



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:33 PM UTC

PDB ID : 6RMO / pdb_00006rmo
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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

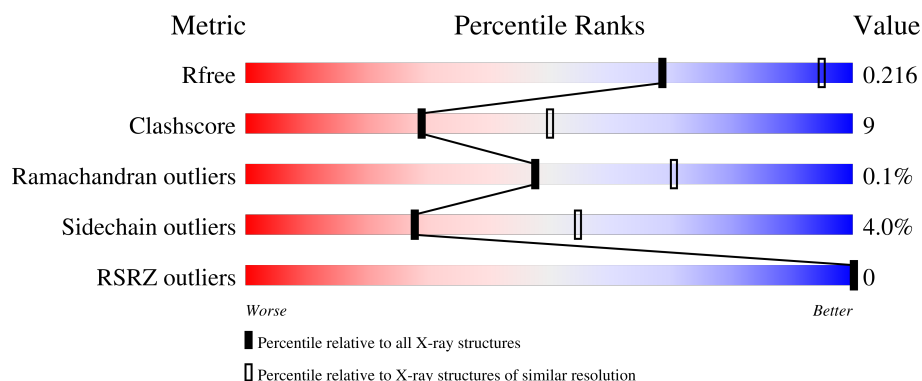
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



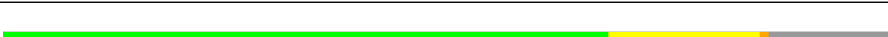
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	444	 75% 17% • 7%
1	B	444	 68% 14% • 17%
1	C	444	 70% 20% • 8%
1	D	444	 66% 16% • 17%
1	E	444	 74% 16% • 8%

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Mol	Chain	Length	Quality of chain
1	F	444	
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			

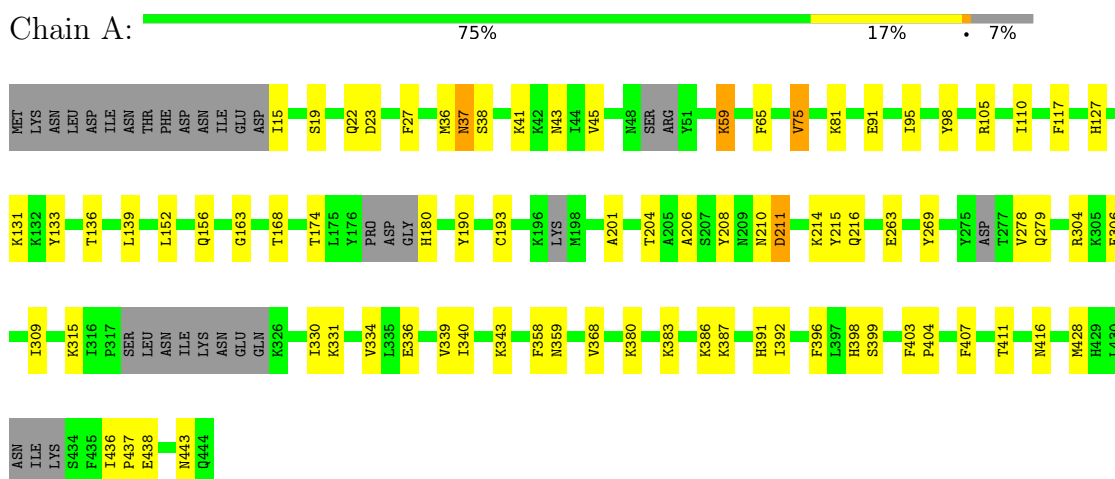
- Molecule 2 is water.

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

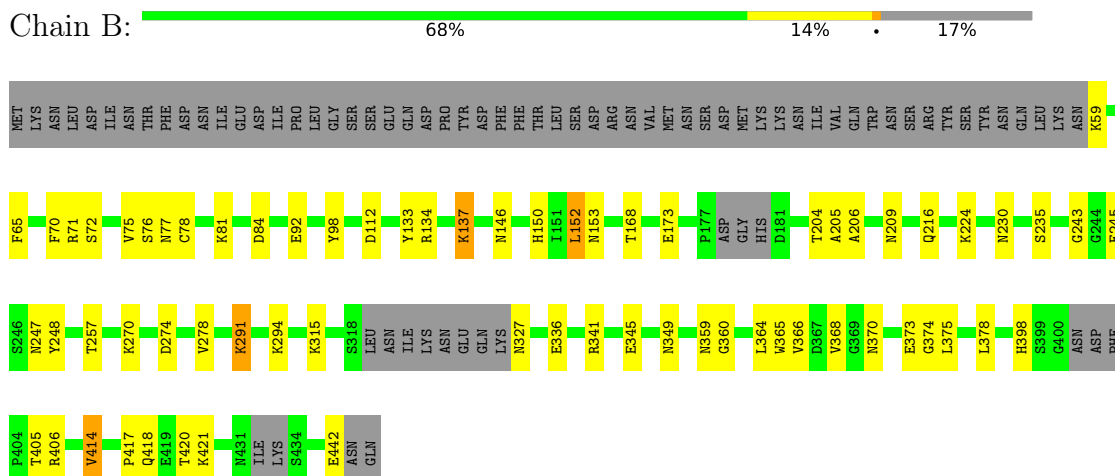
3 Residue-property plots

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

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

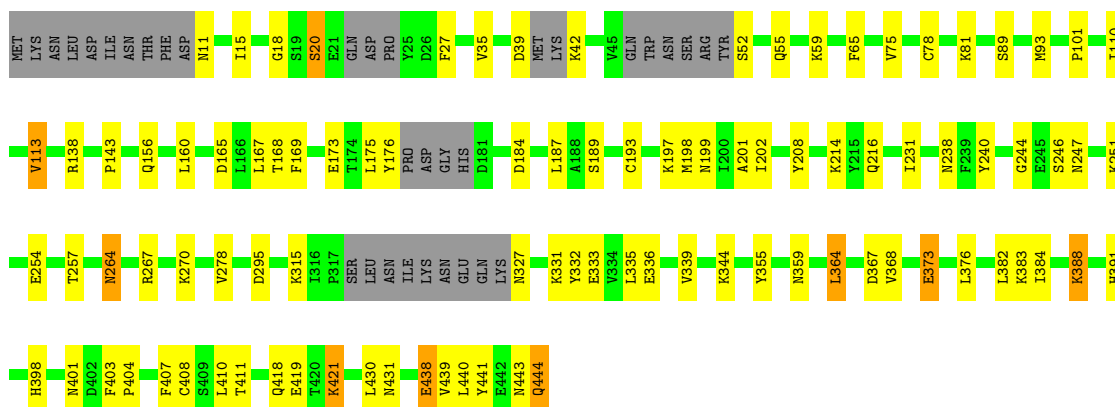


- Molecule 1: IMP-specific 5'-nucleotidase, putative



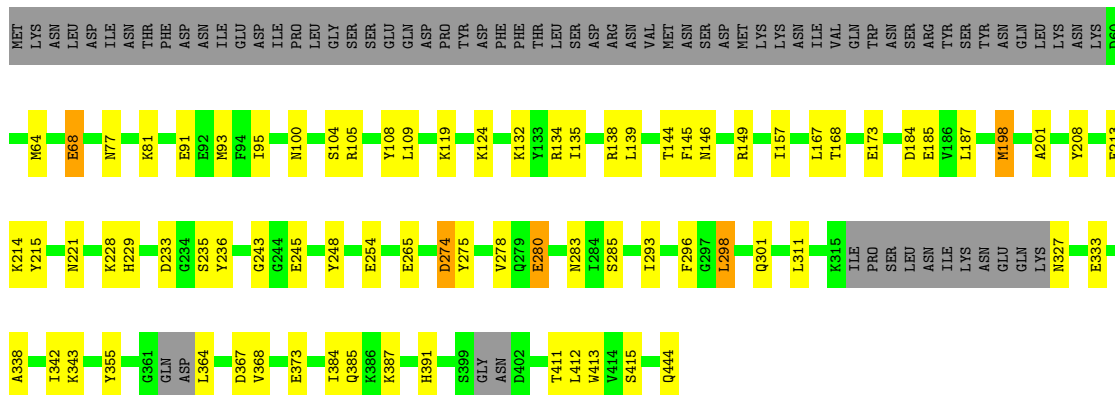
- Molecule 1: IMP-specific 5'-nucleotidase, putative





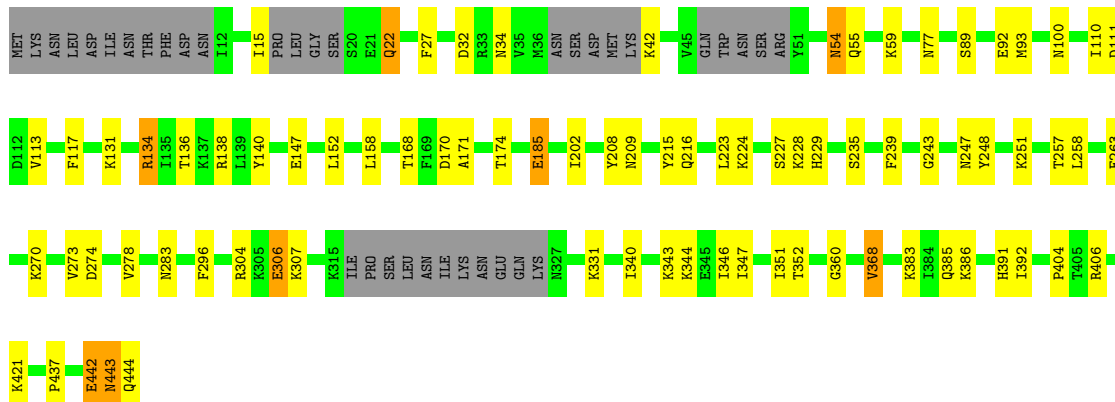
- Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain D: 66% 16% 17%



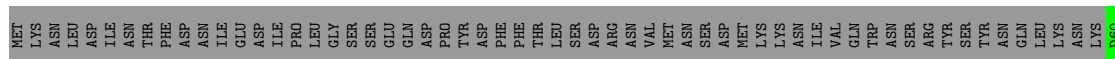
- Molecule 1: IMP-specific 5'-nucleotidase, putative

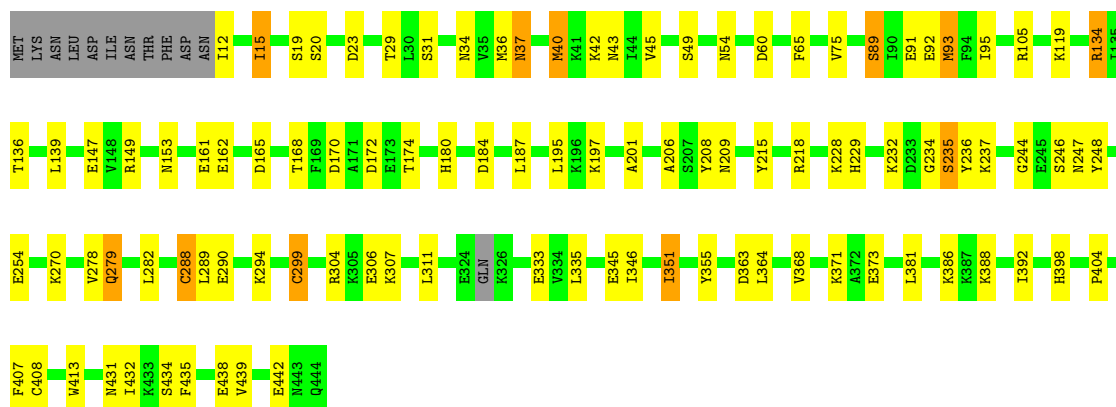
Chain E: 74% 16% 8%



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

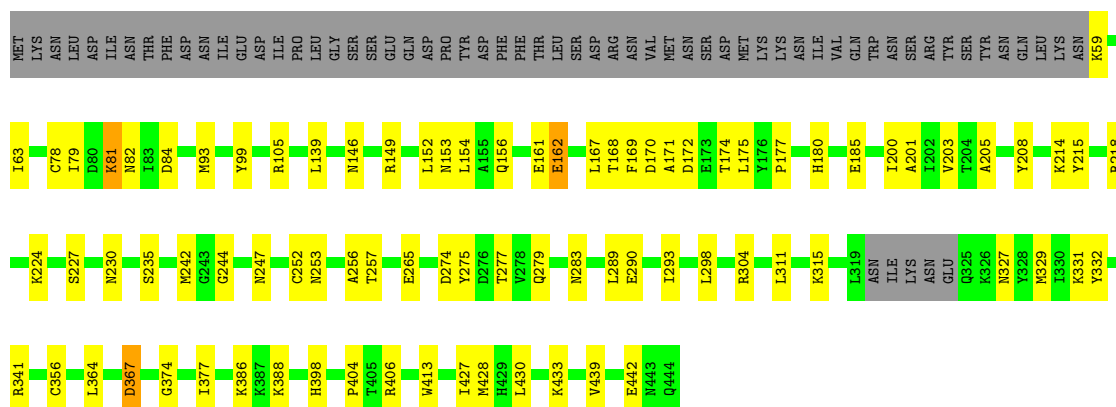
Chain F: 63% 16% 18%





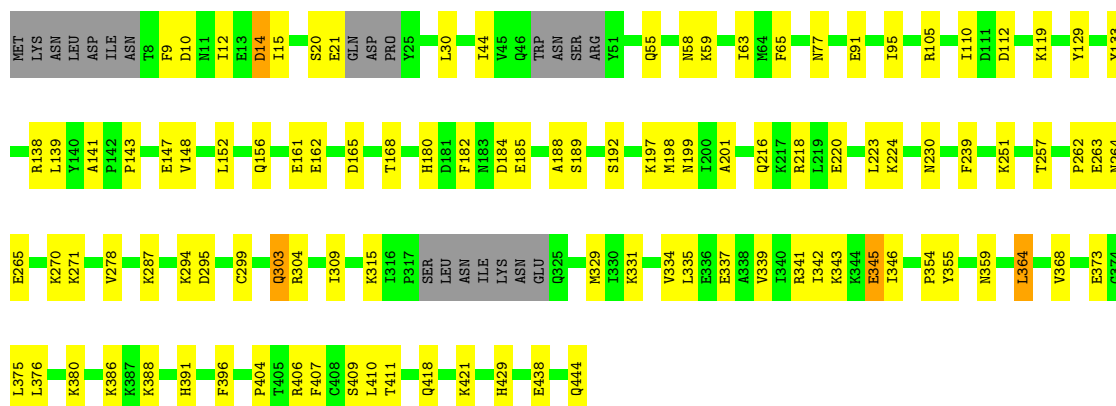
- Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain J: 67% 18% 14%



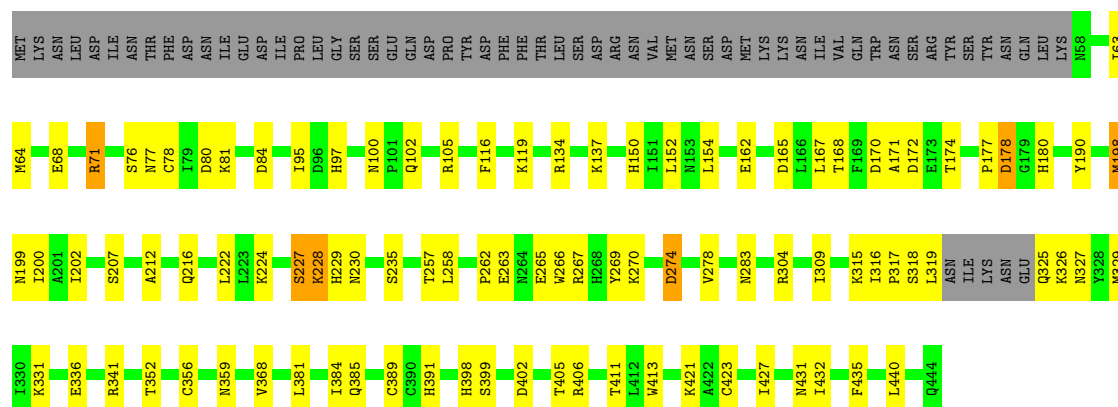
- Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain K: 72% 23% 5%



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

Chain L: 64% 20% 14%



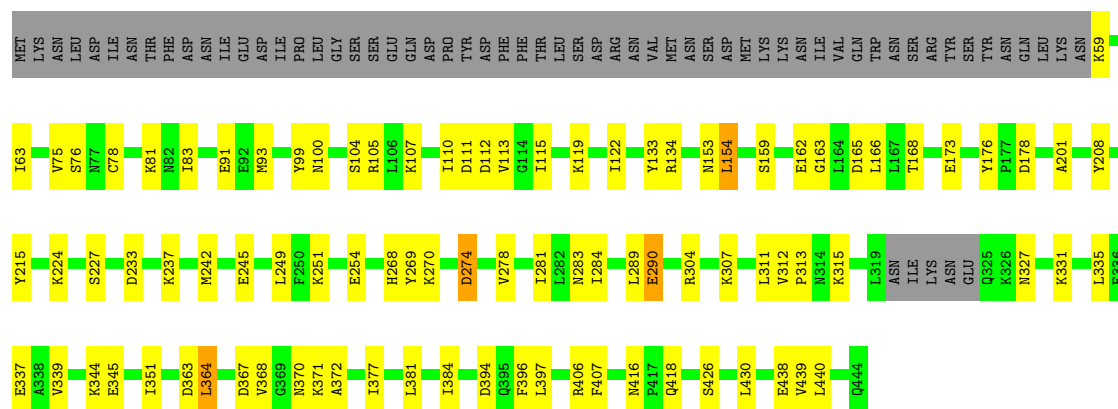
- Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain M: 77% 19% ..



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

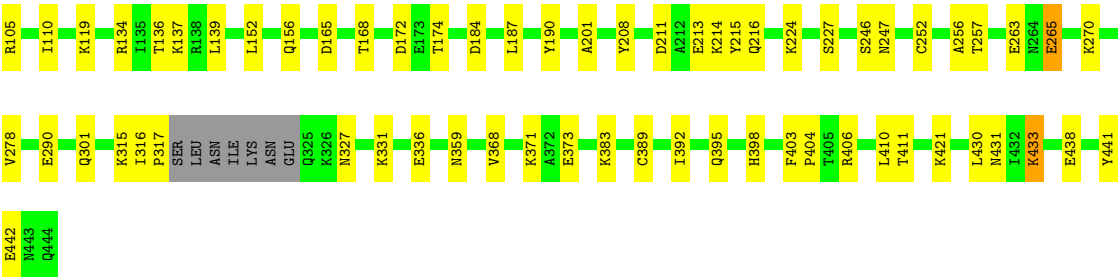
Chain N: 65% 20% • 14%



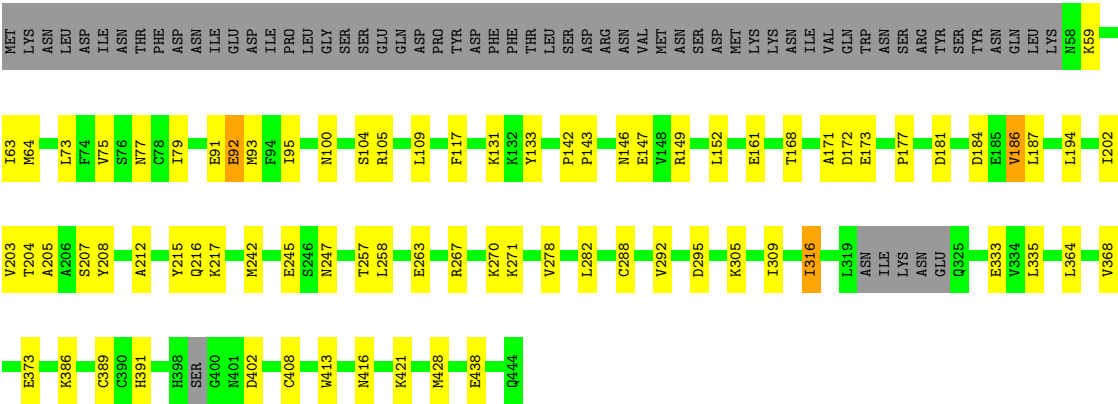
- Molecule 1: IMP-specific 5'-nucleotidase, putative

Chain O: 76% 19% • 5%





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



4 Data and refinement statistics

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 48.30 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.7 (48.30-2.60) 91.2 (48.30-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.230 , 0.253 0.208 , 0.216	Depositor DCC
R_{free} test set	12515 reflections (4.64%)	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)	0.30 , 23.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	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	0.97	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.13	0/3390	0.32	0/4577
1	B	0.10	0/2993	0.30	0/4050
1	C	0.12	0/3394	0.30	0/4579
1	D	0.11	0/3027	0.28	0/4093
1	E	0.13	0/3345	0.32	0/4519
1	F	0.12	0/3007	0.28	0/4058
1	G	0.14	0/3326	0.31	0/4485
1	H	0.14	0/2918	0.30	0/3949
1	I	0.11	0/3558	0.28	0/4806
1	J	0.13	0/3151	0.27	0/4255
1	K	0.11	0/3518	0.30	0/4746
1	L	0.13	0/3173	0.31	0/4287
1	M	0.12	0/3587	0.30	0/4844
1	N	0.10	0/3146	0.28	0/4248
1	O	0.12	0/3504	0.30	0/4730
1	P	0.11	0/3148	0.28	0/4254
All	All	0.12	0/52185	0.30	0/70480

There are no bond length outliers.

There are no bond angle outliers.

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	49	0
1	B	2932	0	2884	48	0
1	C	3328	0	3309	70	0
1	D	2965	0	2911	53	0
1	E	3279	0	3217	55	1
1	F	2950	0	2951	54	0
1	G	3264	0	3194	56	0
1	H	2863	0	2802	62	0
1	I	3486	0	3438	66	0
1	J	3085	0	3078	52	0
1	K	3447	0	3427	71	0
1	L	3106	0	3086	75	1
1	M	3512	0	3479	60	0
1	N	3080	0	3081	58	0
1	O	3433	0	3405	62	0
1	P	3083	0	3054	54	0
2	A	93	0	0	14	0
2	B	59	0	0	9	0
2	C	103	0	0	16	0
2	D	65	0	0	19	0
2	E	105	0	0	22	1
2	F	57	0	0	9	0
2	G	95	0	0	22	0
2	H	75	0	0	23	0
2	I	97	0	0	20	1
2	J	53	0	0	10	0
2	K	112	0	0	21	0
2	L	74	0	0	26	0
2	M	95	0	0	22	0
2	N	60	0	0	19	0
2	O	99	0	0	23	0
2	P	63	0	0	14	0
All	All	52441	0	50594	889	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 9.

All (889) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:275:TYR:OH	2:D:501:HOH:O	1.87	0.92
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: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
1:M:236:TYR:O	2:M:503:HOH:O	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:81:LYS:NZ	2:D:514:HOH:O	2.22	0.72
1:D:293:ILE:HD11	1:D:311:LEU:HD11	1.71	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:92:GLU:OE1	2:G:507:HOH:O	2.08	0.72
1:G:133:TYR:OH	2:G:508: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:L:167:LEU:HB2	1:L:198:MET:HE2	1.72	0.71
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:K:10:ASP:O	1:K:380:LYS:NZ	2.26	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
1:G:96:ASP:OD2	2:G:509:HOH:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:36:MET:HE1	1:A:45:VAL:HG21	1.74	0.68
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: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:I:246:SER:OG	2:I:507:HOH:O	2.11	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:N	1:G:37:ASN:OD1	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:279:GLN:OE1	1:L:385:GLN:NE2	2.27	0.67
1:H:441:TYR:O	2:H:508:HOH:O	2.12	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:G:197:LYS:NZ	2:G:506:HOH:O	2.04	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:N:307:LYS:NZ	2:N:513: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:OD1	1:L:274:ASP:N	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: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:82:ASN:OD1	2:H:510:HOH:O	2.14	0.65
1:H:385:GLN:OE1	2:H:509:HOH:O	2.14	0.65
1:K:278:VAL:HG22	1:K:368:VAL:HG11	1.79	0.65
1:I:34:ASN:O	1:I:37:ASN:ND2	2.30	0.65
1:I:247:ASN:OD1	1:I:270:LYS:NZ	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: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:C:383:LYS:NZ	2:C:516:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:294:LYS:NZ	2:K:518:HOH:O	2.31	0.63
1:I:161:GLU:O	1:I:431:ASN:ND2	2.31	0.63
1:C:101:PRO:HB3	2:C:517:HOH:O	1.99	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:OD1	1:C:264:ASN:N	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:F:291:LYS:NZ	2:F:503:HOH:O	2.14	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:100:ASN:C	2:L:504:HOH:O	2.44	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:H:259:TYR:OH	2:H:503:HOH:O	2.00	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:N:268:HIS:NE2	2:N:514:HOH:O	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	1:K:55:GLN:OE1	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:I:165:ASP:CG	1:I:388:LYS:HZ2	2.11	0.58
1:H:167:LEU:HB2	1:H:198:MET:HE2	1.84	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:64:MET:HE3	1:D:145:PHE:HD2	1.68	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:OD1	1:N:274:ASP:N	2.16	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:M:278:VAL:HG23	1:M:368:VAL:HG21	1.87	0.57
1:P:207:SER:O	1:P:305:LYS:NZ	2.35	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:95:ILE:HD12	1:K:119:LYS:HD2	1.87	0.57
1:K:165:ASP:O	1:K:199:ASN:ND2	2.37	0.57
1:J:329:MET:SD	2:J:550:HOH:O	2.58	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:C:27:PHE:O	1:D:144:THR:OG1	2.23	0.55
1:F:293:ILE:HA	1:F:298:LEU:HB2	1.87	0.55
1:I:363:ASP:N	1:I:363:ASP:OD1	2.37	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:A:193:CYS:HB2	1:A:428:MET:HE2	1.88	0.55
1:C:398:HIS:CE1	1:C:403:PHE:HB3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:133:TYR:OH	1:P:438:GLU:OE2	2.15	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
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:C:331:LYS:NZ	2:C:508:HOH:O	2.41	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:O:80:ASP:CG	2:O:504:HOH:O	2.47	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:H:119:LYS:NZ	2:H:523:HOH:O	2.40	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:D:167:LEU:HB2	1:D:198:MET:HE2	1.89	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:O:36:MET:HE1	1:O:45:VAL:HG21	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:84:ASP:HB3	1:F:88:LEU:HD23	1.90	0.52
1:F:304:ARG:HD2	1:F:309:ILE:HD12	1.92	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:L:178:ASP:C	2:L:510:HOH:O	2.52	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
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:G:306:GLU:CD	1:G:306:GLU:H	2.18	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: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:H:135:ILE:O	2:H:513:HOH:O	2.19	0.51
1:I:246:SER:O	1:I:270:LYS:NZ	2.38	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:E:224:LYS:O	1:E:227:SER:OG	2.26	0.51
1:I:91:GLU:O	1:I:95:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:L:270:LYS:NZ	2:L:516:HOH:O	2.35	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
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:D:274:ASP:OD1	1:D:274:ASP:N	2.43	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:174:THR:HG21	1:I:392:ILE:HG22	1.94	0.50
1:I:244:GLY:N	2:I:512:HOH:O	2.35	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:P:131:LYS:NZ	2:P:512:HOH:O	2.25	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:F:386:LYS:NZ	2:F:522:HOH:O	2.44	0.49
1:K:20:SER:OG	1:K:355:TYR:OH	2.26	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:O:442:GLU:HB2	2:O:505:HOH:O	2.11	0.49
1:P:93:MET:HE1	1:P:109:LEU:HD12	1.93	0.49
1:B:205:ALA:HA	1:B:245:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:186:VAL:HG13	1:P:421:LYS:HE2	1.95	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:M:133:TYR:HB3	1:N:331:LYS:HZ1	1.78	0.49
1:O:184:ASP:OD2	1:O:421:LYS:NZ	2.46	0.49
1:B:98:TYR:OH	1:N:290:GLU:OE2	2.23	0.48
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: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:O:119:LYS:NZ	2:O:524:HOH:O	2.45	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:F:192:SER:HB2	1:F:230:ASN:ND2	2.29	0.48
1:G:246:SER:OG	2:G:513:HOH:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:M:386:LYS:NZ	2:M:522:HOH:O	2.46	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:HD2	1:H:387:LYS:N	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
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:L:266:TRP:C	2:L:507:HOH:O	2.55	0.47
1:N:224:LYS:O	1:N:227:SER:OG	2.31	0.47
1:D:91:GLU:O	1:D:95:ILE:HG12	2.15	0.47
1:E:343:LYS:NZ	2:E:519:HOH:O	2.48	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:L:398:HIS:O	1:L:398:HIS:ND1	2.48	0.47
1:O:246:SER:O	1:O:270:LYS:NZ	2.32	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:O:331:LYS:NZ	1:P:147:GLU:OE2	2.43	0.47
1:P:149:ARG:HD2	1:P:413:TRP:CG	2.50	0.47
1:P:168:THR:OG1	1:P:391:HIS:ND1	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:117:PHE:CZ	1:A:386:LYS:HD3	2.50	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:E:442:GLU:O	1:E:443:ASN:C	2.58	0.47
1:I:172:ASP:OD2	1:I:371:LYS:NZ	2.47	0.47
1:K:138:ARG:NH1	1:K:141:ALA:O	2.46	0.47
1:H:265:GLU:OE2	1:H:265:GLU:N	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:43:ASN:HB3	1:J:332:TYR:CZ	2.50	0.46
1:I:254:GLU:OE1	1:I:254:GLU:N	2.47	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:N:76:SER:HB3	1:O:69:ILE:HD13	1.98	0.46
1:O:214:LYS:HA	2:O:502:HOH:O	2.16	0.46
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:78:CYS:HA	1:C:81:LYS:HD2	1.97	0.46
1:C:278:VAL:HG22	1:C:368:VAL:HG11	1.98	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:41:LYS:HE3	1:N:397:LEU:HD21	1.98	0.46
1:M:299:CYS:HB3	1:M:328:TYR:CG	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:M:379:GLN:CD	2:M:506:HOH:O	2.57	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:L:102:GLN:H	1:L:102:GLN:CD	2.24	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:388:LYS:HB3	1:C:388:LYS:HE2	1.78	0.45
1:D:228:LYS:HE3	1:D:229:HIS:HE1	1.81	0.45
1:A:190:TYR:HA	1:A:428:MET:HE3	1.98	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
1:C:335:LEU:O	1:C:339:VAL:HG23	2.16	0.45
1:D:132:LYS:NZ	1:D:444:GLN:O	2.40	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:N:254:GLU:H	1:N:254:GLU:CD	2.25	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:35:VAL:HG13	1:D:415:SER:HB2	1.99	0.45
1:C:156:GLN:NE2	1:C:411:THR:O	2.46	0.45
1:J:224:LYS:O	1:J:227:SER:OG	2.32	0.45
1:K:138:ARG:HH22	1:K:147:GLU:CD	2.23	0.45
1:K:287:LYS:HA	1:K:287:LYS:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:38:SER:HB2	1:A:41:LYS:HG3	1.99	0.45
1:A:269:TYR:HB3	1:A:380:LYS:HD2	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
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:K:9:PHE:O	1:K:386:LYS:NZ	2.40	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:H:242:MET:HE3	1:H:246:SER:HA	1.99	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:I:197:LYS:NZ	2:I:508:HOH:O	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:93:MET:HE1	1:F:109:LEU:HD12	1.99	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:F:380:LYS:HD3	1:J:275:TYR:CE1	2.53	0.44
1:G:93:MET:HG2	1:G:106:LEU:HB2	1.99	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:HD2	1:F:380:LYS:O	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:89:SER:HB3	1:L:76:SER:O	2.18	0.43
1:I:335:LEU:HD22	1:I:364:LEU:HB2	1.99	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: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:M:287:LYS:HA	1:M:287:LYS:HD3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:329:MET:HE2	1:H:329:MET:HB2	1.97	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:154:LEU:HD11	1:H:437:PRO:HB2	2.01	0.43
1:H:425:LYS:HE2	1:H:435:PHE:HE1	1.83	0.43
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:40:MET:HE3	1:O:44:ILE:HD11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:222:LEU:H	1:L:222:LEU:HD23	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:99:TYR:OH	1:N:119:LYS:NZ	2.50	0.42
1:N:407:PHE:HA	2:N:517:HOH:O	2.19	0.42
1:O:136:THR:C	2:O:504:HOH:O	2.61	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:HE2	1:I:294:LYS:HB3	1.69	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:54:ASN:OD1	1:E:54:ASN:N	2.46	0.42
1:E:158:LEU:HD21	1:E:437:PRO:HG2	2.01	0.42
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: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:E:385:GLN:H	1:E:385:GLN:CD	2.24	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:M:93:MET:HE1	1:M:109:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:246:SER:O	1:C:270:LYS:NZ	2.36	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: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:55:GLN:O	1:E:59:LYS:HG3	2.19	0.41
1:E:263:GLU:OE1	1:E:263:GLU:N	2.43	0.41
1:F:263:GLU:HA	1:F:266:TRP:NE1	2.35	0.41
1:H:224:LYS:O	1:H:227:SER:OG	2.37	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:150:HIS:CE1	1:F:440:LEU:HD13	2.56	0.41
1:F:355:TYR:OH	2:F:507:HOH:O	2.22	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: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:HE3	1:G:41:LYS:HB2	1.70	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:B:70:PHE:N	1:B:70:PHE:CD1	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:15:ILE:HG12	1:I:407:PHE:HB3	2.01	0.41
1:I:209:ASN:HA	1:I:248:TYR:CZ	2.56	0.41
1:K:15:ILE:HD12	1:K:376:LEU:HD11	2.02	0.41
1:K:343:LYS:C	2:K:503:HOH:O	2.63	0.41
1:N:254:GLU:OE2	1:N:254:GLU:N	2.49	0.41
1:P:171:ALA:HB2	1:P:202:ILE:HG23	2.02	0.41
1:B:84:ASP:OD1	1:B:84:ASP:N	2.53	0.41
1:C:156:GLN:HB3	1:C:410:LEU:HD13	2.02	0.41
1:C:167:LEU:HD22	1:C:169:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LEU:HD11	1:C:202:ILE:HD12	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:224:LYS:O	1:O:227:SER:OG	2.30	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:82:ASN:ND2	1:J:84:ASP:OD2	2.53	0.41
1:J:208:TYR:HB2	1:J:215:TYR:CE1	2.55	0.41
1:L:413:TRP:CD1	1:L:413:TRP:C	2.99	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:331:LYS:HE2	1:F:133:TYR:CD1	2.56	0.41
1:E:344:LYS:HD3	1:E:344:LYS:HA	1.89	0.41
1:I:93:MET:SD	1:I:105:ARG:HG2	2.60	0.41
1:K:44:ILE:HG23	1:L:399:SER:HB2	2.03	0.41
1:K:303:GLN:HG3	2:K:517:HOH:O	2.20	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:G:171:ALA:HB2	1:G:202:ILE:HG23	2.02	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: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:M:138:ARG:HD2	1:N:337:GLU:HB2	2.01	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:117:PHE:CE1	1:E:386:LYS:HD3	2.56	0.41
1:E:228:LYS:HB2	1:E:229:HIS:CE1	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:315:LYS:HA	1:O:327:ASN:HA	2.03	0.41
1:O:316:ILE:HA	1:O:317:PRO:HD3	1.93	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:168:THR:HG23	1:E:391:HIS:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:ASP:O	1:E:174:THR:HG22	2.21	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:HD13	1:E:347:ILE:HA	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:P:59:LYS:NZ	2:P:516:HOH:O	2.41	0.40
1:P:305:LYS:NZ	2:P:507:HOH:O	2.13	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: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: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:H:82:ASN:ND2	1:H:84:ASP:OD2	2.54	0.40
1:J:93:MET:HE3	1:K:77:ASN:HB2	2.03	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
1:P:278:VAL:HG22	1:P:368:VAL:HG11	2.02	0.40
1:P:288:CYS:O	1:P:292:VAL:HG23	2.22	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 ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	398/444 (90%)	383 (96%)	14 (4%)	1 (0%)	36	58
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%)	12	28
1	F	356/444 (80%)	338 (95%)	17 (5%)	1 (0%)	36	58
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%)	36	58
1	K	415/444 (94%)	395 (95%)	19 (5%)	1 (0%)	43	66
1	L	378/444 (85%)	363 (96%)	15 (4%)	0	100	100
1	M	427/444 (96%)	406 (95%)	20 (5%)	1 (0%)	43	66
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%)	48	70

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 ⓘ

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%)	352 (96%)	13 (4%)	31	58
1	B	314/413 (76%)	305 (97%)	9 (3%)	37	65
1	C	368/413 (89%)	353 (96%)	15 (4%)	27	54
1	D	318/413 (77%)	305 (96%)	13 (4%)	27	54
1	E	358/413 (87%)	345 (96%)	13 (4%)	31	58
1	F	325/413 (79%)	309 (95%)	16 (5%)	22	47
1	G	353/413 (86%)	338 (96%)	15 (4%)	26	52
1	H	307/413 (74%)	295 (96%)	12 (4%)	28	55
1	I	385/413 (93%)	362 (94%)	23 (6%)	17	37
1	J	338/413 (82%)	328 (97%)	10 (3%)	36	64
1	K	382/413 (92%)	364 (95%)	18 (5%)	23	48
1	L	342/413 (83%)	329 (96%)	13 (4%)	29	56
1	M	391/413 (95%)	376 (96%)	15 (4%)	29	56
1	N	337/413 (82%)	320 (95%)	17 (5%)	22	46
1	O	379/413 (92%)	367 (97%)	12 (3%)	34	62
1	P	337/413 (82%)	325 (96%)	12 (4%)	31	58
All	All	5599/6608 (85%)	5373 (96%)	226 (4%)	28	55

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
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

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Mol	Chain	Res	Type
1	A	306	GLU
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	294	LYS
1	B	366	VAL
1	B	405	THR
1	B	414	VAL
1	B	418	GLN
1	B	442	GLU
1	C	20	SER
1	C	113	VAL
1	C	189	SER
1	C	264	ASN
1	C	267	ARG
1	C	344	LYS
1	C	364	LEU
1	C	367	ASP
1	C	373	GLU
1	C	388	LYS
1	C	418	GLN
1	C	421	LYS
1	C	438	GLU
1	C	443	ASN
1	C	444	GLN
1	D	68	GLU
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	298	LEU
1	D	327	ASN
1	D	373	GLU
1	D	384	ILE

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Mol	Chain	Res	Type
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	185	GLU
1	E	235	SER
1	E	306	GLU
1	E	392	ILE
1	E	442	GLU
1	E	444	GLN
1	F	75	VAL
1	F	88	LEU
1	F	91	GLU
1	F	207	SER
1	F	235	SER
1	F	251	LYS
1	F	273	VAL
1	F	284	ILE
1	F	350	LYS
1	F	367	ASP
1	F	373	GLU
1	F	376	LEU
1	F	380	LYS
1	F	385	GLN
1	F	406	ARG
1	F	418	GLN
1	G	15	ILE
1	G	37	ASN
1	G	63	ILE
1	G	71	ARG
1	G	75	VAL
1	G	113	VAL
1	G	132	LYS
1	G	146	ASN
1	G	156	GLN
1	G	172	ASP
1	G	203	VAL
1	G	264	ASN
1	G	279	GLN

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Mol	Chain	Res	Type
1	G	294	LYS
1	G	418	GLN
1	H	68	GLU
1	H	197	LYS
1	H	264	ASN
1	H	280	GLU
1	H	294	LYS
1	H	358	PHE
1	H	377	ILE
1	H	409	SER
1	H	410	LEU
1	H	430	LEU
1	H	431	ASN
1	H	442	GLU
1	I	15	ILE
1	I	36	MET
1	I	37	ASN
1	I	40	MET
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	232	LYS
1	I	235	SER
1	I	237	LYS
1	I	279	GLN
1	I	282	LEU
1	I	288	CYS
1	I	290	GLU
1	I	299	CYS
1	I	351	ILE
1	I	381	LEU
1	I	434	SER
1	I	438	GLU
1	I	442	GLU
1	J	81	LYS
1	J	161	GLU
1	J	162	GLU
1	J	172	ASP
1	J	185	GLU

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Mol	Chain	Res	Type
1	J	290	GLU
1	J	356	CYS
1	J	367	ASP
1	J	433	LYS
1	J	442	GLU
1	K	14	ASP
1	K	30	LEU
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	303	GLN
1	K	315	LYS
1	K	329	MET
1	K	345	GLU
1	K	364	LEU
1	K	375	LEU
1	K	406	ARG
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	227	SER
1	L	228	LYS
1	L	274	ASP
1	L	352	THR
1	L	402	ASP
1	L	405	THR
1	L	431	ASN
1	M	12	ILE
1	M	30	LEU
1	M	33	ARG
1	M	44	ILE
1	M	59	LYS
1	M	75	VAL

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Mol	Chain	Res	Type
1	M	92	GLU
1	M	154	LEU
1	M	278	VAL
1	M	282	LEU
1	M	305	LYS
1	M	323	ASN
1	M	324	GLU
1	M	345	GLU
1	M	418	GLN
1	N	75	VAL
1	N	93	MET
1	N	122	ILE
1	N	154	LEU
1	N	159	SER
1	N	162	GLU
1	N	233	ASP
1	N	237	LYS
1	N	242	MET
1	N	249	LEU
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	58	ASN
1	O	211	ASP
1	O	263	GLU
1	O	265	GLU
1	O	301	GLN
1	O	373	GLU
1	O	383	LYS
1	O	433	LYS
1	P	64	MET
1	P	75	VAL
1	P	92	GLU
1	P	161	GLU

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Mol	Chain	Res	Type
1	P	186	VAL
1	P	203	VAL
1	P	204	THR
1	P	217	LYS
1	P	242	MET
1	P	271	LYS
1	P	316	ILE
1	P	408	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	HIS
1	A	418	GLN
1	B	127	HIS
1	C	103	HIS
1	C	130	ASN
1	C	391	HIS
1	D	210	ASN
1	D	229	HIS
1	E	103	HIS
1	E	127	HIS
1	E	216	GLN
1	E	221	ASN
1	F	82	ASN
1	F	100	ASN
1	G	11	ASN
1	G	82	ASN
1	G	156	GLN
1	H	130	ASN
1	H	199	ASN
1	H	279	GLN
1	I	43	ASN
1	I	100	ASN
1	I	103	HIS
1	I	130	ASN
1	I	279	GLN
1	I	301	GLN
1	I	303	GLN
1	I	395	GLN
1	I	401	ASN
1	J	82	ASN

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Mol	Chain	Res	Type
1	J	156	GLN
1	J	180	HIS
1	J	303	GLN
1	K	46	GLN
1	K	216	GLN
1	K	395	GLN
1	L	362	GLN
1	L	385	GLN
1	L	395	GLN
1	M	102	GLN
1	M	199	ASN
1	M	238	ASN
1	N	103	HIS
1	N	130	ASN
1	N	146	ASN
1	N	229	HIS
1	N	429	HIS
1	O	82	ASN
1	P	100	ASN
1	P	221	ASN
1	P	247	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	412/444 (92%)	-1.37	0 100 100	38, 52, 73, 96	0
1	B	368/444 (82%)	-1.31	0 100 100	38, 59, 79, 112	0
1	C	410/444 (92%)	-1.37	0 100 100	37, 52, 76, 89	0
1	D	370/444 (83%)	-1.31	0 100 100	38, 58, 82, 113	0
1	E	408/444 (91%)	-1.35	0 100 100	35, 51, 78, 96	0
1	F	364/444 (81%)	-1.31	0 100 100	35, 58, 85, 112	0
1	G	407/444 (91%)	-1.34	0 100 100	38, 52, 71, 88	0
1	H	361/444 (81%)	-1.29	0 100 100	37, 59, 89, 108	0
1	I	432/444 (97%)	-1.31	0 100 100	33, 53, 100, 140	0
1	J	381/444 (85%)	-1.28	0 100 100	34, 60, 88, 137	0
1	K	423/444 (95%)	-1.34	0 100 100	36, 51, 77, 141	0
1	L	382/444 (86%)	-1.29	0 100 100	34, 56, 83, 118	0
1	M	431/444 (97%)	-1.31	0 100 100	35, 52, 103, 165	0
1	N	381/444 (85%)	-1.26	0 100 100	38, 61, 90, 169	0
1	O	423/444 (95%)	-1.31	0 100 100	36, 53, 85, 120	0
1	P	381/444 (85%)	-1.31	0 100 100	37, 60, 86, 142	0
All	All	6334/7104 (89%)	-1.32	0 100 100	33, 55, 86, 169	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.