Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 09:12 AM EDT

PDB ID	:	3EOO
Title	:	2.9A crystal structure of methyl-isocitrate lyase from Burkholderia pseudomallei
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2008-09-28
Resolution	:	2.90 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:

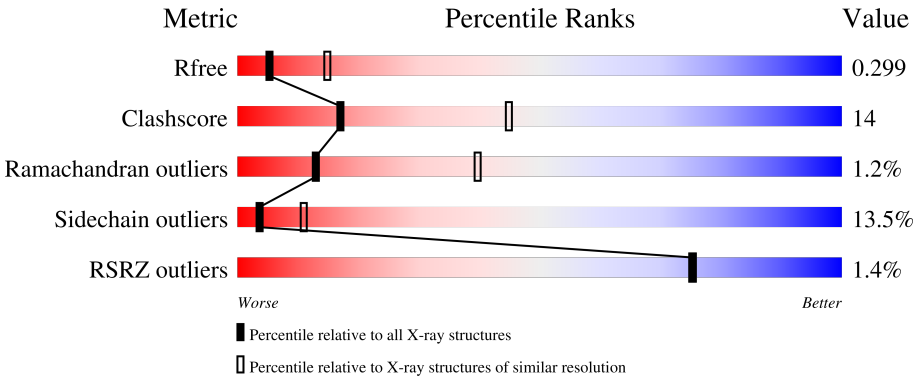
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	298	68% 24% 5% ·
1	B	298	70% 22% · ·
1	C	298	70% 22% · ·
1	D	298	71% 20% 5% ·
1	E	298	68% 24% · ·

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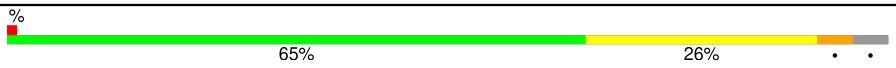
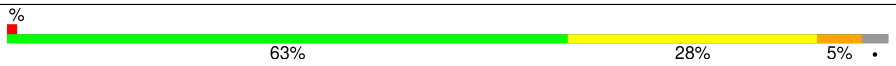
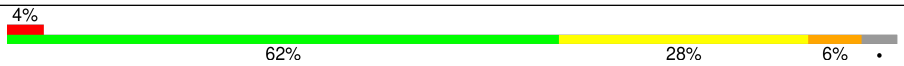
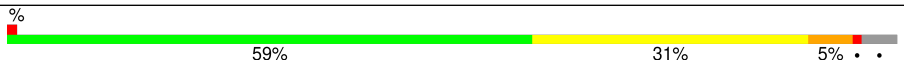
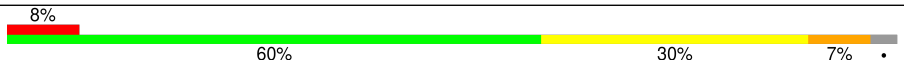
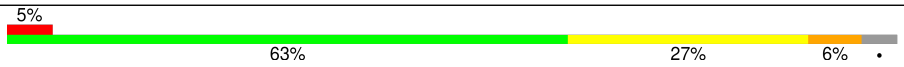
Mol	Chain	Length	Quality of chain
1	F	298	
1	G	298	
1	H	298	
1	I	298	
1	J	298	
1	K	298	
1	L	298	
1	M	298	
1	N	298	
1	O	298	
1	P	298	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 34623 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 Methylisocitrate lyase.

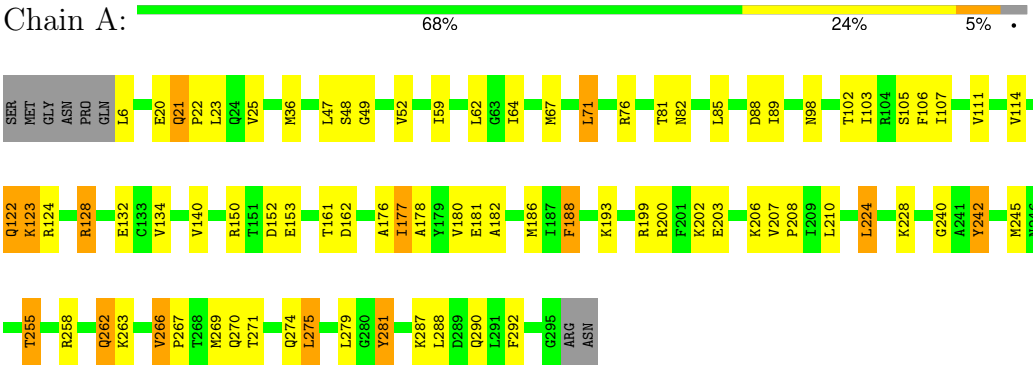
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2183	1379	376	416	12			
1	B	286	Total	C	N	O	S	0	0	0
			2154	1362	370	410	12			
1	C	287	Total	C	N	O	S	0	0	0
			2162	1366	372	412	12			
1	D	287	Total	C	N	O	S	0	0	0
			2162	1368	371	411	12			
1	E	288	Total	C	N	O	S	0	0	0
			2170	1372	373	413	12			
1	F	286	Total	C	N	O	S	0	0	0
			2154	1362	370	410	12			
1	G	287	Total	C	N	O	S	0	0	0
			2162	1368	371	411	12			
1	H	288	Total	C	N	O	S	0	0	0
			2170	1372	373	413	12			
1	I	289	Total	C	N	O	S	0	0	0
			2179	1377	375	415	12			
1	J	288	Total	C	N	O	S	0	0	0
			2171	1373	373	413	12			
1	K	286	Total	C	N	O	S	0	0	0
			2154	1362	370	410	12			
1	L	286	Total	C	N	O	S	0	0	0
			2154	1362	370	410	12			
1	M	287	Total	C	N	O	S	0	0	0
			2162	1366	372	412	12			
1	N	287	Total	C	N	O	S	0	0	0
			2162	1368	371	411	12			
1	O	288	Total	C	N	O	S	0	0	0
			2170	1372	373	413	12			
1	P	286	Total	C	N	O	S	0	0	0
			2154	1362	370	410	12			

3 Residue-property plots (i)

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.

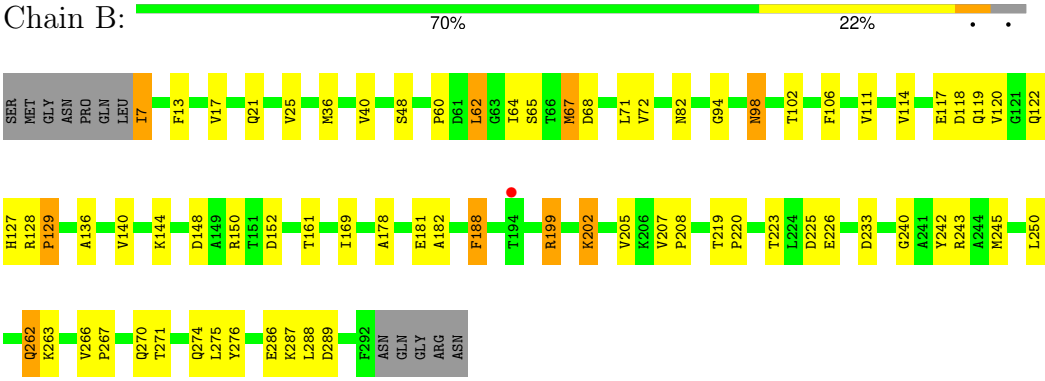
• Molecule 1: Methylisocitrate lyase

Chain A:



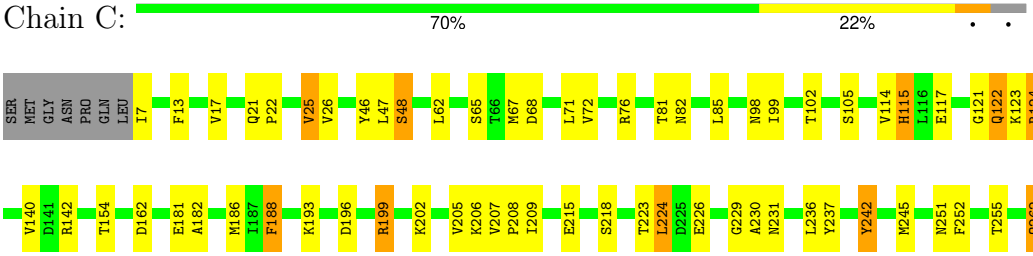
• Molecule 1: Methylisocitrate lyase

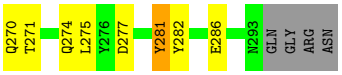
Chain B:



• Molecule 1: Methylisocitrate lyase

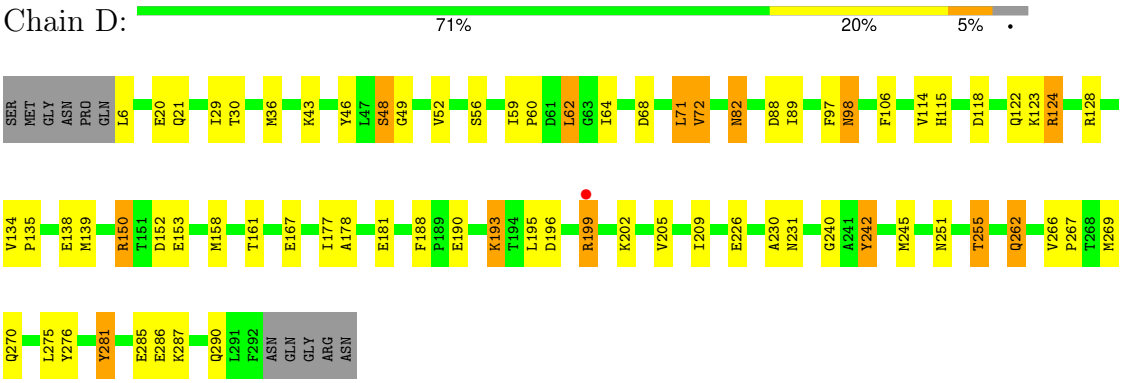
Chain C:





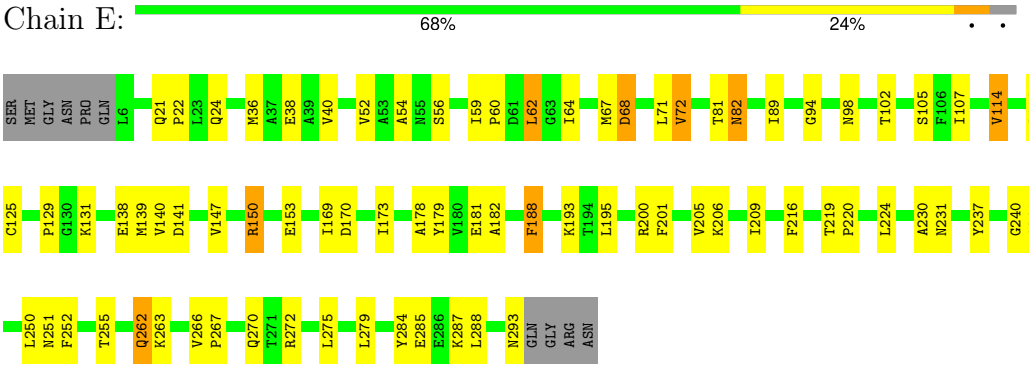
• Molecule 1: Methylisocitrate lyase

Chain D:



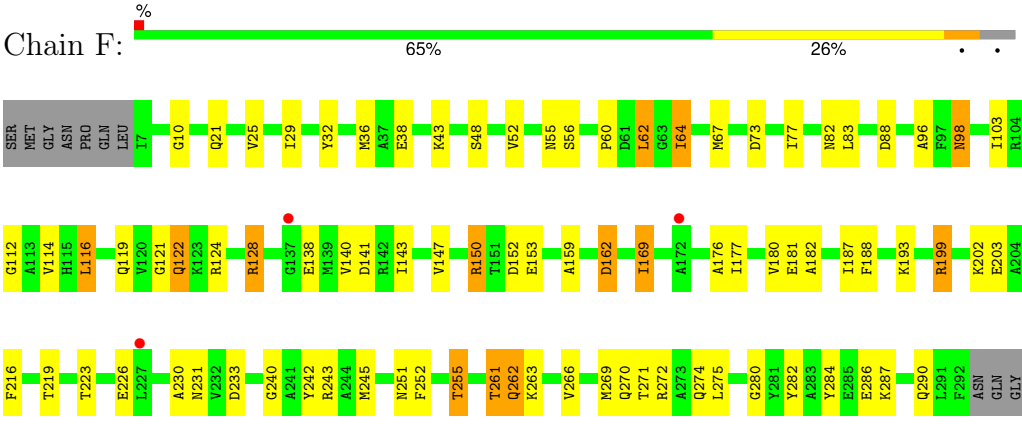
• Molecule 1: Methylisocitrate lyase

Chain E:



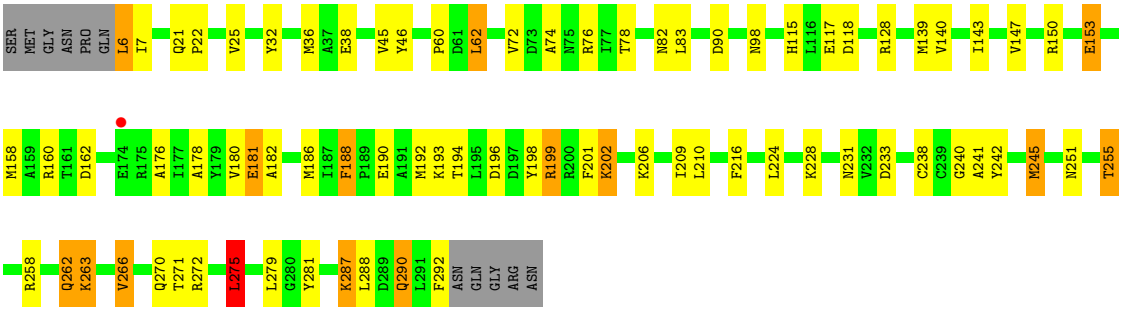
• Molecule 1: Methylisocitrate lyase

Chain F:



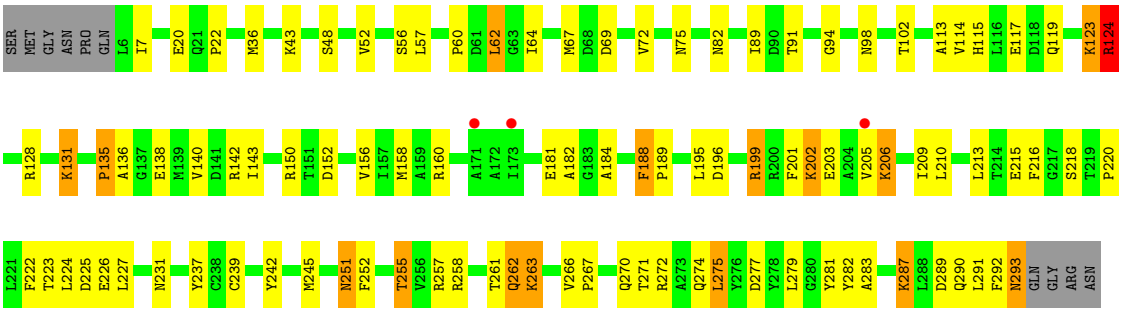
• Molecule 1: Methylisocitrate lyase

Chain G:



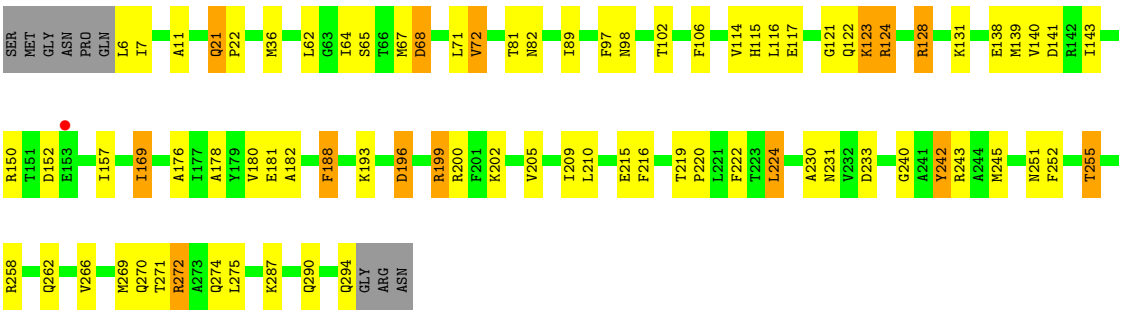
• Molecule 1: Methylisocitrate lyase

Chain H:



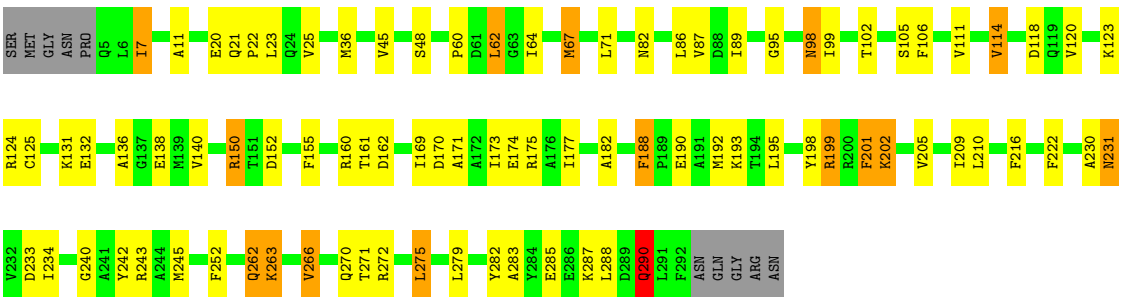
• Molecule 1: Methylisocitrate lyase

Chain I:



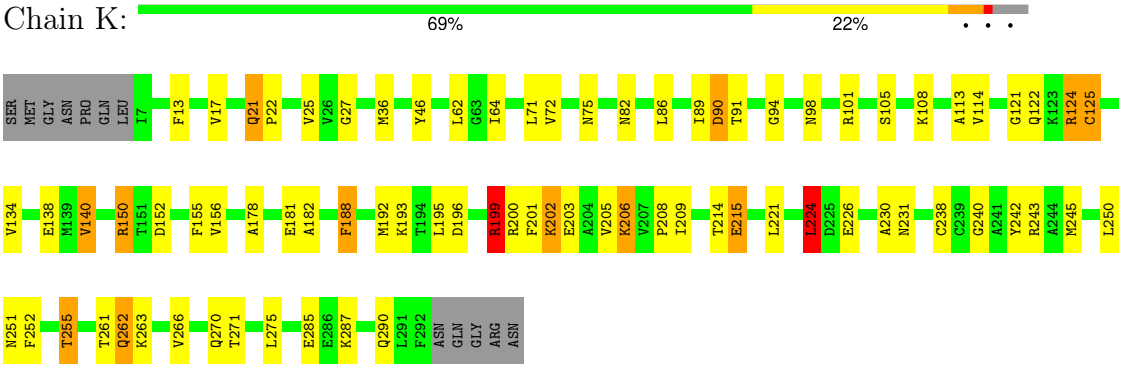
• Molecule 1: Methylisocitrate lyase

Chain J:



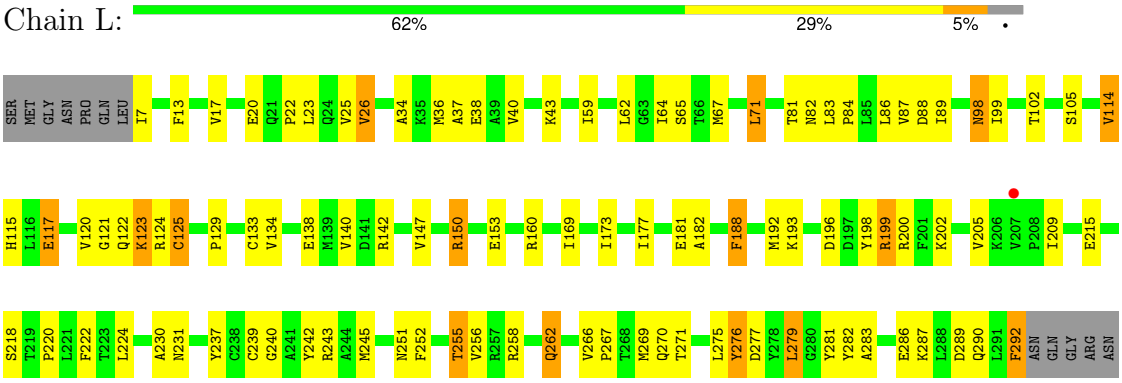
• Molecule 1: Methylisocitrate lyase

Chain K:



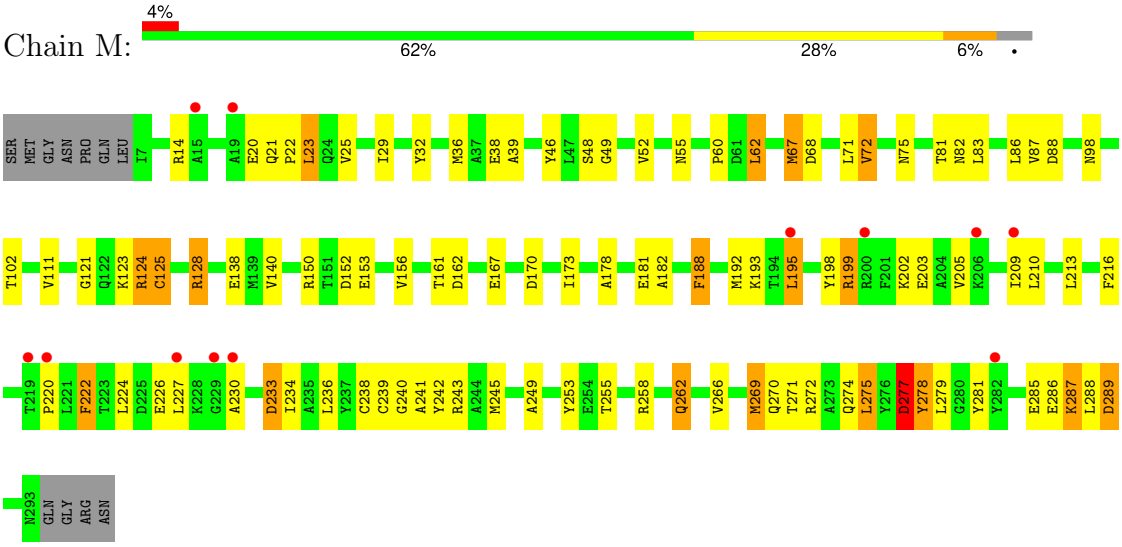
• Molecule 1: Methylisocitrate lyase

Chain L:



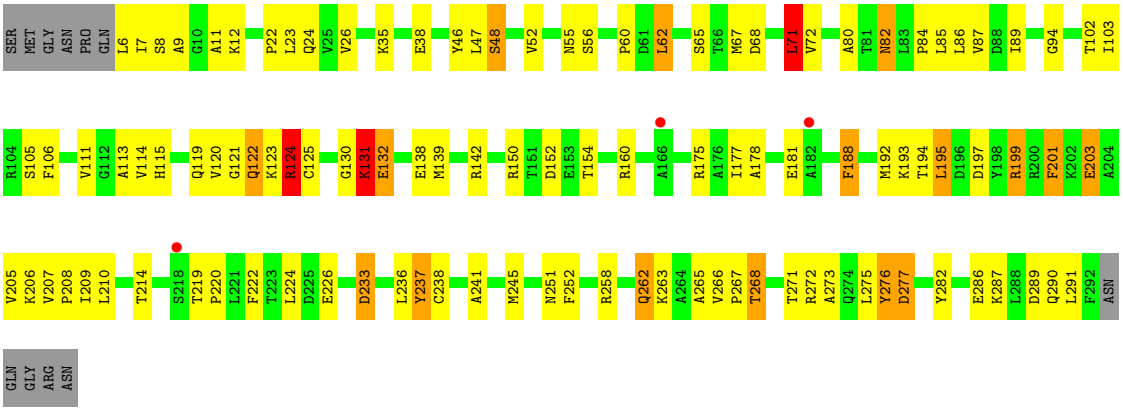
• Molecule 1: Methylisocitrate lyase

Chain M:



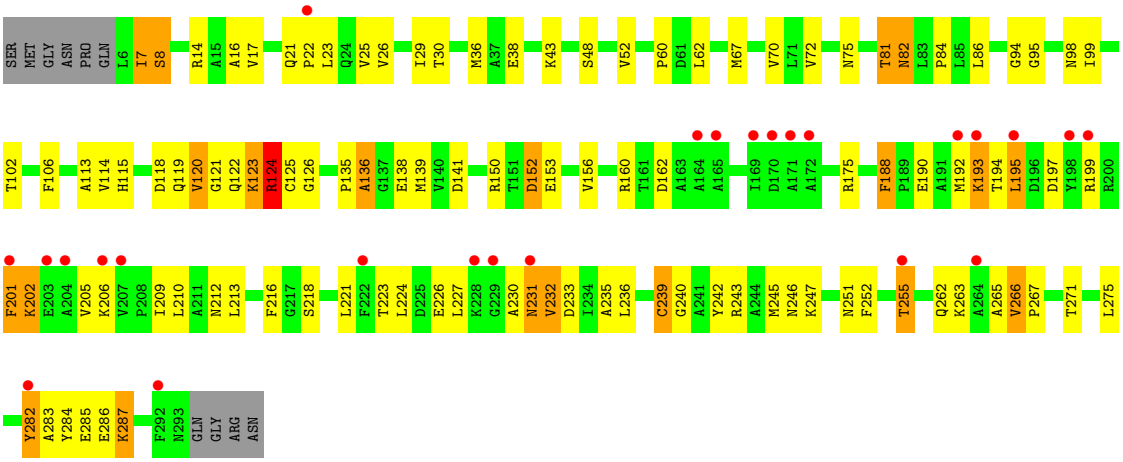
• Molecule 1: Methylisocitrate lyase

Chain N:



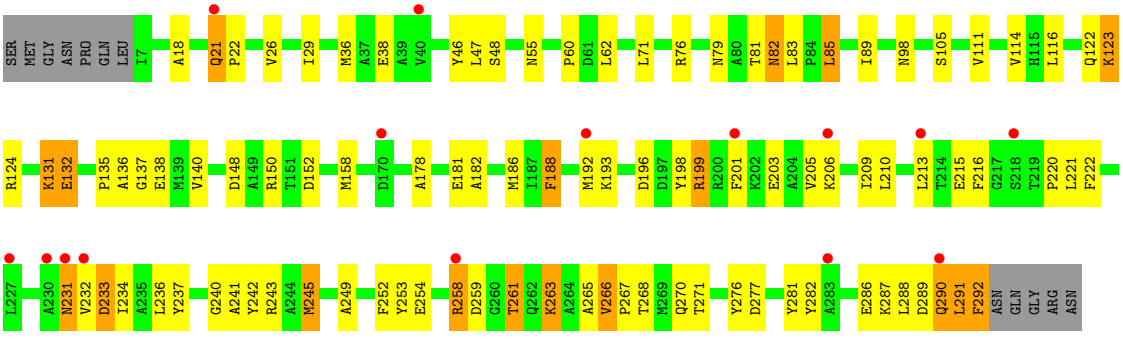
• Molecule 1: Methylisocitrate lyase

Chain O:



• Molecule 1: Methylisocitrate lyase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	163.81Å 172.40Å 179.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.90 46.49 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.00-2.90) 98.5 (46.49-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.237 , 0.299 0.237 , 0.299	Depositor DCC
R_{free} test set	5514 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 27.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	34623	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.69	0/2218	0.80	2/3005 (0.1%)
1	B	0.67	0/2189	0.78	0/2966
1	C	0.65	0/2197	0.78	0/2977
1	D	0.64	0/2197	0.74	0/2977
1	E	0.67	0/2205	0.78	0/2988
1	F	0.67	0/2189	0.75	2/2966 (0.1%)
1	G	0.64	0/2197	0.77	2/2977 (0.1%)
1	H	0.69	1/2205 (0.0%)	0.75	0/2988
1	I	0.65	0/2214	0.77	1/3000 (0.0%)
1	J	0.67	0/2206	0.77	0/2989
1	K	0.70	0/2189	0.77	2/2966 (0.1%)
1	L	0.68	1/2189 (0.0%)	0.77	2/2966 (0.1%)
1	M	0.74	0/2197	0.81	0/2977
1	N	0.75	0/2197	0.83	1/2977 (0.0%)
1	O	0.83	1/2205 (0.0%)	0.79	1/2988 (0.0%)
1	P	0.74	0/2189	0.75	0/2966
All	All	0.69	3/35183 (0.0%)	0.78	13/47673 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	239	CYS	CB-SG	-10.33	1.64	1.82
1	H	239	CYS	CB-SG	-5.44	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	239	CYS	CB-SG	-5.28	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	279	LEU	CA-CB-CG	6.08	129.29	115.30
1	A	76	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	K	199	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	L	71	LEU	CA-CB-CG	5.65	128.30	115.30
1	G	275	LEU	CA-CB-CG	5.61	128.19	115.30
1	A	118	ASP	CB-CG-OD1	5.41	123.17	118.30
1	F	88	ASP	CB-CG-OD1	5.37	123.14	118.30
1	G	245	MET	CA-CB-CG	5.35	122.40	113.30
1	K	224	LEU	CA-CB-CG	5.25	127.38	115.30
1	F	116	LEU	CA-CB-CG	5.19	127.24	115.30
1	I	116	LEU	CA-CB-CG	5.17	127.19	115.30
1	O	36	MET	CG-SD-CE	5.12	108.40	100.20
1	N	71	LEU	CB-CG-CD2	-5.10	102.33	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	121	GLY	Peptide
1	N	122	GLN	Peptide

5.2 Too-close contacts (i)

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	2183	0	2179	59	0
1	B	2154	0	2151	59	0
1	C	2162	0	2157	50	0
1	D	2162	0	2162	57	0
1	E	2170	0	2168	65	0
1	F	2154	0	2151	69	0
1	G	2162	0	2162	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2170	0	2168	69	0
1	I	2179	0	2176	55	0
1	J	2171	0	2170	64	0
1	K	2154	0	2151	59	0
1	L	2154	0	2151	64	0
1	M	2162	0	2157	92	0
1	N	2162	0	2162	95	0
1	O	2170	0	2168	91	0
1	P	2154	0	2151	81	0
All	All	34623	0	34584	969	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (969) 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:I:67:MET:HE3	1:I:102:THR:HA	1.23	1.15
1:L:199:ARG:HH11	1:L:199:ARG:HB2	1.14	1.07
1:I:123:LYS:HD2	1:I:124:ARG:H	1.12	1.07
1:I:67:MET:CE	1:I:102:THR:HA	1.85	1.05
1:G:199:ARG:HH11	1:G:199:ARG:HB2	0.88	1.03
1:G:199:ARG:HB2	1:G:199:ARG:NH1	1.74	1.02
1:A:67:MET:HE3	1:A:102:THR:HA	1.42	1.01
1:H:199:ARG:HB2	1:H:199:ARG:HH11	1.25	1.00
1:G:199:ARG:HH11	1:G:199:ARG:CB	1.75	0.99
1:O:67:MET:CE	1:O:102:THR:HA	1.92	0.99
1:J:160:ARG:NH2	1:J:190:GLU:HG3	1.79	0.98
1:E:67:MET:HE3	1:E:102:THR:HA	1.45	0.98
1:C:67:MET:CE	1:C:102:THR:HA	1.96	0.96
1:H:67:MET:HE2	1:H:102:THR:HA	1.46	0.95
1:H:67:MET:CE	1:H:102:THR:HA	1.95	0.95
1:C:223:THR:OG1	1:C:226:GLU:HG3	1.66	0.95
1:I:245:MET:HB2	1:J:245:MET:HB2	1.48	0.93
1:I:128:ARG:H	1:I:128:ARG:HD2	1.29	0.93
1:H:262:GLN:H	1:H:262:GLN:HE21	0.99	0.93
1:B:148:ASP:OD2	1:D:287:LYS:HE2	1.70	0.92
1:L:262:GLN:H	1:L:262:GLN:HE21	1.03	0.92
1:G:251:ASN:O	1:G:255:THR:HG23	1.70	0.91
1:C:245:MET:HB2	1:D:245:MET:HB2	1.51	0.91
1:C:67:MET:HE3	1:C:102:THR:HA	1.48	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:67:MET:HE3	1:O:102:THR:HA	1.52	0.89
1:A:245:MET:HB2	1:B:245:MET:HB2	1.52	0.89
1:O:252:PHE:CE1	1:P:240:GLY:HA3	2.07	0.89
1:I:199:ARG:HH11	1:I:199:ARG:HB2	1.36	0.89
1:N:199:ARG:CB	1:N:199:ARG:HH11	1.86	0.88
1:H:20:GLU:OE1	1:H:43:LYS:HE3	1.74	0.88
1:P:242:TYR:HA	1:P:245:MET:HG3	1.54	0.88
1:C:122:GLN:HG2	1:C:123:LYS:N	1.89	0.88
1:L:199:ARG:HB2	1:L:199:ARG:NH1	1.88	0.87
1:M:67:MET:HE2	1:M:102:THR:HA	1.56	0.87
1:I:36:MET:HE2	1:I:270:GLN:HE22	1.36	0.87
1:I:271:THR:OG1	1:I:274:GLN:HG3	1.74	0.86
1:K:245:MET:HB2	1:L:245:MET:HB2	1.54	0.86
1:F:199:ARG:HH11	1:F:199:ARG:HB2	1.39	0.86
1:E:216:PHE:HB2	1:F:272:ARG:HG3	1.57	0.86
1:H:22:PRO:HG2	1:H:224:LEU:CD2	2.06	0.85
1:A:242:TYR:HA	1:A:245:MET:HG2	1.57	0.85
1:G:245:MET:HB2	1:H:245:MET:HB2	1.58	0.85
1:E:67:MET:CE	1:E:102:THR:HA	2.07	0.84
1:F:251:ASN:O	1:F:255:THR:HG23	1.77	0.84
1:A:271:THR:OG1	1:A:274:GLN:HG3	1.76	0.84
1:N:205:VAL:HG21	1:N:209:ILE:HD11	1.57	0.84
1:B:262:GLN:H	1:B:262:GLN:HE21	1.23	0.84
1:H:203:GLU:O	1:H:206:LYS:HE3	1.77	0.84
1:N:67:MET:CE	1:N:102:THR:HA	2.07	0.84
1:O:160:ARG:HH21	1:O:190:GLU:HG3	1.42	0.84
1:F:242:TYR:HA	1:F:245:MET:HG2	1.57	0.84
1:O:188:PHE:HZ	1:O:212:ASN:HD22	1.23	0.84
1:G:262:GLN:H	1:G:262:GLN:HE21	1.22	0.84
1:P:258:ARG:HA	1:P:258:ARG:NE	1.93	0.83
1:A:67:MET:CE	1:A:102:THR:HA	2.06	0.83
1:F:215:GLU:HG2	1:F:243:ARG:HH21	1.40	0.83
1:J:275:LEU:HD22	1:J:279:LEU:HD22	1.60	0.83
1:N:177:ILE:O	1:N:181:GLU:HG2	1.79	0.83
1:C:122:GLN:HG2	1:C:123:LYS:H	1.40	0.83
1:E:36:MET:CE	1:E:270:GLN:HE22	1.92	0.82
1:J:67:MET:CE	1:J:102:THR:HA	2.09	0.82
1:L:22:PRO:HG2	1:L:224:LEU:HD22	1.62	0.82
1:I:67:MET:HE3	1:I:102:THR:CA	2.07	0.82
1:F:223:THR:OG1	1:F:226:GLU:HG3	1.80	0.81
1:F:60:PRO:HB2	1:F:62:LEU:HD22	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:TYR:HA	1:C:245:MET:HG2	1.60	0.81
1:A:262:GLN:H	1:A:262:GLN:HE21	1.26	0.81
1:O:205:VAL:HG21	1:O:209:ILE:HD11	1.61	0.81
1:B:67:MET:HE2	1:B:102:THR:HA	1.62	0.80
1:N:199:ARG:HH11	1:N:199:ARG:HB2	1.46	0.80
1:L:251:ASN:O	1:L:255:THR:HG23	1.82	0.80
1:J:98:ASN:N	1:J:98:ASN:HD22	1.79	0.80
1:N:219:THR:HG23	1:N:222:PHE:HE1	1.47	0.80
1:N:35:LYS:HE2	1:N:80:ALA:O	1.82	0.79
1:K:89:ILE:HD13	1:K:114:VAL:HG21	1.65	0.79
1:D:98:ASN:N	1:D:98:ASN:HD22	1.79	0.79
1:N:46:TYR:HD1	1:N:86:LEU:HD23	1.47	0.79
1:G:6:LEU:HD12	1:G:7:ILE:H	1.45	0.79
1:E:122:GLN:NE2	1:N:94:GLY:HA2	1.98	0.79
1:I:252:PHE:CE1	1:J:240:GLY:HA3	2.19	0.78
1:M:67:MET:CE	1:M:102:THR:HA	2.13	0.78
1:A:36:MET:HE3	1:A:270:GLN:HE22	1.48	0.78
1:E:252:PHE:CE1	1:F:240:GLY:HA3	2.19	0.78
1:H:262:GLN:H	1:H:262:GLN:NE2	1.80	0.77
1:B:128:ARG:HG2	1:B:129:PRO:HD3	1.66	0.77
1:M:241:ALA:O	1:M:245:MET:HG2	1.84	0.77
1:N:67:MET:HE3	1:N:102:THR:HA	1.67	0.77
1:H:242:TYR:HA	1:H:245:MET:HG2	1.67	0.76
1:E:242:TYR:HA	1:E:245:MET:HG3	1.66	0.76
1:F:262:GLN:H	1:F:262:GLN:HE21	1.33	0.76
1:K:199:ARG:HG2	1:K:199:ARG:HH11	1.51	0.76
1:M:22:PRO:HG2	1:M:224:LEU:HD23	1.66	0.76
1:I:36:MET:CE	1:I:270:GLN:HE22	1.98	0.76
1:E:22:PRO:HG2	1:E:224:LEU:HD22	1.66	0.76
1:C:262:GLN:H	1:C:262:GLN:HE21	1.34	0.76
1:K:242:TYR:HA	1:K:245:MET:HG2	1.66	0.76
1:A:36:MET:CE	1:A:270:GLN:HE22	2.00	0.75
1:N:130:GLY:O	1:N:131:LYS:HB2	1.85	0.75
1:E:293:ASN:HB2	1:H:272:ARG:NH2	2.02	0.75
1:F:98:ASN:H	1:F:98:ASN:HD22	1.33	0.74
1:G:240:GLY:HA3	1:H:252:PHE:CE1	2.22	0.74
1:J:98:ASN:HD22	1:J:98:ASN:H	1.35	0.74
1:I:199:ARG:HB2	1:I:199:ARG:NH1	2.02	0.73
1:M:281:TYR:HD2	1:M:281:TYR:O	1.70	0.73
1:G:262:GLN:H	1:G:262:GLN:NE2	1.87	0.73
1:E:288:LEU:HD13	1:F:128:ARG:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:36:MET:CE	1:K:270:GLN:HE22	2.02	0.73
1:L:64:ILE:HA	1:P:98:ASN:HD21	1.54	0.73
1:D:205:VAL:HG21	1:D:209:ILE:HD11	1.70	0.73
1:F:98:ASN:HD22	1:F:98:ASN:N	1.86	0.73
1:G:6:LEU:HD12	1:G:7:ILE:N	2.03	0.73
1:J:242:TYR:HA	1:J:245:MET:HG2	1.70	0.73
1:E:241:ALA:O	1:E:245:MET:HG2	1.88	0.72
1:F:177:ILE:O	1:F:181:GLU:HG2	1.88	0.72
1:I:22:PRO:HG2	1:I:224:LEU:HD22	1.71	0.72
1:J:160:ARG:HH21	1:J:190:GLU:HG3	1.52	0.72
1:H:251:ASN:O	1:H:255:THR:HG23	1.90	0.72
1:O:201:PHE:O	1:O:205:VAL:HG22	1.89	0.72
1:A:251:ASN:O	1:A:255:THR:HG23	1.90	0.72
1:N:219:THR:CG2	1:N:222:PHE:HE1	2.03	0.72
1:G:242:TYR:HA	1:G:245:MET:HG2	1.70	0.72
1:K:262:GLN:H	1:K:262:GLN:HE21	1.37	0.72
1:I:242:TYR:HA	1:I:245:MET:HG2	1.72	0.71
1:N:273:ALA:O	1:N:277:ASP:OD1	2.09	0.71
1:M:242:TYR:HA	1:M:245:MET:CG	2.21	0.71
1:P:213:LEU:HD12	1:P:237:TYR:CE2	2.26	0.71
1:B:98:ASN:H	1:B:98:ASN:HD22	1.39	0.70
1:M:22:PRO:HG2	1:M:224:LEU:CD2	2.21	0.70
1:O:251:ASN:O	1:O:255:THR:HG23	1.91	0.70
1:J:60:PRO:HG2	1:J:62:LEU:HD22	1.73	0.70
1:B:242:TYR:HA	1:B:245:MET:HG2	1.73	0.70
1:J:262:GLN:H	1:J:262:GLN:HE21	1.40	0.70
1:G:251:ASN:O	1:G:255:THR:CG2	2.40	0.70
1:O:150:ARG:HD3	1:O:153:GLU:HA	1.73	0.69
1:E:140:VAL:HG13	1:E:182:ALA:HB2	1.73	0.69
1:O:193:LYS:H	1:O:193:LYS:HD2	1.58	0.69
1:H:262:GLN:HE21	1:H:262:GLN:N	1.82	0.69
1:K:287:LYS:HE3	1:K:290:GLN:NE2	2.06	0.69
1:B:271:THR:OG1	1:B:274:GLN:HG3	1.91	0.69
1:H:199:ARG:HB2	1:H:199:ARG:NH1	2.05	0.69
1:J:290:GLN:O	1:J:290:GLN:HG2	1.93	0.69
1:L:262:GLN:H	1:L:262:GLN:NE2	1.86	0.69
1:M:262:GLN:H	1:M:262:GLN:HE21	1.38	0.69
1:A:123:LYS:H	1:A:123:LYS:HD3	1.58	0.69
1:H:98:ASN:HD21	1:I:64:ILE:HA	1.57	0.69
1:I:230:ALA:O	1:I:231:ASN:HB2	1.91	0.69
1:J:140:VAL:HG13	1:J:182:ALA:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:215:GLU:HG2	1:F:243:ARG:NH2	2.07	0.69
1:J:7:ILE:H	1:J:7:ILE:HD12	1.56	0.69
1:E:242:TYR:HA	1:E:245:MET:CG	2.23	0.68
1:I:128:ARG:HD2	1:I:128:ARG:N	2.05	0.68
1:J:118:ASP:OD1	1:J:161:THR:HA	1.93	0.68
1:N:46:TYR:CD1	1:N:86:LEU:HD23	2.28	0.67
1:M:32:TYR:HE2	1:M:36:MET:CE	2.07	0.67
1:M:195:LEU:HD11	1:M:226:GLU:HB3	1.75	0.67
1:B:251:ASN:O	1:B:255:THR:CG2	2.42	0.67
1:B:251:ASN:O	1:B:255:THR:HG23	1.93	0.67
1:K:199:ARG:HH11	1:K:199:ARG:CG	2.08	0.67
1:E:60:PRO:HB2	1:E:62:LEU:HD22	1.76	0.67
1:L:147:VAL:HG13	1:L:150:ARG:HH12	1.58	0.67
1:L:98:ASN:HD22	1:L:98:ASN:N	1.92	0.67
1:M:14:ARG:NH1	1:M:156:VAL:HG22	2.10	0.67
1:M:281:TYR:O	1:M:281:TYR:CD2	2.48	0.67
1:D:251:ASN:O	1:D:255:THR:HG23	1.95	0.66
1:G:60:PRO:HB3	1:H:281:TYR:CE1	2.30	0.66
1:I:216:PHE:CE1	1:J:271:THR:HG22	2.29	0.66
1:M:249:ALA:O	1:M:253:TYR:CD2	2.48	0.66
1:E:293:ASN:HB2	1:H:272:ARG:HH21	1.59	0.66
1:I:123:LYS:HD2	1:I:124:ARG:N	1.97	0.66
1:K:13:PHE:O	1:K:17:VAL:HG23	1.96	0.66
1:P:29:ILE:HD13	1:P:55:ASN:OD1	1.96	0.66
1:O:210:LEU:HD11	1:O:236:LEU:HD22	1.78	0.66
1:E:38:GLU:OE2	1:E:82:ASN:ND2	2.28	0.66
1:A:240:GLY:HA3	1:B:252:PHE:CE1	2.30	0.65
1:B:199:ARG:HH11	1:B:199:ARG:HB2	1.61	0.65
1:H:22:PRO:HG2	1:H:224:LEU:HD23	1.76	0.65
1:C:67:MET:HE1	1:C:102:THR:HA	1.78	0.65
1:N:67:MET:HE2	1:N:102:THR:HA	1.78	0.65
1:O:202:LYS:HG3	1:O:231:ASN:HB3	1.77	0.65
1:D:178:ALA:O	1:D:181:GLU:HB2	1.96	0.65
1:M:199:ARG:HH11	1:M:199:ARG:HB2	1.60	0.65
1:O:82:ASN:ND2	1:O:82:ASN:H	1.94	0.65
1:O:195:LEU:HD21	1:O:226:GLU:HB3	1.79	0.65
1:B:36:MET:CE	1:B:270:GLN:HE22	2.08	0.65
1:N:60:PRO:HB2	1:N:62:LEU:HD22	1.79	0.65
1:C:22:PRO:HG2	1:C:224:LEU:HD22	1.77	0.65
1:P:199:ARG:HG2	1:P:199:ARG:HH11	1.62	0.65
1:E:119:GLN:HE22	1:E:131:LYS:HA	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:195:LEU:HD12	1:M:222:PHE:CD2	2.32	0.64
1:O:22:PRO:HG2	1:O:224:LEU:CD2	2.27	0.64
1:O:242:TYR:HA	1:O:245:MET:HG2	1.79	0.64
1:C:128:ARG:HH21	1:D:285:GLU:HG3	1.62	0.64
1:E:252:PHE:CZ	1:F:240:GLY:HA3	2.32	0.64
1:J:67:MET:HE3	1:J:102:THR:HA	1.80	0.64
1:O:247:LYS:HE2	1:P:268:THR:HA	1.80	0.64
1:B:67:MET:HE2	1:B:102:THR:CA	2.26	0.64
1:M:140:VAL:HG13	1:M:182:ALA:HB2	1.78	0.64
1:D:123:LYS:O	1:D:124:ARG:O	2.15	0.64
1:L:67:MET:CE	1:L:102:THR:HA	2.27	0.64
1:O:266:VAL:N	1:O:267:PRO:HD2	2.13	0.64
1:A:281:TYR:C	1:A:281:TYR:CD2	2.71	0.64
1:O:152:ASP:OD1	1:O:152:ASP:C	2.36	0.64
1:B:140:VAL:HG13	1:B:182:ALA:HB2	1.81	0.63
1:G:60:PRO:HB2	1:G:62:LEU:HD22	1.80	0.63
1:D:281:TYR:C	1:D:281:TYR:CD2	2.71	0.63
1:N:199:ARG:HB2	1:N:199:ARG:NH1	2.12	0.63
1:F:270:GLN:HG3	1:F:274:GLN:HE21	1.63	0.63
1:M:36:MET:CE	1:M:270:GLN:HE22	2.10	0.63
1:P:71:LEU:HD11	1:P:105:SER:HB3	1.81	0.63
1:C:140:VAL:HG13	1:C:182:ALA:HB2	1.80	0.63
1:K:195:LEU:HD21	1:K:226:GLU:HB3	1.80	0.63
1:I:89:ILE:HG12	1:I:114:VAL:HG13	1.81	0.63
1:D:262:GLN:HE21	1:D:262:GLN:H	1.46	0.63
1:H:62:LEU:HD23	1:I:97:PHE:CE2	2.34	0.62
1:E:36:MET:HE3	1:E:270:GLN:HE22	1.63	0.62
1:F:261:THR:HG23	1:F:263:LYS:H	1.63	0.62
1:C:26:VAL:HG12	1:C:237:TYR:HB2	1.81	0.62
1:L:67:MET:HE3	1:L:102:THR:HA	1.80	0.62
1:O:14:ARG:NH1	1:O:156:VAL:HG22	2.15	0.62
1:K:178:ALA:O	1:K:181:GLU:HB2	2.00	0.62
1:L:138:GLU:OE1	1:L:138:GLU:HA	2.00	0.62
1:F:98:ASN:N	1:F:98:ASN:ND2	2.48	0.62
1:M:32:TYR:HE2	1:M:36:MET:HE1	1.64	0.62
1:O:67:MET:HE3	1:O:102:THR:CA	2.26	0.62
1:O:82:ASN:H	1:O:82:ASN:HD22	1.46	0.62
1:B:64:ILE:HA	1:C:98:ASN:HD21	1.64	0.61
1:D:49:GLY:HA3	1:D:88:ASP:OD2	1.99	0.61
1:O:205:VAL:CG2	1:O:209:ILE:HD11	2.29	0.61
1:C:199:ARG:HG2	1:C:199:ARG:HH11	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:230:ALA:O	1:F:231:ASN:HB2	1.98	0.61
1:G:38:GLU:HG3	1:G:83:LEU:HG	1.83	0.61
1:H:36:MET:CE	1:H:270:GLN:HE22	2.14	0.61
1:I:199:ARG:NH1	1:I:230:ALA:HA	2.15	0.61
1:P:38:GLU:HG3	1:P:83:LEU:HG	1.83	0.61
1:D:242:TYR:HA	1:D:245:MET:HG2	1.82	0.61
1:I:140:VAL:HG13	1:I:182:ALA:HB2	1.82	0.61
1:J:201:PHE:O	1:J:205:VAL:HG22	2.01	0.61
1:M:36:MET:HE2	1:M:270:GLN:NE2	2.15	0.61
1:N:199:ARG:HH11	1:N:199:ARG:CG	2.13	0.61
1:E:272:ARG:HD2	1:F:216:PHE:HB2	1.82	0.61
1:B:140:VAL:HG12	1:B:144:LYS:HE3	1.83	0.61
1:A:178:ALA:HA	1:A:181:GLU:HG3	1.84	0.60
1:M:38:GLU:HG3	1:M:83:LEU:HG	1.82	0.60
1:J:275:LEU:CD2	1:J:279:LEU:HD22	2.30	0.60
1:B:262:GLN:HE21	1:B:262:GLN:N	1.98	0.60
1:D:98:ASN:N	1:D:98:ASN:ND2	2.49	0.60
1:A:120:VAL:HA	1:A:134:VAL:HG13	1.84	0.60
1:M:210:LEU:HD21	1:M:236:LEU:HD23	1.83	0.60
1:D:89:ILE:HD13	1:D:114:VAL:HG11	1.84	0.60
1:I:128:ARG:H	1:I:128:ARG:CD	2.08	0.60
1:J:36:MET:CE	1:J:270:GLN:HE22	2.14	0.60
1:O:245:MET:HB2	1:P:245:MET:HB3	1.84	0.60
1:E:169:ILE:O	1:E:173:ILE:HG13	2.02	0.60
1:F:121:GLY:O	1:F:122:GLN:O	2.18	0.59
1:G:117:GLU:HB3	1:G:160:ARG:HD3	1.83	0.59
1:K:108:LYS:NZ	1:P:79:ASN:OD1	2.35	0.59
1:L:26:VAL:HG12	1:L:237:TYR:HB2	1.83	0.59
1:I:240:GLY:HA3	1:J:252:PHE:CE1	2.37	0.59
1:J:138:GLU:OE1	1:J:138:GLU:HA	2.02	0.59
1:M:249:ALA:O	1:M:253:TYR:HD2	1.85	0.59
1:G:140:VAL:HG13	1:G:182:ALA:HB2	1.84	0.59
1:K:252:PHE:CE1	1:L:240:GLY:HA3	2.37	0.59
1:L:122:GLN:HG2	1:P:122:GLN:HB2	1.84	0.59
1:G:147:VAL:HG13	1:G:150:ARG:HH12	1.67	0.59
1:E:293:ASN:CB	1:H:272:ARG:HH21	2.16	0.59
1:J:120:VAL:CG2	1:J:132:GLU:HB3	2.33	0.59
1:K:200:ARG:O	1:K:203:GLU:HB3	2.03	0.59
1:B:136:ALA:O	1:B:140:VAL:HG23	2.02	0.59
1:G:158:MET:HG3	1:G:186:MET:HB2	1.84	0.59
1:M:245:MET:HB2	1:N:245:MET:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:38:GLU:OE2	1:N:82:ASN:ND2	2.35	0.59
1:L:262:GLN:HE21	1:L:262:GLN:N	1.87	0.59
1:F:242:TYR:HA	1:F:245:MET:CG	2.29	0.59
1:M:253:TYR:CD1	1:N:26:VAL:HG21	2.38	0.59
1:C:252:PHE:CE1	1:D:240:GLY:HA3	2.38	0.58
1:E:24:GLN:HG2	1:E:237:TYR:HE1	1.68	0.58
1:B:98:ASN:HD22	1:B:98:ASN:N	2.00	0.58
1:J:202:LYS:HE2	1:J:231:ASN:O	2.02	0.58
1:J:120:VAL:HG23	1:J:132:GLU:HB3	1.84	0.58
1:K:22:PRO:HG2	1:K:224:LEU:HD22	1.85	0.58
1:A:242:TYR:HA	1:A:245:MET:CG	2.30	0.58
1:A:36:MET:CE	1:B:250:LEU:HB2	2.33	0.58
1:O:282:TYR:CZ	1:O:286:GLU:HG2	2.39	0.58
1:M:242:TYR:HA	1:M:245:MET:HG3	1.85	0.58
1:N:203:GLU:O	1:N:206:LYS:HE2	2.04	0.58
1:G:242:TYR:HA	1:G:245:MET:CG	2.34	0.58
1:L:220:PRO:HB2	1:L:222:PHE:CE2	2.39	0.58
1:O:38:GLU:OE2	1:O:82:ASN:ND2	2.36	0.58
1:B:276:TYR:N	1:B:276:TYR:HD1	2.01	0.58
1:P:266:VAL:N	1:P:267:PRO:HD2	2.19	0.58
1:B:67:MET:CE	1:B:102:THR:HA	2.33	0.58
1:E:250:LEU:HD22	1:F:36:MET:HE2	1.85	0.57
1:M:266:VAL:HA	1:M:269:MET:HG3	1.87	0.57
1:H:263:LYS:O	1:H:266:VAL:HG22	2.04	0.57
1:D:150:ARG:HD3	1:D:152:ASP:O	2.04	0.57
1:M:216:PHE:CE2	1:N:271:THR:HA	2.39	0.57
1:G:216:PHE:O	1:H:272:ARG:NH1	2.37	0.57
1:N:67:MET:HE3	1:N:102:THR:CA	2.35	0.57
1:D:60:PRO:HG2	1:D:62:LEU:HD22	1.86	0.57
1:F:143:ILE:O	1:F:147:VAL:HG23	2.03	0.57
1:K:251:ASN:O	1:K:255:THR:HG23	2.05	0.57
1:O:70:VAL:HG12	1:O:106:PHE:HZ	1.69	0.57
1:M:253:TYR:CE1	1:N:26:VAL:HG21	2.40	0.57
1:B:7:ILE:HD13	1:B:7:ILE:N	2.20	0.57
1:M:87:VAL:HG23	1:M:111:VAL:HG11	1.87	0.57
1:M:178:ALA:O	1:M:181:GLU:HB2	2.04	0.57
1:O:120:VAL:HB	1:O:123:LYS:HE3	1.86	0.56
1:C:25:VAL:HG22	1:C:236:LEU:HD12	1.87	0.56
1:J:199:ARG:HB2	1:J:199:ARG:NH1	2.20	0.56
1:O:265:ALA:C	1:O:267:PRO:HD2	2.26	0.56
1:B:263:LYS:HB2	1:B:263:LYS:NZ	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:MET:CE	1:H:102:THR:CA	2.80	0.56
1:C:47:LEU:HB2	1:C:85:LEU:HD11	1.88	0.56
1:F:67:MET:HE3	1:F:105:SER:HB2	1.86	0.56
1:P:18:ALA:O	1:P:21:GLN:NE2	2.39	0.56
1:E:170:ASP:OD2	1:E:200:ARG:NH2	2.39	0.56
1:A:252:PHE:CE1	1:B:240:GLY:HA3	2.41	0.56
1:J:199:ARG:HH12	1:J:230:ALA:HA	1.71	0.56
1:J:111:VAL:O	1:J:155:PHE:HE1	1.89	0.56
1:N:119:GLN:OE1	1:N:131:LYS:HA	2.06	0.55
1:O:160:ARG:NH2	1:O:190:GLU:HG3	2.18	0.55
1:A:150:ARG:HD3	1:A:153:GLU:HA	1.87	0.55
1:D:29:ILE:HG13	1:D:30:THR:HG23	1.88	0.55
1:I:215:GLU:HG2	1:I:243:ARG:HE	1.71	0.55
1:J:282:TYR:O	1:J:285:GLU:N	2.39	0.55
1:I:71:LEU:HD23	1:I:106:PHE:CE1	2.42	0.55
1:K:140:VAL:HG22	1:K:182:ALA:HB2	1.88	0.55
1:K:240:GLY:HA3	1:L:252:PHE:CE1	2.41	0.55
1:O:240:GLY:HA3	1:P:252:PHE:CE1	2.41	0.55
1:H:223:THR:OG1	1:H:226:GLU:HG3	2.07	0.55
1:N:192:MET:SD	1:N:197:ASP:HB3	2.46	0.55
1:L:242:TYR:HA	1:L:245:MET:HG2	1.88	0.55
1:M:36:MET:CE	1:M:270:GLN:NE2	2.70	0.55
1:B:117:GLU:HG3	1:B:119:GLN:HG2	1.87	0.55
1:B:150:ARG:HD3	1:B:152:ASP:O	2.06	0.55
1:K:89:ILE:HD13	1:K:114:VAL:CG2	2.35	0.55
1:O:82:ASN:ND2	1:O:82:ASN:N	2.55	0.55
1:A:118:ASP:OD1	1:A:161:THR:HA	2.06	0.55
1:C:123:LYS:HD3	1:C:124:ARG:H	1.71	0.55
1:I:266:VAL:HA	1:I:269:MET:HG3	1.88	0.55
1:C:252:PHE:CZ	1:D:240:GLY:HA3	2.41	0.55
1:P:215:GLU:HG2	1:P:243:ARG:HH21	1.71	0.55
1:B:276:TYR:N	1:B:276:TYR:CD1	2.73	0.55
1:J:67:MET:HE2	1:J:102:THR:HA	1.86	0.55
1:K:287:LYS:HE3	1:K:290:GLN:HE22	1.69	0.55
1:M:46:TYR:HD1	1:M:86:LEU:HG	1.70	0.55
1:I:7:ILE:HG23	1:I:11:ALA:HB3	1.89	0.54
1:A:119:GLN:HE22	1:A:132:GLU:H	1.56	0.54
1:B:128:ARG:HG2	1:B:129:PRO:CD	2.35	0.54
1:H:113:ALA:HB2	1:H:156:VAL:HB	1.89	0.54
1:H:117:GLU:HB3	1:H:160:ARG:HD3	1.89	0.54
1:N:219:THR:HG23	1:N:222:PHE:CE1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:249:ALA:O	1:P:253:TYR:CD2	2.61	0.54
1:E:245:MET:CB	1:F:245:MET:HB2	2.36	0.54
1:G:192:MET:HG3	1:G:198:TYR:CE1	2.43	0.54
1:N:265:ALA:O	1:N:268:THR:HG23	2.08	0.54
1:A:275:LEU:O	1:A:279:LEU:HB2	2.07	0.54
1:B:127:HIS:ND1	1:B:128:ARG:O	2.35	0.54
1:H:271:THR:HG23	1:H:274:GLN:OE1	2.07	0.54
1:K:287:LYS:CE	1:K:290:GLN:HE22	2.21	0.54
1:E:243:ARG:HB2	1:F:269:MET:HG2	1.90	0.54
1:L:117:GLU:HB3	1:L:160:ARG:HD3	1.90	0.54
1:O:29:ILE:HD13	1:O:242:TYR:HB2	1.89	0.54
1:P:85:LEU:HD23	1:P:111:VAL:HG22	1.88	0.54
1:M:170:ASP:HA	1:M:173:ILE:HD12	1.90	0.54
1:B:98:ASN:N	1:B:98:ASN:ND2	2.55	0.54
1:L:266:VAL:HA	1:L:269:MET:HG3	1.90	0.54
1:N:203:GLU:O	1:N:206:LYS:CE	2.56	0.54
1:B:223:THR:OG1	1:B:226:GLU:HG3	2.08	0.54
1:G:98:ASN:HD21	1:J:64:ILE:HA	1.73	0.54
1:G:143:ILE:O	1:G:147:VAL:HG23	2.08	0.54
1:F:36:MET:HE3	1:F:270:GLN:HE22	1.73	0.54
1:N:86:LEU:HA	1:N:113:ALA:O	2.08	0.54
1:C:230:ALA:O	1:C:231:ASN:HB2	2.08	0.53
1:D:281:TYR:C	1:D:281:TYR:HD2	2.12	0.53
1:J:199:ARG:HB2	1:J:199:ARG:HH11	1.73	0.53
1:J:170:ASP:HA	1:J:173:ILE:HD12	1.89	0.53
1:J:195:LEU:HD12	1:J:222:PHE:CE2	2.42	0.53
1:K:202:LYS:HG2	1:K:209:ILE:HG12	1.90	0.53
1:L:147:VAL:HG13	1:L:150:ARG:NH1	2.22	0.53
1:B:40:VAL:HG12	1:B:40:VAL:O	2.07	0.53
1:H:123:LYS:O	1:H:124:ARG:C	2.47	0.53
1:I:139:MET:HG3	1:I:143:ILE:HD11	1.89	0.53
1:J:98:ASN:N	1:J:98:ASN:ND2	2.47	0.53
1:J:120:VAL:HG11	1:J:123:LYS:HD3	1.89	0.53
1:D:36:MET:CE	1:D:270:GLN:HE22	2.20	0.53
1:D:193:LYS:HD2	1:D:193:LYS:N	2.23	0.53
1:K:86:LEU:HA	1:K:113:ALA:O	2.08	0.53
1:N:233:ASP:N	1:N:233:ASP:OD2	2.38	0.53
1:N:237:TYR:N	1:N:237:TYR:CD1	2.77	0.53
1:P:291:LEU:HB3	1:P:292:PHE:CE2	2.44	0.53
1:E:36:MET:CE	1:E:270:GLN:NE2	2.67	0.53
1:K:205:VAL:HG21	1:K:209:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:205:VAL:HG21	1:M:209:ILE:HD11	1.90	0.53
1:N:150:ARG:HD3	1:N:152:ASP:O	2.07	0.53
1:O:245:MET:HB2	1:P:245:MET:CB	2.38	0.53
1:F:106:PHE:HD1	1:F:111:VAL:HG21	1.74	0.53
1:C:207:VAL:HB	1:C:208:PRO:HD2	1.91	0.53
1:I:251:ASN:O	1:I:255:THR:HG23	2.08	0.53
1:K:94:GLY:HA2	1:O:122:GLN:NE2	2.24	0.53
1:L:20:GLU:HG2	1:L:23:LEU:HA	1.91	0.53
1:M:60:PRO:HG2	1:M:62:LEU:HD22	1.91	0.53
1:K:114:VAL:HG13	1:K:155:PHE:CZ	2.44	0.52
1:M:255:THR:HG22	1:M:258:ARG:HH22	1.74	0.52
1:B:120:VAL:HG11	1:B:123:LYS:HD2	1.91	0.52
1:D:123:LYS:O	1:D:124:ARG:C	2.47	0.52
1:O:271:THR:HG22	1:P:216:PHE:CE1	2.44	0.52
1:A:281:TYR:CD2	1:A:281:TYR:O	2.62	0.52
1:E:262:GLN:H	1:E:262:GLN:HE21	1.56	0.52
1:A:22:PRO:HD2	1:A:224:LEU:HD22	1.91	0.52
1:N:8:SER:O	1:N:11:ALA:N	2.41	0.52
1:O:194:THR:N	1:O:197:ASP:OD2	2.34	0.52
1:B:223:THR:H	1:B:226:GLU:HG3	1.75	0.52
1:C:271:THR:H	1:C:274:GLN:NE2	2.07	0.52
1:D:177:ILE:O	1:D:181:GLU:HG2	2.09	0.52
1:J:210:LEU:HD12	1:J:234:ILE:HG21	1.90	0.52
1:L:251:ASN:O	1:L:255:THR:CG2	2.56	0.52
1:L:283:ALA:HA	1:L:286:GLU:HG2	1.92	0.52
1:N:262:GLN:H	1:N:262:GLN:HE21	1.56	0.52
1:O:70:VAL:HG12	1:O:106:PHE:CZ	2.44	0.52
1:K:215:GLU:HG3	1:K:243:ARG:HE	1.75	0.52
1:N:195:LEU:HD21	1:N:226:GLU:HB3	1.91	0.52
1:P:47:LEU:HB2	1:P:85:LEU:HD11	1.92	0.52
1:A:269:MET:HB3	1:B:243:ARG:HB3	1.92	0.52
1:D:68:ASP:O	1:D:72:VAL:HG13	2.10	0.52
1:F:282:TYR:CE2	1:F:286:GLU:OE2	2.62	0.52
1:J:36:MET:HE2	1:J:270:GLN:HE22	1.74	0.52
1:C:99:ILE:HD11	1:C:142:ARG:HG2	1.91	0.52
1:E:262:GLN:H	1:E:262:GLN:NE2	2.08	0.52
1:L:140:VAL:HG13	1:L:182:ALA:HB2	1.92	0.52
1:M:195:LEU:HD12	1:M:222:PHE:CE2	2.46	0.52
1:E:250:LEU:HD22	1:F:36:MET:CE	2.39	0.51
1:M:39:ALA:CB	1:M:278:TYR:HE1	2.23	0.51
1:P:241:ALA:O	1:P:245:MET:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASN:HD21	1:D:64:ILE:HA	1.75	0.51
1:H:150:ARG:HD3	1:H:152:ASP:O	2.10	0.51
1:K:243:ARG:HB3	1:L:269:MET:HB3	1.92	0.51
1:J:150:ARG:HD3	1:J:152:ASP:O	2.09	0.51
1:P:209:ILE:N	1:P:233:ASP:OD2	2.31	0.51
1:A:67:MET:HE2	1:A:105:SER:CB	2.39	0.51
1:A:177:ILE:O	1:A:181:GLU:HG3	2.10	0.51
1:K:71:LEU:HD11	1:K:105:SER:HB3	1.91	0.51
1:B:94:GLY:HA2	1:C:122:GLN:NE2	2.25	0.51
1:L:205:VAL:HG21	1:L:209:ILE:HD11	1.91	0.51
1:M:255:THR:HG22	1:M:258:ARG:NH2	2.26	0.51
1:D:46:TYR:HE2	1:D:48:SER:HB2	1.76	0.51
1:E:245:MET:HB3	1:F:245:MET:HB2	1.91	0.51
1:I:128:ARG:N	1:I:128:ARG:CD	2.70	0.51
1:J:192:MET:HG3	1:J:198:TYR:CE1	2.46	0.51
1:M:199:ARG:HB2	1:M:199:ARG:NH1	2.25	0.51
1:A:36:MET:HE2	1:B:250:LEU:HB2	1.92	0.51
1:F:36:MET:CE	1:F:270:GLN:HE22	2.24	0.51
1:F:60:PRO:CB	1:F:62:LEU:HD22	2.39	0.51
1:H:94:GLY:HA2	1:I:122:GLN:NE2	2.25	0.51
1:P:265:ALA:C	1:P:267:PRO:HD2	2.31	0.51
1:F:67:MET:HE3	1:F:105:SER:CB	2.41	0.51
1:F:150:ARG:HD3	1:F:152:ASP:O	2.11	0.51
1:J:290:GLN:O	1:J:290:GLN:CG	2.58	0.51
1:N:271:THR:OG1	1:N:273:ALA:HB3	2.10	0.51
1:B:266:VAL:N	1:B:267:PRO:CD	2.74	0.51
1:P:258:ARG:HA	1:P:258:ARG:HE	1.74	0.51
1:G:46:TYR:CE2	1:G:238:CYS:HB2	2.45	0.50
1:K:113:ALA:HB2	1:K:156:VAL:HB	1.94	0.50
1:F:73:ASP:O	1:F:77:ILE:HG13	2.11	0.50
1:G:22:PRO:HG2	1:G:224:LEU:HD22	1.93	0.50
1:K:199:ARG:HG2	1:K:199:ARG:NH1	2.22	0.50
1:L:125:CYS:HB3	1:P:138:GLU:OE2	2.11	0.50
1:E:24:GLN:HG2	1:E:237:TYR:CE1	2.46	0.50
1:I:219:THR:HG22	1:I:220:PRO:O	2.11	0.50
1:M:202:LYS:HE3	1:M:233:ASP:OD2	2.11	0.50
1:A:85:LEU:O	1:A:111:VAL:HG13	2.11	0.50
1:C:99:ILE:CD1	1:C:142:ARG:HG2	2.41	0.50
1:N:175:ARG:O	1:N:178:ALA:HB3	2.11	0.50
1:B:120:VAL:HG11	1:B:123:LYS:CD	2.42	0.50
1:F:67:MET:CE	1:F:105:SER:CB	2.89	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:169:ILE:HG12	1:L:173:ILE:HD11	1.93	0.50
1:N:89:ILE:HG12	1:N:114:VAL:HG22	1.93	0.50
1:F:140:VAL:HG13	1:F:182:ALA:HB2	1.92	0.50
1:C:13:PHE:O	1:C:17:VAL:HG23	2.12	0.50
1:M:216:PHE:HB2	1:N:272:ARG:HG3	1.93	0.50
1:O:262:GLN:NE2	1:P:221:LEU:HB3	2.26	0.50
1:N:47:LEU:HD23	1:N:87:VAL:HG13	1.93	0.50
1:N:236:LEU:HD21	1:N:238:CYS:HB3	1.94	0.50
1:A:49:GLY:HA3	1:A:88:ASP:OD2	2.12	0.49
1:J:263:LYS:O	1:J:266:VAL:HG13	2.12	0.49
1:L:192:MET:HB2	1:L:198:TYR:CE2	2.47	0.49
1:M:150:ARG:HD3	1:M:152:ASP:O	2.12	0.49
1:E:284:TYR:CD1	1:F:60:PRO:HG3	2.47	0.49
1:N:220:PRO:HD2	1:N:222:PHE:CZ	2.47	0.49
1:P:192:MET:HG3	1:P:198:TYR:CE1	2.47	0.49
1:F:270:GLN:HG3	1:F:274:GLN:NE2	2.27	0.49
1:A:281:TYR:C	1:A:281:TYR:HD2	2.13	0.49
1:D:20:GLU:OE1	1:D:43:LYS:HE2	2.11	0.49
1:E:59:ILE:CD1	1:E:64:ILE:HB	2.42	0.49
1:L:290:GLN:O	1:L:290:GLN:HG2	2.12	0.49
1:N:71:LEU:HD11	1:N:105:SER:HB3	1.93	0.49
1:O:223:THR:OG1	1:O:226:GLU:HG3	2.13	0.49
1:F:121:GLY:O	1:F:122:GLN:C	2.50	0.49
1:J:95:GLY:O	1:J:99:ILE:HG13	2.12	0.49
1:M:213:LEU:HD11	1:M:227:LEU:HD11	1.94	0.49
1:O:284:TYR:CE1	1:P:60:PRO:CD	2.95	0.49
1:A:128:ARG:HH22	1:B:289:ASP:CG	2.16	0.49
1:F:64:ILE:HA	1:M:98:ASN:HD21	1.77	0.49
1:J:136:ALA:HB2	1:J:175:ARG:HG2	1.93	0.49
1:J:171:ALA:O	1:J:174:GLU:HB3	2.12	0.49
1:P:258:ARG:HB3	1:P:259:ASP:OD1	2.12	0.49
1:G:90:ASP:HA	1:G:117:GLU:OE1	2.13	0.49
1:M:49:GLY:HA3	1:M:88:ASP:OD2	2.12	0.49
1:F:10:GLY:HA2	1:F:112:GLY:O	2.12	0.49
1:H:136:ALA:O	1:H:140:VAL:HG23	2.12	0.49
1:J:199:ARG:NH1	1:J:230:ALA:HA	2.28	0.49
1:B:13:PHE:O	1:B:17:VAL:HG23	2.13	0.49
1:O:22:PRO:HG2	1:O:224:LEU:HD23	1.94	0.49
1:P:89:ILE:HG12	1:P:114:VAL:HG22	1.94	0.49
1:A:22:PRO:HD3	1:A:228:LYS:HB2	1.95	0.49
1:L:71:LEU:HD21	1:L:105:SER:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:ILE:HA	1:I:98:ASN:HD21	1.78	0.48
1:I:176:ALA:O	1:I:180:VAL:HG23	2.13	0.48
1:J:160:ARG:CZ	1:J:190:GLU:HG3	2.41	0.48
1:J:169:ILE:HG12	1:J:173:ILE:HD11	1.95	0.48
1:P:220:PRO:HD2	1:P:222:PHE:CZ	2.48	0.48
1:A:103:ILE:O	1:A:107:ILE:HG13	2.13	0.48
1:A:266:VAL:N	1:A:267:PRO:CD	2.75	0.48
1:B:124:ARG:O	1:B:125:CYS:C	2.51	0.48
1:G:290:GLN:O	1:G:290:GLN:HG2	2.13	0.48
1:H:275:LEU:HD22	1:H:279:LEU:HD11	1.95	0.48
1:L:13:PHE:O	1:L:17:VAL:HG23	2.13	0.48
1:I:205:VAL:HG21	1:I:209:ILE:HD11	1.94	0.48
1:L:59:ILE:HD12	1:L:64:ILE:HB	1.94	0.48
1:O:72:VAL:HG22	1:P:76:ARG:HH22	1.79	0.48
1:O:119:GLN:HE22	1:O:162:ASP:HB2	1.78	0.48
1:P:178:ALA:O	1:P:181:GLU:HB2	2.12	0.48
1:P:188:PHE:C	1:P:188:PHE:CD2	2.86	0.48
1:I:22:PRO:HG2	1:I:224:LEU:CD2	2.42	0.48
1:K:208:PRO:O	1:K:209:ILE:HD13	2.14	0.48
1:O:263:LYS:O	1:O:266:VAL:HG13	2.14	0.48
1:P:276:TYR:N	1:P:276:TYR:HD1	2.11	0.48
1:A:67:MET:HE2	1:A:105:SER:HB2	1.95	0.48
1:H:242:TYR:HA	1:H:245:MET:CG	2.40	0.48
1:K:250:LEU:HB2	1:L:36:MET:CE	2.44	0.48
1:N:203:GLU:O	1:N:206:LYS:NZ	2.45	0.48
1:P:188:PHE:C	1:P:188:PHE:HD2	2.17	0.48
1:A:89:ILE:HG12	1:A:114:VAL:HG22	1.95	0.48
1:E:178:ALA:O	1:E:181:GLU:HB2	2.13	0.48
1:E:250:LEU:HB2	1:F:36:MET:HE1	1.96	0.48
1:F:52:VAL:O	1:F:56:SER:HB2	2.13	0.48
1:K:36:MET:HE1	1:K:270:GLN:HE22	1.77	0.48
1:C:266:VAL:N	1:C:267:PRO:CD	2.76	0.48
1:E:68:ASP:O	1:E:72:VAL:HG13	2.14	0.48
1:E:251:ASN:O	1:E:255:THR:HG23	2.13	0.48
1:G:115:HIS:HA	1:G:158:MET:O	2.14	0.48
1:J:89:ILE:HG12	1:J:114:VAL:HG13	1.94	0.48
1:M:222:PHE:HA	1:M:226:GLU:OE1	2.14	0.48
1:M:240:GLY:HA3	1:N:252:PHE:CE1	2.49	0.48
1:O:216:PHE:CE1	1:P:271:THR:HG22	2.48	0.48
1:P:199:ARG:HH11	1:P:199:ARG:CG	2.27	0.48
1:A:152:ASP:OD1	1:A:152:ASP:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASP:OD2	1:D:287:LYS:CE	2.53	0.48
1:G:38:GLU:HG3	1:G:83:LEU:CG	2.43	0.48
1:L:88:ASP:OD1	1:L:115:HIS:CE1	2.67	0.48
1:N:131:LYS:O	1:N:132:GLU:CB	2.61	0.48
1:P:140:VAL:HG13	1:P:182:ALA:HB2	1.95	0.48
1:A:71:LEU:HD23	1:A:106:PHE:CE1	2.49	0.48
1:A:140:VAL:HG13	1:A:182:ALA:HB2	1.95	0.48
1:C:215:GLU:HG3	1:D:269:MET:SD	2.54	0.48
1:D:195:LEU:HD21	1:D:226:GLU:HB3	1.96	0.48
1:F:38:GLU:HA	1:F:83:LEU:HD11	1.95	0.48
1:M:262:GLN:NE2	1:N:237:TYR:CD2	2.81	0.48
1:P:249:ALA:O	1:P:253:TYR:HD2	1.97	0.48
1:H:266:VAL:N	1:H:267:PRO:CD	2.76	0.48
1:O:16:ALA:C	1:O:23:LEU:HD22	2.34	0.48
1:D:230:ALA:O	1:D:231:ASN:HB2	2.14	0.47
1:L:43:LYS:O	1:L:84:PRO:HD2	2.14	0.47
1:M:29:ILE:HG21	1:M:55:ASN:ND2	2.28	0.47
1:O:72:VAL:HG22	1:P:76:ARG:NH2	2.29	0.47
1:F:205:VAL:HG21	1:F:209:ILE:HD11	1.95	0.47
1:J:152:ASP:OD1	1:J:152:ASP:C	2.51	0.47
1:K:114:VAL:CG1	1:K:155:PHE:HZ	2.27	0.47
1:L:150:ARG:HD3	1:L:153:GLU:HA	1.94	0.47
1:O:188:PHE:HZ	1:O:212:ASN:ND2	2.02	0.47
1:P:276:TYR:N	1:P:276:TYR:CD1	2.82	0.47
1:G:279:LEU:HA	1:G:279:LEU:HD12	1.50	0.47
1:I:124:ARG:HH12	1:I:128:ARG:HH21	1.63	0.47
1:M:238:CYS:SG	1:M:239:CYS:N	2.87	0.47
1:N:123:LYS:O	1:N:124:ARG:C	2.52	0.47
1:O:17:VAL:HG23	1:O:23:LEU:HD23	1.97	0.47
1:F:169:ILE:O	1:F:169:ILE:HG13	2.13	0.47
1:G:36:MET:CE	1:G:270:GLN:HE22	2.27	0.47
1:O:86:LEU:HA	1:O:113:ALA:O	2.14	0.47
1:O:192:MET:HE2	1:O:201:PHE:CD1	2.49	0.47
1:G:176:ALA:O	1:G:180:VAL:HG23	2.14	0.47
1:K:114:VAL:CG1	1:K:155:PHE:CZ	2.97	0.47
1:A:98:ASN:ND2	1:D:64:ILE:HA	2.29	0.47
1:A:177:ILE:O	1:A:181:GLU:CG	2.62	0.47
1:B:36:MET:HE2	1:B:270:GLN:HE22	1.77	0.47
1:D:98:ASN:HD22	1:D:98:ASN:H	1.58	0.47
1:F:36:MET:HE3	1:F:270:GLN:NE2	2.30	0.47
1:G:118:ASP:HB3	1:G:139:MET:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:150:ARG:HD3	1:K:152:ASP:O	2.15	0.47
1:L:64:ILE:HA	1:P:98:ASN:ND2	2.27	0.47
1:M:242:TYR:HA	1:M:245:MET:HG2	1.95	0.47
1:N:71:LEU:HA	1:N:71:LEU:HD23	1.13	0.47
1:N:263:LYS:O	1:N:266:VAL:HG22	2.14	0.47
1:O:188:PHE:C	1:O:188:PHE:CD2	2.88	0.47
1:D:266:VAL:HG22	1:D:267:PRO:HD3	1.97	0.47
1:H:115:HIS:HA	1:H:158:MET:O	2.15	0.47
1:L:266:VAL:N	1:L:267:PRO:HD2	2.30	0.47
1:M:262:GLN:HE21	1:M:262:GLN:N	2.09	0.47
1:D:89:ILE:HD13	1:D:114:VAL:CG1	2.44	0.47
1:E:122:GLN:HB2	1:N:122:GLN:HB2	1.97	0.47
1:H:20:GLU:OE1	1:H:43:LYS:CE	2.53	0.47
1:L:276:TYR:HA	1:L:281:TYR:HD1	1.79	0.47
1:A:200:ARG:O	1:A:203:GLU:HB3	2.14	0.47
1:J:71:LEU:HD11	1:J:105:SER:HB3	1.96	0.47
1:M:138:GLU:OE1	1:M:138:GLU:HA	2.15	0.47
1:A:122:GLN:HB2	1:D:122:GLN:OE1	2.14	0.46
1:F:159:ALA:HB3	1:F:187:ILE:CD1	2.45	0.46
1:L:38:GLU:HA	1:L:83:LEU:HD11	1.96	0.46
1:N:178:ALA:O	1:N:181:GLU:HB2	2.15	0.46
1:A:279:LEU:HD23	1:A:279:LEU:HA	1.73	0.46
1:H:213:LEU:HD11	1:H:227:LEU:HD11	1.97	0.46
1:O:188:PHE:C	1:O:188:PHE:HD2	2.18	0.46
1:B:251:ASN:O	1:B:255:THR:HG22	2.14	0.46
1:P:241:ALA:O	1:P:245:MET:CG	2.64	0.46
1:K:250:LEU:HB2	1:L:36:MET:HE2	1.96	0.46
1:M:36:MET:HE2	1:M:270:GLN:HE22	1.74	0.46
1:N:85:LEU:O	1:N:111:VAL:HG13	2.15	0.46
1:B:68:ASP:HA	1:B:71:LEU:HB2	1.97	0.46
1:G:188:PHE:C	1:G:188:PHE:HD2	2.19	0.46
1:J:160:ARG:NH2	1:J:190:GLU:CG	2.66	0.46
1:O:239:CYS:O	1:O:243:ARG:HG3	2.15	0.46
1:C:122:GLN:CG	1:C:123:LYS:H	2.19	0.46
1:C:281:TYR:C	1:C:281:TYR:CD2	2.89	0.46
1:G:188:PHE:C	1:G:188:PHE:CD2	2.87	0.46
1:H:225:ASP:OD1	1:H:225:ASP:N	2.49	0.46
1:H:237:TYR:N	1:H:237:TYR:CD1	2.84	0.46
1:J:106:PHE:HD1	1:J:111:VAL:HG21	1.80	0.46
1:N:160:ARG:HA	1:N:188:PHE:HB3	1.98	0.46
1:O:67:MET:HE3	1:O:102:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:38:GLU:HG3	1:P:83:LEU:CG	2.44	0.46
1:G:192:MET:HE3	1:G:198:TYR:CD1	2.50	0.46
1:M:20:GLU:HG2	1:M:23:LEU:HA	1.96	0.46
1:B:202:LYS:HD2	1:B:202:LYS:O	2.15	0.46
1:D:251:ASN:O	1:D:255:THR:CG2	2.63	0.46
1:F:103:ILE:O	1:F:107:ILE:HG13	2.15	0.46
1:O:213:LEU:HD11	1:O:235:ALA:HB1	1.98	0.46
1:A:288:LEU:HD23	1:A:292:PHE:HE1	1.81	0.46
1:D:285:GLU:N	1:D:285:GLU:OE1	2.49	0.46
1:E:67:MET:HE2	1:E:105:SER:CB	2.46	0.46
1:G:263:LYS:O	1:G:266:VAL:HG13	2.15	0.46
1:J:7:ILE:HG22	1:J:11:ALA:HB3	1.98	0.46
1:K:27:GLY:HA2	1:K:46:TYR:HB3	1.98	0.46
1:M:46:TYR:HE2	1:M:48:SER:HB3	1.80	0.46
1:M:87:VAL:HG23	1:M:111:VAL:CG1	2.45	0.46
1:M:220:PRO:HB2	1:M:222:PHE:CE1	2.50	0.46
1:A:176:ALA:O	1:A:180:VAL:HG23	2.15	0.45
1:D:266:VAL:N	1:D:267:PRO:CD	2.79	0.45
1:G:178:ALA:O	1:G:181:GLU:HB2	2.16	0.45
1:H:140:VAL:HG13	1:H:182:ALA:HB2	1.98	0.45
1:L:89:ILE:HG12	1:L:114:VAL:HG13	1.98	0.45
1:O:242:TYR:HA	1:O:245:MET:CG	2.45	0.45
1:G:181:GLU:HA	1:G:181:GLU:OE1	2.16	0.45
1:I:68:ASP:O	1:I:72:VAL:HG12	2.16	0.45
1:K:188:PHE:C	1:K:188:PHE:CD2	2.88	0.45
1:O:266:VAL:N	1:O:267:PRO:CD	2.78	0.45
1:C:188:PHE:C	1:C:188:PHE:CD2	2.90	0.45
1:C:215:GLU:CD	1:C:215:GLU:H	2.20	0.45
1:G:46:TYR:HE2	1:G:238:CYS:HB2	1.80	0.45
1:M:128:ARG:NH2	1:N:289:ASP:OD1	2.49	0.45
1:N:241:ALA:O	1:N:245:MET:HG3	2.15	0.45
1:O:227:LEU:HD22	1:O:232:VAL:HG11	1.98	0.45
1:B:118:ASP:OD1	1:B:161:THR:HA	2.17	0.45
1:C:205:VAL:HG21	1:C:209:ILE:HD11	1.99	0.45
1:E:216:PHE:CB	1:F:272:ARG:HG3	2.36	0.45
1:F:176:ALA:O	1:F:180:VAL:HG23	2.16	0.45
1:H:275:LEU:HD22	1:H:279:LEU:CD1	2.47	0.45
1:I:220:PRO:HG2	1:I:222:PHE:CZ	2.52	0.45
1:K:21:GLN:HA	1:K:22:PRO:HA	1.81	0.45
1:K:90:ASP:HB3	1:K:91:THR:H	1.55	0.45
1:K:125:CYS:HB3	1:O:138:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:188:PHE:C	1:K:188:PHE:HD2	2.19	0.45
1:M:220:PRO:O	1:M:222:PHE:HD1	1.99	0.45
1:A:266:VAL:HG22	1:A:267:PRO:HD3	1.99	0.45
1:H:91:THR:HG22	1:H:142:ARG:NH1	2.32	0.45
1:E:89:ILE:HG23	1:E:114:VAL:HG22	1.98	0.45
1:L:200:ARG:HE	1:L:200:ARG:HB3	1.60	0.45
1:M:123:LYS:O	1:M:124:ARG:C	2.55	0.45
1:C:251:ASN:O	1:C:255:THR:HG23	2.16	0.45
1:F:138:GLU:O	1:F:141:ASP:HB2	2.16	0.45
1:I:178:ALA:O	1:I:181:GLU:HB2	2.16	0.45
1:M:32:TYR:CE2	1:M:36:MET:CE	2.93	0.45
1:M:199:ARG:HD3	1:M:230:ALA:HA	1.98	0.45
1:O:81:THR:OG1	1:O:82:ASN:N	2.50	0.45
1:P:261:THR:HG23	1:P:263:LYS:H	1.82	0.45
1:A:48:SER:O	1:A:52:VAL:HG23	2.16	0.45
1:B:178:ALA:O	1:B:181:GLU:HB2	2.16	0.45
1:E:284:TYR:CE1	1:F:60:PRO:CG	3.00	0.45
1:G:210:LEU:HD23	1:G:210:LEU:C	2.37	0.45
1:G:271:THR:HG22	1:H:216:PHE:CE1	2.52	0.45
1:K:122:GLN:NE2	1:O:94:GLY:HA2	2.32	0.45
1:N:46:TYR:CE2	1:N:48:SER:HA	2.52	0.45
1:N:194:THR:O	1:N:197:ASP:HB2	2.17	0.45
1:N:219:THR:CG2	1:N:222:PHE:CE1	2.92	0.45
1:O:230:ALA:O	1:O:231:ASN:HB2	2.16	0.45
1:O:284:TYR:HE1	1:P:60:PRO:CD	2.30	0.45
1:E:52:VAL:O	1:E:56:SER:HB2	2.17	0.45
1:E:138:GLU:O	1:E:141:ASP:HB2	2.18	0.44
1:L:230:ALA:O	1:L:231:ASN:HB2	2.16	0.44
1:P:46:TYR:CE2	1:P:48:SER:HA	2.52	0.44
1:G:32:TYR:HE2	1:G:36:MET:HE3	1.82	0.44
1:H:89:ILE:HG23	1:H:114:VAL:CG2	2.46	0.44
1:M:192:MET:HB2	1:M:198:TYR:CE2	2.52	0.44
1:N:201:PHE:O	1:N:205:VAL:HG22	2.17	0.44
1:O:72:VAL:CG2	1:P:76:ARG:NH2	2.80	0.44
1:E:150:ARG:HD3	1:E:153:GLU:HA	2.00	0.44
1:F:271:THR:OG1	1:F:274:GLN:HG3	2.17	0.44
1:I:188:PHE:CD2	1:I:210:LEU:HD22	2.52	0.44
1:E:94:GLY:HA3	1:E:98:ASN:OD1	2.17	0.44
1:E:266:VAL:N	1:E:267:PRO:CD	2.80	0.44
1:F:64:ILE:HA	1:M:98:ASN:ND2	2.32	0.44
1:F:67:MET:CE	1:F:105:SER:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:GLN:HE22	1:H:131:LYS:HG3	1.82	0.44
1:L:86:LEU:HD12	1:L:87:VAL:H	1.82	0.44
1:N:115:HIS:ND1	1:N:115:HIS:O	2.49	0.44
1:O:60:PRO:HB2	1:O:62:LEU:HD13	2.00	0.44
1:P:231:ASN:HD22	1:P:231:ASN:HA	1.65	0.44
1:J:7:ILE:HD12	1:J:7:ILE:N	2.29	0.44
1:O:136:ALA:HA	1:O:175:ARG:NH1	2.32	0.44
1:A:274:GLN:HE21	1:A:274:GLN:HB3	1.58	0.44
1:D:199:ARG:HH11	1:D:199:ARG:HB2	1.82	0.44
1:E:188:PHE:C	1:E:188:PHE:CD2	2.91	0.44
1:G:287:LYS:HE3	1:G:290:GLN:HE22	1.82	0.44
1:H:291:LEU:HD23	1:H:291:LEU:HA	1.76	0.44
1:K:262:GLN:H	1:K:262:GLN:NE2	2.10	0.44
1:M:239:CYS:SG	1:M:242:TYR:CE1	3.11	0.44
1:O:52:VAL:HG21	1:O:70:VAL:HG22	1.99	0.44
1:B:288:LEU:HG	1:D:97:PHE:CZ	2.53	0.44
1:M:188:PHE:C	1:M:188:PHE:CD2	2.91	0.44
1:M:274:GLN:HA	1:M:277:ASP:HB2	2.00	0.44
1:O:246:ASN:HB3	1:P:36:MET:HE3	1.99	0.44
1:C:46:TYR:HE2	1:C:48:SER:HB2	1.82	0.44
1:C:270:GLN:HG3	1:C:274:GLN:HE21	1.83	0.44
1:F:119:GLN:HE22	1:F:162:ASP:HB2	1.83	0.44
1:I:71:LEU:HD23	1:I:71:LEU:HA	1.80	0.44
1:K:46:TYR:HE2	1:K:238:CYS:HB2	1.83	0.44
1:M:202:LYS:HG2	1:M:209:ILE:CG1	2.48	0.44
1:N:138:GLU:HA	1:N:138:GLU:OE1	2.18	0.44
1:O:284:TYR:CE1	1:P:60:PRO:CG	3.01	0.44
1:G:38:GLU:HA	1:G:83:LEU:HD11	2.00	0.44
1:M:46:TYR:CE2	1:M:48:SER:HB3	2.53	0.44
1:C:76:ARG:HH22	1:D:72:VAL:HG22	1.84	0.43
1:D:193:LYS:HD2	1:D:193:LYS:H	1.83	0.43
1:K:46:TYR:CE2	1:K:238:CYS:HB2	2.52	0.43
1:M:233:ASP:C	1:M:234:ILE:HG13	2.38	0.43
1:N:192:MET:CE	1:N:201:PHE:CD1	3.01	0.43
1:O:124:ARG:O	1:O:126:GLY:N	2.50	0.43
1:C:115:HIS:O	1:C:115:HIS:ND1	2.51	0.43
1:L:40:VAL:O	1:L:40:VAL:HG12	2.18	0.43
1:M:68:ASP:HA	1:M:71:LEU:HB2	2.00	0.43
1:M:262:GLN:NE2	1:N:237:TYR:HD2	2.16	0.43
1:P:135:PRO:O	1:P:136:ALA:C	2.56	0.43
1:A:59:ILE:CD1	1:A:64:ILE:HB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:279:LEU:HD23	1:E:279:LEU:HA	1.84	0.43
1:H:57:LEU:HD11	1:H:69:ASP:HB3	2.01	0.43
1:H:89:ILE:CG2	1:H:114:VAL:CG2	2.96	0.43
1:K:287:LYS:HE2	1:P:148:ASP:OD2	2.18	0.43
1:M:253:TYR:HE1	1:N:26:VAL:CG2	2.32	0.43
1:P:210:LEU:HD12	1:P:234:ILE:HG21	2.00	0.43
1:B:60:PRO:HG2	1:B:62:LEU:HD22	2.00	0.43
1:B:106:PHE:HD1	1:B:111:VAL:HG21	1.83	0.43
1:C:124:ARG:O	1:C:126:GLY:N	2.52	0.43
1:E:40:VAL:HG12	1:E:40:VAL:O	2.18	0.43
1:F:128:ARG:HD3	1:H:282:TYR:CZ	2.53	0.43
1:G:150:ARG:HD3	1:G:153:GLU:HA	2.00	0.43
1:H:89:ILE:HG12	1:H:114:VAL:HG22	1.99	0.43
1:K:203:GLU:O	1:K:206:LYS:HE2	2.18	0.43
1:L:276:TYR:HA	1:L:281:TYR:CD1	2.53	0.43
1:C:67:MET:HE2	1:C:105:SER:HB2	2.00	0.43
1:E:230:ALA:O	1:E:231:ASN:HB2	2.17	0.43
1:H:289:ASP:O	1:H:293:ASN:HB3	2.18	0.43
1:N:131:LYS:O	1:N:132:GLU:HB2	2.19	0.43
1:O:118:ASP:HB3	1:O:139:MET:HG2	2.01	0.43
1:P:21:GLN:HA	1:P:22:PRO:HA	1.86	0.43
1:L:67:MET:HE1	1:L:102:THR:HA	1.99	0.43
1:L:99:ILE:HD11	1:L:142:ARG:HG2	2.00	0.43
1:N:139:MET:HA	1:N:142:ARG:HD2	2.00	0.43
1:E:119:GLN:HE22	1:E:131:LYS:CA	2.31	0.43
1:G:38:GLU:HG3	1:G:83:LEU:CD1	2.49	0.43
1:K:64:ILE:HA	1:O:98:ASN:HD21	1.84	0.43
1:K:192:MET:HE2	1:K:201:PHE:CD1	2.54	0.43
1:L:20:GLU:OE1	1:L:43:LYS:HE2	2.19	0.43
1:L:188:PHE:C	1:L:188:PHE:HD2	2.22	0.43
1:N:12:LYS:HB3	1:N:84:PRO:HG3	2.01	0.43
1:N:192:MET:HE2	1:N:201:PHE:CD1	2.53	0.43
1:C:186:MET:HG2	1:C:208:PRO:HB2	2.00	0.43
1:E:147:VAL:HG13	1:E:150:ARG:NH1	2.33	0.43
1:H:135:PRO:O	1:H:138:GLU:HB3	2.19	0.43
1:I:169:ILE:O	1:I:169:ILE:HG13	2.18	0.43
1:I:196:ASP:O	1:I:200:ARG:HG3	2.19	0.43
1:L:188:PHE:C	1:L:188:PHE:CD2	2.92	0.43
1:M:275:LEU:HD23	1:M:275:LEU:HA	1.93	0.43
1:G:241:ALA:O	1:G:245:MET:HG2	2.18	0.43
1:O:43:LYS:O	1:O:84:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ASP:HB3	1:D:139:MET:HE2	2.00	0.43
1:E:122:GLN:NE2	1:N:94:GLY:CA	2.75	0.43
1:H:202:LYS:HE2	1:H:231:ASN:O	2.19	0.43
1:J:188:PHE:C	1:J:188:PHE:CD2	2.92	0.43
1:L:177:ILE:O	1:L:181:GLU:HG2	2.19	0.43
1:M:195:LEU:HD12	1:M:222:PHE:HD2	1.80	0.43
1:N:60:PRO:CB	1:N:62:LEU:HD22	2.45	0.43
1:C:199:ARG:HH11	1:C:199:ARG:CG	2.29	0.42
1:G:202:LYS:HE2	1:G:233:ASP:OD2	2.19	0.42
1:G:263:LYS:HB2	1:G:263:LYS:NZ	2.34	0.42
1:N:22:PRO:HG2	1:N:224:LEU:CD2	2.49	0.42
1:N:207:VAL:HB	1:N:208:PRO:HD2	2.01	0.42
1:O:98:ASN:N	1:O:98:ASN:HD22	2.17	0.42
1:O:252:PHE:CZ	1:P:240:GLY:HA3	2.51	0.42
1:A:20:GLU:HG2	1:A:23:LEU:HA	2.00	0.42
1:A:188:PHE:CD2	1:A:210:LEU:HD22	2.54	0.42
1:D:36:MET:HE1	1:D:270:GLN:HE22	1.83	0.42
1:C:68:ASP:HA	1:C:71:LEU:HB2	2.01	0.42
1:F:272:ARG:HB3	1:F:272:ARG:NH2	2.34	0.42
1:I:150:ARG:HD3	1:I:152:ASP:O	2.18	0.42
1:M:32:TYR:HB2	1:N:55:ASN:HA	2.01	0.42
1:M:285:GLU:OE2	1:M:285:GLU:HA	2.19	0.42
1:N:24:GLN:HG2	1:N:224:LEU:HD21	2.01	0.42
1:P:192:MET:HE2	1:P:201:PHE:CD1	2.54	0.42
1:A:21:GLN:HA	1:A:22:PRO:HA	1.92	0.42
1:H:143:ILE:HD13	1:H:184:ALA:HB2	2.02	0.42
1:N:208:PRO:O	1:N:209:ILE:HD13	2.19	0.42
1:A:207:VAL:HB	1:A:208:PRO:HD2	2.01	0.42
1:B:208:PRO:HA	1:B:233:ASP:OD2	2.20	0.42
1:N:130:GLY:O	1:N:131:LYS:CB	2.63	0.42
1:O:29:ILE:HG13	1:O:30:THR:HG23	2.02	0.42
1:P:201:PHE:O	1:P:205:VAL:HG22	2.19	0.42
1:A:47:LEU:HB2	1:A:85:LEU:HD11	2.01	0.42
1:C:242:TYR:C	1:C:242:TYR:CD2	2.93	0.42
1:K:94:GLY:HA3	1:K:98:ASN:OD1	2.20	0.42
1:L:181:GLU:HA	1:L:181:GLU:OE1	2.20	0.42
1:L:252:PHE:O	1:L:256:VAL:HG23	2.19	0.42
1:M:48:SER:O	1:M:52:VAL:HG23	2.19	0.42
1:M:210:LEU:HD21	1:M:236:LEU:CD2	2.48	0.42
1:M:216:PHE:HB2	1:N:272:ARG:HD2	2.01	0.42
1:N:71:LEU:CD2	1:N:106:PHE:CE1	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:247:LYS:HB2	1:P:270:GLN:HB2	2.02	0.42
1:P:266:VAL:N	1:P:267:PRO:CD	2.81	0.42
1:H:181:GLU:OE1	1:H:181:GLU:HA	2.20	0.42
1:J:160:ARG:HG3	1:J:188:PHE:CG	2.54	0.42
1:N:207:VAL:HB	1:N:208:PRO:CD	2.49	0.42
1:N:266:VAL:HG23	1:N:267:PRO:HD3	2.01	0.42
1:O:193:LYS:H	1:O:193:LYS:CD	2.30	0.42
1:P:192:MET:CE	1:P:201:PHE:CD1	3.03	0.42
1:P:215:GLU:HG2	1:P:243:ARG:NH2	2.34	0.42
1:B:188:PHE:C	1:B:188:PHE:CD2	2.93	0.42
1:E:188:PHE:C	1:E:188:PHE:HD2	2.22	0.42
1:E:205:VAL:CG2	1:E:209:ILE:HD11	2.50	0.42
1:H:36:MET:HE2	1:H:270:GLN:HE22	1.85	0.42
1:O:192:MET:CE	1:O:201:PHE:CD1	3.02	0.42
1:P:82:ASN:H	1:P:82:ASN:ND2	2.17	0.42
1:G:32:TYR:CE2	1:G:36:MET:HE3	2.54	0.42
1:I:272:ARG:NH1	1:J:216:PHE:O	2.51	0.42
1:J:21:GLN:HA	1:J:22:PRO:HA	1.80	0.42
1:J:86:LEU:HD12	1:J:87:VAL:N	2.34	0.42
1:M:277:ASP:O	1:M:279:LEU:N	2.52	0.42
1:N:82:ASN:ND2	1:N:82:ASN:H	2.17	0.42
1:P:158:MET:HE3	1:P:186:MET:HB2	2.02	0.42
1:G:272:ARG:HG3	1:H:216:PHE:HB2	2.02	0.42
1:H:188:PHE:C	1:H:188:PHE:CD2	2.93	0.42
1:N:52:VAL:O	1:N:56:SER:HB2	2.20	0.42
1:N:282:TYR:O	1:N:286:GLU:HG3	2.19	0.42
1:P:131:LYS:O	1:P:132:GLU:HB2	2.20	0.42
1:D:59:ILE:HB	1:D:60:PRO:HD2	2.02	0.41
1:F:280:GLY:O	1:F:284:TYR:HD1	2.03	0.41
1:I:188:PHE:CD2	1:I:188:PHE:C	2.93	0.41
1:M:216:PHE:HB2	1:N:272:ARG:CD	2.50	0.41
1:M:243:ARG:HG2	1:M:243:ARG:HH11	1.85	0.41
1:O:21:GLN:HA	1:O:22:PRO:HA	1.94	0.41
1:P:123:LYS:HG3	1:P:124:ARG:H	1.85	0.41
1:D:52:VAL:O	1:D:56:SER:HB2	2.20	0.41
1:D:82:ASN:ND2	1:D:82:ASN:H	2.18	0.41
1:D:285:GLU:HG2	1:H:128:ARG:HH22	1.85	0.41
1:G:281:TYR:HD1	1:H:60:PRO:HB3	1.85	0.41
1:H:287:LYS:HE3	1:H:290:GLN:NE2	2.35	0.41
1:N:7:ILE:CG2	1:N:12:LYS:HG2	2.50	0.41
1:N:236:LEU:HD11	1:N:238:CYS:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:259:ASP:OD1	1:P:259:ASP:N	2.53	0.41
1:D:115:HIS:HA	1:D:158:MET:O	2.20	0.41
1:I:138:GLU:O	1:I:141:ASP:HB2	2.21	0.41
1:M:46:TYR:CE2	1:M:48:SER:CB	3.03	0.41
1:O:67:MET:CE	1:O:102:THR:CA	2.81	0.41
1:O:284:TYR:CD1	1:P:60:PRO:HG3	2.54	0.41
1:P:22:PRO:HB3	1:P:232:VAL:O	2.21	0.41
1:E:125:CYS:N	1:N:138:GLU:OE2	2.49	0.41
1:K:261:THR:HG23	1:K:263:LYS:H	1.86	0.41
1:P:55:ASN:HD22	1:P:55:ASN:H	1.68	0.41
1:A:186:MET:HG2	1:A:208:PRO:HB2	2.02	0.41
1:F:272:ARG:HB3	1:F:272:ARG:CZ	2.50	0.41
1:G:76:ARG:NH2	1:H:72:VAL:HG22	2.35	0.41
1:L:34:ALA:O	1:L:37:ALA:HB3	2.21	0.41
1:L:215:GLU:HG2	1:L:243:ARG:HE	1.86	0.41
1:A:262:GLN:HE21	1:A:262:GLN:N	2.04	0.41
1:A:288:LEU:HD23	1:A:292:PHE:CE1	2.56	0.41
1:C:271:THR:OG1	1:C:274:GLN:HG3	2.21	0.41
1:E:59:ILE:HD12	1:E:64:ILE:HB	2.02	0.41
1:E:139:MET:HG2	1:E:179:TYR:CZ	2.55	0.41
1:I:123:LYS:CD	1:I:124:ARG:H	2.03	0.41
1:J:188:PHE:C	1:J:188:PHE:HD2	2.24	0.41
1:P:46:TYR:CG	1:P:236:LEU:HD11	2.56	0.41
1:B:219:THR:HG22	1:B:220:PRO:O	2.21	0.41
1:C:281:TYR:O	1:C:282:TYR:C	2.59	0.41
1:D:71:LEU:HD23	1:D:106:PHE:CZ	2.55	0.41
1:E:240:GLY:HA3	1:F:252:PHE:CE1	2.55	0.41
1:I:89:ILE:HD13	1:I:114:VAL:HG11	2.03	0.41
1:K:230:ALA:O	1:K:231:ASN:HB2	2.21	0.41
1:N:87:VAL:HB	1:N:114:VAL:HG23	2.03	0.41
1:O:22:PRO:HG2	1:O:224:LEU:HD22	2.01	0.41
1:P:291:LEU:HB3	1:P:292:PHE:CD2	2.55	0.41
1:D:134:VAL:HB	1:D:138:GLU:HB3	2.03	0.41
1:E:67:MET:HE1	1:E:102:THR:HA	1.99	0.41
1:F:36:MET:CE	1:F:270:GLN:NE2	2.83	0.41
1:F:96:ALA:HB2	1:M:125:CYS:O	2.21	0.41
1:G:74:ALA:O	1:G:78:THR:HG23	2.20	0.41
1:G:275:LEU:HD22	1:G:279:LEU:HD22	2.02	0.41
1:I:290:GLN:O	1:I:290:GLN:HG2	2.20	0.41
1:J:20:GLU:HG2	1:J:23:LEU:HA	2.02	0.41
1:K:134:VAL:HB	1:K:138:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:287:LYS:O	1:M:289:ASP:N	2.54	0.41
1:O:95:GLY:O	1:O:99:ILE:HD12	2.20	0.41
1:O:115:HIS:O	1:O:115:HIS:ND1	2.54	0.41
1:P:150:ARG:HD3	1:P:152:ASP:O	2.21	0.41
1:P:282:TYR:O	1:P:286:GLU:HG2	2.21	0.41
1:P:289:ASP:C	1:P:291:LEU:H	2.25	0.41
1:C:199:ARG:NH2	1:C:229:GLY:O	2.49	0.41
1:D:46:TYR:CE2	1:D:48:SER:HB2	2.55	0.41
1:E:219:THR:HG22	1:E:220:PRO:O	2.20	0.41
1:G:188:PHE:CG	1:G:210:LEU:HD22	2.56	0.41
1:H:205:VAL:HG21	1:H:209:ILE:HD11	2.03	0.41
1:H:220:PRO:HD2	1:H:222:PHE:CE1	2.57	0.41
1:K:122:GLN:CD	1:O:94:GLY:HA2	2.41	0.41
1:K:290:GLN:HE21	1:K:290:GLN:HB3	1.58	0.41
1:L:40:VAL:O	1:L:40:VAL:CG1	2.68	0.41
1:M:14:ARG:NH2	1:M:153:GLU:O	2.49	0.41
1:B:207:VAL:HB	1:B:208:PRO:HD2	2.03	0.40
1:D:205:VAL:CG2	1:D:209:ILE:HD11	2.46	0.40
1:E:54:ALA:O	1:F:32:TYR:HB2	2.21	0.40
1:F:29:ILE:HG21	1:F:55:ASN:ND2	2.37	0.40
1:G:98:ASN:ND2	1:J:64:ILE:HA	2.36	0.40
1:G:209:ILE:HD13	1:G:209:ILE:HA	1.83	0.40
1:I:150:ARG:HE	1:I:157:ILE:HD12	1.86	0.40
1:N:22:PRO:HG2	1:N:224:LEU:HD22	2.02	0.40
1:O:284:TYR:CE1	1:P:60:PRO:HD2	2.56	0.40
1:B:64:ILE:HA	1:C:98:ASN:ND2	2.33	0.40
1:C:67:MET:HE2	1:C:105:SER:CB	2.52	0.40
1:D:29:ILE:HD11	1:D:245:MET:HE2	2.04	0.40
1:K:215:GLU:CG	1:K:243:ARG:HE	2.34	0.40
1:L:123:LYS:HG3	1:L:124:ARG:H	1.86	0.40
1:L:292:PHE:HE2	1:O:141:ASP:HB3	1.87	0.40
1:M:216:PHE:CZ	1:N:271:THR:HG22	2.56	0.40
1:N:276:TYR:N	1:N:276:TYR:HD1	2.20	0.40
1:O:283:ALA:O	1:O:287:LYS:HB2	2.22	0.40
1:P:199:ARG:CG	1:P:199:ARG:NH1	2.84	0.40
1:H:189:PRO:HD2	1:H:210:LEU:O	2.22	0.40
1:M:67:MET:CE	1:M:102:THR:CA	2.95	0.40
1:D:161:THR:O	1:D:190:GLU:HB2	2.21	0.40
1:H:52:VAL:O	1:H:56:SER:HB2	2.21	0.40
1:I:21:GLN:HA	1:I:22:PRO:HA	1.86	0.40
1:J:202:LYS:HG3	1:J:231:ASN:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:68:ASP:O	1:M:72:VAL:HG12	2.21	0.40
1:N:210:LEU:HD21	1:N:236:LEU:HB3	2.04	0.40

There are no symmetry-related clashes.

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	288/298 (97%)	273 (95%)	13 (4%)	2 (1%)	22	54
1	B	284/298 (95%)	268 (94%)	12 (4%)	4 (1%)	11	36
1	C	285/298 (96%)	266 (93%)	16 (6%)	3 (1%)	14	42
1	D	285/298 (96%)	274 (96%)	9 (3%)	2 (1%)	22	54
1	E	286/298 (96%)	271 (95%)	13 (4%)	2 (1%)	22	54
1	F	284/298 (95%)	268 (94%)	14 (5%)	2 (1%)	22	54
1	G	285/298 (96%)	272 (95%)	13 (5%)	0	100	100
1	H	286/298 (96%)	272 (95%)	12 (4%)	2 (1%)	22	54
1	I	287/298 (96%)	274 (96%)	11 (4%)	2 (1%)	22	54
1	J	286/298 (96%)	274 (96%)	8 (3%)	4 (1%)	11	36
1	K	284/298 (95%)	272 (96%)	10 (4%)	2 (1%)	22	54
1	L	284/298 (95%)	270 (95%)	10 (4%)	4 (1%)	11	36
1	M	285/298 (96%)	262 (92%)	15 (5%)	8 (3%)	5	19
1	N	285/298 (96%)	267 (94%)	12 (4%)	6 (2%)	7	26
1	O	286/298 (96%)	269 (94%)	10 (4%)	7 (2%)	6	22
1	P	284/298 (95%)	271 (95%)	9 (3%)	4 (1%)	11	36
All	All	4564/4768 (96%)	4323 (95%)	187 (4%)	54 (1%)	13	40

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	125	CYS
1	C	281	TYR
1	D	124	ARG
1	E	124	ARG
1	F	122	GLN
1	F	124	ARG
1	M	269	MET
1	N	132	GLU
1	O	7	ILE
1	O	124	ARG
1	O	125	CYS
1	O	136	ALA
1	B	124	ARG
1	C	125	CYS
1	H	124	ARG
1	L	121	GLY
1	M	278	TYR
1	M	289	ASP
1	N	131	LYS
1	O	121	GLY
1	P	132	GLU
1	C	124	ARG
1	H	283	ALA
1	I	121	GLY
1	I	124	ARG
1	J	283	ALA
1	K	124	ARG
1	L	276	TYR
1	L	282	TYR
1	M	124	ARG
1	M	277	ASP
1	M	288	LEU
1	N	121	GLY
1	N	124	ARG
1	N	290	GLN
1	O	8	SER
1	B	65	SER
1	E	129	PRO
1	P	290	GLN
1	A	118	ASP
1	D	135	PRO
1	J	124	ARG

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Mol	Chain	Res	Type
1	J	131	LYS
1	J	290	GLN
1	K	121	GLY
1	M	286	GLU
1	P	281	TYR
1	B	129	PRO
1	L	129	PRO
1	N	9	ALA
1	O	135	PRO
1	A	121	GLY
1	M	121	GLY
1	P	137	GLY

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	216/223 (97%)	186 (86%)	30 (14%)	3 10
1	B	213/223 (96%)	190 (89%)	23 (11%)	6 20
1	C	214/223 (96%)	184 (86%)	30 (14%)	3 10
1	D	214/223 (96%)	189 (88%)	25 (12%)	5 16
1	E	215/223 (96%)	191 (89%)	24 (11%)	6 18
1	F	213/223 (96%)	184 (86%)	29 (14%)	3 11
1	G	214/223 (96%)	182 (85%)	32 (15%)	3 9
1	H	215/223 (96%)	185 (86%)	30 (14%)	3 10
1	I	216/223 (97%)	187 (87%)	29 (13%)	4 11
1	J	215/223 (96%)	185 (86%)	30 (14%)	3 10
1	K	213/223 (96%)	185 (87%)	28 (13%)	4 12
1	L	213/223 (96%)	180 (84%)	33 (16%)	2 8
1	M	214/223 (96%)	187 (87%)	27 (13%)	4 13
1	N	214/223 (96%)	181 (85%)	33 (15%)	2 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	215/223 (96%)	184 (86%)	31 (14%)	3 9
1	P	213/223 (96%)	184 (86%)	29 (14%)	3 11
All	All	3427/3568 (96%)	2964 (86%)	463 (14%)	4 11

All (463) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	21	GLN
1	A	25	VAL
1	A	62	LEU
1	A	71	LEU
1	A	81	THR
1	A	82	ASN
1	A	122	GLN
1	A	123	LYS
1	A	124	ARG
1	A	128	ARG
1	A	162	ASP
1	A	177	ILE
1	A	188	PHE
1	A	193	LYS
1	A	199	ARG
1	A	202	LYS
1	A	206	LYS
1	A	224	LEU
1	A	242	TYR
1	A	247	LYS
1	A	255	THR
1	A	258	ARG
1	A	262	GLN
1	A	263	LYS
1	A	266	VAL
1	A	275	LEU
1	A	281	TYR
1	A	287	LYS
1	A	290	GLN
1	B	7	ILE
1	B	21	GLN
1	B	25	VAL
1	B	48	SER

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Mol	Chain	Res	Type
1	B	62	LEU
1	B	67	MET
1	B	72	VAL
1	B	82	ASN
1	B	98	ASN
1	B	114	VAL
1	B	122	GLN
1	B	124	ARG
1	B	169	ILE
1	B	188	PHE
1	B	199	ARG
1	B	202	LYS
1	B	205	VAL
1	B	225	ASP
1	B	255	THR
1	B	262	GLN
1	B	275	LEU
1	B	286	GLU
1	B	287	LYS
1	C	7	ILE
1	C	21	GLN
1	C	25	VAL
1	C	48	SER
1	C	62	LEU
1	C	65	SER
1	C	72	VAL
1	C	81	THR
1	C	82	ASN
1	C	114	VAL
1	C	115	HIS
1	C	117	GLU
1	C	122	GLN
1	C	154	THR
1	C	162	ASP
1	C	181	GLU
1	C	188	PHE
1	C	193	LYS
1	C	196	ASP
1	C	199	ARG
1	C	202	LYS
1	C	206	LYS
1	C	218	SER

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Mol	Chain	Res	Type
1	C	224	LEU
1	C	242	TYR
1	C	262	GLN
1	C	266	VAL
1	C	275	LEU
1	C	277	ASP
1	C	286	GLU
1	D	6	LEU
1	D	21	GLN
1	D	48	SER
1	D	62	LEU
1	D	71	LEU
1	D	72	VAL
1	D	82	ASN
1	D	98	ASN
1	D	128	ARG
1	D	150	ARG
1	D	153	GLU
1	D	167	GLU
1	D	188	PHE
1	D	193	LYS
1	D	196	ASP
1	D	199	ARG
1	D	202	LYS
1	D	242	TYR
1	D	255	THR
1	D	262	GLN
1	D	275	LEU
1	D	276	TYR
1	D	281	TYR
1	D	286	GLU
1	D	290	GLN
1	E	21	GLN
1	E	62	LEU
1	E	68	ASP
1	E	71	LEU
1	E	72	VAL
1	E	81	THR
1	E	82	ASN
1	E	107	ILE
1	E	114	VAL
1	E	122	GLN

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Mol	Chain	Res	Type
1	E	123	LYS
1	E	150	ARG
1	E	188	PHE
1	E	193	LYS
1	E	195	LEU
1	E	201	PHE
1	E	206	LYS
1	E	242	TYR
1	E	245	MET
1	E	262	GLN
1	E	263	LYS
1	E	275	LEU
1	E	285	GLU
1	E	287	LYS
1	F	21	GLN
1	F	25	VAL
1	F	43	LYS
1	F	48	SER
1	F	62	LEU
1	F	64	ILE
1	F	82	ASN
1	F	98	ASN
1	F	114	VAL
1	F	116	LEU
1	F	128	ARG
1	F	150	ARG
1	F	153	GLU
1	F	162	ASP
1	F	169	ILE
1	F	188	PHE
1	F	193	LYS
1	F	199	ARG
1	F	202	LYS
1	F	203	GLU
1	F	219	THR
1	F	233	ASP
1	F	255	THR
1	F	261	THR
1	F	262	GLN
1	F	266	VAL
1	F	275	LEU
1	F	287	LYS

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Mol	Chain	Res	Type
1	F	290	GLN
1	G	6	LEU
1	G	21	GLN
1	G	25	VAL
1	G	45	VAL
1	G	62	LEU
1	G	72	VAL
1	G	82	ASN
1	G	128	ARG
1	G	153	GLU
1	G	162	ASP
1	G	181	GLU
1	G	188	PHE
1	G	190	GLU
1	G	193	LYS
1	G	194	THR
1	G	196	ASP
1	G	199	ARG
1	G	201	PHE
1	G	202	LYS
1	G	206	LYS
1	G	228	LYS
1	G	231	ASN
1	G	255	THR
1	G	258	ARG
1	G	262	GLN
1	G	263	LYS
1	G	266	VAL
1	G	275	LEU
1	G	287	LYS
1	G	288	LEU
1	G	290	GLN
1	G	292	PHE
1	H	7	ILE
1	H	48	SER
1	H	62	LEU
1	H	75	ASN
1	H	82	ASN
1	H	123	LYS
1	H	124	ARG
1	H	131	LYS
1	H	135	PRO

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Mol	Chain	Res	Type
1	H	188	PHE
1	H	195	LEU
1	H	196	ASP
1	H	199	ARG
1	H	201	PHE
1	H	202	LYS
1	H	206	LYS
1	H	215	GLU
1	H	218	SER
1	H	251	ASN
1	H	255	THR
1	H	257	ARG
1	H	258	ARG
1	H	261	THR
1	H	262	GLN
1	H	263	LYS
1	H	275	LEU
1	H	277	ASP
1	H	287	LYS
1	H	292	PHE
1	H	293	ASN
1	I	6	LEU
1	I	21	GLN
1	I	62	LEU
1	I	65	SER
1	I	68	ASP
1	I	72	VAL
1	I	81	THR
1	I	82	ASN
1	I	115	HIS
1	I	117	GLU
1	I	123	LYS
1	I	128	ARG
1	I	131	LYS
1	I	169	ILE
1	I	188	PHE
1	I	193	LYS
1	I	196	ASP
1	I	199	ARG
1	I	202	LYS
1	I	224	LEU
1	I	233	ASP

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Mol	Chain	Res	Type
1	I	242	TYR
1	I	255	THR
1	I	258	ARG
1	I	262	GLN
1	I	272	ARG
1	I	275	LEU
1	I	287	LYS
1	I	294	GLN
1	J	7	ILE
1	J	25	VAL
1	J	45	VAL
1	J	48	SER
1	J	62	LEU
1	J	67	MET
1	J	82	ASN
1	J	98	ASN
1	J	114	VAL
1	J	125	CYS
1	J	150	ARG
1	J	162	ASP
1	J	177	ILE
1	J	188	PHE
1	J	193	LYS
1	J	199	ARG
1	J	201	PHE
1	J	202	LYS
1	J	209	ILE
1	J	231	ASN
1	J	233	ASP
1	J	243	ARG
1	J	262	GLN
1	J	263	LYS
1	J	266	VAL
1	J	272	ARG
1	J	275	LEU
1	J	287	LYS
1	J	288	LEU
1	J	290	GLN
1	K	21	GLN
1	K	25	VAL
1	K	62	LEU
1	K	72	VAL

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Mol	Chain	Res	Type
1	K	75	ASN
1	K	82	ASN
1	K	90	ASP
1	K	101	ARG
1	K	124	ARG
1	K	125	CYS
1	K	140	VAL
1	K	150	ARG
1	K	188	PHE
1	K	193	LYS
1	K	196	ASP
1	K	199	ARG
1	K	202	LYS
1	K	206	LYS
1	K	214	THR
1	K	215	GLU
1	K	221	LEU
1	K	224	LEU
1	K	255	THR
1	K	262	GLN
1	K	266	VAL
1	K	271	THR
1	K	275	LEU
1	K	285	GLU
1	L	7	ILE
1	L	25	VAL
1	L	26	VAL
1	L	62	LEU
1	L	65	SER
1	L	81	THR
1	L	82	ASN
1	L	98	ASN
1	L	114	VAL
1	L	117	GLU
1	L	120	VAL
1	L	123	LYS
1	L	125	CYS
1	L	133	CYS
1	L	134	VAL
1	L	150	ARG
1	L	188	PHE
1	L	193	LYS

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Mol	Chain	Res	Type
1	L	196	ASP
1	L	199	ARG
1	L	202	LYS
1	L	218	SER
1	L	255	THR
1	L	258	ARG
1	L	262	GLN
1	L	270	GLN
1	L	271	THR
1	L	275	LEU
1	L	277	ASP
1	L	279	LEU
1	L	287	LYS
1	L	289	ASP
1	L	292	PHE
1	M	21	GLN
1	M	23	LEU
1	M	25	VAL
1	M	62	LEU
1	M	67	MET
1	M	72	VAL
1	M	75	ASN
1	M	81	THR
1	M	82	ASN
1	M	125	CYS
1	M	128	ARG
1	M	161	THR
1	M	162	ASP
1	M	167	GLU
1	M	188	PHE
1	M	193	LYS
1	M	195	LEU
1	M	199	ARG
1	M	203	GLU
1	M	222	PHE
1	M	233	ASP
1	M	262	GLN
1	M	271	THR
1	M	272	ARG
1	M	275	LEU
1	M	277	ASP
1	M	287	LYS

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Mol	Chain	Res	Type
1	N	6	LEU
1	N	23	LEU
1	N	48	SER
1	N	62	LEU
1	N	65	SER
1	N	68	ASP
1	N	71	LEU
1	N	72	VAL
1	N	82	ASN
1	N	103	ILE
1	N	120	VAL
1	N	124	ARG
1	N	125	CYS
1	N	131	LYS
1	N	154	THR
1	N	188	PHE
1	N	193	LYS
1	N	195	LEU
1	N	199	ARG
1	N	201	PHE
1	N	203	GLU
1	N	214	THR
1	N	233	ASP
1	N	237	TYR
1	N	251	ASN
1	N	258	ARG
1	N	262	GLN
1	N	268	THR
1	N	275	LEU
1	N	276	TYR
1	N	277	ASP
1	N	287	LYS
1	N	291	LEU
1	O	7	ILE
1	O	8	SER
1	O	25	VAL
1	O	26	VAL
1	O	48	SER
1	O	75	ASN
1	O	81	THR
1	O	82	ASN
1	O	114	VAL

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Mol	Chain	Res	Type
1	O	120	VAL
1	O	123	LYS
1	O	124	ARG
1	O	152	ASP
1	O	188	PHE
1	O	193	LYS
1	O	195	LEU
1	O	199	ARG
1	O	201	PHE
1	O	202	LYS
1	O	206	LYS
1	O	218	SER
1	O	221	LEU
1	O	231	ASN
1	O	232	VAL
1	O	233	ASP
1	O	255	THR
1	O	266	VAL
1	O	275	LEU
1	O	282	TYR
1	O	285	GLU
1	O	287	LYS
1	P	21	GLN
1	P	26	VAL
1	P	62	LEU
1	P	81	THR
1	P	82	ASN
1	P	85	LEU
1	P	116	LEU
1	P	123	LYS
1	P	131	LYS
1	P	188	PHE
1	P	193	LYS
1	P	196	ASP
1	P	199	ARG
1	P	203	GLU
1	P	206	LYS
1	P	231	ASN
1	P	233	ASP
1	P	245	MET
1	P	254	GLU
1	P	258	ARG

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Mol	Chain	Res	Type
1	P	261	THR
1	P	263	LYS
1	P	266	VAL
1	P	277	ASP
1	P	287	LYS
1	P	288	LEU
1	P	290	GLN
1	P	291	LEU
1	P	292	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	119	GLN
1	A	122	GLN
1	A	246	ASN
1	A	262	GLN
1	A	270	GLN
1	A	274	GLN
1	B	98	ASN
1	B	246	ASN
1	B	262	GLN
1	B	270	GLN
1	C	82	ASN
1	C	98	ASN
1	C	122	GLN
1	C	246	ASN
1	C	262	GLN
1	C	274	GLN
1	C	290	GLN
1	D	82	ASN
1	D	98	ASN
1	D	246	ASN
1	D	262	GLN
1	D	270	GLN
1	D	290	GLN
1	E	82	ASN
1	E	119	GLN
1	E	122	GLN
1	E	246	ASN
1	E	262	GLN

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Mol	Chain	Res	Type
1	E	270	GLN
1	F	98	ASN
1	F	119	GLN
1	F	262	GLN
1	F	270	GLN
1	F	274	GLN
1	G	122	GLN
1	G	246	ASN
1	G	262	GLN
1	G	270	GLN
1	G	290	GLN
1	H	98	ASN
1	H	231	ASN
1	H	251	ASN
1	H	262	GLN
1	H	270	GLN
1	H	290	GLN
1	H	293	ASN
1	I	82	ASN
1	I	98	ASN
1	I	122	GLN
1	I	246	ASN
1	I	262	GLN
1	I	270	GLN
1	I	290	GLN
1	J	98	ASN
1	J	246	ASN
1	J	262	GLN
1	J	270	GLN
1	K	246	ASN
1	K	262	GLN
1	K	270	GLN
1	K	290	GLN
1	L	98	ASN
1	L	246	ASN
1	L	262	GLN
1	L	290	GLN
1	M	24	GLN
1	M	82	ASN
1	M	127	HIS
1	M	246	ASN
1	M	262	GLN

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Mol	Chain	Res	Type
1	M	270	GLN
1	N	82	ASN
1	N	122	GLN
1	N	246	ASN
1	N	251	ASN
1	N	262	GLN
1	O	82	ASN
1	O	98	ASN
1	O	119	GLN
1	O	122	GLN
1	O	246	ASN
1	O	262	GLN
1	P	82	ASN
1	P	98	ASN
1	P	231	ASN
1	P	246	ASN
1	P	262	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	290/298 (97%)	0.01	0 100 100	26, 44, 60, 67	0
1	B	286/298 (95%)	0.01	1 (0%) 94 94	28, 45, 60, 67	0
1	C	287/298 (96%)	0.07	0 100 100	29, 46, 61, 69	0
1	D	287/298 (96%)	0.04	1 (0%) 94 94	32, 46, 61, 67	0
1	E	288/298 (96%)	0.03	0 100 100	32, 46, 62, 73	0
1	F	286/298 (95%)	0.13	3 (1%) 82 82	32, 48, 63, 71	0
1	G	287/298 (96%)	-0.03	1 (0%) 94 94	30, 46, 60, 68	0
1	H	288/298 (96%)	-0.00	3 (1%) 82 82	34, 47, 62, 70	0
1	I	289/298 (96%)	-0.05	1 (0%) 94 94	33, 46, 61, 70	0
1	J	288/298 (96%)	-0.14	0 100 100	33, 47, 62, 67	0
1	K	286/298 (95%)	0.06	0 100 100	32, 47, 62, 76	0
1	L	286/298 (95%)	0.16	1 (0%) 94 94	33, 48, 64, 74	0
1	M	287/298 (96%)	0.27	12 (4%) 36 32	33, 49, 65, 80	0
1	N	287/298 (96%)	0.21	3 (1%) 82 82	33, 50, 65, 72	0
1	O	288/298 (96%)	0.44	25 (8%) 10 7	34, 50, 71, 88	0
1	P	286/298 (95%)	0.37	15 (5%) 27 23	33, 49, 69, 78	0
All	All	4596/4768 (96%)	0.10	66 (1%) 75 75	26, 47, 63, 88	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	282	TYR	3.8
1	P	218	SER	3.5
1	P	232	VAL	3.4
1	O	222	PHE	3.4
1	O	164	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	O	199	ARG	3.3
1	P	230	ALA	3.3
1	P	170	ASP	3.3
1	O	169	ILE	3.3
1	O	193	LYS	3.2
1	N	182	ALA	3.2
1	O	171	ALA	3.2
1	P	227	LEU	3.0
1	M	229	GLY	3.0
1	M	209	ILE	2.9
1	M	220	PRO	2.8
1	O	198	TYR	2.8
1	P	283	ALA	2.8
1	O	172	ALA	2.7
1	P	258	ARG	2.7
1	F	227	LEU	2.7
1	M	206	LYS	2.6
1	D	199	ARG	2.6
1	M	195	LEU	2.6
1	O	203	GLU	2.6
1	P	231	ASN	2.6
1	O	192	MET	2.6
1	O	165	ALA	2.5
1	P	290	GLN	2.5
1	O	170	ASP	2.5
1	O	201	PHE	2.5
1	F	172	ALA	2.5
1	P	206	LYS	2.5
1	M	200	ARG	2.4
1	O	195	LEU	2.4
1	P	201	PHE	2.3
1	O	207	VAL	2.3
1	O	22	PRO	2.3
1	H	171	ALA	2.3
1	O	231	ASN	2.3
1	O	282	TYR	2.3
1	M	19	ALA	2.2
1	O	206	LYS	2.2
1	P	192	MET	2.2
1	M	219	THR	2.2
1	M	230	ALA	2.2
1	L	207	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	40	VAL	2.2
1	F	137	GLY	2.1
1	H	173	ILE	2.1
1	O	204	ALA	2.1
1	N	166	ALA	2.1
1	I	153	GLU	2.1
1	O	228	LYS	2.1
1	O	264	ALA	2.1
1	O	229	GLY	2.1
1	B	194	THR	2.1
1	P	213	LEU	2.1
1	P	21	GLN	2.1
1	H	205	VAL	2.1
1	M	227	LEU	2.0
1	O	292	PHE	2.0
1	N	218	SER	2.0
1	G	174	GLU	2.0
1	M	15	ALA	2.0
1	O	255	THR	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.