Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:45 PM BST

PDB ID	:	6RMO
Title	:	Structure of Plasmodium falciparum IMP-nucleotidase
Authors	:	Carrique, L.; Ballut, L.; Violot, S.; Aghajari, N.
Deposited on	:	2019-05-07
Resolution	:	2.60 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 following versions of software and data (see references ⓘ) were used in the production of this report:

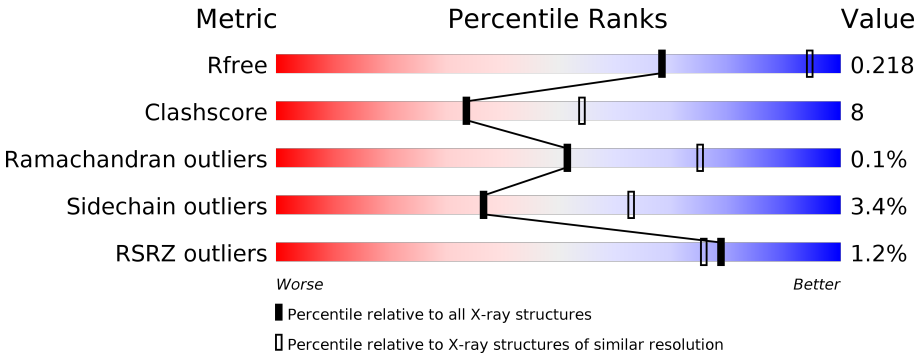
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	444	% 76% 16% • 7%
1	B	444	68% 14% • 17%
1	C	444	% 71% 20% • 8%
1	D	444	67% 16% • 17%
1	E	444	% 74% 16% • 8%
1	F	444	64% 16% • 18%

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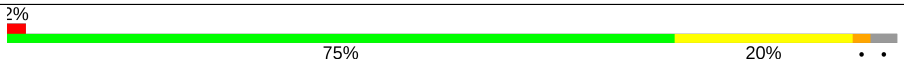
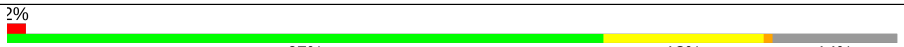
Mol	Chain	Length	Quality of chain
1	G	444	
1	H	444	
1	I	444	
1	J	444	
1	K	444	
1	L	444	
1	M	444	
1	N	444	
1	O	444	
1	P	444	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 52441 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 IMP-specific 5'-nucleotidase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	S	0	0	0
			3323	2149	544	613	17			
1	B	368	Total	C	N	O	S	0	0	0
			2932	1909	475	532	16			
1	C	410	Total	C	N	O	S	0	0	0
			3328	2154	544	613	17			
1	D	370	Total	C	N	O	S	0	0	0
			2965	1927	480	542	16			
1	E	408	Total	C	N	O	S	0	0	0
			3279	2118	534	611	16			
1	F	364	Total	C	N	O	S	0	0	0
			2950	1910	481	543	16			
1	G	407	Total	C	N	O	S	0	0	0
			3264	2109	536	602	17			
1	H	361	Total	C	N	O	S	0	0	0
			2863	1855	466	526	16			
1	I	432	Total	C	N	O	S	0	0	0
			3486	2242	574	652	18			
1	J	381	Total	C	N	O	S	0	0	0
			3085	1999	506	564	16			
1	K	423	Total	C	N	O	S	0	0	0
			3447	2226	566	637	18			
1	L	382	Total	C	N	O	S	0	0	0
			3106	2010	508	572	16			
1	M	431	Total	C	N	O	S	0	0	0
			3512	2263	575	656	18			
1	N	381	Total	C	N	O	S	0	0	0
			3080	1999	506	559	16			
1	O	423	Total	C	N	O	S	0	0	0
			3433	2216	565	634	18			
1	P	381	Total	C	N	O	S	0	0	0
			3083	1995	505	567	16			

- Molecule 2 is water.

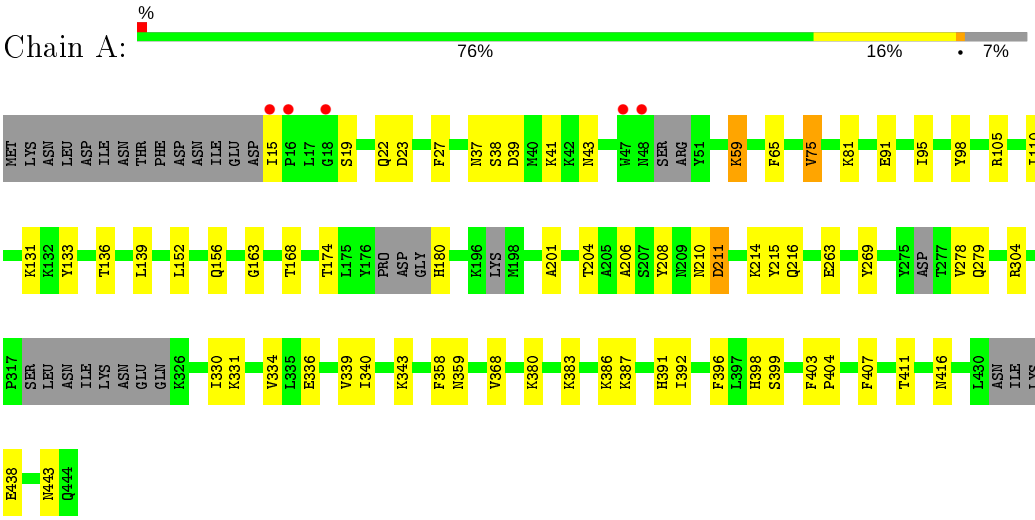
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	93	Total O 93 93	0	0
2	B	59	Total O 59 59	0	0
2	C	103	Total O 103 103	0	0
2	D	65	Total O 65 65	0	0
2	E	105	Total O 105 105	0	0
2	F	57	Total O 57 57	0	0
2	G	95	Total O 95 95	0	0
2	H	75	Total O 75 75	0	0
2	I	97	Total O 97 97	0	0
2	J	53	Total O 53 53	0	0
2	K	112	Total O 112 112	0	0
2	L	74	Total O 74 74	0	0
2	M	95	Total O 95 95	0	0
2	N	60	Total O 60 60	0	0
2	O	99	Total O 99 99	0	0
2	P	63	Total O 63 63	0	0

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.

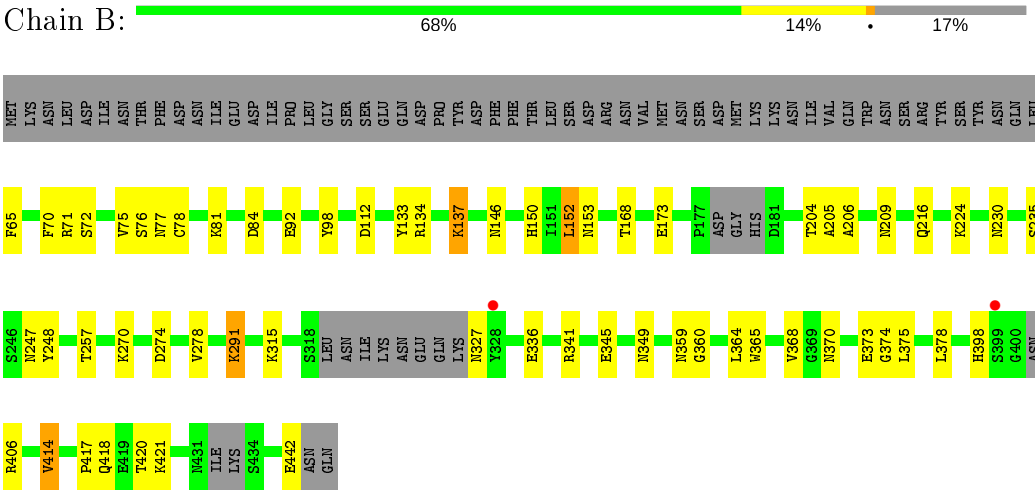
- Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain A:



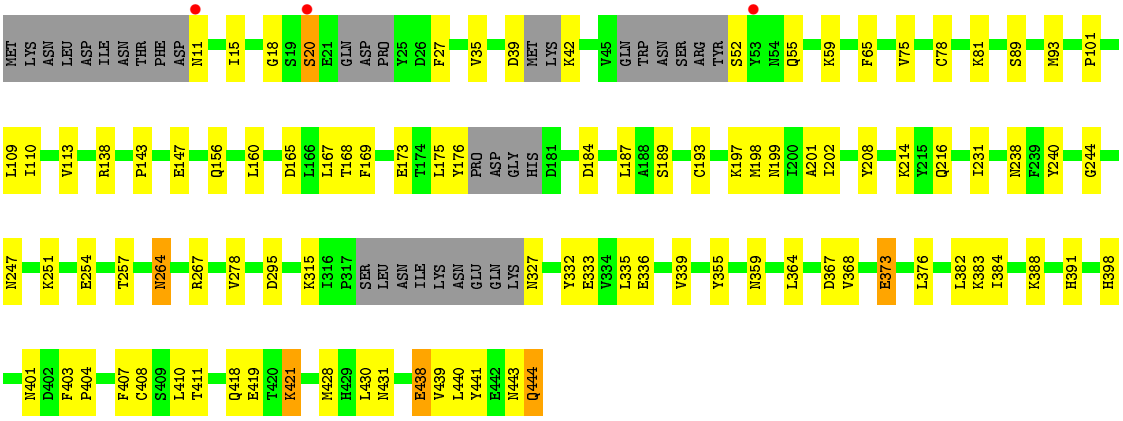
- Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain B:



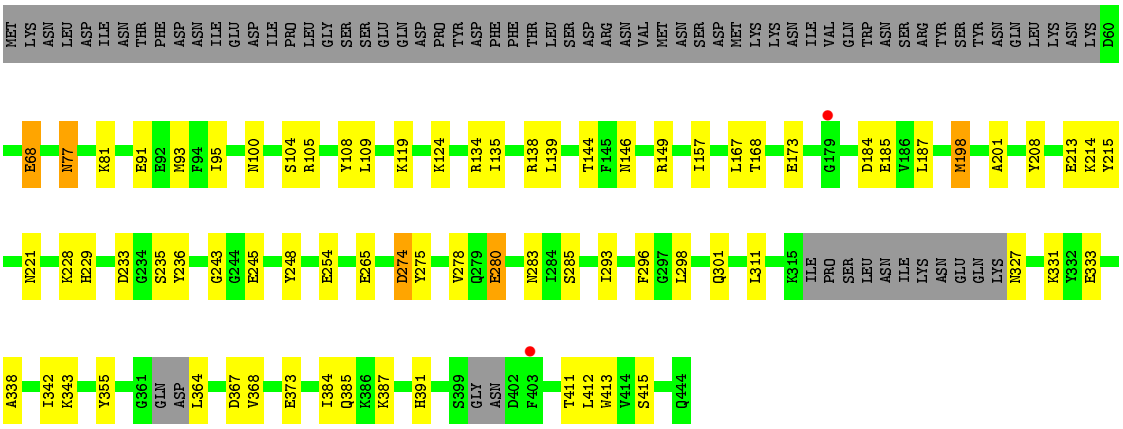
- Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain C:



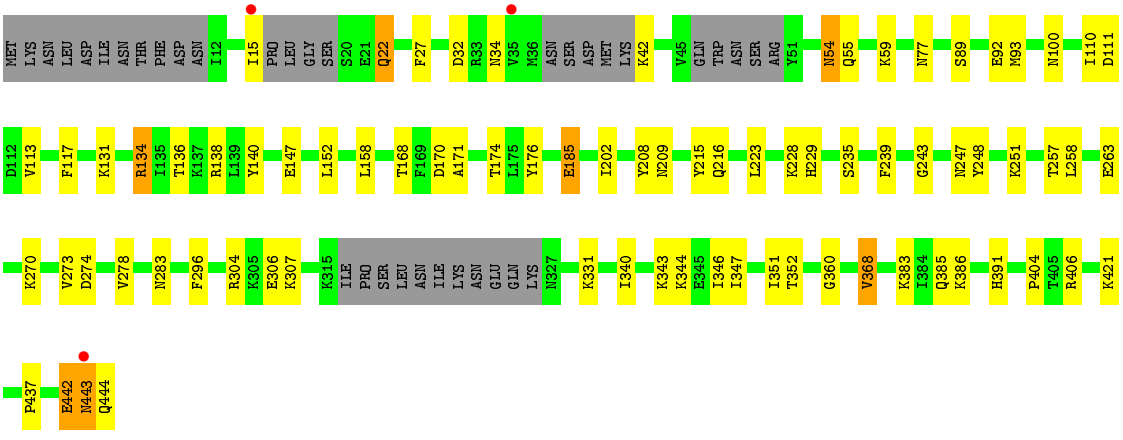
• Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain D:



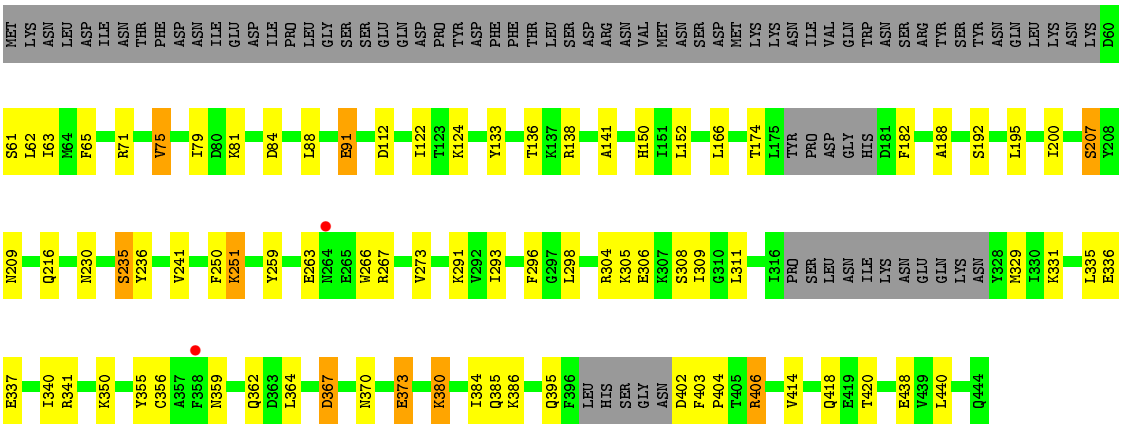
• Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain E:



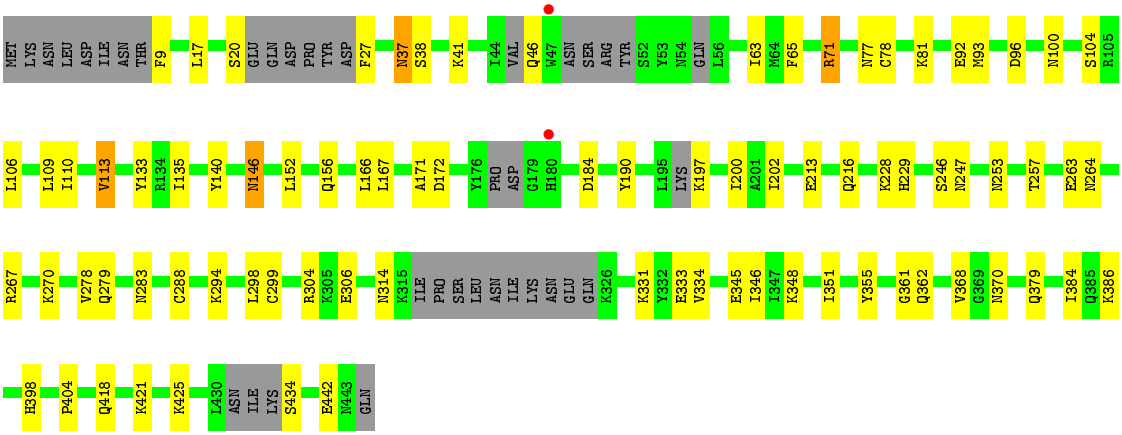
• Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain F:



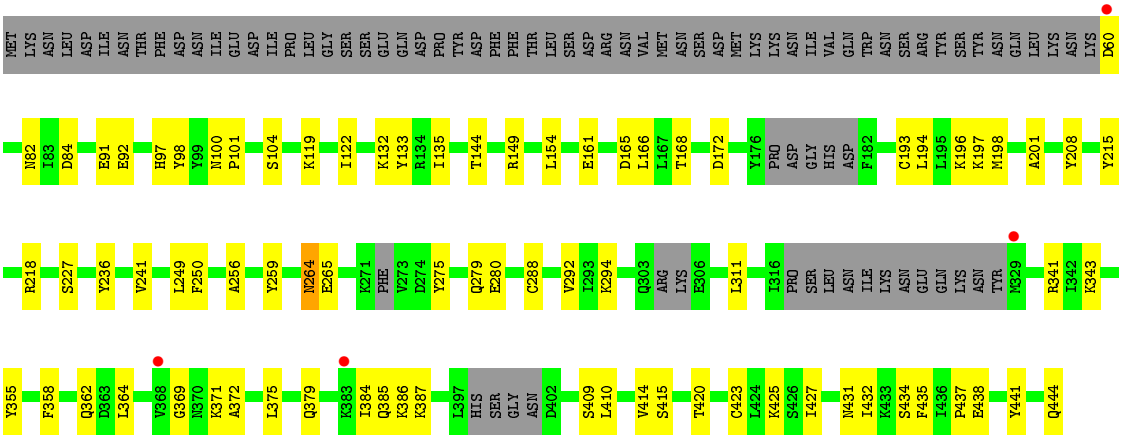
• Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain G:



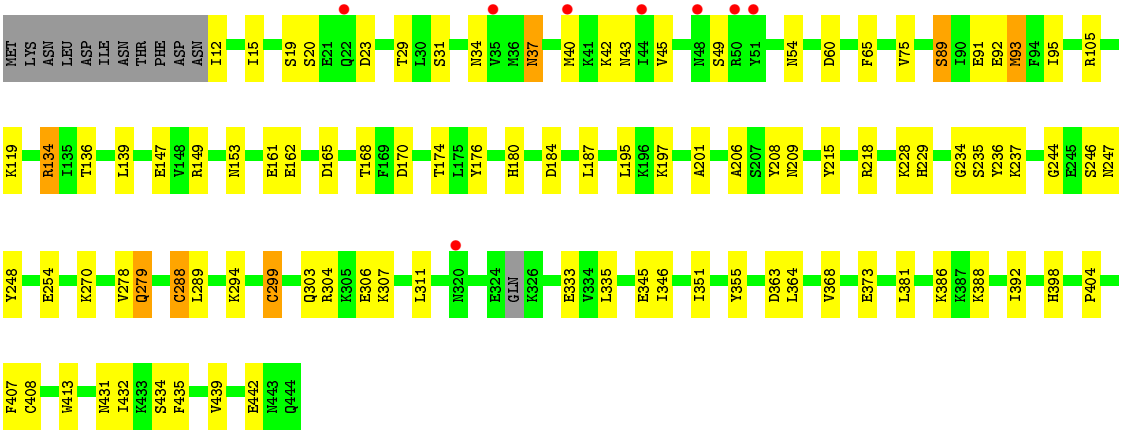
• Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain H:



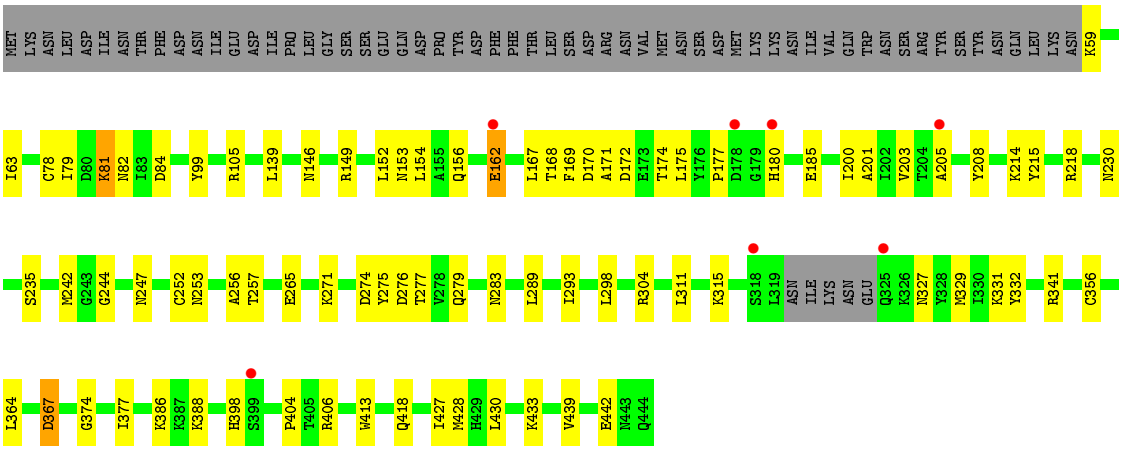
• Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain I:



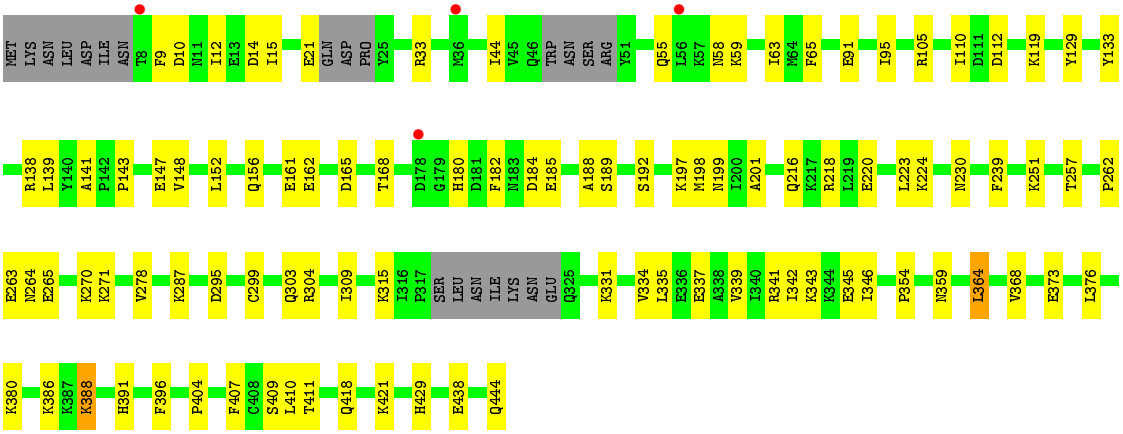
• Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain J:

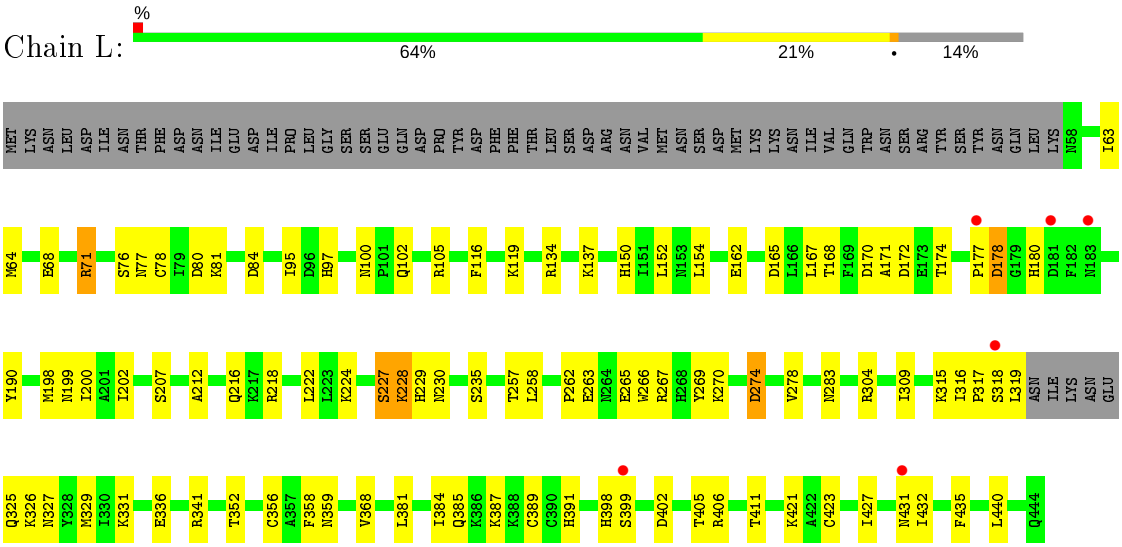


• Molecule 1: IMP-specific 5'-nucleotidase, putative

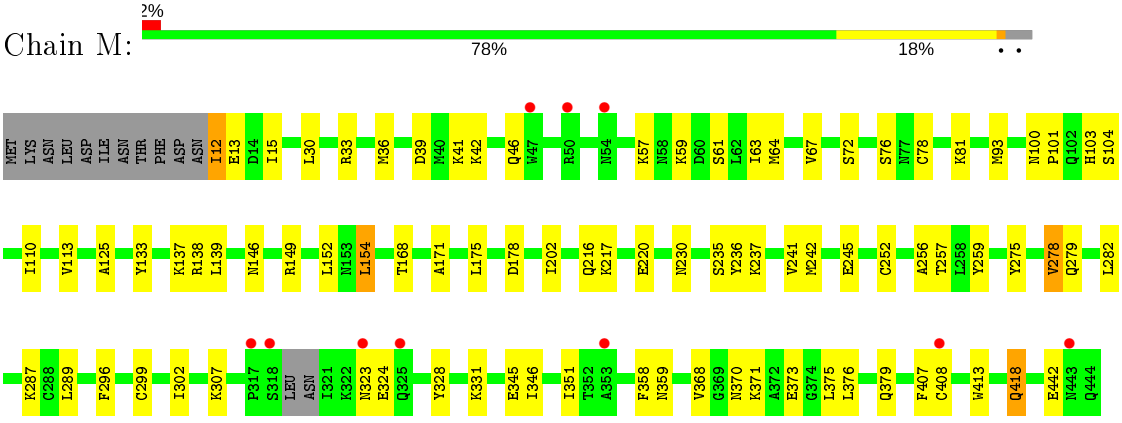
Chain K:



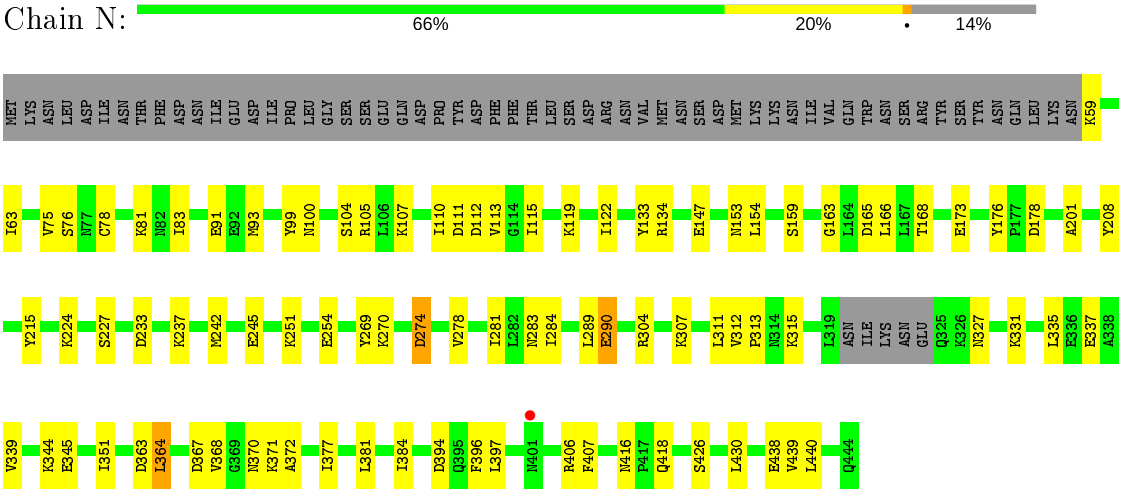
• Molecule 1: IMP-specific 5'-nucleotidase, putative



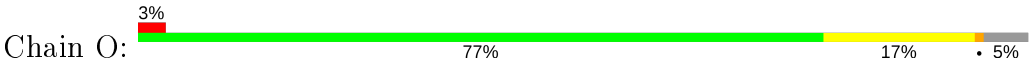
• Molecule 1: IMP-specific 5'-nucleotidase, putative

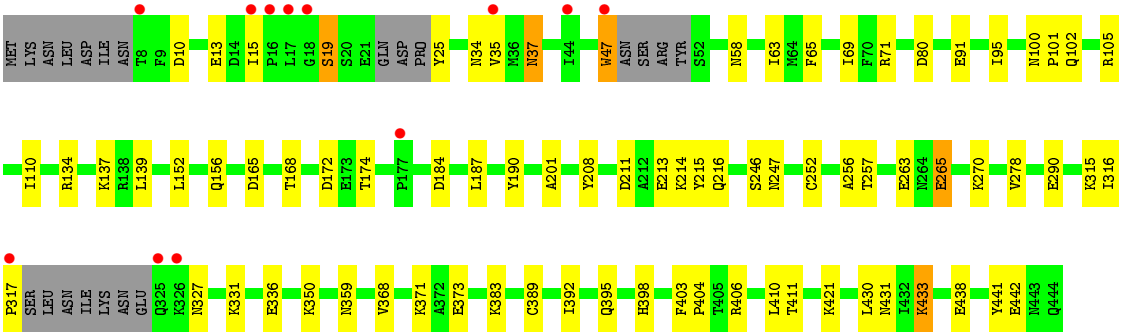


• Molecule 1: IMP-specific 5'-nucleotidase, putative



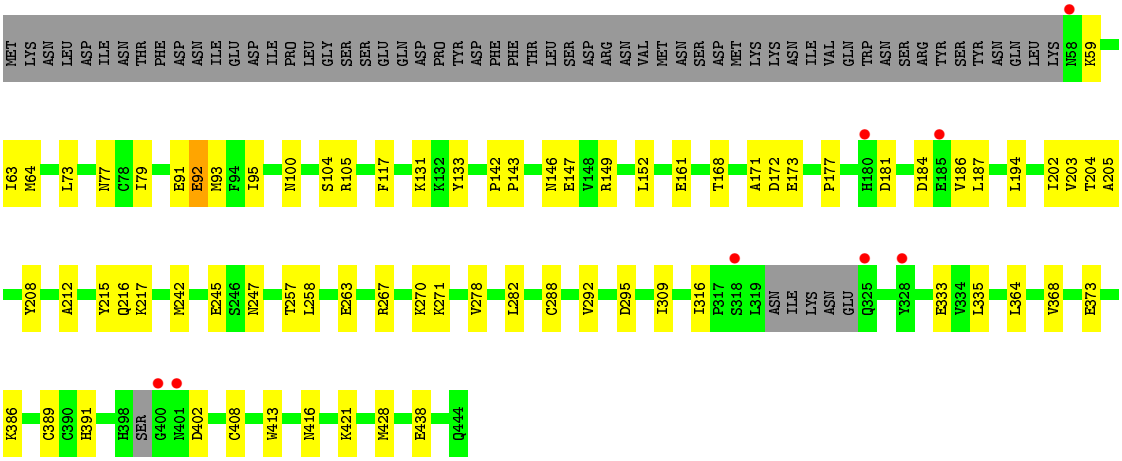
• Molecule 1: IMP-specific 5'-nucleotidase, putative





- Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	148.96Å 204.07Å 149.28Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	48.30 – 2.60 48.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.7 (48.30-2.60) 91.2 (48.34-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.230 , 0.253 0.210 , 0.218	Depositor DCC
R_{free} test set	12515 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 19.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.317 for l,k,-h 0.329 for h,-k,-l 0.399 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	52441	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3947e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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	0.25	0/3390	0.41	0/4577
1	B	0.24	0/2993	0.40	0/4050
1	C	0.25	0/3394	0.42	1/4579 (0.0%)
1	D	0.25	0/3027	0.40	0/4093
1	E	0.25	0/3345	0.42	0/4519
1	F	0.25	0/3007	0.41	0/4058
1	G	0.26	0/3326	0.41	0/4485
1	H	0.26	0/2918	0.42	0/3949
1	I	0.25	0/3558	0.40	0/4806
1	J	0.25	0/3151	0.41	0/4255
1	K	0.25	0/3518	0.41	0/4746
1	L	0.25	0/3173	0.42	0/4287
1	M	0.25	0/3587	0.41	0/4844
1	N	0.25	0/3146	0.41	0/4248
1	O	0.25	0/3504	0.42	0/4730
1	P	0.24	0/3148	0.40	0/4254
All	All	0.25	0/52185	0.41	1/70480 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	109	LEU	CB-CG-CD1	-5.94	100.89	111.00

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	3323	0	3278	46	0
1	B	2932	0	2884	48	0
1	C	3328	0	3309	71	0
1	D	2965	0	2911	52	0
1	E	3279	0	3217	54	1
1	F	2950	0	2951	54	0
1	G	3264	0	3194	58	0
1	H	2863	0	2802	58	0
1	I	3486	0	3438	65	0
1	J	3085	0	3078	51	0
1	K	3447	0	3427	66	0
1	L	3106	0	3086	73	1
1	M	3512	0	3479	59	0
1	N	3080	0	3081	58	0
1	O	3433	0	3405	57	0
1	P	3083	0	3054	51	0
2	A	93	0	0	14	0
2	B	59	0	0	9	0
2	C	103	0	0	15	0
2	D	65	0	0	19	0
2	E	105	0	0	23	1
2	F	57	0	0	10	0
2	G	95	0	0	24	0
2	H	75	0	0	23	0
2	I	97	0	0	20	1
2	J	53	0	0	11	0
2	K	112	0	0	19	0
2	L	74	0	0	26	0
2	M	95	0	0	21	0
2	N	60	0	0	18	0
2	O	99	0	0	21	0
2	P	63	0	0	13	0
All	All	52441	0	50594	864	2

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 8.

All (864) 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:119:LYS:NZ	2:I:501:HOH:O	1.92	1.00
1:A:152:LEU:N	2:A:501:HOH:O	1.88	0.99
1:D:138:ARG:NH1	2:D:503:HOH:O	1.96	0.98
1:H:215:TYR:OH	2:H:501:HOH:O	1.81	0.98
1:K:112:ASP:OD2	2:K:501:HOH:O	1.83	0.97
1:G:434:SER:N	2:G:503:HOH:O	1.95	0.97
1:G:404:PRO:O	2:G:501:HOH:O	1.82	0.96
1:G:333:GLU:OE1	2:G:502:HOH:O	1.84	0.96
1:H:369:GLY:O	2:H:502:HOH:O	1.83	0.95
1:J:341:ARG:NH1	2:J:501:HOH:O	1.87	0.94
2:M:543:HOH:O	1:P:93:MET:SD	2.25	0.94
1:L:116:PHE:O	2:L:501:HOH:O	1.84	0.94
1:M:137:LYS:NZ	2:M:501:HOH:O	1.98	0.94
1:O:290:GLU:OE2	2:O:501:HOH:O	1.88	0.92
1:F:395:GLN:O	2:F:501:HOH:O	1.89	0.90
1:J:79:ILE:O	2:J:502:HOH:O	1.89	0.90
1:E:383:LYS:O	2:E:501:HOH:O	1.90	0.88
1:L:224:LYS:O	2:L:502:HOH:O	1.90	0.88
1:N:134:ARG:NH1	2:N:503:HOH:O	2.04	0.88
1:P:402:ASP:O	2:P:501:HOH:O	1.91	0.87
1:E:77:ASN:OD1	2:E:502:HOH:O	1.93	0.87
1:F:236:TYR:O	2:F:502:HOH:O	1.95	0.85
1:I:355:TYR:O	2:I:502:HOH:O	1.95	0.85
1:C:59:LYS:O	2:C:501:HOH:O	1.94	0.84
1:K:220:GLU:OE1	2:K:502:HOH:O	1.96	0.83
1:O:19:SER:O	2:O:503:HOH:O	1.95	0.83
1:A:81:LYS:O	2:A:502:HOH:O	1.96	0.83
1:I:92:GLU:OE2	2:I:504:HOH:O	1.96	0.82
1:M:104:SER:N	2:M:502:HOH:O	2.12	0.82
1:O:213:GLU:O	2:O:502:HOH:O	1.95	0.82
1:E:89:SER:O	2:E:503:HOH:O	1.97	0.82
1:E:209:ASN:OD1	2:E:504:HOH:O	1.98	0.81
1:N:438:GLU:OE2	2:N:502:HOH:O	1.98	0.81
1:B:247:ASN:ND2	2:B:506:HOH:O	2.12	0.81
1:D:367:ASP:OD1	2:D:502:HOH:O	1.96	0.81
1:F:291:LYS:NZ	2:F:503:HOH:O	2.14	0.81
1:H:149:ARG:NH1	1:H:415:SER:OG	2.13	0.81
1:L:406:ARG:O	2:L:503:HOH:O	1.99	0.81
1:M:100:ASN:O	2:M:502:HOH:O	1.99	0.81
1:N:426:SER:O	2:N:501:HOH:O	1.96	0.81
2:B:501:HOH:O	1:C:81:LYS:NZ	2.13	0.80
1:O:80:ASP:OD1	2:O:504:HOH:O	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:236:TYR:O	2:M:503:HOH:O	1.99	0.80
1:I:65:PHE:O	2:I:505:HOH:O	1.99	0.80
1:J:428:MET:SD	2:J:551:HOH:O	2.38	0.80
1:G:306:GLU:OE2	2:G:504:HOH:O	1.98	0.80
1:O:190:TYR:OH	2:O:505:HOH:O	1.99	0.79
1:K:346:ILE:N	2:K:503:HOH:O	2.01	0.79
1:A:204:THR:HG22	1:A:206:ALA:H	1.47	0.79
1:E:140:TYR:O	2:E:505:HOH:O	1.98	0.79
1:A:59:LYS:NZ	2:A:503:HOH:O	2.08	0.79
1:B:92:GLU:OE1	2:B:501:HOH:O	1.99	0.79
1:J:275:TYR:O	1:J:279:GLN:NE2	2.16	0.79
1:E:111:ASP:O	2:E:507:HOH:O	2.00	0.78
1:H:259:TYR:OH	2:H:503:HOH:O	2.00	0.78
1:K:21:GLU:OE2	2:K:505:HOH:O	2.01	0.78
1:I:12:ILE:HD12	1:I:373:GLU:HB2	1.64	0.78
1:K:342:ILE:O	2:K:503:HOH:O	2.02	0.78
1:F:138:ARG:NH1	1:F:141:ALA:O	2.15	0.78
1:O:19:SER:OG	2:O:506:HOH:O	2.01	0.78
1:G:345:GLU:OE2	2:G:505:HOH:O	2.02	0.78
1:G:348:LYS:NZ	2:G:512:HOH:O	2.15	0.78
1:O:105:ARG:NH1	2:O:507:HOH:O	2.09	0.78
1:J:304:ARG:NH1	2:J:503:HOH:O	1.99	0.78
1:P:181:ASP:OD1	2:P:503:HOH:O	2.02	0.78
1:K:197:LYS:O	2:K:504:HOH:O	2.01	0.77
1:C:176:TYR:O	2:C:502:HOH:O	2.01	0.77
1:J:244:GLY:O	1:J:247:ASN:ND2	2.16	0.77
1:H:387:LYS:H	1:H:387:LYS:HD2	1.49	0.77
1:K:216:GLN:NE2	2:K:508:HOH:O	2.17	0.76
1:P:100:ASN:O	2:P:502:HOH:O	2.01	0.76
1:A:214:LYS:NZ	2:A:506:HOH:O	2.18	0.76
1:K:386:LYS:HD2	2:K:511:HOH:O	1.85	0.76
1:D:108:TYR:OH	2:D:504:HOH:O	2.01	0.76
1:F:166:LEU:HB2	1:F:384:ILE:HD13	1.67	0.76
1:J:99:TYR:OH	2:J:504:HOH:O	2.04	0.76
1:H:166:LEU:HB2	1:H:384:ILE:HD13	1.67	0.75
1:H:362:GLN:OE1	2:H:504:HOH:O	2.05	0.75
1:E:185:GLU:OE1	2:E:509:HOH:O	2.04	0.75
1:K:263:GLU:OE1	2:K:506:HOH:O	2.03	0.75
1:C:208:TYR:HB3	1:C:214:LYS:HD3	1.69	0.74
1:I:153:ASN:OD1	2:I:506:HOH:O	2.04	0.74
1:J:205:ALA:O	2:J:505:HOH:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:GLU:O	2:E:508:HOH:O	2.03	0.74
1:M:42:LYS:HG3	2:M:514:HOH:O	1.87	0.74
1:L:100:ASN:O	2:L:504:HOH:O	2.04	0.74
1:C:444:GLN:O	2:C:503:HOH:O	2.05	0.73
1:D:124:LYS:NZ	2:D:512:HOH:O	2.22	0.73
1:M:39:ASP:HA	1:M:42:LYS:HB2	1.69	0.73
1:P:247:ASN:OD1	2:P:504:HOH:O	2.07	0.73
1:J:386:LYS:O	2:J:506:HOH:O	2.06	0.73
1:B:173:GLU:OE1	2:B:502:HOH:O	2.06	0.73
1:G:398:HIS:NE2	2:G:515:HOH:O	2.22	0.72
1:N:163:GLY:N	2:N:506:HOH:O	2.14	0.72
1:L:180:HIS:ND1	2:L:510:HOH:O	2.21	0.72
1:D:293:ILE:HD11	1:D:311:LEU:HD11	1.71	0.72
1:D:81:LYS:NZ	2:D:514:HOH:O	2.22	0.72
1:F:112:ASP:O	1:F:406:ARG:NH1	2.23	0.72
1:K:444:GLN:NE2	1:L:329:MET:O	2.21	0.72
1:J:367:ASP:OD2	2:J:505:HOH:O	2.06	0.72
1:D:245:GLU:OE2	2:D:507:HOH:O	2.08	0.72
1:G:133:TYR:OH	2:G:508:HOH:O	2.08	0.72
1:G:92:GLU:OE1	2:G:507:HOH:O	2.08	0.72
1:B:341:ARG:O	2:B:503:HOH:O	2.06	0.72
1:C:11:ASN:N	2:C:512:HOH:O	2.22	0.72
1:C:373:GLU:OE2	2:C:504:HOH:O	2.07	0.72
1:D:173:GLU:O	2:D:505:HOH:O	2.08	0.71
1:O:430:LEU:O	1:O:431:ASN:ND2	2.23	0.71
1:E:93:MET:HB2	2:E:520:HOH:O	1.90	0.71
1:K:429:HIS:NE2	2:K:509:HOH:O	2.22	0.71
1:N:168:THR:HG22	1:N:201:ALA:HB3	1.73	0.71
1:G:38:SER:N	2:G:517:HOH:O	2.24	0.70
1:D:367:ASP:OD2	2:D:506:HOH:O	2.08	0.70
1:P:131:LYS:NZ	2:P:511:HOH:O	2.23	0.70
1:E:283:ASN:OD1	1:E:304:ARG:NH2	2.25	0.70
1:K:239:PHE:O	2:K:507:HOH:O	2.08	0.70
1:H:97:HIS:O	2:H:505:HOH:O	2.08	0.70
1:A:336:GLU:OE2	1:A:359:ASN:ND2	2.22	0.70
1:J:253:ASN:ND2	1:J:257:THR:O	2.25	0.70
1:A:98:TYR:OH	1:A:387:LYS:NZ	2.24	0.69
1:D:146:ASN:ND2	2:D:515:HOH:O	2.24	0.69
1:N:270:LYS:HD3	1:N:377:ILE:HD11	1.74	0.69
1:C:20:SER:HG	1:C:355:TYR:HH	1.36	0.69
1:M:307:LYS:NZ	2:M:510:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:ASP:OD2	2:G:509:HOH:O	2.09	0.69
1:L:411:THR:OG1	2:L:506:HOH:O	2.10	0.69
1:N:176:TYR:O	2:N:505:HOH:O	2.11	0.69
1:O:247:ASN:OD1	1:O:270:LYS:NZ	2.25	0.69
1:F:124:LYS:NZ	2:F:511:HOH:O	2.25	0.69
1:H:355:TYR:O	2:H:506:HOH:O	2.10	0.69
1:I:168:THR:HG22	1:I:201:ALA:HB3	1.74	0.69
1:J:59:LYS:NZ	1:J:153:ASN:OD1	2.23	0.69
1:B:173:GLU:OE2	2:B:504:HOH:O	2.09	0.69
1:H:249:LEU:O	2:H:507:HOH:O	2.11	0.68
1:J:162:GLU:HB2	1:J:388:LYS:HE3	1.74	0.68
1:M:245:GLU:HG2	1:M:371:LYS:HG3	1.74	0.68
1:N:91:GLU:OE1	2:N:504:HOH:O	2.10	0.68
1:P:131:LYS:NZ	2:P:512:HOH:O	2.25	0.68
1:P:316:ILE:O	2:P:505:HOH:O	2.10	0.68
1:M:379:GLN:NE2	2:M:506:HOH:O	2.26	0.68
1:N:339:VAL:HG23	1:N:364:LEU:HD11	1.76	0.68
1:P:216:GLN:HE22	1:P:257:THR:HA	1.59	0.68
1:A:139:LEU:O	1:D:105:ARG:NH2	2.23	0.68
1:F:329:MET:SD	1:F:362:GLN:NE2	2.66	0.68
1:G:299:CYS:O	1:G:314:ASN:ND2	2.27	0.68
1:O:404:PRO:O	2:O:509:HOH:O	2.12	0.68
1:C:160:LEU:HD21	1:C:410:LEU:HD21	1.75	0.68
1:F:370:ASN:HB3	1:F:373:GLU:HB2	1.75	0.67
1:A:216:GLN:OE1	2:A:504:HOH:O	2.10	0.67
1:F:209:ASN:ND2	2:F:510:HOH:O	2.24	0.67
1:G:37:ASN:OD1	1:G:37:ASN:N	2.26	0.67
1:B:360:GLY:O	2:B:505:HOH:O	2.12	0.67
1:B:398:HIS:HE1	2:B:502:HOH:O	1.77	0.67
1:H:441:TYR:O	2:H:508:HOH:O	2.12	0.67
1:H:279:GLN:OE1	1:L:385:GLN:NE2	2.27	0.67
1:I:20:SER:HG	1:I:355:TYR:HH	1.43	0.67
1:N:112:ASP:O	1:N:406:ARG:NH1	2.28	0.67
1:J:283:ASN:OD1	1:J:304:ARG:NH2	2.27	0.67
1:L:178:ASP:HB2	2:L:510:HOH:O	1.95	0.67
1:E:100:ASN:ND2	2:E:518:HOH:O	2.28	0.67
1:O:265:GLU:O	2:O:508:HOH:O	2.11	0.67
1:B:336:GLU:OE1	1:B:359:ASN:ND2	2.28	0.67
1:A:105:ARG:NH2	1:D:139:LEU:O	2.21	0.66
1:M:13:GLU:OE1	2:M:504:HOH:O	2.11	0.66
1:C:408:CYS:O	2:C:505:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:427:ILE:O	2:L:508:HOH:O	2.12	0.66
1:P:373:GLU:OE1	2:P:506:HOH:O	2.13	0.66
1:D:168:THR:HG22	1:D:201:ALA:HB3	1.77	0.66
1:E:147:GLU:OE1	1:F:331:LYS:NZ	2.28	0.66
1:D:68:GLU:OE2	2:D:508:HOH:O	2.12	0.66
1:L:274:ASP:N	1:L:274:ASP:OD1	2.17	0.66
1:N:281:ILE:HD11	1:N:351:ILE:HG21	1.78	0.66
1:M:103:HIS:N	2:M:502:HOH:O	2.16	0.66
1:G:135:ILE:O	2:G:511:HOH:O	2.14	0.66
1:A:380:LYS:NZ	2:A:505:HOH:O	2.14	0.65
1:B:247:ASN:OD1	1:B:270:LYS:NZ	2.29	0.65
1:G:190:TYR:OH	2:G:510:HOH:O	2.12	0.65
1:I:398:HIS:NE2	2:I:520:HOH:O	2.28	0.65
1:E:247:ASN:OD1	1:E:270:LYS:NZ	2.28	0.65
1:M:149:ARG:NH1	1:M:413:TRP:O	2.29	0.65
1:A:174:THR:HG21	1:A:392:ILE:HG22	1.79	0.65
1:H:385:GLN:OE1	2:H:509:HOH:O	2.14	0.65
1:H:82:ASN:OD1	2:H:510:HOH:O	2.14	0.65
1:K:278:VAL:HG22	1:K:368:VAL:HG11	1.79	0.65
1:I:247:ASN:OD1	1:I:270:LYS:NZ	2.30	0.65
1:I:34:ASN:O	1:I:37:ASN:ND2	2.30	0.65
1:K:265:GLU:N	2:K:513:HOH:O	2.28	0.65
1:N:430:LEU:N	2:N:501:HOH:O	2.30	0.65
1:F:138:ARG:HD2	1:F:141:ALA:HB3	1.79	0.64
1:N:105:ARG:NH2	1:O:139:LEU:O	2.26	0.64
1:O:442:GLU:OE2	2:O:505:HOH:O	2.14	0.64
1:B:345:GLU:O	1:B:349:ASN:ND2	2.30	0.64
1:E:421:LYS:HB3	1:E:442:GLU:HG3	1.78	0.64
1:H:435:PHE:N	2:H:516:HOH:O	2.28	0.64
1:K:409:SER:HA	2:K:511:HOH:O	1.96	0.64
1:J:146:ASN:OD1	1:J:149:ARG:NH1	2.23	0.64
1:M:370:ASN:HB3	1:M:373:GLU:HG2	1.78	0.64
1:O:336:GLU:OE1	1:O:359:ASN:ND2	2.30	0.64
1:C:404:PRO:HB2	1:C:407:PHE:HD2	1.63	0.64
1:N:165:ASP:OD1	2:N:507:HOH:O	2.15	0.64
1:P:133:TYR:OH	1:P:438:GLU:OE2	2.15	0.63
1:C:439:VAL:O	2:C:506:HOH:O	2.15	0.63
1:E:239:PHE:O	2:E:511:HOH:O	2.15	0.63
1:J:168:THR:HG22	1:J:201:ALA:HB3	1.79	0.63
1:A:168:THR:HG22	1:A:201:ALA:HB3	1.80	0.63
1:I:161:GLU:O	1:I:431:ASN:ND2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:PRO:HB3	2:C:517:HOH:O	1.99	0.63
1:K:10:ASP:O	1:K:380:LYS:NZ	2.26	0.63
1:G:197:LYS:NZ	2:G:506:HOH:O	2.04	0.63
1:C:168:THR:HG22	1:C:201:ALA:HB3	1.81	0.62
1:M:12:ILE:N	2:M:504:HOH:O	2.32	0.62
1:G:27:PHE:O	1:H:144:THR:OG1	2.17	0.62
1:L:278:VAL:HG22	1:L:368:VAL:HG11	1.80	0.62
1:C:264:ASN:N	1:C:264:ASN:OD1	2.33	0.62
1:K:264:ASN:ND2	2:K:513:HOH:O	2.31	0.62
1:L:216:GLN:HE22	1:L:257:THR:HA	1.64	0.62
1:M:101:PRO:HB3	2:M:547:HOH:O	2.00	0.62
1:A:331:LYS:HE3	1:A:334:VAL:HG21	1.81	0.61
1:F:133:TYR:OH	1:F:438:GLU:OE2	2.17	0.61
1:P:104:SER:N	2:P:502:HOH:O	2.33	0.61
1:L:356:CYS:SG	2:L:523:HOH:O	2.56	0.61
1:D:364:LEU:N	2:D:521:HOH:O	2.32	0.61
1:E:113:VAL:O	1:E:406:ARG:NE	2.32	0.61
1:O:278:VAL:HG22	1:O:368:VAL:HG11	1.82	0.61
1:E:296:PHE:O	2:E:512:HOH:O	2.16	0.61
1:H:132:LYS:NZ	1:H:444:GLN:O	2.30	0.61
1:H:208:TYR:OH	1:H:218:ARG:NH2	2.33	0.61
1:I:299:CYS:SG	2:I:589:HOH:O	2.56	0.61
1:H:414:VAL:HG21	1:H:420:THR:HG22	1.82	0.60
1:I:60:ASP:OD2	2:I:511:HOH:O	2.16	0.60
1:C:110:ILE:HB	1:C:113:VAL:HG22	1.83	0.60
1:L:266:TRP:O	2:L:507:HOH:O	2.16	0.60
1:C:438:GLU:OE2	1:C:441:TYR:N	2.20	0.60
1:K:262:PRO:HB2	2:K:513:HOH:O	2.00	0.60
1:E:251:LYS:NZ	2:E:521:HOH:O	2.33	0.60
1:G:110:ILE:HB	1:G:113:VAL:HG22	1.82	0.60
1:A:22:GLN:HG3	1:A:340:ILE:HG13	1.82	0.60
1:J:171:ALA:HA	1:J:175:LEU:HD13	1.85	0.59
1:L:84:ASP:OD1	1:L:84:ASP:N	2.35	0.59
1:G:247:ASN:OD1	1:G:270:LYS:NZ	2.34	0.59
1:I:345:GLU:OE1	2:I:510:HOH:O	2.16	0.59
1:O:37:ASN:OD1	1:O:37:ASN:N	2.36	0.59
1:H:264:ASN:OD1	1:H:264:ASN:N	2.34	0.59
1:I:54:ASN:O	2:I:513:HOH:O	2.17	0.59
1:M:46:GLN:OE1	1:M:146:ASN:ND2	2.35	0.59
1:F:174:THR:O	2:F:505:HOH:O	2.17	0.59
1:G:63:ILE:HD13	1:G:152:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLN:NE2	1:A:411:THR:O	2.27	0.59
1:G:253:ASN:OD1	1:G:257:THR:N	2.28	0.59
1:G:346:ILE:HG23	1:G:351:ILE:HB	1.85	0.59
1:I:206:ALA:O	2:I:512:HOH:O	2.16	0.59
1:L:134:ARG:HB3	1:L:137:LYS:HG3	1.85	0.59
1:O:100:ASN:HB2	2:O:527:HOH:O	2.01	0.59
1:A:330:ILE:HA	2:A:540:HOH:O	2.03	0.58
1:D:278:VAL:HG22	1:D:368:VAL:HG11	1.85	0.58
1:F:414:VAL:HG21	1:F:420:THR:HG22	1.84	0.58
1:N:370:ASN:HD21	1:N:372:ALA:HB3	1.67	0.58
1:J:59:LYS:HB2	1:J:63:ILE:HG13	1.86	0.58
1:P:335:LEU:HD22	1:P:364:LEU:HB2	1.85	0.58
1:J:78:CYS:HA	1:J:81:LYS:HD3	1.85	0.58
1:K:55:GLN:OE1	1:K:55:GLN:N	2.36	0.58
1:K:270:LYS:NZ	2:K:506:HOH:O	2.30	0.58
1:M:346:ILE:HG23	1:M:351:ILE:HB	1.85	0.58
1:O:71:ARG:NH1	2:O:519:HOH:O	2.36	0.58
1:B:230:ASN:HB3	1:B:235:SER:HB2	1.85	0.58
1:K:63:ILE:HG23	1:K:148:VAL:HG13	1.85	0.58
1:L:228:LYS:N	2:L:502:HOH:O	2.19	0.58
1:D:391:HIS:HB3	1:D:411:THR:HG22	1.84	0.58
1:L:318:SER:HA	2:L:513:HOH:O	2.03	0.58
1:M:168:THR:HG21	1:M:375:LEU:HD22	1.86	0.58
1:E:22:GLN:HG2	1:E:340:ILE:HG13	1.85	0.58
1:F:195:LEU:HD13	1:F:200:ILE:HB	1.85	0.58
1:O:100:ASN:OD1	1:O:102:GLN:NE2	2.36	0.58
1:G:41:LYS:HB3	2:G:517:HOH:O	2.04	0.58
1:N:274:ASP:N	1:N:274:ASP:OD1	2.16	0.58
1:C:383:LYS:NZ	2:C:516:HOH:O	2.31	0.57
1:D:77:ASN:OD1	2:D:511:HOH:O	2.17	0.57
1:I:278:VAL:HG22	1:I:368:VAL:HG11	1.86	0.57
1:K:156:GLN:NE2	1:K:411:THR:O	2.37	0.57
1:N:154:LEU:HD13	1:N:439:VAL:HG13	1.86	0.57
1:L:71:ARG:NH1	2:L:518:HOH:O	2.37	0.57
1:B:173:GLU:OE2	1:B:398:HIS:ND1	2.30	0.57
1:N:367:ASP:OD2	2:N:508:HOH:O	2.18	0.57
1:L:97:HIS:HA	2:L:504:HOH:O	2.03	0.57
1:M:442:GLU:HG3	2:M:508:HOH:O	2.03	0.57
1:K:133:TYR:OH	1:K:438:GLU:OE2	2.20	0.57
1:B:204:THR:HG22	1:B:206:ALA:H	1.68	0.57
1:B:278:VAL:HG22	1:B:368:VAL:HG11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:278:VAL:HG23	1:M:368:VAL:HG21	1.87	0.57
1:G:78:CYS:HA	1:G:81:LYS:HD2	1.85	0.57
1:J:230:ASN:HB3	1:J:235:SER:HB2	1.86	0.57
1:K:337:GLU:OE1	1:K:341:ARG:NE	2.38	0.57
1:L:71:ARG:NH2	2:L:517:HOH:O	2.36	0.57
1:B:134:ARG:HB3	1:B:137:LYS:HG3	1.86	0.57
1:K:165:ASP:O	1:K:199:ASN:ND2	2.37	0.57
1:K:95:ILE:HD12	1:K:119:LYS:HD2	1.87	0.57
1:J:329:MET:SD	2:J:550:HOH:O	2.58	0.56
1:L:100:ASN:C	2:L:504:HOH:O	2.44	0.56
1:L:315:LYS:HA	1:L:327:ASN:HA	1.86	0.56
1:E:15:ILE:HG22	1:E:404:PRO:HG2	1.86	0.56
1:H:275:TYR:O	1:H:279:GLN:HG2	2.04	0.56
1:D:157:ILE:HD11	1:D:412:LEU:HD11	1.87	0.56
1:L:269:TYR:N	2:L:507:HOH:O	2.11	0.56
1:F:306:GLU:OE2	2:F:506:HOH:O	2.18	0.56
1:H:194:LEU:O	1:H:198:MET:HG2	2.06	0.56
1:N:315:LYS:HA	1:N:327:ASN:HA	1.87	0.56
1:A:278:VAL:HG22	1:A:368:VAL:HG11	1.87	0.56
1:O:411:THR:HG21	2:O:523:HOH:O	2.06	0.56
1:J:180:HIS:O	1:J:218:ARG:NH2	2.32	0.55
1:L:336:GLU:HG2	1:L:359:ASN:HD22	1.72	0.55
1:E:216:GLN:HE21	1:E:258:LEU:H	1.55	0.55
1:I:31:SER:OG	2:I:503:HOH:O	1.96	0.55
1:N:396:PHE:HD2	2:N:520:HOH:O	1.89	0.55
1:P:389:CYS:O	2:P:508:HOH:O	2.18	0.55
1:F:293:ILE:HA	1:F:298:LEU:HB2	1.87	0.55
1:I:363:ASP:OD1	1:I:363:ASP:N	2.37	0.55
1:I:388:LYS:HZ3	1:I:388:LYS:HB3	1.70	0.55
1:C:52:SER:N	2:C:520:HOH:O	2.40	0.55
1:K:295:ASP:O	1:L:134:ARG:NH1	2.39	0.55
1:B:315:LYS:HA	1:B:327:ASN:HA	1.88	0.55
1:H:161:GLU:HA	2:H:527:HOH:O	2.07	0.55
1:C:398:HIS:CE1	1:C:403:PHE:HB3	2.42	0.55
1:I:289:LEU:HD22	1:I:311:LEU:HD22	1.88	0.55
1:P:184:ASP:HB3	1:P:187:LEU:HB3	1.87	0.55
1:B:112:ASP:O	1:B:406:ARG:NH2	2.40	0.55
1:C:27:PHE:O	1:D:144:THR:OG1	2.23	0.55
1:H:133:TYR:OH	1:H:438:GLU:OE2	2.16	0.54
1:M:30:LEU:O	1:M:36:MET:HG3	2.07	0.54
1:B:216:GLN:HE22	1:B:257:THR:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:ASN:ND2	2:A:508:HOH:O	2.20	0.54
1:J:398:HIS:O	1:J:398:HIS:ND1	2.40	0.54
1:K:168:THR:HG22	1:K:201:ALA:HB3	1.90	0.54
1:L:391:HIS:HB3	2:L:506:HOH:O	2.07	0.54
1:B:65:PHE:HE1	1:C:75:VAL:HG12	1.72	0.54
1:K:345:GLU:N	2:K:503:HOH:O	2.39	0.54
1:M:408:CYS:O	2:M:506:HOH:O	2.18	0.54
1:L:319:LEU:N	2:L:513:HOH:O	2.27	0.54
1:D:301:GLN:HA	2:D:520:HOH:O	2.06	0.54
1:E:385:GLN:NE2	2:E:527:HOH:O	2.41	0.54
1:D:243:GLY:N	1:D:248:TYR:O	2.33	0.54
1:B:146:ASN:O	1:B:150:HIS:ND1	2.41	0.54
1:E:93:MET:HG3	2:E:503:HOH:O	2.07	0.54
1:F:305:LYS:HE3	1:F:308:SER:HB3	1.89	0.54
1:G:20:SER:OG	1:G:355:TYR:OH	2.19	0.54
1:M:110:ILE:HB	1:M:113:VAL:HB	1.89	0.54
1:C:138:ARG:HH11	1:D:333:GLU:HB3	1.73	0.54
1:G:166:LEU:HB2	1:G:384:ILE:HD13	1.90	0.53
1:O:406:ARG:N	2:O:523:HOH:O	2.42	0.53
1:A:127:HIS:O	1:A:131:LYS:HG2	2.08	0.53
1:B:59:LYS:HD2	1:B:152:LEU:HD13	1.88	0.53
1:B:78:CYS:HA	1:B:81:LYS:HD2	1.89	0.53
1:G:362:GLN:N	2:G:524:HOH:O	2.33	0.53
1:I:15:ILE:HG23	1:I:404:PRO:HG2	1.90	0.53
1:H:236:TYR:O	2:H:511:HOH:O	2.18	0.53
1:H:241:VAL:HB	1:H:250:PHE:HB2	1.89	0.53
1:D:254:GLU:OE2	2:D:510:HOH:O	2.19	0.53
1:K:162:GLU:OE1	1:K:388:LYS:NZ	2.42	0.53
1:A:180:HIS:N	2:A:517:HOH:O	2.40	0.53
1:J:149:ARG:HD2	1:J:413:TRP:CG	2.44	0.53
1:G:140:TYR:HE2	1:H:341:ARG:HD3	1.74	0.53
1:F:304:ARG:HD2	1:F:309:ILE:HD12	1.92	0.52
1:F:84:ASP:HB3	1:F:88:LEU:HD23	1.90	0.52
1:P:59:LYS:NZ	2:P:516:HOH:O	2.41	0.52
1:F:91:GLU:HG3	1:F:122:ILE:HG22	1.91	0.52
1:G:379:GLN:OE1	1:G:386:LYS:NZ	2.41	0.52
1:J:427:ILE:HA	1:J:430:LEU:HG	1.91	0.52
1:P:92:GLU:OE1	2:P:509:HOH:O	2.19	0.52
1:M:139:LEU:O	1:P:105:ARG:NH2	2.32	0.52
1:D:236:TYR:OH	2:D:510:HOH:O	2.17	0.52
1:I:40:MET:HA	1:I:43:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:GLU:O	1:O:95:ILE:HG12	2.08	0.52
1:I:95:ILE:HD12	1:I:119:LYS:HB3	1.91	0.52
1:B:370:ASN:OD1	1:B:373:GLU:N	2.37	0.52
1:K:129:TYR:OH	1:L:331:LYS:NZ	2.41	0.52
1:M:373:GLU:OE1	2:M:507:HOH:O	2.19	0.52
1:N:278:VAL:HG22	1:N:368:VAL:HG11	1.91	0.52
1:A:391:HIS:HB3	1:A:411:THR:HG22	1.92	0.52
1:G:37:ASN:N	2:G:517:HOH:O	2.43	0.52
1:I:279:GLN:HG3	1:I:304:ARG:HH21	1.75	0.52
1:G:213:GLU:HA	1:G:216:GLN:HB3	1.91	0.51
1:G:9:PHE:N	2:G:530:HOH:O	2.43	0.51
1:H:92:GLU:OE2	2:H:512:HOH:O	2.19	0.51
1:N:345:GLU:HG2	2:N:540:HOH:O	2.09	0.51
1:D:274:ASP:OD1	1:D:274:ASP:N	2.43	0.51
1:F:291:LYS:HE3	1:F:341:ARG:HD3	1.91	0.51
1:F:402:ASP:OD1	1:F:403:PHE:N	2.40	0.51
1:N:173:GLU:HB3	1:N:394:ASP:HB3	1.91	0.51
1:A:37:ASN:OD1	1:A:37:ASN:N	2.44	0.51
1:C:247:ASN:ND2	2:C:524:HOH:O	2.44	0.51
1:D:228:LYS:HB2	1:D:229:HIS:CE1	2.45	0.51
1:P:172:ASP:OD1	2:P:510:HOH:O	2.19	0.51
1:E:93:MET:HE2	2:E:520:HOH:O	2.09	0.51
1:H:135:ILE:O	2:H:513:HOH:O	2.19	0.51
1:J:139:LEU:O	1:K:105:ARG:NH2	2.43	0.51
1:B:278:VAL:HG13	1:B:368:VAL:HG21	1.93	0.51
1:G:283:ASN:OD1	1:G:304:ARG:NH2	2.36	0.51
1:E:216:GLN:NE2	1:E:257:THR:HA	2.26	0.51
1:I:91:GLU:O	1:I:95:ILE:HG12	2.10	0.51
1:C:359:ASN:N	2:C:507:HOH:O	2.19	0.51
1:N:178:ASP:O	2:N:509:HOH:O	2.19	0.51
1:D:413:TRP:HA	2:D:519:HOH:O	2.11	0.50
1:K:216:GLN:HE22	1:K:257:THR:HG23	1.75	0.50
1:M:78:CYS:HA	1:M:81:LYS:HD2	1.92	0.50
1:N:307:LYS:NZ	2:N:513:HOH:O	2.28	0.50
1:D:208:TYR:HB2	1:D:215:TYR:CE1	2.46	0.50
1:I:439:VAL:HG22	2:I:509:HOH:O	2.11	0.50
1:J:169:PHE:HB3	1:J:175:LEU:HD11	1.93	0.50
1:C:339:VAL:HG22	1:C:364:LEU:HD21	1.94	0.50
1:D:280:GLU:HA	1:D:283:ASN:HB2	1.93	0.50
1:K:139:LEU:HG	1:L:341:ARG:HH21	1.76	0.50
1:L:432:ILE:HG22	1:L:435:PHE:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LYS:N	2:J:504:HOH:O	2.44	0.50
1:F:207:SER:O	1:F:207:SER:OG	2.26	0.50
1:F:296:PHE:HB2	1:F:298:LEU:HD13	1.94	0.50
1:G:288:CYS:SG	1:G:345:GLU:HG3	2.51	0.50
1:I:95:ILE:HG23	1:I:119:LYS:HD2	1.94	0.50
1:C:165:ASP:HB3	1:C:384:ILE:HD12	1.94	0.50
1:I:162:GLU:OE1	1:I:162:GLU:N	2.39	0.50
1:I:288:CYS:SG	1:I:345:GLU:HG3	2.51	0.50
1:C:441:TYR:HB3	1:C:444:GLN:HB2	1.93	0.50
1:I:244:GLY:N	2:I:512:HOH:O	2.35	0.50
1:I:174:THR:HG21	1:I:392:ILE:HG22	1.94	0.50
1:L:170:ASP:O	1:L:174:THR:HG22	2.11	0.50
1:I:228:LYS:HB2	1:I:229:HIS:CE1	2.45	0.50
1:H:60:ASP:N	2:H:528:HOH:O	2.45	0.50
1:I:180:HIS:O	1:I:218:ARG:NH2	2.40	0.50
1:D:149:ARG:HD2	1:D:413:TRP:CG	2.47	0.49
1:K:184:ASP:OD2	1:K:421:LYS:NZ	2.45	0.49
1:O:47:TRP:HZ2	1:P:333:GLU:HG3	1.77	0.49
1:M:133:TYR:HB3	1:N:331:LYS:NZ	2.26	0.49
1:E:42:LYS:N	2:E:530:HOH:O	2.46	0.49
1:L:389:CYS:SG	2:L:535:HOH:O	2.59	0.49
1:M:331:LYS:NZ	1:N:147:GLU:OE2	2.39	0.49
1:O:442:GLU:HB2	2:O:505:HOH:O	2.11	0.49
1:B:205:ALA:HA	1:B:245:GLU:HG2	1.93	0.49
1:D:95:ILE:HG23	1:D:119:LYS:HD3	1.95	0.49
1:I:386:LYS:NZ	1:I:408:CYS:O	2.43	0.49
1:M:15:ILE:HD12	1:M:376:LEU:HD11	1.93	0.49
1:O:403:PHE:HE1	2:O:523:HOH:O	1.94	0.49
1:L:227:SER:N	2:L:502:HOH:O	2.45	0.49
1:P:270:LYS:NZ	1:P:373:GLU:OE2	2.41	0.49
1:E:278:VAL:HG13	1:E:368:VAL:HG11	1.94	0.49
1:H:91:GLU:HG3	1:H:122:ILE:HG22	1.94	0.49
1:K:12:ILE:HD13	1:K:373:GLU:HB2	1.94	0.49
1:L:150:HIS:CE1	1:L:440:LEU:HD13	2.47	0.49
1:M:61:SER:N	2:M:519:HOH:O	2.39	0.49
1:B:65:PHE:CE1	1:C:75:VAL:HG12	2.46	0.49
1:C:333:GLU:OE2	2:C:508:HOH:O	2.19	0.49
1:F:335:LEU:HD22	1:F:364:LEU:HB2	1.95	0.49
1:H:168:THR:HA	1:H:201:ALA:O	2.13	0.49
1:I:346:ILE:HG23	1:I:351:ILE:HB	1.93	0.49
1:J:271:LYS:NZ	2:J:512:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:186:VAL:HG13	1:P:421:LYS:HE2	1.95	0.49
1:F:386:LYS:NZ	2:F:522:HOH:O	2.44	0.49
1:H:208:TYR:HB2	1:H:215:TYR:CE2	2.47	0.49
1:I:289:LEU:HD13	1:I:311:LEU:HB2	1.93	0.49
1:I:306:GLU:HG2	1:I:307:LYS:HG3	1.95	0.49
1:L:263:GLU:O	1:L:267:ARG:N	2.46	0.49
1:O:184:ASP:OD2	1:O:421:LYS:NZ	2.46	0.49
1:I:29:THR:OG1	1:J:146:ASN:ND2	2.45	0.48
1:K:91:GLU:O	1:K:95:ILE:HG12	2.13	0.48
1:B:98:TYR:OH	1:N:290:GLU:OE2	2.23	0.48
1:M:15:ILE:HG12	1:M:407:PHE:HB3	1.95	0.48
1:A:404:PRO:O	2:A:507:HOH:O	2.20	0.48
1:E:138:ARG:HD2	1:F:337:GLU:HB2	1.95	0.48
1:J:289:LEU:HD13	1:J:311:LEU:HB2	1.95	0.48
1:M:125:ALA:HB1	1:M:154:LEU:HB3	1.95	0.48
1:C:193:CYS:O	1:C:197:LYS:NZ	2.46	0.48
1:G:425:LYS:HB2	2:G:510:HOH:O	2.13	0.48
1:K:216:GLN:HG3	1:K:223:LEU:HD13	1.94	0.48
1:M:275:TYR:O	1:M:279:GLN:HG2	2.13	0.48
1:O:80:ASP:CG	2:O:504:HOH:O	2.47	0.48
1:F:192:SER:HB2	1:F:230:ASN:ND2	2.29	0.48
1:M:63:ILE:HG12	1:M:152:LEU:HD12	1.94	0.48
1:N:313:PRO:HG3	2:N:518:HOH:O	2.14	0.48
1:L:165:ASP:O	1:L:199:ASN:ND2	2.46	0.48
1:O:246:SER:O	1:O:270:LYS:NZ	2.32	0.48
1:O:34:ASN:O	1:P:416:ASN:ND2	2.47	0.48
1:A:208:TYR:O	1:A:211:ASP:HB2	2.13	0.48
1:C:244:GLY:O	1:C:247:ASN:ND2	2.44	0.48
1:D:275:TYR:OH	2:D:501:HOH:O	1.87	0.48
1:L:230:ASN:HB3	1:L:235:SER:HB2	1.94	0.48
1:E:352:THR:HG22	2:E:533:HOH:O	2.14	0.48
1:L:178:ASP:C	2:L:510:HOH:O	2.52	0.48
1:A:27:PHE:CZ	1:B:71:ARG:HG3	2.49	0.47
1:F:195:LEU:HG	1:F:235:SER:HB2	1.96	0.47
1:K:9:PHE:HA	1:K:14:ASP:HB2	1.95	0.47
1:C:15:ILE:HD12	1:C:376:LEU:HD11	1.96	0.47
1:F:195:LEU:HA	1:F:200:ILE:HD13	1.96	0.47
1:H:387:LYS:N	1:H:387:LYS:HD2	2.25	0.47
1:I:147:GLU:OE1	1:J:331:LYS:NZ	2.42	0.47
1:M:175:LEU:HD11	1:M:202:ILE:HD12	1.96	0.47
1:N:100:ASN:O	1:N:104:SER:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:134:ARG:NH1	1:P:295:ASP:O	2.46	0.47
1:O:389:CYS:O	2:O:510:HOH:O	2.20	0.47
1:D:233:ASP:OD1	1:D:233:ASP:N	2.46	0.47
1:E:346:ILE:HG23	1:E:351:ILE:HB	1.96	0.47
1:G:146:ASN:ND2	2:G:520:HOH:O	2.28	0.47
1:M:39:ASP:HA	1:M:42:LYS:HD2	1.97	0.47
1:N:110:ILE:HB	1:N:113:VAL:HB	1.96	0.47
1:H:444:GLN:O	2:H:508:HOH:O	2.20	0.47
1:N:224:LYS:O	1:N:227:SER:OG	2.31	0.47
1:E:343:LYS:NZ	2:E:519:HOH:O	2.48	0.47
1:G:306:GLU:H	1:G:306:GLU:CD	2.18	0.47
1:G:331:LYS:HD2	1:H:133:TYR:CD1	2.50	0.47
1:H:165:ASP:OD1	2:H:515:HOH:O	2.21	0.47
1:H:372:ALA:HA	1:H:375:LEU:HD12	1.96	0.47
1:I:42:LYS:HA	1:I:45:VAL:HG22	1.96	0.47
1:K:59:LYS:HZ3	1:K:396:PHE:HA	1.79	0.47
1:L:168:THR:OG1	1:L:391:HIS:HB2	2.15	0.47
1:D:91:GLU:O	1:D:95:ILE:HG12	2.15	0.47
1:L:398:HIS:O	1:L:398:HIS:ND1	2.48	0.47
1:C:55:GLN:N	1:C:55:GLN:OE1	2.48	0.47
1:C:295:ASP:O	1:D:134:ARG:HD2	2.15	0.47
1:G:442:GLU:HG3	2:G:510:HOH:O	2.13	0.47
1:P:168:THR:OG1	1:P:391:HIS:ND1	2.37	0.47
1:P:149:ARG:HD2	1:P:413:TRP:CG	2.50	0.47
1:A:117:PHE:CZ	1:A:386:LYS:HD3	2.50	0.47
1:A:59:LYS:HE3	1:A:396:PHE:HA	1.97	0.47
1:A:91:GLU:O	1:A:95:ILE:HG12	2.15	0.47
1:C:173:GLU:OE1	2:C:509:HOH:O	2.20	0.47
1:A:339:VAL:O	1:A:343:LYS:HG3	2.15	0.47
1:K:138:ARG:NH1	1:K:141:ALA:O	2.46	0.47
1:H:265:GLU:N	1:H:265:GLU:OE2	2.48	0.46
1:L:317:PRO:HA	1:L:325:GLN:HA	1.97	0.46
1:M:230:ASN:HB3	1:M:235:SER:HB2	1.96	0.46
1:I:254:GLU:OE1	1:I:254:GLU:N	2.47	0.46
1:I:43:ASN:HB3	1:J:332:TYR:CZ	2.50	0.46
1:O:172:ASP:OD2	1:O:371:LYS:NZ	2.48	0.46
1:D:385:GLN:HG3	1:D:387:LYS:H	1.80	0.46
1:K:65:PHE:CG	1:K:110:ILE:HD11	2.50	0.46
1:K:192:SER:OG	1:K:230:ASN:OD1	2.22	0.46
1:O:214:LYS:HA	2:O:502:HOH:O	2.16	0.46
1:N:76:SER:HB3	1:O:69:ILE:HD13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:98:TYR:O	2:H:514:HOH:O	2.20	0.46
1:K:143:PRO:HA	1:K:147:GLU:OE2	2.16	0.46
1:M:289:LEU:HB2	1:M:302:ILE:HD11	1.97	0.46
1:N:284:ILE:HD11	1:N:345:GLU:HB3	1.97	0.46
1:C:278:VAL:HG22	1:C:368:VAL:HG11	1.98	0.46
1:C:78:CYS:HA	1:C:81:LYS:HD2	1.97	0.46
1:I:23:ASP:OD2	2:I:514:HOH:O	2.20	0.46
1:K:133:TYR:CD1	1:L:331:LYS:HD2	2.50	0.46
1:M:418:GLN:OE1	2:M:508:HOH:O	2.20	0.46
1:L:64:MET:O	1:L:68:GLU:HG3	2.16	0.46
1:G:184:ASP:OD1	1:G:421:LYS:NZ	2.48	0.46
1:J:374:GLY:HA2	1:J:377:ILE:HD12	1.97	0.46
1:M:299:CYS:HB3	1:M:328:TYR:CG	2.49	0.46
1:M:41:LYS:HE3	1:N:397:LEU:HD21	1.98	0.46
1:O:65:PHE:CG	1:O:110:ILE:HD11	2.50	0.46
1:O:80:ASP:OD2	1:O:137:LYS:NZ	2.48	0.46
1:O:156:GLN:HB3	1:O:410:LEU:HD21	1.97	0.46
1:P:212:ALA:HB1	1:P:258:LEU:HB3	1.98	0.46
1:C:184:ASP:HB3	1:C:187:LEU:HB3	1.97	0.46
1:J:274:ASP:HB3	1:J:277:THR:HG23	1.97	0.46
1:M:42:LYS:O	1:M:46:GLN:HG3	2.15	0.46
1:D:285:SER:HA	1:D:342:ILE:HD12	1.98	0.46
1:G:298:LEU:HD11	1:G:334:VAL:HG11	1.98	0.46
1:J:404:PRO:HB2	1:J:406:ARG:HG2	1.98	0.46
1:L:316:ILE:N	1:L:326:LYS:O	2.41	0.46
1:O:184:ASP:HB3	1:O:187:LEU:HB3	1.98	0.46
1:O:216:GLN:HE22	1:O:257:THR:HG23	1.81	0.46
1:F:241:VAL:HG13	1:F:250:PHE:HB2	1.98	0.46
1:N:115:ILE:N	2:N:517:HOH:O	2.37	0.46
1:P:91:GLU:O	1:P:95:ILE:HG12	2.15	0.46
1:B:274:ASP:OD1	1:B:274:ASP:N	2.49	0.45
1:I:333:GLU:OE2	2:I:515:HOH:O	2.21	0.45
1:M:63:ILE:O	1:M:67:VAL:HG23	2.16	0.45
1:P:73:LEU:HB2	1:P:79:ILE:HD13	1.98	0.45
1:A:23:ASP:OD2	1:A:399:SER:OG	2.26	0.45
1:C:147:GLU:OE1	1:D:331:LYS:NZ	2.43	0.45
1:C:388:LYS:HE2	1:C:388:LYS:HB3	1.78	0.45
1:D:228:LYS:HE3	1:D:229:HIS:HE1	1.81	0.45
1:C:199:ASN:HA	1:C:238:ASN:HB3	1.98	0.45
1:E:243:GLY:N	1:E:248:TYR:O	2.47	0.45
1:K:391:HIS:HB3	1:K:411:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:LEU:O	1:C:339:VAL:HG23	2.16	0.45
1:E:216:GLN:NE2	1:E:223:LEU:HD13	2.31	0.45
1:J:170:ASP:O	1:J:174:THR:OG1	2.31	0.45
1:K:404:PRO:HB2	1:K:407:PHE:CD2	2.51	0.45
1:L:172:ASP:O	1:L:177:PRO:HA	2.16	0.45
1:M:72:SER:O	1:M:76:SER:OG	2.25	0.45
1:L:77:ASN:OD1	2:L:509:HOH:O	2.20	0.45
1:L:78:CYS:HA	1:L:81:LYS:HD2	1.98	0.45
1:O:174:THR:HG21	1:O:392:ILE:HG22	1.98	0.45
1:A:437:PRO:O	2:A:509:HOH:O	2.20	0.45
1:C:156:GLN:NE2	1:C:411:THR:O	2.46	0.45
1:C:35:VAL:HG13	1:D:415:SER:HB2	1.99	0.45
1:K:287:LYS:HD3	1:K:287:LYS:HA	1.81	0.45
1:N:59:LYS:N	2:N:525:HOH:O	2.49	0.45
1:C:138:ARG:HH22	1:C:143:PRO:HA	1.82	0.45
1:D:338:ALA:O	1:D:342:ILE:HG12	2.16	0.45
1:G:46:GLN:NE2	1:G:146:ASN:OD1	2.49	0.45
1:M:252:CYS:SG	1:M:256:ALA:HA	2.57	0.45
1:M:376:LEU:HD23	2:M:506:HOH:O	2.17	0.45
1:P:216:GLN:NE2	1:P:257:THR:HA	2.29	0.45
1:B:209:ASN:HA	1:B:248:TYR:CZ	2.52	0.45
1:B:243:GLY:N	1:B:248:TYR:O	2.49	0.45
1:F:81:LYS:NZ	2:F:512:HOH:O	2.27	0.45
1:L:262:PRO:HG2	1:L:265:GLU:HG3	1.99	0.45
1:M:171:ALA:HA	1:M:175:LEU:HG	1.99	0.45
1:B:168:THR:HG21	1:B:375:LEU:HD22	1.98	0.45
1:G:246:SER:OG	2:G:513:HOH:O	2.20	0.45
1:N:107:LYS:NZ	1:N:111:ASP:O	2.50	0.45
1:P:143:PRO:HA	1:P:147:GLU:OE1	2.17	0.45
1:P:282:LEU:HD22	1:P:309:ILE:HG22	1.99	0.45
1:A:269:TYR:HB3	1:A:380:LYS:HD2	1.99	0.45
1:A:38:SER:HB2	1:A:41:LYS:HG3	1.99	0.45
1:C:18:GLY:O	1:C:401:ASN:HB3	2.16	0.45
1:E:274:ASP:N	2:E:510:HOH:O	2.15	0.45
1:H:168:THR:HG22	1:H:201:ALA:HB3	1.98	0.45
1:M:237:LYS:NZ	1:M:259:TYR:OH	2.50	0.45
1:A:133:TYR:OH	1:A:438:GLU:OE1	2.33	0.44
1:L:167:LEU:HB3	1:L:200:ILE:HD13	1.99	0.44
1:O:15:ILE:HG23	1:O:404:PRO:HG2	1.99	0.44
1:O:35:VAL:HG11	1:P:146:ASN:HD21	1.82	0.44
1:F:311:LEU:HB3	1:F:364:LEU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:17:LEU:HD11	1:G:370:ASN:HD22	1.82	0.44
1:G:71:ARG:HE	1:G:71:ARG:HB3	1.65	0.44
1:K:331:LYS:HB2	1:K:334:VAL:HG23	1.98	0.44
1:H:432:ILE:O	2:H:516:HOH:O	2.21	0.44
1:J:154:LEU:HD13	1:J:439:VAL:HG13	1.98	0.44
1:L:228:LYS:HB2	1:L:229:HIS:CE1	2.52	0.44
1:G:77:ASN:OD1	2:G:514:HOH:O	2.21	0.44
1:I:134:ARG:NH1	2:I:534:HOH:O	2.49	0.44
1:K:156:GLN:HB3	1:K:410:LEU:HD11	1.99	0.44
1:K:339:VAL:HG12	1:K:343:LYS:HE2	2.00	0.44
1:N:59:LYS:O	1:N:63:ILE:N	2.38	0.44
1:O:63:ILE:HG12	1:O:152:LEU:HD12	1.99	0.44
1:A:75:VAL:HG22	1:D:109:LEU:HD22	1.99	0.44
1:M:296:PHE:HA	1:N:134:ARG:HD2	1.98	0.44
1:D:221:ASN:HB2	2:D:509:HOH:O	2.16	0.44
1:F:336:GLU:O	1:F:340:ILE:HG13	2.18	0.44
1:P:263:GLU:O	1:P:267:ARG:N	2.50	0.44
1:B:77:ASN:HB2	1:C:93:MET:SD	2.58	0.44
1:C:391:HIS:HD2	1:C:411:THR:HG23	1.83	0.44
1:E:110:ILE:HB	1:E:113:VAL:HB	1.99	0.44
1:G:93:MET:HG2	1:G:106:LEU:HB2	1.99	0.44
1:F:380:LYS:HD3	1:J:275:TYR:CE1	2.53	0.44
1:K:335:LEU:HD22	1:K:364:LEU:HB3	2.00	0.44
1:N:166:LEU:HB2	1:N:384:ILE:HD13	1.99	0.44
1:O:101:PRO:HB3	2:O:537:HOH:O	2.16	0.44
1:O:168:THR:HG22	1:O:201:ALA:HB3	1.99	0.44
1:A:65:PHE:CG	1:A:110:ILE:HD11	2.53	0.44
1:B:414:VAL:HG11	1:B:420:THR:OG1	2.18	0.44
1:F:251:LYS:NZ	1:F:259:TYR:OH	2.26	0.44
1:L:423:CYS:O	1:L:427:ILE:HG13	2.17	0.44
1:N:283:ASN:OD1	1:N:304:ARG:NH2	2.37	0.44
1:P:59:LYS:HE3	1:P:59:LYS:HB2	1.56	0.44
1:C:315:LYS:HA	1:C:327:ASN:HA	2.00	0.44
1:F:380:LYS:O	1:F:380:LYS:HD2	2.17	0.44
1:H:101:PRO:HB3	2:H:505:HOH:O	2.18	0.44
1:J:315:LYS:HA	1:J:327:ASN:HA	2.00	0.44
1:O:208:TYR:HB2	1:O:215:TYR:CE1	2.52	0.44
1:A:19:SER:O	1:A:343:LYS:HD2	2.18	0.43
1:C:240:TYR:CE2	1:C:251:LYS:HE2	2.53	0.43
1:G:278:VAL:HG13	1:G:368:VAL:HG21	1.99	0.43
1:I:335:LEU:HD22	1:I:364:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:89:SER:HB3	1:L:76:SER:O	2.18	0.43
1:P:173:GLU:HA	1:P:177:PRO:HB3	2.00	0.43
1:A:210:ASN:O	2:A:511:HOH:O	2.21	0.43
1:B:398:HIS:HB3	2:B:504:HOH:O	2.18	0.43
1:D:167:LEU:HB2	1:D:198:MET:HE2	2.00	0.43
1:E:34:ASN:HA	2:E:532:HOH:O	2.18	0.43
1:N:208:TYR:HB2	1:N:215:TYR:CE1	2.52	0.43
1:C:333:GLU:OE1	2:C:510:HOH:O	2.21	0.43
1:F:61:SER:OG	1:F:112:ASP:OD2	2.31	0.43
1:L:266:TRP:C	2:L:507:HOH:O	2.55	0.43
1:M:287:LYS:HD3	1:M:287:LYS:HA	1.82	0.43
1:B:59:LYS:NZ	1:B:153:ASN:OD1	2.52	0.43
1:F:62:LEU:O	1:F:65:PHE:HB3	2.18	0.43
1:H:311:LEU:HB3	1:H:364:LEU:HB3	2.00	0.43
1:N:78:CYS:HA	1:N:81:LYS:HD2	2.00	0.43
1:P:208:TYR:HB2	1:P:215:TYR:CE1	2.53	0.43
1:A:436:ILE:O	2:A:510:HOH:O	2.20	0.43
1:B:417:PRO:O	1:B:421:LYS:HG3	2.18	0.43
1:C:167:LEU:HB2	1:C:198:MET:SD	2.59	0.43
1:C:430:LEU:O	1:C:431:ASN:HB3	2.19	0.43
1:I:184:ASP:HB3	1:I:187:LEU:HB3	2.00	0.43
1:I:197:LYS:NZ	2:I:508:HOH:O	2.12	0.43
1:L:212:ALA:HB1	1:L:258:LEU:HB2	2.01	0.43
1:N:289:LEU:HD22	1:N:311:LEU:HD22	2.00	0.43
1:O:165:ASP:OD1	2:O:511:HOH:O	2.21	0.43
1:P:194:LEU:HD21	1:P:428:MET:HG2	1.99	0.43
1:C:231:ILE:HG23	1:C:254:GLU:HG2	2.00	0.43
1:K:251:LYS:HE2	1:K:251:LYS:HB3	1.92	0.43
1:H:193:CYS:O	1:H:196:LYS:HG2	2.17	0.43
1:I:149:ARG:HD2	1:I:413:TRP:CG	2.54	0.43
1:J:203:VAL:HG12	1:J:242:MET:HB3	2.00	0.43
1:J:289:LEU:HD22	1:J:311:LEU:HD22	1.99	0.43
1:O:35:VAL:HG11	1:P:146:ASN:ND2	2.34	0.43
1:K:354:PRO:HB2	2:K:520:HOH:O	2.19	0.43
1:M:358:PHE:HA	2:M:545:HOH:O	2.17	0.43
1:B:364:LEU:HD23	1:B:365:TRP:N	2.34	0.43
1:H:100:ASN:O	1:H:104:SER:HB3	2.19	0.43
1:P:278:VAL:O	1:P:282:LEU:HG	2.18	0.43
1:E:306:GLU:HG2	1:E:307:LYS:HG3	2.01	0.43
1:H:425:LYS:HE2	1:H:435:PHE:HE1	1.83	0.43
1:H:154:LEU:HD11	1:H:437:PRO:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:GLN:HE22	1:C:257:THR:HA	1.84	0.42
1:G:278:VAL:HG22	1:G:368:VAL:HG11	2.01	0.42
1:O:395:GLN:HA	1:O:398:HIS:CD2	2.54	0.42
1:C:20:SER:OG	1:C:355:TYR:OH	2.17	0.42
1:D:100:ASN:O	1:D:104:SER:HB3	2.19	0.42
1:G:228:LYS:HG3	1:G:229:HIS:ND1	2.34	0.42
1:J:208:TYR:CD2	1:J:214:LYS:HB3	2.54	0.42
1:J:265:GLU:OE2	1:J:265:GLU:N	2.52	0.42
1:J:293:ILE:HG23	1:J:298:LEU:HB2	2.01	0.42
1:K:304:ARG:HG3	1:K:309:ILE:HD12	2.01	0.42
1:L:263:GLU:HB3	1:L:267:ARG:HD3	2.01	0.42
1:P:63:ILE:HG12	1:P:152:LEU:HD12	1.99	0.42
2:A:528:HOH:O	1:B:137:LYS:HE3	2.18	0.42
1:C:332:TYR:O	1:C:336:GLU:HG2	2.19	0.42
1:D:184:ASP:HB3	1:D:187:LEU:HB3	2.00	0.42
1:L:222:LEU:HD23	1:L:222:LEU:H	1.84	0.42
1:N:269:TYR:HE2	1:N:381:LEU:HD12	1.83	0.42
1:B:76:SER:OG	1:B:78:CYS:SG	2.69	0.42
1:C:138:ARG:NH1	1:D:333:GLU:HB3	2.34	0.42
1:H:172:ASP:OD2	1:H:371:LYS:NZ	2.42	0.42
1:H:379:GLN:OE1	1:H:386:LYS:HG2	2.19	0.42
1:J:105:ARG:NH2	1:K:139:LEU:O	2.45	0.42
1:N:407:PHE:HA	2:N:517:HOH:O	2.19	0.42
1:N:99:TYR:OH	1:N:119:LYS:NZ	2.50	0.42
1:B:72:SER:HA	1:B:75:VAL:HG22	2.01	0.42
1:F:263:GLU:HG2	1:F:267:ARG:HB2	2.02	0.42
1:I:294:LYS:HB3	1:I:294:LYS:HE2	1.69	0.42
1:I:165:ASP:CG	1:I:388:LYS:HZ2	2.23	0.42
1:L:283:ASN:OD1	1:L:304:ARG:NH2	2.37	0.42
1:M:93:MET:SD	1:P:77:ASN:HB2	2.59	0.42
1:A:15:ILE:HD12	1:A:407:PHE:HB3	2.02	0.42
1:A:331:LYS:HD3	1:B:133:TYR:CD1	2.54	0.42
1:C:65:PHE:CG	1:C:110:ILE:HD11	2.55	0.42
1:E:134:ARG:NH1	2:E:540:HOH:O	2.52	0.42
1:G:263:GLU:HG2	1:G:267:ARG:HB2	2.01	0.42
1:H:227:SER:HB3	1:H:256:ALA:HB2	2.01	0.42
1:K:63:ILE:HG12	1:K:152:LEU:HD12	2.02	0.42
1:L:269:TYR:CE2	1:L:381:LEU:HA	2.54	0.42
1:M:216:GLN:HE22	1:M:257:THR:HA	1.85	0.42
1:E:158:LEU:HD21	1:E:437:PRO:HG2	2.01	0.42
1:E:54:ASN:OD1	1:E:54:ASN:N	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:ILE:HG12	1:L:152:LEU:HD12	2.02	0.42
1:L:180:HIS:CG	2:L:510:HOH:O	2.71	0.42
1:O:438:GLU:HG2	1:O:441:TYR:O	2.20	0.42
1:B:224:LYS:HA	1:B:224:LYS:HD3	1.75	0.42
1:E:442:GLU:O	1:E:443:ASN:C	2.58	0.42
1:F:75:VAL:HG23	1:G:109:LEU:HD22	2.02	0.42
1:G:167:LEU:HB3	1:G:200:ILE:HD13	2.02	0.42
1:J:311:LEU:HB3	1:J:364:LEU:HB3	2.01	0.42
1:N:335:LEU:HD22	1:N:364:LEU:HB2	2.01	0.42
1:A:398:HIS:CE1	1:A:403:PHE:HB3	2.55	0.42
1:C:39:ASP:O	1:C:42:LYS:N	2.53	0.42
1:E:273:VAL:HA	2:E:510:HOH:O	2.20	0.42
1:I:170:ASP:O	1:I:174:THR:OG1	2.33	0.42
1:K:278:VAL:HG13	1:K:368:VAL:HG21	2.02	0.42
1:O:331:LYS:HD2	1:P:133:TYR:CD1	2.54	0.42
1:P:146:ASN:HD22	1:P:149:ARG:HH21	1.66	0.42
1:C:419:GLU:HG2	1:C:440:LEU:HA	2.01	0.42
1:E:27:PHE:CZ	1:F:71:ARG:HG3	2.54	0.42
1:H:119:LYS:NZ	2:H:523:HOH:O	2.40	0.42
1:H:343:LYS:HA	1:H:355:TYR:OH	2.20	0.42
1:I:19:SER:OG	2:I:502:HOH:O	2.22	0.42
1:O:252:CYS:SG	1:O:256:ALA:HA	2.59	0.42
1:D:208:TYR:HB3	1:D:214:LYS:HD3	2.02	0.41
1:D:343:LYS:HA	1:D:355:TYR:OH	2.20	0.41
1:E:263:GLU:N	1:E:263:GLU:OE1	2.43	0.41
1:E:55:GLN:O	1:E:59:LYS:HG3	2.19	0.41
1:F:263:GLU:HA	1:F:266:TRP:NE1	2.35	0.41
1:H:432:ILE:HG22	1:H:434:SER:H	1.83	0.41
1:J:152:LEU:O	1:J:156:GLN:HG3	2.20	0.41
1:J:167:LEU:HB3	1:J:200:ILE:HD13	2.01	0.41
1:E:208:TYR:HB2	1:E:215:TYR:CE2	2.54	0.41
1:F:355:TYR:OH	2:F:507:HOH:O	2.22	0.41
1:F:150:HIS:CE1	1:F:440:LEU:HD13	2.56	0.41
1:H:288:CYS:O	1:H:292:VAL:HG23	2.20	0.41
1:L:165:ASP:HB3	1:L:384:ILE:HD12	2.00	0.41
1:M:379:GLN:CD	2:M:506:HOH:O	2.57	0.41
1:N:245:GLU:HG2	1:N:371:LYS:HG2	2.02	0.41
1:N:416:ASN:OD1	1:N:418:GLN:HG2	2.19	0.41
1:D:135:ILE:O	2:D:513:HOH:O	2.22	0.41
1:E:171:ALA:HB2	1:E:202:ILE:HG23	2.02	0.41
1:G:41:LYS:HB2	1:G:41:LYS:HE3	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:270:LYS:NZ	2:L:516:HOH:O	2.35	0.41
1:L:304:ARG:HD2	1:L:309:ILE:HD12	2.02	0.41
1:J:252:CYS:SG	1:J:256:ALA:HA	2.60	0.41
1:O:331:LYS:NZ	1:P:147:GLU:OE2	2.43	0.41
1:B:70:PHE:CD1	1:B:70:PHE:N	2.88	0.41
1:B:76:SER:O	1:C:89:SER:OG	2.32	0.41
1:F:356:CYS:SG	1:F:367:ASP:HB2	2.60	0.41
1:I:209:ASN:HA	1:I:248:TYR:CZ	2.56	0.41
1:I:246:SER:OG	2:I:507:HOH:O	2.11	0.41
1:I:15:ILE:HG12	1:I:407:PHE:HB3	2.01	0.41
1:K:15:ILE:HD12	1:K:376:LEU:HD11	2.02	0.41
1:N:254:GLU:N	1:N:254:GLU:OE2	2.49	0.41
1:P:171:ALA:HB2	1:P:202:ILE:HG23	2.02	0.41
1:B:84:ASP:N	1:B:84:ASP:OD1	2.53	0.41
1:C:167:LEU:HD22	1:C:169:PHE:CE1	2.55	0.41
1:C:175:LEU:HD11	1:C:202:ILE:HD12	2.02	0.41
1:C:156:GLN:HB3	1:C:410:LEU:HD13	2.02	0.41
1:F:182:PHE:HE2	1:F:188:ALA:HB2	1.84	0.41
1:M:202:ILE:HB	1:M:241:VAL:HG22	2.02	0.41
1:O:25:TYR:CE2	1:P:142:PRO:HD2	2.55	0.41
1:O:433:LYS:H	1:O:433:LYS:HG3	1.57	0.41
1:C:184:ASP:OD2	1:C:421:LYS:HE3	2.21	0.41
1:H:387:LYS:HD3	2:H:509:HOH:O	2.21	0.41
1:I:234:GLY:HA2	1:I:236:TYR:CE1	2.55	0.41
1:J:208:TYR:HB2	1:J:215:TYR:CE1	2.55	0.41
1:J:82:ASN:ND2	1:J:84:ASP:OD2	2.53	0.41
1:M:57:LYS:HB2	1:M:64:MET:HG2	2.03	0.41
1:N:83:ILE:N	2:N:526:HOH:O	2.53	0.41
1:B:374:GLY:O	1:B:378:LEU:HG	2.21	0.41
1:E:344:LYS:HA	1:E:344:LYS:HD3	1.89	0.41
1:E:331:LYS:HE2	1:F:133:TYR:CD1	2.56	0.41
1:I:93:MET:SD	1:I:105:ARG:HG2	2.60	0.41
1:K:303:GLN:HG3	2:K:517:HOH:O	2.20	0.41
1:K:44:ILE:HG23	1:L:399:SER:HB2	2.03	0.41
1:L:168:THR:OG1	1:L:391:HIS:ND1	2.46	0.41
1:M:220:GLU:HB3	2:M:509:HOH:O	2.19	0.41
1:F:402:ASP:O	1:F:404:PRO:HD3	2.20	0.41
1:G:100:ASN:O	1:G:104:SER:HB3	2.21	0.41
1:I:208:TYR:HB2	1:I:215:TYR:CE1	2.55	0.41
1:K:59:LYS:HZ2	1:K:396:PHE:HD1	1.67	0.41
1:L:102:GLN:H	1:L:102:GLN:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:138:ARG:HD2	1:N:337:GLU:HB2	2.01	0.41
1:C:193:CYS:HB3	1:C:428:MET:HE1	2.03	0.41
1:G:171:ALA:HB2	1:G:202:ILE:HG23	2.02	0.41
1:K:138:ARG:NH2	1:K:147:GLU:OE1	2.54	0.41
1:L:171:ALA:HB2	1:L:202:ILE:HG23	2.02	0.41
1:N:59:LYS:NZ	1:N:153:ASN:OD1	2.54	0.41
1:C:336:GLU:OE1	1:C:359:ASN:ND2	2.54	0.41
1:E:228:LYS:HB2	1:E:229:HIS:CE1	2.56	0.41
1:E:117:PHE:CE1	1:E:386:LYS:HD3	2.56	0.41
1:F:350:LYS:HE2	1:F:350:LYS:HB2	1.70	0.41
1:G:65:PHE:CG	1:G:110:ILE:HD11	2.55	0.41
1:O:316:ILE:HA	1:O:317:PRO:HD3	1.93	0.41
1:O:315:LYS:HA	1:O:327:ASN:HA	2.03	0.41
1:A:304:ARG:HD2	1:A:309:ILE:HD12	2.03	0.40
1:D:296:PHE:HB2	1:D:298:LEU:HD13	2.02	0.40
1:E:170:ASP:O	1:E:174:THR:HG22	2.21	0.40
1:E:168:THR:HG23	1:E:391:HIS:HA	2.03	0.40
1:F:79:ILE:HG13	1:F:136:THR:HG22	2.03	0.40
1:G:361:GLY:HA3	2:G:524:HOH:O	2.20	0.40
1:L:80:ASP:OD1	1:L:137:LYS:NZ	2.51	0.40
1:A:208:TYR:HB2	1:A:215:TYR:CE1	2.56	0.40
1:E:347:ILE:HA	1:E:347:ILE:HD13	1.86	0.40
1:I:195:LEU:HG	1:I:235:SER:HB2	2.03	0.40
1:I:432:ILE:HG22	1:I:435:PHE:H	1.86	0.40
1:A:278:VAL:HG13	1:A:368:VAL:HG21	2.03	0.40
1:H:423:CYS:O	1:H:427:ILE:HG12	2.22	0.40
1:K:138:ARG:HH22	1:K:147:GLU:CD	2.23	0.40
1:N:254:GLU:CD	1:N:254:GLU:H	2.25	0.40
1:P:205:ALA:HA	1:P:245:GLU:HG3	2.03	0.40
1:F:63:ILE:HG12	1:F:152:LEU:HD12	2.04	0.40
1:I:139:LEU:O	1:L:105:ARG:NH2	2.47	0.40
1:K:182:PHE:CE2	1:K:188:ALA:HB2	2.57	0.40
1:L:95:ILE:HG23	1:L:119:LYS:HD3	2.03	0.40
1:L:190:TYR:HE2	1:L:421:LYS:HB3	1.85	0.40
1:M:133:TYR:HB3	1:N:331:LYS:HZ2	1.85	0.40
1:N:133:TYR:CZ	1:N:440:LEU:HD23	2.55	0.40
1:C:240:TYR:CZ	1:C:382:LEU:HD21	2.57	0.40
1:C:93:MET:HB3	1:C:93:MET:HE2	1.87	0.40
1:H:82:ASN:ND2	1:H:84:ASP:OD2	2.54	0.40
1:K:180:HIS:O	1:K:218:ARG:NH2	2.54	0.40
1:P:117:PHE:CE1	1:P:386:LYS:HD3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:288:CYS:O	1:P:292:VAL:HG23	2.22	0.40
1:P:278:VAL:HG22	1:P:368:VAL:HG11	2.02	0.40

All (2) 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)
2:E:595:HOH:O	2:I:578:HOH:O[1_655]	1.92	0.28
1:E:216:GLN:OE1	1:L:228:LYS:NZ[2_655]	2.16	0.04

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	398/444 (90%)	383 (96%)	14 (4%)	1 (0%)	41 64
1	B	358/444 (81%)	344 (96%)	14 (4%)	0	100 100
1	C	398/444 (90%)	381 (96%)	17 (4%)	0	100 100
1	D	362/444 (82%)	348 (96%)	14 (4%)	0	100 100
1	E	398/444 (90%)	381 (96%)	13 (3%)	4 (1%)	15 32
1	F	356/444 (80%)	338 (95%)	17 (5%)	1 (0%)	41 64
1	G	389/444 (88%)	372 (96%)	17 (4%)	0	100 100
1	H	349/444 (79%)	338 (97%)	11 (3%)	0	100 100
1	I	428/444 (96%)	404 (94%)	24 (6%)	0	100 100
1	J	377/444 (85%)	356 (94%)	20 (5%)	1 (0%)	41 64
1	K	415/444 (94%)	395 (95%)	19 (5%)	1 (0%)	47 71
1	L	378/444 (85%)	363 (96%)	15 (4%)	0	100 100
1	M	427/444 (96%)	406 (95%)	20 (5%)	1 (0%)	47 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	N	377/444 (85%)	362 (96%)	15 (4%)	0	100 100
1	O	415/444 (94%)	397 (96%)	18 (4%)	0	100 100
1	P	375/444 (84%)	359 (96%)	16 (4%)	0	100 100
All	All	6200/7104 (87%)	5927 (96%)	264 (4%)	9 (0%)	51 75

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	443	ASN
1	F	359	ASN
1	M	359	ASN
1	E	32	ASP
1	A	163	GLY
1	K	359	ASN
1	E	368	VAL
1	J	177	PRO
1	E	360	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	365/413 (88%)	353 (97%)	12 (3%)	38 64
1	B	314/413 (76%)	307 (98%)	7 (2%)	52 76
1	C	368/413 (89%)	357 (97%)	11 (3%)	41 67
1	D	318/413 (77%)	305 (96%)	13 (4%)	30 56
1	E	358/413 (87%)	346 (97%)	12 (3%)	37 63
1	F	325/413 (79%)	312 (96%)	13 (4%)	31 57
1	G	353/413 (86%)	343 (97%)	10 (3%)	43 69
1	H	307/413 (74%)	299 (97%)	8 (3%)	46 72
1	I	385/413 (93%)	369 (96%)	16 (4%)	30 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	338/413 (82%)	328 (97%)	10 (3%)	41	67
1	K	382/413 (92%)	369 (97%)	13 (3%)	37	63
1	L	342/413 (83%)	326 (95%)	16 (5%)	26	50
1	M	391/413 (95%)	378 (97%)	13 (3%)	38	64
1	N	337/413 (82%)	323 (96%)	14 (4%)	30	55
1	O	379/413 (92%)	366 (97%)	13 (3%)	37	63
1	P	337/413 (82%)	328 (97%)	9 (3%)	44	71
All	All	5599/6608 (85%)	5409 (97%)	190 (3%)	37	63

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	43	ASN
1	A	59	LYS
1	A	75	VAL
1	A	136	THR
1	A	211	ASP
1	A	263	GLU
1	A	279	GLN
1	A	315	LYS
1	A	358	PHE
1	A	383	LYS
1	A	443	ASN
1	B	137	LYS
1	B	152	LEU
1	B	291	LYS
1	B	405	THR
1	B	414	VAL
1	B	418	GLN
1	B	442	GLU
1	C	20	SER
1	C	189	SER
1	C	264	ASN
1	C	267	ARG
1	C	367	ASP
1	C	373	GLU
1	C	418	GLN
1	C	421	LYS
1	C	438	GLU

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Mol	Chain	Res	Type
1	C	443	ASN
1	C	444	GLN
1	D	68	GLU
1	D	77	ASN
1	D	93	MET
1	D	185	GLU
1	D	198	MET
1	D	213	GLU
1	D	235	SER
1	D	265	GLU
1	D	274	ASP
1	D	280	GLU
1	D	327	ASN
1	D	373	GLU
1	D	384	ILE
1	E	22	GLN
1	E	54	ASN
1	E	92	GLU
1	E	131	LYS
1	E	134	ARG
1	E	136	THR
1	E	152	LEU
1	E	176	TYR
1	E	185	GLU
1	E	235	SER
1	E	442	GLU
1	E	444	GLN
1	F	75	VAL
1	F	91	GLU
1	F	207	SER
1	F	216	GLN
1	F	235	SER
1	F	251	LYS
1	F	273	VAL
1	F	367	ASP
1	F	373	GLU
1	F	380	LYS
1	F	385	GLN
1	F	406	ARG
1	F	418	GLN
1	G	37	ASN
1	G	71	ARG

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Mol	Chain	Res	Type
1	G	113	VAL
1	G	146	ASN
1	G	156	GLN
1	G	172	ASP
1	G	264	ASN
1	G	279	GLN
1	G	294	LYS
1	G	418	GLN
1	H	197	LYS
1	H	264	ASN
1	H	280	GLU
1	H	294	LYS
1	H	358	PHE
1	H	409	SER
1	H	410	LEU
1	H	431	ASN
1	I	37	ASN
1	I	49	SER
1	I	75	VAL
1	I	89	SER
1	I	93	MET
1	I	134	ARG
1	I	136	THR
1	I	176	TYR
1	I	237	LYS
1	I	279	GLN
1	I	288	CYS
1	I	299	CYS
1	I	303	GLN
1	I	381	LEU
1	I	434	SER
1	I	442	GLU
1	J	81	LYS
1	J	162	GLU
1	J	172	ASP
1	J	185	GLU
1	J	276	ASP
1	J	356	CYS
1	J	367	ASP
1	J	418	GLN
1	J	433	LYS
1	J	442	GLU

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Mol	Chain	Res	Type
1	K	33	ARG
1	K	58	ASN
1	K	161	GLU
1	K	185	GLU
1	K	189	SER
1	K	198	MET
1	K	224	LYS
1	K	271	LYS
1	K	299	CYS
1	K	315	LYS
1	K	364	LEU
1	K	388	LYS
1	K	418	GLN
1	L	71	ARG
1	L	154	LEU
1	L	162	GLU
1	L	178	ASP
1	L	198	MET
1	L	207	SER
1	L	218	ARG
1	L	227	SER
1	L	228	LYS
1	L	274	ASP
1	L	352	THR
1	L	358	PHE
1	L	387	LYS
1	L	402	ASP
1	L	405	THR
1	L	431	ASN
1	M	12	ILE
1	M	33	ARG
1	M	59	LYS
1	M	154	LEU
1	M	178	ASP
1	M	217	LYS
1	M	242	MET
1	M	278	VAL
1	M	282	LEU
1	M	323	ASN
1	M	324	GLU
1	M	345	GLU
1	M	418	GLN

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Mol	Chain	Res	Type
1	N	75	VAL
1	N	93	MET
1	N	122	ILE
1	N	159	SER
1	N	233	ASP
1	N	237	LYS
1	N	242	MET
1	N	251	LYS
1	N	274	ASP
1	N	290	GLU
1	N	312	VAL
1	N	344	LYS
1	N	363	ASP
1	N	364	LEU
1	O	10	ASP
1	O	13	GLU
1	O	19	SER
1	O	37	ASN
1	O	47	TRP
1	O	58	ASN
1	O	211	ASP
1	O	263	GLU
1	O	265	GLU
1	O	350	LYS
1	O	373	GLU
1	O	383	LYS
1	O	433	LYS
1	P	64	MET
1	P	92	GLU
1	P	161	GLU
1	P	203	VAL
1	P	204	THR
1	P	217	LYS
1	P	242	MET
1	P	271	LYS
1	P	408	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	229	HIS
1	E	216	GLN

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Mol	Chain	Res	Type
1	H	279	GLN
1	K	216	GLN
1	L	385	GLN
1	N	146	ASN
1	P	247	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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

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	412/444 (92%)	-0.01	5 (1%)	79	76	38, 52, 73, 96	0
1	B	368/444 (82%)	-0.07	2 (0%)	91	89	38, 59, 79, 112	0
1	C	410/444 (92%)	0.00	3 (0%)	87	86	37, 52, 76, 89	0
1	D	370/444 (83%)	0.00	2 (0%)	91	89	38, 58, 82, 113	0
1	E	408/444 (91%)	-0.04	3 (0%)	87	86	35, 51, 78, 96	0
1	F	364/444 (81%)	-0.02	2 (0%)	91	89	35, 58, 85, 112	0
1	G	407/444 (91%)	-0.01	2 (0%)	91	89	38, 52, 71, 88	0
1	H	361/444 (81%)	-0.04	4 (1%)	80	78	37, 59, 89, 108	0
1	I	432/444 (97%)	0.03	8 (1%)	66	62	33, 53, 100, 140	0
1	J	381/444 (85%)	0.09	7 (1%)	68	64	34, 60, 88, 137	0
1	K	423/444 (95%)	-0.01	4 (0%)	84	82	36, 51, 77, 141	0
1	L	382/444 (86%)	0.00	6 (1%)	72	68	34, 56, 83, 118	0
1	M	431/444 (97%)	0.07	10 (2%)	60	54	35, 52, 103, 165	0
1	N	381/444 (85%)	0.04	1 (0%)	94	93	38, 61, 90, 169	0
1	O	423/444 (95%)	0.09	12 (2%)	53	46	36, 53, 85, 120	0
1	P	381/444 (85%)	0.00	8 (2%)	63	58	37, 60, 86, 142	0
All	All	6334/7104 (89%)	0.01	79 (1%)	79	76	33, 55, 86, 169	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	325	GLN	5.8
1	O	8	THR	5.4
1	O	325	GLN	5.1
1	G	47	TRP	4.6
1	M	317	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	I	320	ASN	4.5
1	J	180	HIS	4.3
1	M	47	TRP	4.3
1	K	8	THR	4.2
1	I	48	ASN	4.1
1	P	401	ASN	4.0
1	J	399	SER	3.8
1	M	318	SER	3.7
1	L	399	SER	3.6
1	O	16	PRO	3.6
1	D	403	PHE	3.6
1	A	15	ILE	3.6
1	E	443	ASN	3.6
1	I	50	ARG	3.6
1	P	328	TYR	3.6
1	I	40	MET	3.5
1	J	178	ASP	3.4
1	L	181	ASP	3.4
1	O	47	TRP	3.3
1	A	47	TRP	3.3
1	M	323	ASN	3.2
1	I	51	TYR	3.2
1	D	179	GLY	3.2
1	L	431	ASN	3.2
1	H	60	ASP	3.1
1	L	318	SER	3.1
1	O	18	GLY	2.9
1	I	44	ILE	2.9
1	M	54	ASN	2.9
1	P	318	SER	2.8
1	E	15	ILE	2.8
1	A	18	GLY	2.8
1	G	180	HIS	2.7
1	H	368	VAL	2.7
1	I	35	VAL	2.7
1	P	400	GLY	2.7
1	L	177	PRO	2.6
1	P	58	ASN	2.6
1	K	178	ASP	2.5
1	P	185	GLU	2.5
1	A	16	PRO	2.5
1	J	205	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	408	CYS	2.5
1	B	328	TYR	2.4
1	B	399	SER	2.4
1	C	20	SER	2.4
1	H	329	MET	2.3
1	E	35	VAL	2.3
1	P	180	HIS	2.3
1	O	17	LEU	2.3
1	O	44	ILE	2.3
1	C	53	TYR	2.3
1	O	177	PRO	2.3
1	J	162	GLU	2.3
1	F	264	ASN	2.2
1	K	36	MET	2.2
1	O	35	VAL	2.2
1	A	48	ASN	2.2
1	C	11	ASN	2.2
1	J	318	SER	2.2
1	O	326	LYS	2.1
1	F	358	PHE	2.1
1	P	325	GLN	2.1
1	L	183	ASN	2.1
1	N	401	ASN	2.1
1	O	317	PRO	2.1
1	M	325	GLN	2.1
1	H	383	LYS	2.1
1	M	443	ASN	2.1
1	O	15	ILE	2.0
1	M	50	ARG	2.0
1	M	353	ALA	2.0
1	K	56	LEU	2.0
1	I	22	GLN	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.