3:C:54:GLU:H	1.84	0.43
2:B:21:PRO:HD3	3:C:7:TYR:CG	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HG2	1:A:42:ARG:HH11	1.84	0.43
4:P:68:PHE:CZ	4:P:72:VAL:HG21	2.54	0.43
1:M:448:TRP:CG	1:M:449:ALA:N	2.87	0.43
1:A:289:LYS:HG3	1:A:290:VAL:N	2.34	0.43
3:C:63:LEU:HA	3:C:68:ILE:HG21	2.00	0.43
1:M:223:LEU:HB3	1:M:226:MET:HG3	2.01	0.43
3:C:123:ILE:H	3:C:123:ILE:CD1	2.31	0.43
1:M:34:LEU:O	1:M:152:PHE:N	2.50	0.42
2:B:151:CYS:SG	2:B:153:LEU:HD12	2.59	0.42
4:P:105:ALA:O	4:P:109:VAL:HG23	2.18	0.42
1:M:469:PRO:O	1:M:473:GLN:HB2	2.19	0.42
2:B:69:VAL:O	2:B:72:VAL:HG23	2.18	0.42
1:M:528:SER:CB	1:M:539:CYS:O	2.67	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:A:75:TRP:NE1	1:A:575:PRO:HA	2.34	0.42
3:O:45:GLY:HA3	3:O:59:PHE:CE1	2.54	0.42
1:A:65:HIS:ND1	1:A:86:VAL:HG13	2.34	0.42
1:A:448:TRP:CG	1:A:449:ALA:N	2.86	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
3:C:28:ARG:O	3:C:31:THR:HG22	2.19	0.42
1:A:292:GLN:CB	1:A:466:TYR:HE1	2.32	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
2:N:68:MET:HB2	2:N:91:GLU:O	2.19	0.42
1:A:139:LEU:HA	1:A:139:LEU:HD23	1.87	0.42
1:A:15:ALA:HB2	1:A:399:LEU:CD2	2.36	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
2:N:93:LEU:HD11	2:N:153:LEU:HD23	1.99	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
1:M:54:ALA:H	1:M:123:ARG:HG3	1.83	0.42
4:D:117:THR:O	4:D:118:ILE:HG12	2.20	0.42
4:D:71:ILE:HG22	4:D:75:LEU:HD11	2.01	0.42
1:A:12:ALA:CB	1:A:17:LEU:HD21	2.36	0.42
3:O:31:THR:O	3:O:34:PRO:HD2	2.19	0.42
1:A:97:GLU:OE2	2:B:131:THR:HB	2.19	0.42
1:A:250:GLU:HB3	1:A:323:LYS:HZ3	1.75	0.42
1:M:105:ARG:NH1	2:N:132:ASN:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:223:LEU:HB3	1:M:226:MET:SD	2.60	0.42
2:B:8:ILE:HD11	2:B:81:LEU:CD1	2.48	0.42
1:A:146:PHE:HA	1:A:147:PRO:HD2	1.86	0.42
1:M:212:GLY:HA2	1:M:215:MET:HE2	2.01	0.42
1:M:211:ASP:OD1	1:M:510:HIS:CD2	2.73	0.42
1:M:83:ASP:O	1:M:87:HIS:CD2	2.72	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:480:ALA:O	1:A:483:GLN:HB2	2.20	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:N:135:THR:OG1	2:N:138:GLN:NE2	2.50	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
1:M:444:GLY:HA3	1:M:488:ARG:C	2.40	0.42
2:N:165:PRO:C	2:N:167:PHE:H	2.22	0.42
1:M:361:ILE:HG21	1:M:369:THR:HG21	2.02	0.42
2:B:169:GLY:O	2:B:172:ALA:HB3	2.18	0.42
1:M:201:TYR:CE2	1:M:238:GLY:CA	3.03	0.42
3:C:128:LEU:O	4:D:45:PRO:HG2	2.19	0.42
2:B:60:ALA:HA	5:B:244:FES:S1	2.60	0.42
1:M:497:VAL:HG21	2:N:15:PRO:HG2	1.93	0.42
1:M:386:HIS:CE1	1:M:390:ARG:HG3	2.55	0.42
4:D:117:THR:C	4:D:118:ILE:HG12	2.40	0.42
3:C:106:GLU:CD	3:C:107:PRO:HD2	2.40	0.42
1:M:228:PHE:HB2	1:M:358:MET:CB	2.50	0.42
4:D:73:LEU:HA	4:D:73:LEU:HD23	1.72	0.42
2:B:92:ALA:CB	2:B:98:ILE:CD1	2.96	0.42
1:A:448:TRP:CD2	1:A:449:ALA:N	2.88	0.42
1:A:204:ASN:HB3	1:A:208:VAL:HB	2.01	0.42
1:A:194:GLY:O	1:A:208:VAL:CG1	2.67	0.42
2:B:3:MET:HA	2:B:4:LYS:NZ	2.34	0.42
1:A:248:ARG:HG3	1:A:252:GLY:O	2.19	0.42
2:N:24:ALA:CB	2:N:26:TYR:OH	2.68	0.42
1:A:298:TRP:N	1:A:298:TRP:CD1	2.88	0.41
1:A:201:TYR:C	1:A:353:THR:OG1	2.59	0.41
1:M:145:GLN:HB3	2:N:119:TYR:CE2	2.55	0.41
2:B:236:LEU:CD2	2:B:236:LEU:C	2.88	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:60:ALA:HA	5:N:244:FES:S1	2.60	0.41
2:N:9:GLU:OE2	2:N:89:LYS:HE3	2.20	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
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:A:213:MET:CE	1:A:226:MET:SD	3.09	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:228:PHE:HB2	1:A:358:MET:HG3	2.02	0.41
1:M:226:MET:HE2	1:M:514:VAL:HG13	2.02	0.41
1:M:84:TYR:CZ	1:M:405:LEU:HD22	2.56	0.41
1:A:64:TYR:CD2	1:A:120:LYS:HE2	2.56	0.41
1:M:111:VAL:HG23	1:M:111:VAL:O	2.21	0.41
1:A:199:TYR:HB2	1:A:202:ASN:HD22	1.85	0.41
1:M:11:GLY:HA2	8:M:601:FAD:C1B	2.51	0.41
1:M:59:HIS:CE1	1:M:121:ILE:HD12	2.56	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
1:A:90:PRO:O	1:A:94:THR:OG1	2.36	0.41
4:P:48:ALA:O	4:P:49:LEU:HD23	2.21	0.41
2:B:92:ALA:HB3	2:B:98:ILE:HG12	2.03	0.41
3:C:130:TRP:O	4:D:53:ARG:NE	2.54	0.41
3:O:81:LEU:HD12	3:O:85:THR:CG2	2.48	0.41
1:A:211:ASP:O	1:A:214:GLY:N	2.54	0.41
2:N:236:LEU:HD23	2:N:236:LEU:C	2.40	0.41
1:M:484:GLU:HA	1:M:484:GLU:OE1	2.19	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
1:A:57:GLN:NE2	1:A:122:GLU:CG	2.80	0.41
4:D:97:LYS:HB2	4:D:97:LYS:HZ3	1.80	0.41
4:P:109:VAL:O	4:P:112:LEU:HB3	2.20	0.41
1:A:37:LYS:NZ	1:A:507:GLU:OE2	2.40	0.41
2:N:120:ILE:HD13	2:N:120:ILE:HA	1.88	0.41
1:A:502:LEU:O	1:A:506:ILE:HG13	2.20	0.41
1:M:9:ILE:HG22	1:M:10:VAL:N	2.36	0.41
1:A:328:LEU:HB3	1:A:331:ILE:CB	2.47	0.41
1:M:69:THR:HA	1:M:391:LEU:HD22	2.02	0.41
2:B:173:ILE:HG23	2:B:195:LEU:CD2	2.51	0.41
1:M:41:MET:HG2	1:M:42:ARG:HD2	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:M:468:THR:O	1:M:472:MET:CB	2.68	0.41
1:M:203:THR:C	1:M:204:ASN:HD22	2.24	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:M:83:ASP:O	1:M:87:HIS:HD2	2.04	0.41
1:M:375:PHE:N	1:M:375:PHE:CD1	2.88	0.41
1:A:16:GLY:O	1:A:19:ALA:HB3	2.20	0.41
2:N:28:VAL:HA	2:N:29:PRO:HD3	1.83	0.41
1:M:12:ALA:HB3	1:M:43:SER:OG	2.21	0.41
3:C:125:PHE:CE1	3:C:129:TYR:CZ	3.09	0.41
2:N:206:PHE:HD2	2:N:206:PHE:C	2.24	0.41
1:A:4:GLN:HA	1:A:4:GLN:OE1	2.20	0.41
2:N:73:PRO:CA	2:N:153:LEU:HD22	2.50	0.41
1:M:225:ASP:C	1:M:227:GLU:H	2.23	0.41
2:N:149:ILE:HD11	2:N:151:CYS:HB3	2.01	0.41
1:A:157:VAL:HG12	1:A:215:MET:SD	2.60	0.41
1:A:332:CYS:CA	1:A:343:PRO:HG2	2.16	0.41
1:M:10:VAL:HG12	1:M:10:VAL:O	2.20	0.41
2:N:16:GLU:CG	3:O:5:LYS:HZ3	2.25	0.41
1:A:526:LYS:HA	1:A:534:ARG:HH11	1.85	0.41
1:M:361:ILE:HG21	1:M:369:THR:CG2	2.51	0.41
1:M:85:PHE:HB2	1:M:402:PHE:CE1	2.56	0.41
2:N:202:TRP:CZ2	4:P:11:PRO:HG3	2.55	0.41
3:O:42:LEU:HA	3:O:42:LEU:HD23	1.85	0.41
1:M:372:LYS:HE3	1:M:413:ARG:NE	2.36	0.40
1:M:0:MET:HE1	1:M:180:LEU:HB3	2.04	0.40
3:C:121:ILE:HD12	3:C:121:ILE:H	1.86	0.40
1:M:227:GLU:OE2	1:M:525:ARG:NE	2.39	0.40
2:B:155:TYR:HE1	2:B:171:ALA:HB3	1.86	0.40
4:D:42:GLY:HA2	4:D:44:PHE:CE2	2.56	0.40
1:A:204:ASN:HB3	1:A:208:VAL:CB	2.52	0.40
3:O:5:LYS:HB3	3:O:5:LYS:HZ2	1.87	0.40
4:D:73:LEU:HB2	4:D:74:PRO:HD3	2.03	0.40
3:C:28:ARG:NH1	3:C:89:LEU:HD11	2.37	0.40
4:D:93:VAL:H	2:N:243:ARG:C	2.23	0.40
4:D:9:ASP:OD1	4:D:9:ASP:N	2.53	0.40
1:A:526:LYS:HG2	1:A:534:ARG:HH12	1.87	0.40
1:A:147:PRO:CD	1:A:148:GLN:OE1	2.69	0.40
1:M:434:GLN:HA	1:M:434:GLN:HE21	1.85	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:M:12:ALA:HB3	8:M:601:FAD:O3B	2.22	0.40
1:M:53:ALA:N	1:M:393:SER:O	2.54	0.40
1:A:438:ASP:HA	1:A:441:ASN:HD22	1.87	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
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:HA	2:B:195:LEU:HD23	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%)	15 61
1	M	494/602 (82%)	437 (88%)	44 (9%)	13 (3%)	7 48
2	B	241/243 (99%)	220 (91%)	19 (8%)	2 (1%)	24 70
2	N	241/243 (99%)	204 (85%)	30 (12%)	7 (3%)	6 47
3	C	128/130 (98%)	113 (88%)	13 (10%)	2 (2%)	12 58
3	O	128/130 (98%)	116 (91%)	9 (7%)	3 (2%)	8 52
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%)	11 57

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%)	17 59
1	M	355/474 (75%)	331 (93%)	24 (7%)	20 62
2	B	205/205 (100%)	195 (95%)	10 (5%)	31 71
2	N	205/205 (100%)	197 (96%)	8 (4%)	39 77
3	C	111/111 (100%)	101 (91%)	10 (9%)	12 50
3	O	111/111 (100%)	104 (94%)	7 (6%)	22 65
4	D	97/97 (100%)	90 (93%)	7 (7%)	18 59
4	P	97/97 (100%)	97 (100%)	0	100 100
All	All	1605/1774 (90%)	1508 (94%)	97 (6%)	24 66

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

Some 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

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 carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
8	FAD	A	601	-	48,58,58	3.56	23 (47%)	54,89,89	2.30	11 (20%)
5	FES	B	244	2	0,4,4	0.00	-	0,4,4	0.00	-
6	F3S	B	245	2	0,9,9	0.00	-	0,15,15	0.00	-
7	SF4	B	246	2	0,12,12	0.00	-	0,24,24	0.00	-
8	FAD	M	601	-	48,58,58	4.10	29 (60%)	54,89,89	2.93	17 (31%)
5	FES	N	244	2	0,4,4	0.00	-	0,4,4	0.00	-
6	F3S	N	245	2	0,9,9	0.00	-	0,15,15	0.00	-
7	SF4	N	246	2	0,12,12	0.00	-	0,24,24	0.00	-

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
8	FAD	A	601	-	-	0/30/50/50	0/6/6/6
5	FES	B	244	2	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	F3S	B	245	2	-	0/0/24/24	0/0/3/3
7	SF4	B	246	2	-	0/0/48/48	0/6/5/5
8	FAD	M	601	-	-	0/30/50/50	0/6/6/6
5	FES	N	244	2	-	0/0/4/4	0/1/1/1
6	F3S	N	245	2	-	0/0/24/24	0/0/3/3
7	SF4	N	246	2	-	0/0/48/48	0/6/5/5

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	601	FAD	C2B-C3B	-5.00	1.39	1.53
8	M	601	FAD	C5B-C4B	-4.05	1.38	1.51
8	A	601	FAD	C5A-C4A	-3.66	1.32	1.40
8	M	601	FAD	C5A-C4A	-3.42	1.32	1.40
8	M	601	FAD	C7M-C7	-3.20	1.44	1.51
8	A	601	FAD	C7M-C7	-3.11	1.44	1.51
8	M	601	FAD	C8A-N7A	-2.80	1.29	1.34
8	A	601	FAD	C8M-C8	-2.75	1.45	1.51
8	A	601	FAD	C8A-N7A	-2.62	1.29	1.34
8	A	601	FAD	P-O5'	-2.12	1.49	1.59
8	A	601	FAD	C2B-C3B	-2.09	1.47	1.53
8	M	601	FAD	C8M-C8	-2.09	1.46	1.51
8	M	601	FAD	O2B-C2B	2.23	1.48	1.43
8	M	601	FAD	O5B-C5B	2.24	1.54	1.44
8	A	601	FAD	C2A-N1A	2.38	1.38	1.33
8	M	601	FAD	P-O1P	2.51	1.60	1.51
8	M	601	FAD	C9-C9A	2.51	1.46	1.40
8	A	601	FAD	C9-C8	2.57	1.44	1.37
8	M	601	FAD	C2A-N1A	2.61	1.38	1.33
8	M	601	FAD	C9-C8	2.65	1.45	1.37
8	A	601	FAD	C9-C9A	2.78	1.46	1.40
8	M	601	FAD	C3B-C4B	2.93	1.60	1.53
8	A	601	FAD	C5X-N5	2.94	1.40	1.35
8	M	601	FAD	C5X-N5	3.09	1.40	1.35
8	M	601	FAD	C4-C4X	3.16	1.47	1.41
8	A	601	FAD	C4-C4X	3.23	1.47	1.41
8	M	601	FAD	C6-C7	3.87	1.48	1.37
8	A	601	FAD	C6-C7	4.05	1.49	1.37
8	A	601	FAD	C1'-N10	4.69	1.53	1.48
8	M	601	FAD	C5'-C4'	4.74	1.58	1.51
8	A	601	FAD	C8-C7	4.97	1.54	1.41
8	A	601	FAD	C4X-C10	5.24	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	601	FAD	C10-N1	5.27	1.44	1.35
8	M	601	FAD	C1'-N10	5.50	1.54	1.48
8	M	601	FAD	O4B-C1B	5.95	1.48	1.41
8	A	601	FAD	C9A-C5X	6.01	1.54	1.42
8	M	601	FAD	C8-C7	6.06	1.57	1.41
8	M	601	FAD	C4X-C10	6.14	1.52	1.41
8	M	601	FAD	C10-N1	6.30	1.46	1.35
8	M	601	FAD	C9A-N10	6.60	1.47	1.38
8	A	601	FAD	C2A-N3A	6.63	1.43	1.32
8	A	601	FAD	C4-N3	6.63	1.45	1.33
8	M	601	FAD	C9A-C5X	6.82	1.56	1.42
8	M	601	FAD	C2A-N3A	6.98	1.44	1.32
8	M	601	FAD	C4-N3	7.22	1.46	1.33
8	A	601	FAD	C4A-N3A	7.24	1.46	1.35
8	A	601	FAD	C9A-N10	7.63	1.49	1.38
8	M	601	FAD	C4A-N3A	7.80	1.47	1.35
8	M	601	FAD	C4X-N5	8.55	1.46	1.33
8	A	601	FAD	C4X-N5	8.66	1.46	1.33
8	A	601	FAD	C10-N10	8.94	1.49	1.39
8	M	601	FAD	C10-N10	10.53	1.51	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	M	601	FAD	C4B-O4B-C1B	-8.93	99.91	109.72
8	M	601	FAD	O3P-PA-O5B	-8.17	81.25	102.94
8	A	601	FAD	N3A-C2A-N1A	-7.79	122.93	128.89
8	M	601	FAD	N3A-C2A-N1A	-6.53	123.89	128.89
8	A	601	FAD	C4-C4X-C10	-5.54	116.40	119.94
8	A	601	FAD	C4X-C10-N10	-5.45	117.31	120.52
8	M	601	FAD	C4X-C10-N10	-5.26	117.42	120.52
8	M	601	FAD	C4-C4X-C10	-5.01	116.73	119.94
8	A	601	FAD	O3P-PA-O5B	-4.23	91.70	102.94
8	A	601	FAD	O4'-C4'-C5'	-3.32	102.95	110.19
8	M	601	FAD	C2B-C1B-N9A	-3.26	109.31	114.29
8	M	601	FAD	C4X-C4-N3	-3.07	119.39	123.59
8	A	601	FAD	C4X-C4-N3	-2.83	119.72	123.59
8	M	601	FAD	O4'-C4'-C5'	-2.75	104.21	110.19
8	M	601	FAD	O5B-C5B-C4B	-2.56	99.69	109.12
8	M	601	FAD	O5B-PA-O1A	-2.48	100.00	109.62
8	A	601	FAD	C1'-C2'-C3'	2.27	116.31	109.82
8	M	601	FAD	C4-C4X-N5	2.55	121.82	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	601	FAD	C4-C4X-N5	2.70	122.00	118.72
8	M	601	FAD	O2A-PA-O3P	2.99	118.68	105.09
8	A	601	FAD	O3P-P-O5'	3.10	111.17	102.94
8	M	601	FAD	P-O3P-PA	3.88	143.62	132.73
8	A	601	FAD	C4X-N5-C5X	4.00	121.37	116.76
8	M	601	FAD	C4X-N5-C5X	4.01	121.38	116.76
8	M	601	FAD	O3P-P-O5'	4.11	113.84	102.94
8	M	601	FAD	O4B-C4B-C3B	4.14	113.49	105.15
8	A	601	FAD	C4-N3-C2	7.05	121.34	115.25
8	M	601	FAD	C4-N3-C2	8.29	122.42	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	601	FAD	12	0
5	B	244	FES	1	0
6	B	245	F3S	1	0
7	B	246	SF4	2	0
8	M	601	FAD	26	0
5	N	244	FES	1	0
6	N	245	F3S	1	0
7	N	246	SF4	1	0

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, 95^{th} 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%)	-0.20	41 (7%) 17 9	23, 82, 161, 206	0
1	M	504/602 (83%)	0.67	82 (16%) 2 2	117, 184, 208, 208	0
2	B	243/243 (100%)	-0.70	1 (0%) 93 88	19, 76, 126, 205	0
2	N	243/243 (100%)	-0.22	5 (2%) 67 50	100, 161, 195, 206	0
3	C	130/130 (100%)	-0.81	0 100 100	38, 87, 136, 196	0
3	O	130/130 (100%)	-0.52	1 (0%) 87 76	44, 105, 153, 182	0
4	D	119/119 (100%)	-0.90	0 100 100	24, 84, 143, 159	0
4	P	119/119 (100%)	-0.76	1 (0%) 87 76	47, 90, 131, 208	0
All	All	2029/2188 (92%)	-0.18	131 (6%) 22 12	19, 113, 201, 208	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	326	GLU	16.3
1	M	325	HIS	10.0
1	M	238	GLY	9.3
1	A	307	PRO	8.1
1	M	237	PRO	6.2
1	M	334	LEU	5.9
1	A	306	THR	5.9
1	M	335	ALA	5.6
1	M	287	ARG	5.6
1	M	291	SER	5.6
1	M	338	TYR	5.5
1	M	551	THR	5.2
1	M	117	GLY	5.2
1	A	348	ILE	5.1
1	A	302	ASN	5.1
1	A	237	PRO	4.9

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Mol	Chain	Res	Type	RSRZ
1	M	465	ILE	4.8
1	M	336	LYS	4.8
1	A	293	ALA	4.7
1	A	326	GLU	4.6
1	M	349	PRO	4.6
1	A	305	SER	4.6
1	M	330	PHE	4.5
1	M	192	THR	4.4
1	M	293	ALA	4.4
1	M	461	GLU	4.4
1	M	337	ALA	4.4
1	M	292	GLN	4.3
1	M	491	ILE	4.3
1	A	341	VAL	4.2
1	M	544	ASP	4.1
1	M	193	GLY	3.9
1	M	548	LEU	3.9
1	A	238	GLY	3.9
1	M	247	CYS	3.8
1	A	350	VAL	3.8
1	M	490	ARG	3.7
1	M	75	TRP	3.7
1	A	347	PRO	3.7
1	A	327	ARG	3.6
1	A	340	GLY	3.6
1	M	187	ALA	3.6
1	M	378	GLY	3.6
1	A	315	ASP	3.5
1	M	234	ALA	3.5
1	M	324	LEU	3.5
1	M	246	GLY	3.4
1	A	329	PRO	3.4
1	A	314	LEU	3.4
1	A	337	ALA	3.4
1	A	297	GLU	3.4
1	A	351	ARG	3.3
1	M	243	MET	3.3
1	A	253	ILE	3.3
1	A	342	ASP	3.3
1	M	333	GLU	3.2
1	M	332	CYS	3.2
3	O	1	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	252	GLY	3.2
1	A	322	LYS	3.2
1	M	322	LYS	3.2
1	M	13	GLY	3.1
1	M	554	PHE	3.1
1	A	292	GLN	3.1
1	M	11	GLY	3.0
2	B	243	ARG	3.0
1	M	239	SER	3.0
1	A	290	VAL	3.0
1	M	299	ARG	3.0
1	A	298	TRP	2.9
1	M	45	THR	2.9
1	A	246	GLY	2.8
1	A	295	TRP	2.8
1	A	301	GLY	2.8
1	M	231	TYR	2.7
1	M	295	TRP	2.7
1	A	319	LEU	2.7
1	M	288	ASP	2.7
1	M	294	PHE	2.6
1	M	63	GLU	2.6
1	M	553	ALA	2.6
1	A	235	GLY	2.6
1	A	296	HIS	2.6
1	A	193	GLY	2.6
1	M	179	THR	2.6
4	P	0	MET	2.5
2	N	2	GLU	2.5
1	M	245	GLU	2.5
1	A	249	GLY	2.5
1	M	209	THR	2.5
1	M	0	MET	2.5
1	M	442	GLN	2.5
1	A	308	ARG	2.4
1	M	14	GLY	2.4
1	M	206	GLY	2.4
1	M	416	THR	2.4
1	M	227	GLU	2.4
1	M	44	HIS	2.4
1	M	373	GLY	2.3
1	M	183	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	412	GLU	2.3
1	A	239	SER	2.3
1	M	538	GLY	2.3
2	N	6	LEU	2.3
1	A	250	GLU	2.3
1	M	305	SER	2.3
1	M	6	ASP	2.3
1	A	318	HIS	2.3
1	M	395	SER	2.2
1	M	79	GLN	2.2
1	M	49	GLU	2.2
1	M	72	GLY	2.2
1	M	244	THR	2.2
1	M	365	GLN	2.2
1	M	380	CYS	2.2
1	M	191	ALA	2.2
1	M	562	ARG	2.2
1	M	379	GLU	2.2
1	M	537	GLU	2.2
1	A	313	TYR	2.2
1	M	522	ALA	2.2
1	M	290	VAL	2.2
1	M	296	HIS	2.1
1	A	294	PHE	2.1
1	M	7	LEU	2.1
2	N	88	MET	2.1
2	N	64	SER	2.1
1	M	536	ASP	2.1
2	N	1	ALA	2.0
1	M	303	THR	2.0
1	M	289	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 carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
7	SF4	B	246	8/8	0.99	0.32	2.33	111,123,129,129	0
6	F3S	B	245	7/7	0.99	0.27	2.11	109,113,117,126	0
6	F3S	N	245	7/7	0.99	0.22	0.47	116,118,131,151	0
5	FES	B	244	4/4	0.99	0.33	0.21	102,105,107,110	0
7	SF4	N	246	8/8	0.99	0.25	-0.16	122,131,151,155	0
8	FAD	A	601	53/53	0.95	0.23	-0.42	37,41,51,56	0
5	FES	N	244	4/4	0.98	0.21	-0.81	123,126,146,154	0
8	FAD	M	601	53/53	0.86	0.18	-1.57	55,71,78,80	0

6.5 Other polymers

There are no such residues in this entry.