Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2023 – 07:19 pm BST

PDB ID	:	8ASC
Title	:	Ku70/80 binds to the Ku-binding motif of PAXX
Authors	:	Seif El Dahan, M.; Ropars, V.; Charbonnier, J.B.
Deposited on	:	2022-08-19
Resolution	:	2.95 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 (i) 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 (1)) were used in the production of this report:

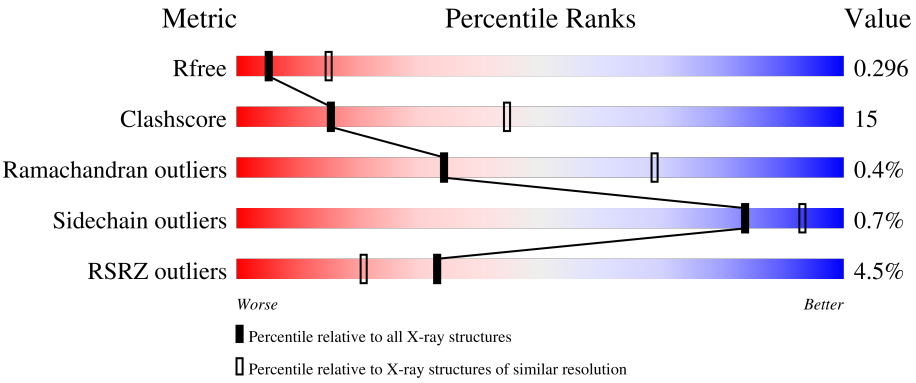
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	544	7% 64% 27% • 8%
1	E	544	% 60% 30% • 9%
1	K	544	8% 61% 30% • 8%
1	O	544	2% 61% 30% • 8%
2	B	572	5% 65% 27% • 7%

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Mol	Chain	Length	Quality of chain
2	F	572	2% 67% 26% 6%
2	L	572	8% 66% 26% 7%
2	P	572	3% 63% 29% 7%
3	C	30	33% 30% 37%
3	G	30	47% 20% 33%
3	M	30	33% 30% 37%
3	Q	30	47% 20% 33%
4	D	15	40% 53% 7%
4	H	15	60% 33% 7%
4	N	15	47% 47% 7%
4	R	15	60% 40%
5	J	28	64% 36%
5	T	28	4% 71% 29%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 36383 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4027	2576	681	752	18			
1	E	497	Total	C	N	O	S	0	0	0
			4015	2569	683	745	18			
1	K	502	Total	C	N	O	S	0	0	0
			4052	2590	686	758	18			
1	O	498	Total	C	N	O	S	0	0	0
			4023	2575	684	746	18			

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	531	Total	C	N	O	S	0	0	0
			4248	2720	715	790	23			
2	F	537	Total	C	N	O	S	0	0	0
			4282	2736	720	803	23			
2	L	530	Total	C	N	O	S	0	0	0
			4238	2712	715	788	23			
2	P	531	Total	C	N	O	S	0	0	0
			4242	2714	713	792	23			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP P13010
B	-15	HIS	-	expression tag	UNP P13010
B	-14	HIS	-	expression tag	UNP P13010
B	-13	HIS	-	expression tag	UNP P13010
B	-12	HIS	-	expression tag	UNP P13010
B	-11	HIS	-	expression tag	UNP P13010
B	-10	HIS	-	expression tag	UNP P13010
B	-9	HIS	-	expression tag	UNP P13010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP P13010
B	-7	HIS	-	expression tag	UNP P13010
B	-6	HIS	-	expression tag	UNP P13010
B	-5	GLU	-	expression tag	UNP P13010
B	-4	ASN	-	expression tag	UNP P13010
B	-3	LEU	-	expression tag	UNP P13010
B	-2	TYR	-	expression tag	UNP P13010
B	-1	PHE	-	expression tag	UNP P13010
B	0	GLN	-	expression tag	UNP P13010
B	1	GLY	-	expression tag	UNP P13010
F	-16	MET	-	initiating methionine	UNP P13010
F	-15	HIS	-	expression tag	UNP P13010
F	-14	HIS	-	expression tag	UNP P13010
F	-13	HIS	-	expression tag	UNP P13010
F	-12	HIS	-	expression tag	UNP P13010
F	-11	HIS	-	expression tag	UNP P13010
F	-10	HIS	-	expression tag	UNP P13010
F	-9	HIS	-	expression tag	UNP P13010
F	-8	HIS	-	expression tag	UNP P13010
F	-7	HIS	-	expression tag	UNP P13010
F	-6	HIS	-	expression tag	UNP P13010
F	-5	GLU	-	expression tag	UNP P13010
F	-4	ASN	-	expression tag	UNP P13010
F	-3	LEU	-	expression tag	UNP P13010
F	-2	TYR	-	expression tag	UNP P13010
F	-1	PHE	-	expression tag	UNP P13010
F	0	GLN	-	expression tag	UNP P13010
F	1	GLY	-	expression tag	UNP P13010
L	-16	MET	-	initiating methionine	UNP P13010
L	-15	HIS	-	expression tag	UNP P13010
L	-14	HIS	-	expression tag	UNP P13010
L	-13	HIS	-	expression tag	UNP P13010
L	-12	HIS	-	expression tag	UNP P13010
L	-11	HIS	-	expression tag	UNP P13010
L	-10	HIS	-	expression tag	UNP P13010
L	-9	HIS	-	expression tag	UNP P13010
L	-8	HIS	-	expression tag	UNP P13010
L	-7	HIS	-	expression tag	UNP P13010
L	-6	HIS	-	expression tag	UNP P13010
L	-5	GLU	-	expression tag	UNP P13010
L	-4	ASN	-	expression tag	UNP P13010
L	-3	LEU	-	expression tag	UNP P13010

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	TYR	-	expression tag	UNP P13010
L	-1	PHE	-	expression tag	UNP P13010
L	0	GLN	-	expression tag	UNP P13010
L	1	GLY	-	expression tag	UNP P13010
P	-16	MET	-	initiating methionine	UNP P13010
P	-15	HIS	-	expression tag	UNP P13010
P	-14	HIS	-	expression tag	UNP P13010
P	-13	HIS	-	expression tag	UNP P13010
P	-12	HIS	-	expression tag	UNP P13010
P	-11	HIS	-	expression tag	UNP P13010
P	-10	HIS	-	expression tag	UNP P13010
P	-9	HIS	-	expression tag	UNP P13010
P	-8	HIS	-	expression tag	UNP P13010
P	-7	HIS	-	expression tag	UNP P13010
P	-6	HIS	-	expression tag	UNP P13010
P	-5	GLU	-	expression tag	UNP P13010
P	-4	ASN	-	expression tag	UNP P13010
P	-3	LEU	-	expression tag	UNP P13010
P	-2	TYR	-	expression tag	UNP P13010
P	-1	PHE	-	expression tag	UNP P13010
P	0	GLN	-	expression tag	UNP P13010
P	1	GLY	-	expression tag	UNP P13010

- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*G P*GP*CP*CP*CP*GP*AP*TP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	19	Total	C	N	O	P	0	0	0
			393	185	76	113	19			
3	G	20	Total	C	N	O	P	0	0	0
			412	194	79	119	20			
3	M	19	Total	C	N	O	P	0	0	0
			393	185	76	113	19			
3	Q	20	Total	C	N	O	P	0	0	0
			412	194	79	119	20			

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*GP*GP*CP*CP*CP*TP*CP*GP*AP *TP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	14	Total	C	N	O	P	0	0	0
			285	134	52	85	14			

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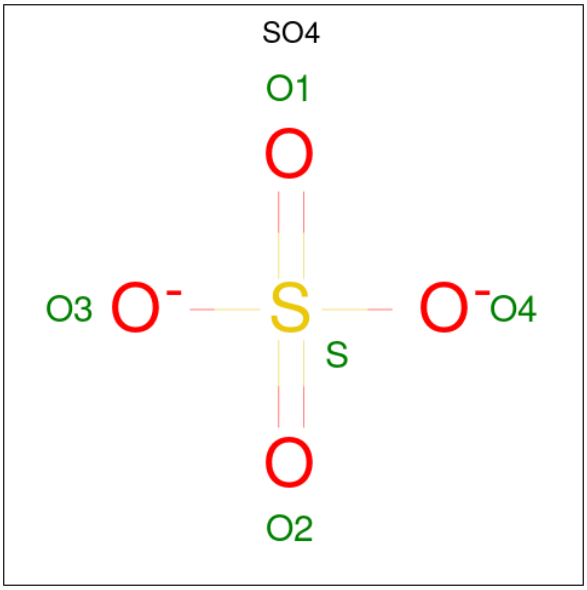
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	15	Total	C	N	O	P	0	0	0
			304	143	55	91	15			
4	N	14	Total	C	N	O	P	0	0	0
			285	134	52	85	14			
4	R	15	Total	C	N	O	P	0	0	0
			304	143	55	91	15			

- Molecule 5 is a protein called Protein PAXX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	J	28	Total	C	N	O	S	0	0	0
			214	132	41	40	1			
5	T	28	Total	C	N	O	S	0	0	0
			214	132	41	40	1			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	O	S		0	0
			5	4	1			
6	F	1	Total	O	S		0	0
			5	4	1			
6	K	1	Total	O	S		0	0
			5	4	1			
6	P	1	Total	O	S		0	0
			5	4	1			

- Molecule 7 is water.

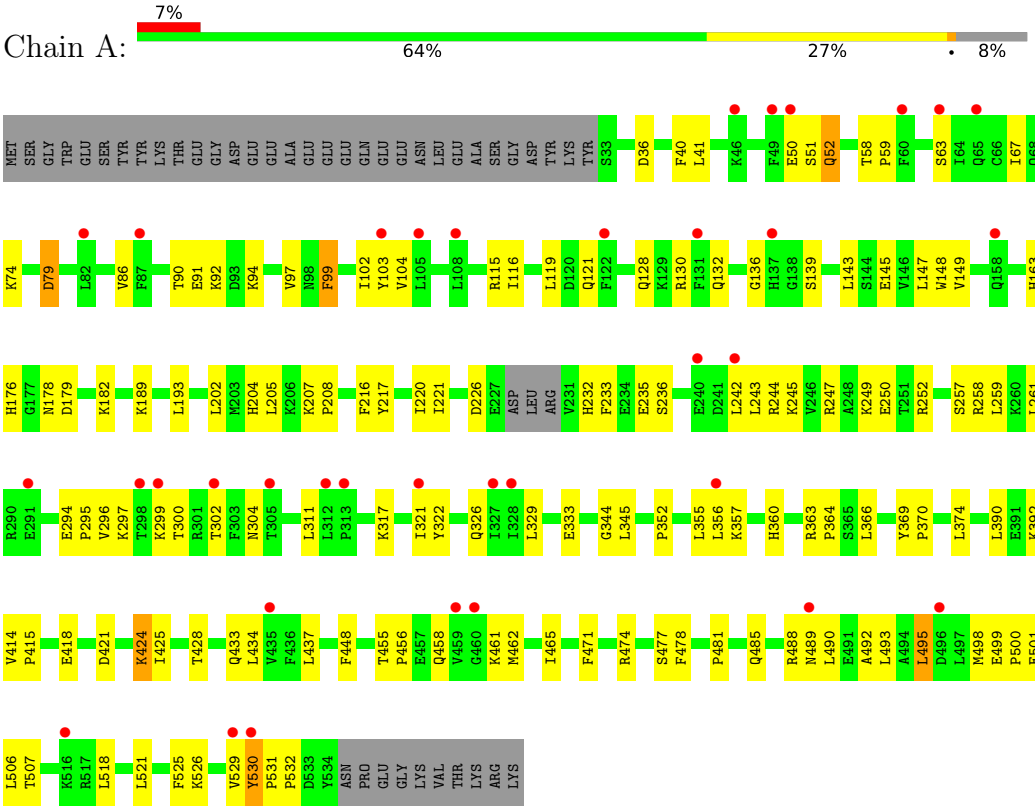
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O 1 1	0	0
7	E	6	Total O 6 6	0	0
7	F	3	Total O 3 3	0	0
7	K	4	Total O 4 4	0	0
7	L	2	Total O 2 2	0	0
7	N	1	Total O 1 1	0	0
7	O	3	Total O 3 3	0	0

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.

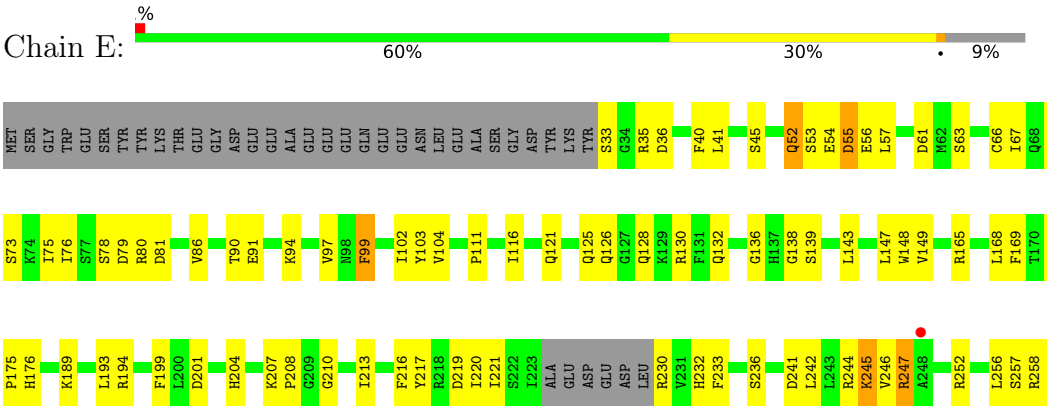
• Molecule 1: X-ray repair cross-complementing protein 6

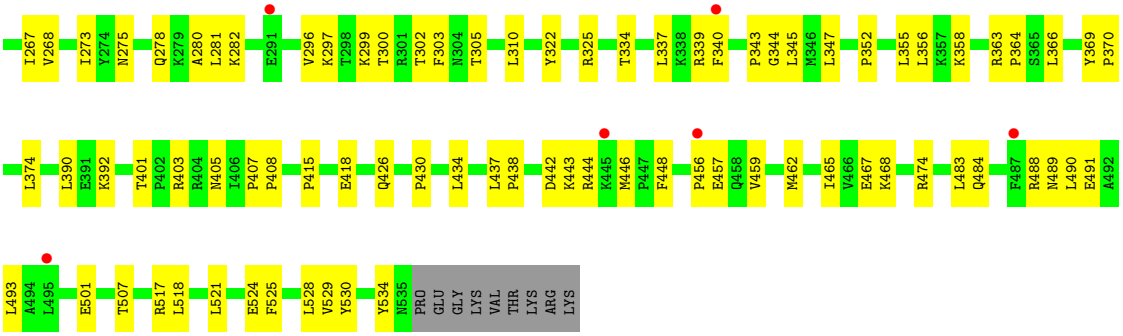
Chain A:



• Molecule 1: X-ray repair cross-complementing protein 6

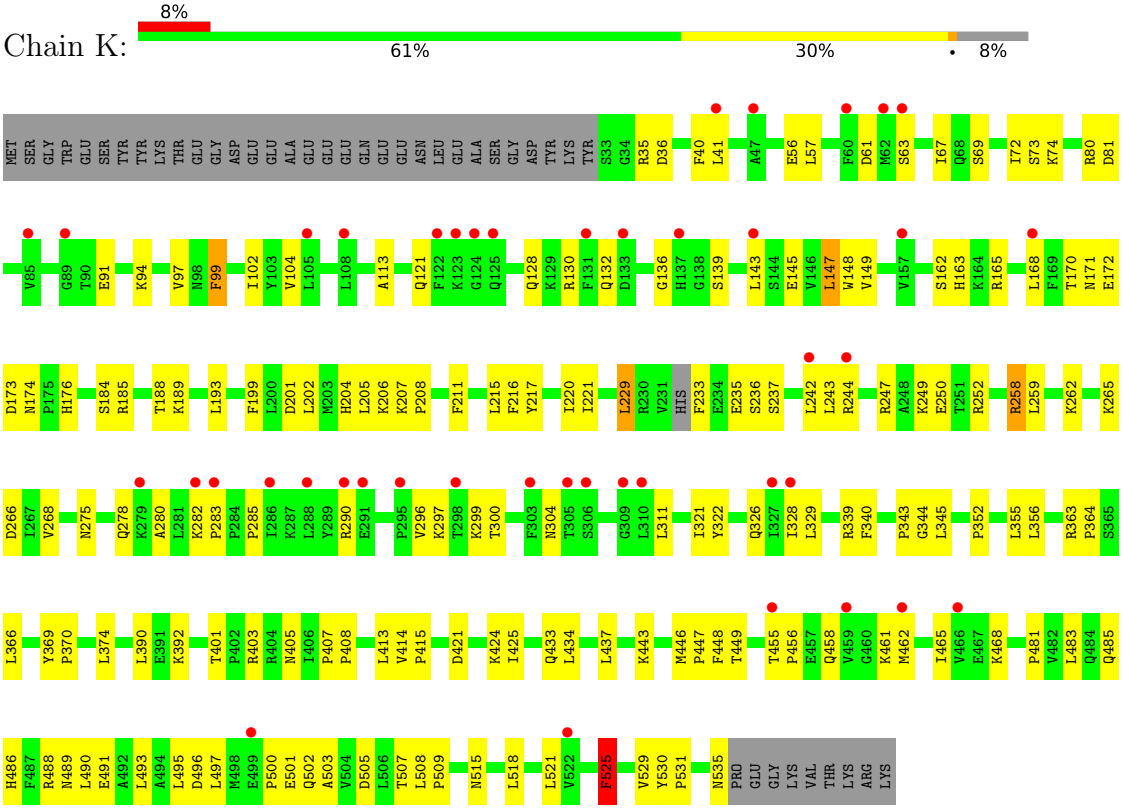
Chain E:





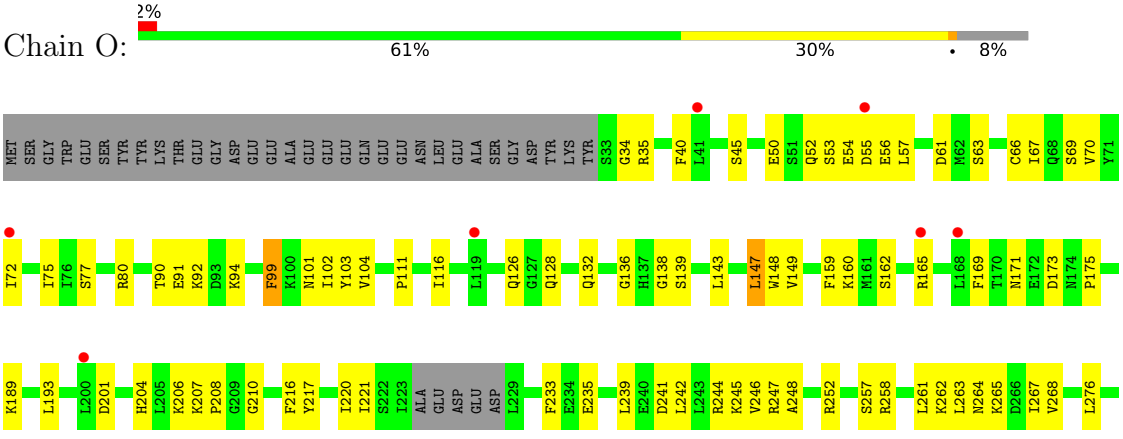
• Molecule 1: X-ray repair cross-complementing protein 6

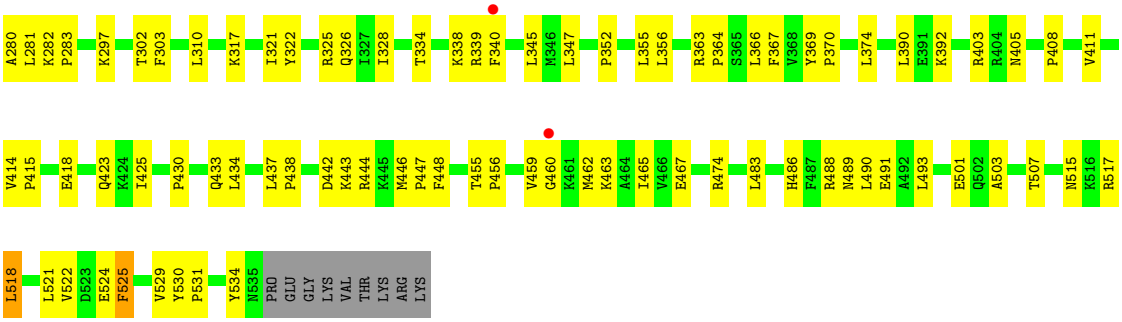
Chain K:



• Molecule 1: X-ray repair cross-complementing protein 6

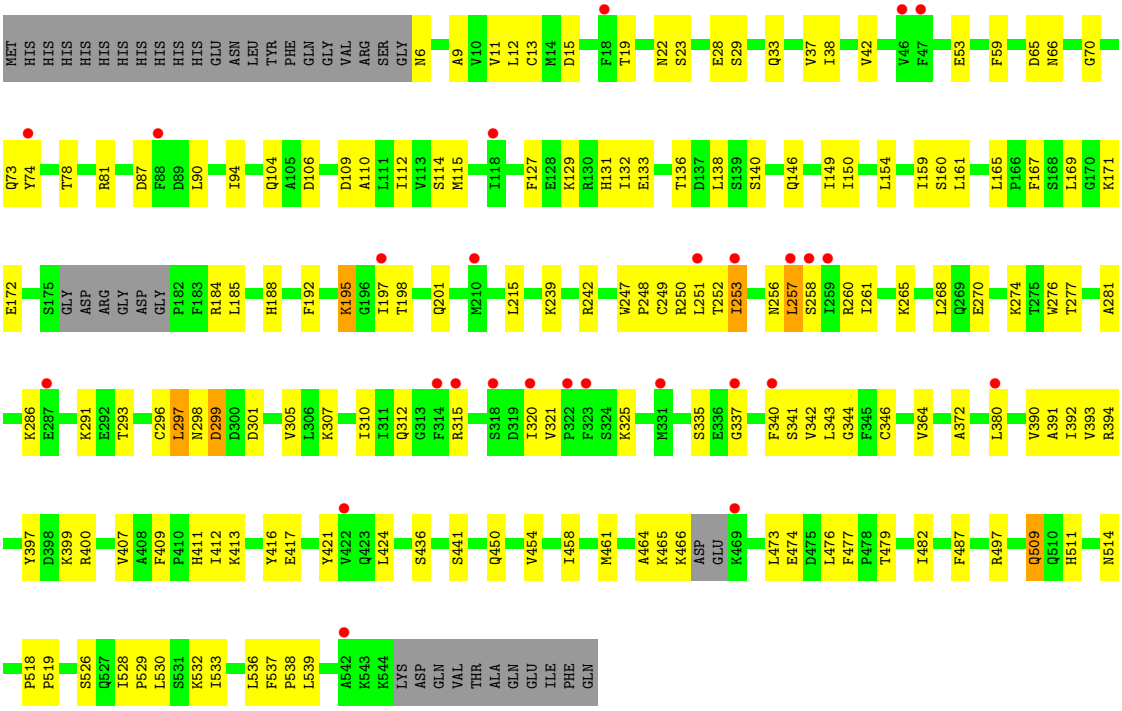
Chain O:





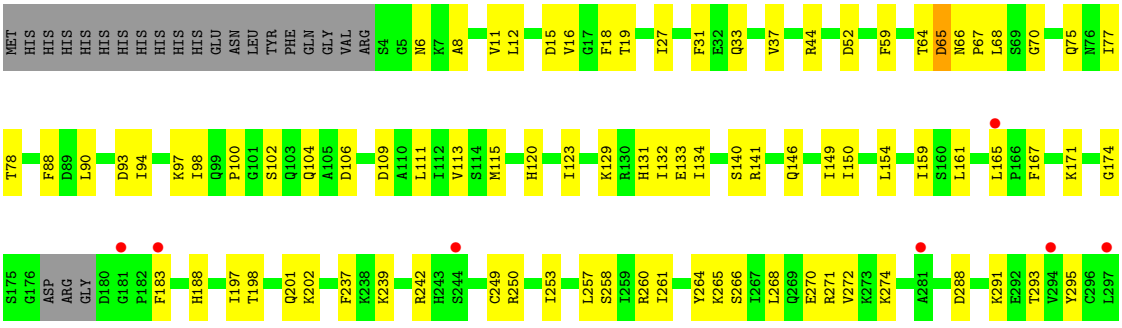
• Molecule 2: X-ray repair cross-complementing protein 5

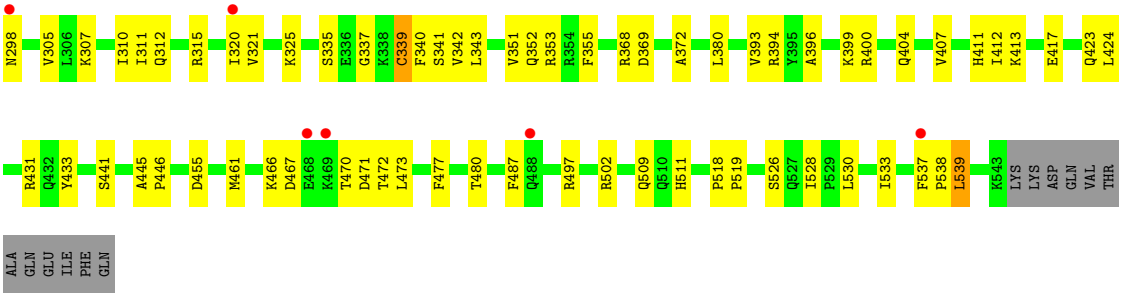
Chain B:



• Molecule 2: X-ray repair cross-complementing protein 5

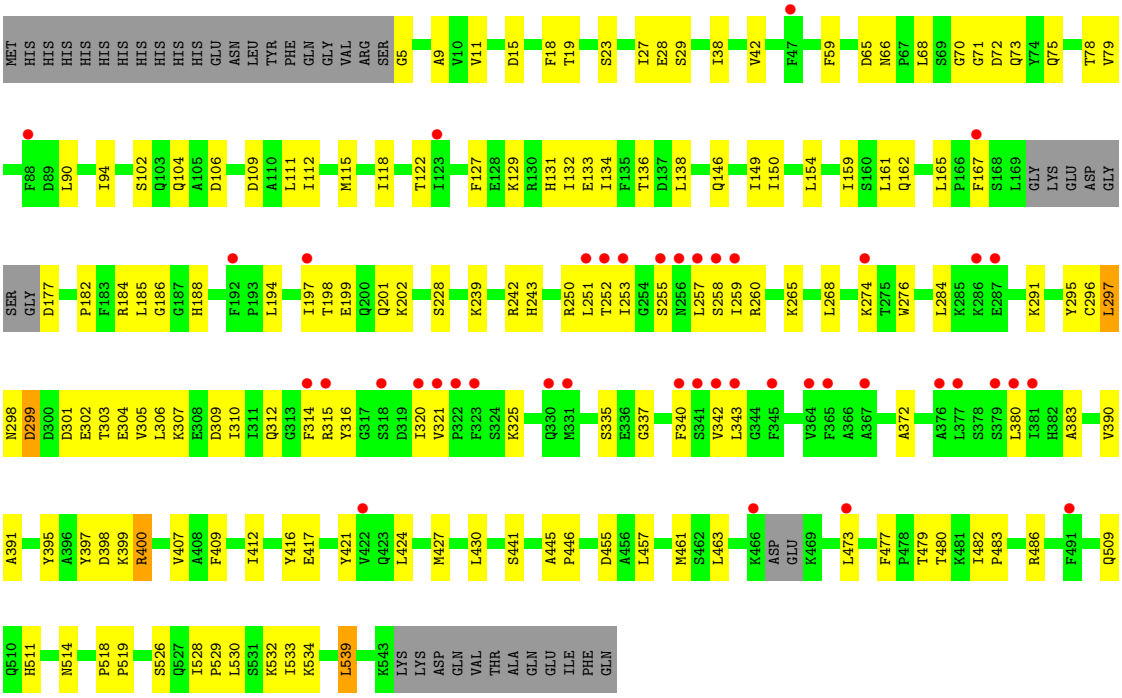
Chain F:





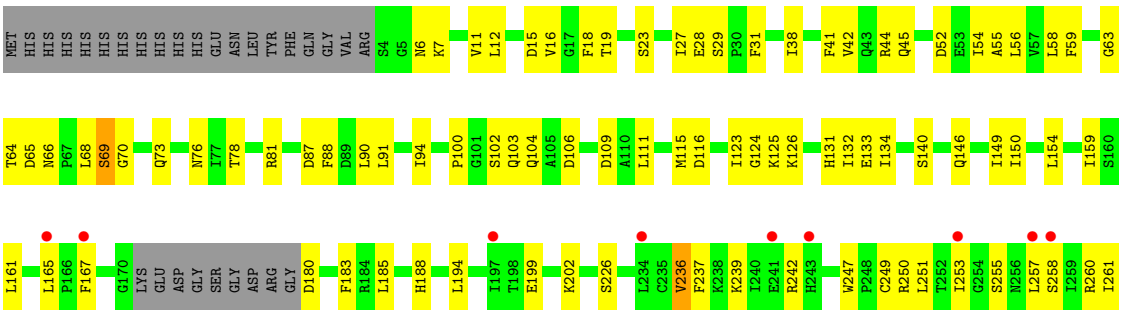
• Molecule 2: X-ray repair cross-complementing protein 5

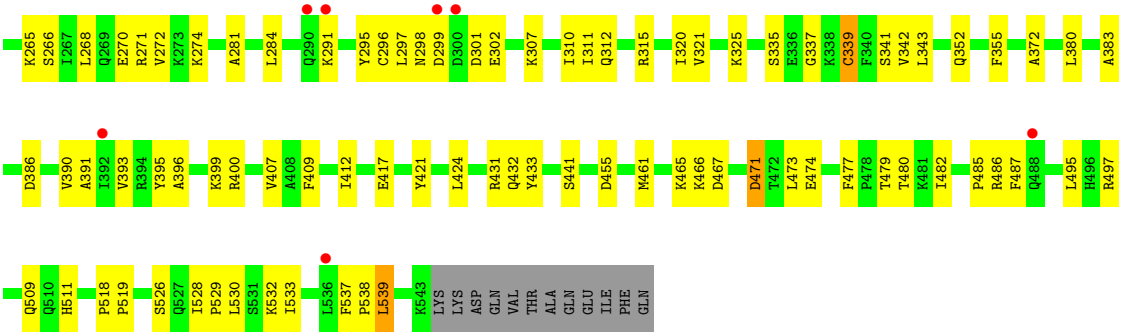
Chain L:



• Molecule 2: X-ray repair cross-complementing protein 5

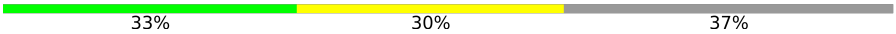
Chain P:

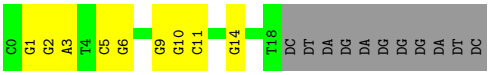




• Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*AP*TP*AP*T)-3')

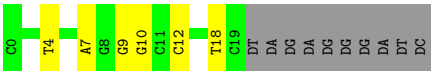
Chain C:





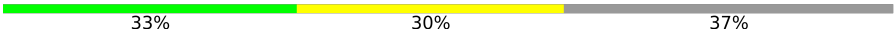
• Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*AP*TP*AP*T)-3')

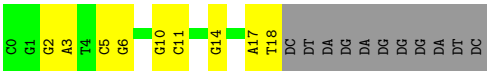
Chain G:



• Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*AP*TP*AP*T)-3')

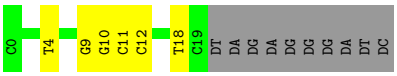
Chain M:





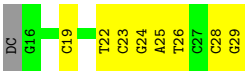
• Molecule 3: DNA (5'-D(P*CP*GP*GP*AP*TP*CP*GP*AP*GP*GP*GP*CP*CP*CP*GP*AP*TP*AP*T)-3')

Chain Q:



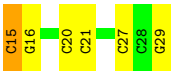
• Molecule 4: DNA (5'-D(P*GP*GP*GP*CP*CP*CP*TP*CP*GP*AP*TP*CP*CP*G)-3')

Chain D:



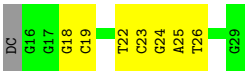
• Molecule 4: DNA (5'-D(P*GP*GP*GP*CP*CP*CP*TP*CP*GP*AP*TP*CP*CP*G)-3')

Chain H:



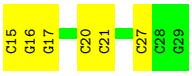
• Molecule 4: DNA (5'-D(P*GP*GP*GP*CP*CP*CP*TP*CP*GP*AP*TP*CP*CP*G)-3')

Chain N:



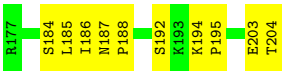
• Molecule 4: DNA (5'-D(P*GP*GP*GP*CP*CP*CP*TP*CP*GP*AP*TP*CP*CP*G)-3')

Chain R:



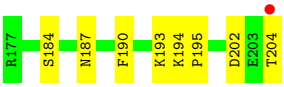
• Molecule 5: Protein PAXX

Chain J:



• Molecule 5: Protein PAXX

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.02Å 428.57Å 96.06Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	45.32 – 2.95 47.73 – 2.95	Depositor EDS
% Data completeness (in resolution range)	23.9 (45.32-2.95) 21.9 (47.73-2.95)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.252 , 0.298 0.253 , 0.296	Depositor DCC
R_{free} test set	2001 reflections (5.85%)	wwPDB-VP
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	1.703	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.358 for h,-k,-l	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	36383	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.37	0/4105	0.75	4/5529 (0.1%)
1	E	0.33	0/4093	0.71	0/5512
1	K	0.37	0/4129	0.75	3/5561 (0.1%)
1	O	0.37	1/4101 (0.0%)	0.74	1/5523 (0.0%)
2	B	0.34	0/4334	0.70	4/5842 (0.1%)
2	F	0.33	0/4369	0.70	2/5892 (0.0%)
2	L	0.35	1/4324 (0.0%)	0.68	3/5831 (0.1%)
2	P	0.32	0/4329	0.69	1/5840 (0.0%)
3	C	0.50	0/441	0.84	0/679
3	G	0.55	0/462	0.83	0/711
3	M	0.51	0/441	0.86	0/679
3	Q	0.54	0/462	0.84	0/711
4	D	0.56	0/318	0.88	0/488
4	H	0.59	0/339	0.94	1/520 (0.2%)
4	N	0.56	0/318	0.86	0/488
4	R	0.62	0/339	0.92	0/520
5	J	0.25	0/218	0.59	0/290
5	T	0.27	0/218	0.58	0/290
All	All	0.37	2/37340 (0.0%)	0.73	19/50906 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	F	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	400	ARG	CB-CG	-5.52	1.37	1.52
1	O	525	PHE	CE2-CZ	5.30	1.47	1.37

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	495	LEU	CB-CG-CD2	8.39	125.27	111.00
2	F	339	CYS	CA-CB-SG	8.08	128.54	114.00
2	P	339	CYS	CA-CB-SG	7.54	127.58	114.00
1	K	258	ARG	CG-CD-NE	7.42	127.37	111.80
2	L	400	ARG	NE-CZ-NH2	-6.73	116.94	120.30
2	B	253	ILE	CG1-CB-CG2	-6.34	97.45	111.40
2	F	141	ARG	CG-CD-NE	6.04	124.49	111.80
2	B	257	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	424	LYS	CD-CE-NZ	6.02	125.54	111.70
2	L	400	ARG	CG-CD-NE	-5.71	99.80	111.80
1	K	147	LEU	CB-CG-CD1	5.39	120.16	111.00
1	K	525	PHE	CD1-CE1-CZ	-5.38	113.65	120.10
1	A	499	GLU	N-CA-C	-5.34	96.59	111.00
2	B	297	LEU	CA-CB-CG	5.27	127.41	115.30
2	L	297	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	79	ASP	CB-CG-OD2	-5.12	113.69	118.30
2	B	195	LYS	CA-CB-CG	-5.08	102.22	113.40
4	H	15	DC	O4'-C1'-N1	5.04	111.53	108.00
1	O	147	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	65	ASP	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4101	148	0
1	E	4015	0	4099	156	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	4052	0	4128	166	0
1	O	4023	0	4110	163	0
2	B	4248	0	4299	125	0
2	F	4282	0	4312	127	0
2	L	4238	0	4281	121	0
2	P	4242	0	4278	133	0
3	C	393	0	213	13	0
3	G	412	0	224	11	0
3	M	393	0	213	18	0
3	Q	412	0	224	10	0
4	D	285	0	157	10	0
4	H	304	0	168	10	0
4	N	285	0	157	8	0
4	R	304	0	168	8	0
5	J	214	0	212	11	0
5	T	214	0	212	9	0
6	A	5	0	0	0	0
6	F	5	0	0	0	0
6	K	5	0	0	0	0
6	P	5	0	0	0	0
7	B	1	0	0	0	0
7	E	6	0	0	0	0
7	F	3	0	0	0	0
7	K	4	0	0	1	0
7	L	2	0	0	0	0
7	N	1	0	0	0	0
7	O	3	0	0	0	0
All	All	36383	0	35556	1063	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1063) 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)
2:F:250:ARG:HD3	2:F:258:SER:HB3	1.37	1.06
2:L:400:ARG:NH2	3:M:10:DG:O3'	1.93	1.02
1:O:339:ARG:HA	1:O:405:ASN:HA	1.44	0.99
1:A:207:LYS:HD2	1:A:208:PRO:HD2	1.48	0.96
1:A:493:LEU:HD13	2:B:321:VAL:HG11	1.46	0.96
1:K:493:LEU:HD13	2:L:321:VAL:HG11	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:72:ILE:HD11	1:O:245:LYS:HG2	1.44	0.96
1:O:207:LYS:HD2	1:O:208:PRO:HD2	1.50	0.94
1:O:493:LEU:HD13	2:P:321:VAL:HG11	1.48	0.94
1:K:300:THR:HG21	2:L:291:LYS:HE3	1.49	0.93
2:L:27:ILE:HD11	2:L:182:PRO:HB2	1.51	0.91
1:E:207:LYS:HD2	1:E:208:PRO:HD2	1.53	0.90
1:E:493:LEU:HD13	2:F:321:VAL:HG11	1.51	0.90
2:L:400:ARG:HH22	3:M:10:DG:H4'	1.36	0.90
2:F:70:GLY:HA3	1:K:148:TRP:HE1	1.35	0.89
1:K:207:LYS:HD2	1:K:208:PRO:HD2	1.56	0.87
3:C:2:DG:H1	4:D:26:DT:H3	1.22	0.86
3:M:2:DG:H1	4:N:26:DT:H3	1.24	0.86
1:K:102:ILE:HG21	1:K:149:VAL:HG11	1.58	0.85
2:L:400:ARG:NH2	3:M:10:DG:H4'	1.90	0.85
1:K:339:ARG:HA	1:K:405:ASN:HA	1.56	0.84
1:E:165:ARG:NH1	1:E:201:ASP:OD2	2.08	0.84
1:O:488:ARG:HH11	1:O:501:GLU:HG3	1.42	0.84
1:K:275:ASN:HD22	1:K:278:GLN:HG3	1.42	0.83
3:M:6:DG:H1	4:N:22:DT:H3	1.25	0.83
1:K:488:ARG:HH11	1:K:501:GLU:HG2	1.43	0.83
2:B:66:ASN:ND2	2:B:74:TYR:O	2.12	0.81
1:A:97:VAL:HG21	1:A:148:TRP:HZ3	1.44	0.81
2:P:65:ASP:HB2	2:P:78:THR:HG23	1.60	0.81
1:A:488:ARG:HB3	1:A:501:GLU:HB2	1.60	0.81
1:E:302:THR:HG22	2:F:291:LYS:HG3	1.62	0.81
1:A:392:LYS:HD2	2:B:458:ILE:HD12	1.60	0.81
1:E:72:ILE:HD11	1:E:245:LYS:HG2	1.61	0.81
1:K:99:PHE:CE2	1:K:145:GLU:HG2	2.16	0.80
2:P:6:ASN:HB2	2:P:242:ARG:HG2	1.63	0.80
1:O:263:LEU:HD22	1:O:347:LEU:HD22	1.64	0.80
2:B:171:LYS:HB3	2:B:192:PHE:HZ	1.45	0.80
1:A:363:ARG:HG2	1:A:364:PRO:HD2	1.65	0.79
2:B:6:ASN:HB2	2:B:242:ARG:HG2	1.62	0.79
1:K:363:ARG:HG2	1:K:364:PRO:HD2	1.65	0.79
1:K:465:ILE:HG13	1:K:525:PHE:HE2	1.45	0.79
1:E:194:ARG:NH2	1:E:219:ASP:O	2.16	0.78
1:E:300:THR:HG23	2:F:293:THR:HG22	1.66	0.78
2:B:411:HIS:NE2	2:B:416:TYR:OH	2.15	0.78
1:E:247:ARG:NH1	1:E:488:ARG:HG3	1.98	0.77
2:L:197:ILE:HG12	2:L:202:LYS:HG3	1.66	0.77
2:F:400:ARG:HD2	3:G:12:DC:H4'	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ILE:HG21	1:A:149:VAL:HG11	1.67	0.77
2:B:253:ILE:HA	2:B:342:VAL:HG12	1.67	0.77
2:P:123:ILE:O	2:P:126:LYS:NZ	2.18	0.76
1:E:97:VAL:HG21	1:E:148:TRP:HZ3	1.49	0.76
2:F:123:ILE:HD11	1:K:184:SER:HB2	1.66	0.76
1:A:36:ASP:OD1	1:A:163:HIS:HB2	1.84	0.76
2:L:5:GLY:HA3	2:L:242:ARG:HA	1.68	0.76
2:B:65:ASP:HB3	2:B:78:THR:HG23	1.68	0.76
1:E:258:ARG:HD2	1:E:374:LEU:HD11	1.67	0.76
1:E:263:LEU:HD22	1:E:347:LEU:HD22	1.68	0.75
1:A:526:LYS:HD3	2:B:256:ASN:HB3	1.68	0.75
2:B:335:SER:OG	2:B:399:LYS:O	2.04	0.75
2:L:199:GLU:HA	2:L:202:LYS:HE3	1.67	0.75
1:E:247:ARG:NH2	1:E:491:GLU:OE2	2.19	0.75
1:A:258:ARG:HD2	1:A:374:LEU:HD11	1.69	0.74
2:L:65:ASP:HB3	2:L:78:THR:HG23	1.69	0.74
1:A:300:THR:HG21	2:B:291:LYS:HE3	1.69	0.74
2:L:337:GLY:HA2	2:L:399:LYS:HG2	1.69	0.74
2:F:253:ILE:HA	2:F:342:VAL:HG12	1.68	0.74
1:A:217:TYR:HA	1:A:220:ILE:HG12	1.68	0.74
1:E:102:ILE:HG21	1:E:149:VAL:HG11	1.69	0.74
1:K:390:LEU:HG	1:K:415:PRO:HB2	1.70	0.74
1:K:57:LEU:HB3	1:K:61:ASP:HB3	1.70	0.73
2:P:253:ILE:HA	2:P:342:VAL:HG12	1.69	0.73
1:K:262:LYS:HE2	1:K:265:LYS:HA	1.70	0.73
1:E:217:TYR:HA	1:E:220:ILE:HG12	1.71	0.73
1:O:126:GLN:N	1:O:126:GLN:OE1	2.22	0.73
1:O:217:TYR:HA	1:O:220:ILE:HG12	1.71	0.73
2:P:335:SER:OG	2:P:399:LYS:O	2.06	0.73
1:K:465:ILE:HG13	1:K:525:PHE:CE2	2.22	0.73
4:R:15:DC:H4'	4:R:16:DG:H5'	1.71	0.73
1:E:126:GLN:OE1	1:E:126:GLN:N	2.22	0.72
2:L:335:SER:OG	2:L:399:LYS:O	2.07	0.72
1:E:488:ARG:HB3	1:E:501:GLU:O	1.90	0.72
1:A:233:PHE:CD2	1:A:245:LYS:HE2	2.24	0.72
1:E:363:ARG:HG2	1:E:364:PRO:HD2	1.70	0.72
1:K:36:ASP:OD1	1:K:162:SER:OG	2.08	0.72
1:A:97:VAL:HG21	1:A:148:TRP:CZ3	2.25	0.71
2:F:64:THR:OG1	2:F:75:GLN:O	2.07	0.71
2:F:70:GLY:HA3	1:K:148:TRP:NE1	2.05	0.71
1:K:247:ARG:HA	1:K:250:GLU:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:363:ARG:HG2	1:O:364:PRO:HD2	1.71	0.71
1:A:495:LEU:HB3	1:A:498:MET:HG3	1.72	0.71
2:F:339:CYS:HB3	2:F:396:ALA:O	1.91	0.71
2:B:315:ARG:HG2	2:B:320:ILE:HG22	1.73	0.71
1:E:488:ARG:HH11	1:E:501:GLU:HG3	1.54	0.71
2:F:249:CYS:SG	2:F:250:ARG:N	2.63	0.71
2:L:19:THR:H	2:L:104:GLN:HE22	1.36	0.70
2:L:315:ARG:HG2	2:L:320:ILE:HG22	1.73	0.70
3:M:5:DC:O2	4:N:24:DG:N2	2.24	0.70
1:A:217:TYR:HD1	1:A:220:ILE:HD11	1.56	0.70
1:O:525:PHE:CD1	1:O:525:PHE:N	2.56	0.70
1:E:97:VAL:HG21	1:E:148:TRP:CZ3	2.27	0.70
1:K:204:HIS:HE1	1:K:233:PHE:CD1	2.10	0.70
1:K:340:PHE:CZ	2:L:486:ARG:HA	2.27	0.70
1:K:262:LYS:HG3	1:K:268:VAL:HG22	1.74	0.69
2:P:337:GLY:HA3	2:P:399:LYS:HG3	1.74	0.69
1:A:202:LEU:O	1:A:233:PHE:HZ	1.74	0.69
2:F:335:SER:OG	2:F:399:LYS:O	2.11	0.69
1:O:258:ARG:HD2	1:O:374:LEU:HD11	1.74	0.69
2:P:19:THR:H	2:P:104:GLN:NE2	1.90	0.69
1:A:489:ASN:O	1:A:493:LEU:HG	1.93	0.69
1:O:460:GLY:O	1:O:463:LYS:HB2	1.92	0.69
2:B:136:THR:HG23	2:B:138:LEU:HD12	1.73	0.69
1:O:102:ILE:HG21	1:O:149:VAL:HG11	1.75	0.69
1:O:165:ARG:NH1	1:O:201:ASP:OD2	2.23	0.69
1:A:529:VAL:O	1:A:531:PRO:HD3	1.92	0.69
1:A:465:ILE:HD11	1:A:525:PHE:HD2	1.58	0.68
1:E:217:TYR:HD1	1:E:220:ILE:HD11	1.58	0.68
1:K:217:TYR:HA	1:K:220:ILE:HG12	1.76	0.68
2:F:90:LEU:O	2:F:94:ILE:HG13	1.94	0.68
2:L:136:THR:HG23	2:L:138:LEU:HD12	1.74	0.68
1:O:462:MET:HG2	2:P:380:LEU:HA	1.76	0.67
2:B:19:THR:H	2:B:104:GLN:NE2	1.92	0.67
1:K:352:PRO:HG2	2:L:473:LEU:HD21	1.76	0.67
2:L:90:LEU:O	2:L:94:ILE:HG13	1.94	0.67
1:K:97:VAL:HG21	1:K:148:TRP:CZ3	2.29	0.67
2:L:66:ASN:HA	2:L:79:VAL:HG12	1.77	0.67
3:C:5:DC:O2	4:D:24:DG:N2	2.27	0.67
2:L:265:LYS:HD3	2:L:268:LEU:HD13	1.77	0.67
1:O:262:LYS:HE2	1:O:265:LYS:HA	1.76	0.67
2:B:261:ILE:HD13	2:B:364:VAL:HG13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:SER:OG	1:A:247:ARG:NH2	2.25	0.67
2:F:19:THR:H	2:F:104:GLN:NE2	1.92	0.66
2:L:19:THR:H	2:L:104:GLN:NE2	1.93	0.66
2:B:346:CYS:SG	2:B:392:ILE:HD11	2.36	0.66
1:K:233:PHE:HA	1:K:424:LYS:HB2	1.75	0.66
2:B:337:GLY:HA2	2:B:399:LYS:HG2	1.77	0.66
2:B:19:THR:H	2:B:104:GLN:HE22	1.44	0.66
1:K:74:LYS:NZ	1:K:81:ASP:OD2	2.27	0.66
1:E:275:ASN:HD22	1:E:278:GLN:HG3	1.60	0.66
1:E:339:ARG:HA	1:E:405:ASN:HA	1.78	0.66
1:A:493:LEU:HD13	2:B:321:VAL:CG1	2.24	0.66
1:O:217:TYR:HD1	1:O:220:ILE:HD11	1.61	0.66
2:L:301:ASP:O	2:L:303:THR:N	2.30	0.65
1:K:35:ARG:HG2	1:K:80:ARG:HB3	1.79	0.65
2:B:253:ILE:HA	2:B:342:VAL:CG1	2.26	0.65
1:E:244:ARG:HD2	5:J:195:PRO:HG3	1.79	0.65
2:P:249:CYS:SG	2:P:250:ARG:N	2.69	0.65
2:P:339:CYS:HB3	2:P:396:ALA:O	1.96	0.65
1:A:363:ARG:CG	1:A:364:PRO:HD2	2.27	0.65
1:E:390:LEU:HG	1:E:415:PRO:HB2	1.79	0.65
1:K:525:PHE:N	1:K:525:PHE:CD1	2.64	0.65
1:K:535:ASN:ND2	7:K:701:HOH:O	2.29	0.65
1:O:94:LYS:O	1:O:104:VAL:HG12	1.97	0.65
1:A:244:ARG:NH2	1:A:421:ASP:OD2	2.29	0.65
1:K:258:ARG:HD2	1:K:374:LEU:HD11	1.77	0.64
2:B:131:HIS:CE1	2:B:239:LYS:HG3	2.32	0.64
2:B:454:VAL:O	2:B:458:ILE:HG12	1.98	0.64
1:E:57:LEU:HB3	1:E:61:ASP:HB3	1.80	0.64
2:F:197:ILE:HG12	2:F:202:LYS:HG3	1.78	0.64
1:E:91:GLU:HG2	1:E:136:GLY:HA3	1.78	0.64
1:A:207:LYS:CD	1:A:208:PRO:HD2	2.24	0.64
1:E:52:GLN:OE1	1:E:208:PRO:HD3	1.97	0.64
1:O:77:SER:HA	1:O:248:ALA:O	1.97	0.64
2:B:184:ARG:HD3	2:B:514:ASN:ND2	2.13	0.64
1:E:443:LYS:HD2	2:F:480:THR:HB	1.80	0.64
1:K:204:HIS:CD2	1:K:235:GLU:HA	2.33	0.64
1:K:449:THR:H	2:L:416:TYR:HE1	1.44	0.64
1:O:302:THR:HG23	2:P:291:LYS:HE3	1.77	0.64
2:L:9:ALA:HB2	2:L:127:PHE:CD1	2.32	0.64
1:K:485:GLN:OE1	1:K:503:ALA:N	2.19	0.64
2:P:431:ARG:NH1	3:Q:4:DT:OP1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASN:O	1:A:207:LYS:HD3	1.99	0.63
1:E:241:ASP:HB3	5:J:185:LEU:HD23	1.81	0.63
2:P:90:LEU:O	2:P:94:ILE:HG13	1.98	0.63
1:A:357:LYS:HB2	1:A:360:HIS:CD2	2.34	0.63
2:F:131:HIS:CE1	2:F:239:LYS:HG3	2.33	0.63
2:L:184:ARG:HD3	2:L:514:ASN:ND2	2.13	0.63
1:E:247:ARG:CZ	1:E:488:ARG:HG3	2.28	0.63
2:F:146:GLN:HG2	2:F:149:ILE:HD13	1.80	0.63
1:K:363:ARG:CG	1:K:364:PRO:HD2	2.28	0.63
1:K:449:THR:N	2:L:416:TYR:HE1	1.97	0.63
1:O:147:LEU:HB3	1:O:193:LEU:HD11	1.79	0.63
2:L:28:GLU:HB2	2:L:185:LEU:HD11	1.81	0.62
1:O:52:GLN:NE2	1:O:206:LYS:O	2.31	0.62
1:O:518:LEU:HD22	1:O:521:LEU:HD13	1.80	0.62
1:A:488:ARG:HD2	1:A:503:ALA:HB2	1.81	0.62
2:F:249:CYS:HB3	2:F:261:ILE:HD11	1.81	0.62
1:O:340:PHE:CZ	2:P:486:ARG:HA	2.35	0.62
1:O:363:ARG:CG	1:O:364:PRO:HD2	2.29	0.62
1:A:525:PHE:O	1:A:529:VAL:HG22	2.00	0.62
2:L:400:ARG:CZ	3:M:10:DG:H4'	2.30	0.62
2:F:315:ARG:HG2	2:F:320:ILE:HG22	1.81	0.62
1:O:217:TYR:O	1:O:221:ILE:HG12	2.00	0.62
1:E:488:ARG:HG2	1:E:501:GLU:HG3	1.81	0.62
5:T:184:SER:HB3	5:T:187:ASN:O	1.99	0.62
1:E:456:PRO:HA	1:E:459:VAL:HG22	1.82	0.62
2:F:342:VAL:HA	2:F:393:VAL:HG22	1.82	0.62
1:E:232:HIS:CE1	1:E:236:SER:HA	2.34	0.61
1:O:462:MET:HB3	2:P:383:ALA:HB2	1.82	0.61
1:O:534:TYR:OH	2:P:260:ARG:HD3	2.00	0.61
1:A:304:ASN:HD21	1:A:311:LEU:HD13	1.65	0.61
2:B:412:ILE:HG23	2:B:417:GLU:HG3	1.83	0.61
1:E:210:GLY:HA2	1:E:233:PHE:HA	1.82	0.61
1:E:246:VAL:HG21	5:J:186:ILE:HD13	1.82	0.61
1:K:217:TYR:CD1	1:K:220:ILE:HD11	2.35	0.61
3:C:3:DA:H61	4:D:25:DA:H61	1.47	0.61
1:E:363:ARG:CG	1:E:364:PRO:HD2	2.29	0.61
4:H:15:DC:H4'	4:H:16:DG:H5'	1.80	0.61
2:P:337:GLY:HA3	2:P:399:LYS:CG	2.29	0.61
1:A:414:VAL:CG2	1:A:433:GLN:HB3	2.30	0.61
1:E:488:ARG:HG2	1:E:501:GLU:CG	2.30	0.61
1:E:217:TYR:O	1:E:221:ILE:HG12	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:400:ARG:NH1	3:G:12:DC:O4'	2.33	0.61
2:P:11:VAL:HG22	2:P:55:ALA:HB3	1.83	0.61
2:B:106:ASP:HB3	2:B:109:ASP:HB2	1.83	0.61
2:L:298:ASN:O	2:L:299:ASP:HB2	2.01	0.61
1:E:297:LYS:HE3	1:E:299:LYS:HE3	1.82	0.61
1:O:54:GLU:O	1:O:56:GLU:HG2	2.01	0.61
1:O:34:GLY:HA3	1:O:162:SER:HB3	1.83	0.60
1:E:534:TYR:OH	2:F:260:ARG:HD3	2.01	0.60
1:K:163:HIS:NE2	1:K:252:ARG:HG2	2.16	0.60
1:O:390:LEU:HG	1:O:415:PRO:HB2	1.83	0.60
1:O:507:THR:O	2:P:343:LEU:HD21	2.01	0.60
1:A:471:PHE:CE1	2:B:392:ILE:HD13	2.35	0.60
2:B:265:LYS:HD3	2:B:268:LEU:HD13	1.82	0.60
1:E:128:GLN:O	1:E:132:GLN:HG3	2.00	0.60
2:L:146:GLN:HG2	2:L:149:ILE:HD13	1.82	0.60
1:O:317:LYS:HD2	2:P:281:ALA:HA	1.81	0.60
2:P:131:HIS:CE1	2:P:239:LYS:HG3	2.36	0.60
2:F:68:LEU:HD12	2:F:113:VAL:HG22	1.84	0.60
1:K:414:VAL:CG2	1:K:433:GLN:HB3	2.32	0.60
1:E:76:ILE:HG21	1:E:247:ARG:O	2.00	0.60
1:A:490:LEU:HA	1:A:493:LEU:HD11	1.84	0.60
1:O:414:VAL:CG2	1:O:433:GLN:HB3	2.30	0.60
2:P:315:ARG:HG2	2:P:320:ILE:HG22	1.83	0.60
2:L:253:ILE:HA	2:L:342:VAL:HG12	1.83	0.60
4:R:15:DC:H4'	4:R:16:DG:C5'	2.30	0.60
2:B:104:GLN:OE1	2:B:140:SER:OG	2.15	0.60
3:C:14:DG:H1	3:G:18:DT:C7	2.15	0.60
1:A:366:LEU:HD12	1:A:434:LEU:HD22	1.83	0.60
2:L:398:ASP:OD2	2:L:400:ARG:HG3	2.02	0.60
1:O:465:ILE:HG13	1:O:525:PHE:HE2	1.66	0.60
2:F:412:ILE:HG23	2:F:417:GLU:HG3	1.82	0.59
1:K:91:GLU:HG2	1:K:136:GLY:HA3	1.83	0.59
1:K:304:ASN:HD21	1:K:311:LEU:HD13	1.66	0.59
2:P:307:LYS:HA	2:P:310:ILE:HD12	1.84	0.59
1:A:390:LEU:HG	1:A:415:PRO:HB2	1.83	0.59
1:E:99:PHE:CE2	1:E:148:TRP:HE3	2.20	0.59
2:P:16:VAL:HG13	2:P:31:PHE:HE1	1.67	0.59
2:P:68:LEU:O	2:P:70:GLY:N	2.35	0.59
2:L:295:TYR:HE1	2:L:307:LYS:HE2	1.67	0.59
2:B:464:ALA:HB1	2:B:473:LEU:HD11	1.83	0.59
1:O:340:PHE:HB3	1:O:408:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:460:GLY:HA2	1:O:463:LYS:HD2	1.83	0.59
1:K:143:LEU:H	1:K:176:HIS:HE1	1.49	0.59
2:P:295:TYR:HE2	2:P:307:LYS:HE2	1.66	0.59
1:A:488:ARG:HG2	1:A:501:GLU:OE1	2.03	0.59
2:F:341:SER:O	2:F:393:VAL:HG13	2.03	0.59
1:O:488:ARG:HB3	1:O:501:GLU:O	2.01	0.59
1:E:217:TYR:CD1	1:E:220:ILE:HD11	2.38	0.59
1:A:461:LYS:HG2	1:A:525:PHE:CE1	2.39	0.58
1:A:91:GLU:HG2	1:A:136:GLY:HA3	1.84	0.58
2:B:90:LEU:O	2:B:94:ILE:HG13	2.02	0.58
1:K:94:LYS:O	1:K:104:VAL:HG12	2.03	0.58
2:B:154:LEU:HD23	2:B:159:ILE:HB	1.85	0.58
1:E:94:LYS:O	1:E:104:VAL:HG12	2.02	0.58
1:K:343:PRO:HG3	1:K:403:ARG:HA	1.84	0.58
2:B:411:HIS:CD2	2:B:416:TYR:HE2	2.21	0.58
2:F:295:TYR:HE2	2:F:307:LYS:HE2	1.69	0.58
1:A:302:THR:HG22	2:B:291:LYS:HB2	1.86	0.58
2:P:265:LYS:HD3	2:P:268:LEU:HD13	1.86	0.58
1:A:217:TYR:CD1	1:A:220:ILE:HD11	2.38	0.58
2:L:461:MET:HG2	2:L:526:SER:HB3	1.85	0.58
1:O:99:PHE:HB3	1:O:102:ILE:HD12	1.84	0.58
1:O:257:SER:HB3	1:O:403:ARG:HH22	1.68	0.58
1:E:325:ARG:HD2	2:F:88:PHE:CG	2.39	0.58
1:E:446:MET:HB3	2:F:264:TYR:OH	2.03	0.58
1:A:414:VAL:HG23	1:A:433:GLN:HB3	1.85	0.58
1:E:54:GLU:O	1:E:56:GLU:N	2.36	0.57
2:F:188:HIS:HB2	2:F:519:PRO:HG3	1.85	0.57
1:O:91:GLU:HG2	1:O:136:GLY:HA3	1.86	0.57
5:J:184:SER:HB3	5:J:188:PRO:HA	1.85	0.57
1:K:296:VAL:HG22	2:L:297:LEU:HD13	1.86	0.57
4:N:23:DC:H2"	4:N:24:DG:C8	2.39	0.57
1:K:275:ASN:ND2	1:K:278:GLN:HG3	2.15	0.57
2:L:198:THR:HG23	2:L:201:GLN:OE1	2.05	0.57
1:O:252:ARG:HD2	5:T:190:PHE:HZ	1.69	0.57
2:B:466:LYS:HA	2:B:473:LEU:HA	1.85	0.57
1:O:217:TYR:CD1	1:O:220:ILE:HD11	2.40	0.57
1:E:73:SER:HB3	1:E:246:VAL:HB	1.86	0.57
2:L:68:LEU:C	2:L:70:GLY:H	2.06	0.57
4:D:23:DC:H2"	4:D:24:DG:C8	2.40	0.57
1:E:33:SER:HG	4:H:29:DG:HO3'	1.52	0.57
2:F:16:VAL:HG13	2:F:31:PHE:HE1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:265:LYS:HD3	2:F:268:LEU:HD13	1.86	0.56
2:L:68:LEU:C	2:L:70:GLY:N	2.59	0.56
2:L:250:ARG:HG3	2:L:260:ARG:HA	1.86	0.56
1:A:492:ALA:HA	1:A:498:MET:HB2	1.87	0.56
1:K:300:THR:CG2	2:L:291:LYS:HE3	2.29	0.56
1:K:488:ARG:NH1	1:K:501:GLU:HG2	2.18	0.56
1:A:163:HIS:NE2	1:A:252:ARG:HG2	2.20	0.56
1:A:478:PHE:HA	1:A:506:LEU:HD23	1.87	0.56
1:A:493:LEU:CD1	2:B:321:VAL:HG11	2.29	0.56
2:B:297:LEU:HB3	2:B:301:ASP:O	2.05	0.56
2:B:307:LYS:HA	2:B:310:ILE:HD12	1.86	0.56
2:B:411:HIS:CD2	2:B:416:TYR:HH	2.17	0.56
2:F:461:MET:HG2	2:F:526:SER:HB3	1.88	0.56
1:K:99:PHE:CD2	1:K:145:GLU:HB3	2.40	0.56
1:K:290:ARG:NH2	2:L:309:ASP:HA	2.20	0.56
2:L:131:HIS:CE1	2:L:239:LYS:HG3	2.40	0.56
2:L:400:ARG:HH22	3:M:10:DG:C4'	2.14	0.56
2:B:461:MET:HG2	2:B:526:SER:HB3	1.85	0.56
2:F:106:ASP:HB3	2:F:109:ASP:HB2	1.86	0.56
2:F:312:GLN:HG2	2:F:325:LYS:HG3	1.86	0.56
3:M:14:DG:H1	3:Q:18:DT:C7	2.18	0.56
1:A:490:LEU:HD23	1:A:493:LEU:HD11	1.88	0.56
2:B:342:VAL:HA	2:B:393:VAL:HG12	1.87	0.56
1:E:507:THR:O	2:F:343:LEU:HD21	2.05	0.56
2:F:337:GLY:HA3	2:F:399:LYS:CG	2.36	0.56
1:A:59:PRO:HB3	1:A:205:LEU:HD13	1.88	0.56
1:A:492:ALA:CB	1:A:500:PRO:HA	2.35	0.56
1:K:462:MET:HG2	2:L:380:LEU:HA	1.88	0.56
3:C:6:DG:H1	4:D:22:DT:H3	1.52	0.56
2:L:400:ARG:NH2	3:M:10:DG:C4'	2.65	0.56
1:O:262:LYS:HG3	1:O:268:VAL:HG22	1.88	0.56
2:P:66:ASN:HA	2:P:69:SER:HB3	1.88	0.56
2:P:432:GLN:HE21	5:T:193:LYS:HE3	1.71	0.56
1:A:147:LEU:HB3	1:A:193:LEU:HD11	1.87	0.55
1:A:300:THR:CG2	2:B:291:LYS:HE3	2.36	0.55
2:B:312:GLN:HG2	2:B:325:LYS:HG3	1.88	0.55
1:K:147:LEU:HB3	1:K:193:LEU:HD11	1.88	0.55
1:O:488:ARG:HD2	1:O:503:ALA:HB2	1.88	0.55
1:K:128:GLN:O	1:K:132:GLN:HG3	2.07	0.55
1:E:259:LEU:HB3	1:E:344:GLY:HA2	1.88	0.55
1:K:530:TYR:CD1	2:L:372:ALA:HB1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:251:LEU:O	2:L:259:ILE:N	2.40	0.55
2:L:397:TYR:CE2	4:N:19:DC:H4'	2.41	0.55
1:O:518:LEU:O	1:O:522:VAL:HG23	2.05	0.55
2:P:341:SER:O	2:P:393:VAL:HG13	2.06	0.55
1:A:357:LYS:HB2	1:A:360:HIS:HD2	1.70	0.55
2:F:70:GLY:HA2	1:K:148:TRP:HZ2	1.70	0.55
1:A:322:TYR:OH	2:B:274:LYS:HG3	2.06	0.55
1:E:121:GLN:O	1:E:130:ARG:HD2	2.06	0.55
1:E:403:ARG:HE	4:H:27:DC:H4'	1.72	0.55
2:F:470:THR:HG23	2:F:472:THR:H	1.71	0.55
1:K:244:ARG:NH1	1:K:425:ILE:HD12	2.22	0.55
1:O:456:PRO:HA	1:O:459:VAL:HG22	1.88	0.55
1:A:94:LYS:O	1:A:104:VAL:HG12	2.07	0.55
1:O:352:PRO:HD2	1:O:355:LEU:HD12	1.88	0.55
1:E:489:ASN:O	1:E:493:LEU:HG	2.07	0.55
1:K:217:TYR:HD1	1:K:220:ILE:HD11	1.71	0.55
2:B:337:GLY:HA2	2:B:399:LYS:CG	2.37	0.54
2:F:337:GLY:HA2	2:F:399:LYS:HA	1.90	0.54
1:E:524:GLU:O	1:E:528:LEU:HD13	2.07	0.54
2:F:337:GLY:HA3	2:F:399:LYS:HG2	1.89	0.54
2:P:400:ARG:NE	3:Q:12:DC:H4'	2.22	0.54
2:P:461:MET:HG2	2:P:526:SER:HB3	1.87	0.54
1:K:507:THR:O	2:L:343:LEU:HD21	2.08	0.54
1:K:99:PHE:HB3	1:K:102:ILE:HD12	1.90	0.54
2:P:16:VAL:HG13	2:P:31:PHE:CE1	2.42	0.54
2:B:167:PHE:CE2	2:B:197:ILE:HD12	2.42	0.54
1:E:275:ASN:ND2	1:E:278:GLN:HG3	2.21	0.54
1:E:392:LYS:HZ1	2:F:455:ASP:CG	2.10	0.54
1:A:488:ARG:CB	1:A:501:GLU:HB2	2.35	0.54
1:E:322:TYR:OH	2:F:274:LYS:HG3	2.08	0.54
1:K:448:PHE:HB2	2:L:416:TYR:OH	2.07	0.54
2:L:118:ILE:O	2:L:122:THR:OG1	2.18	0.54
1:E:165:ARG:HG3	1:E:199:PHE:HB2	1.89	0.54
2:L:301:ASP:C	2:L:303:THR:H	2.11	0.54
2:B:390:VAL:HG23	2:B:409:PHE:HB3	1.89	0.54
1:E:99:PHE:HB3	1:E:102:ILE:HD12	1.88	0.54
1:A:296:VAL:HG22	2:B:305:VAL:HG21	1.90	0.53
2:B:11:VAL:CG1	2:B:132:ILE:HG12	2.38	0.53
1:E:213:ILE:HG21	1:E:230:ARG:N	2.23	0.53
1:A:247:ARG:HA	1:A:250:GLU:HB2	1.89	0.53
1:A:529:VAL:C	1:A:531:PRO:HD3	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:236:SER:OG	1:K:242:LEU:HG	2.08	0.53
1:A:357:LYS:HD2	1:A:360:HIS:CD2	2.44	0.53
2:F:307:LYS:HA	2:F:310:ILE:HD12	1.88	0.53
1:K:490:LEU:HA	1:K:493:LEU:HG	1.88	0.53
2:L:115:MET:HE2	2:L:150:ILE:HG23	1.90	0.53
2:L:390:VAL:HG23	2:L:409:PHE:HB3	1.90	0.53
1:E:75:ILE:HG12	1:E:111:PRO:HB2	1.90	0.53
2:L:11:VAL:CG1	2:L:132:ILE:HG12	2.39	0.53
2:L:528:ILE:HD12	2:L:528:ILE:H	1.74	0.53
1:O:40:PHE:HZ	1:O:70:VAL:HG11	1.73	0.53
1:E:189:LYS:NZ	1:E:193:LEU:HD21	2.24	0.53
1:O:297:LYS:HB2	2:P:298:ASN:HA	1.91	0.53
2:B:528:ILE:HD12	2:B:528:ILE:H	1.74	0.53
2:F:16:VAL:HG13	2:F:31:PHE:CE1	2.44	0.53
2:F:65:ASP:HB3	2:F:78:THR:HG23	1.90	0.53
2:L:106:ASP:HB3	2:L:109:ASP:HB2	1.91	0.53
1:K:488:ARG:O	1:K:491:GLU:HG2	2.09	0.53
1:O:465:ILE:HG13	1:O:525:PHE:CE2	2.44	0.53
2:P:251:LEU:HB2	2:P:261:ILE:HD13	1.90	0.53
2:B:250:ARG:HH21	2:B:260:ARG:HD2	1.74	0.53
1:K:282:LYS:HE3	1:K:486:HIS:CD2	2.44	0.53
1:O:34:GLY:HA2	1:O:160:LYS:HE3	1.91	0.53
2:P:247:TRP:HH2	2:P:395:TYR:HE1	1.57	0.52
1:A:236:SER:OG	1:A:242:LEU:HG	2.09	0.52
2:B:171:LYS:HB3	2:B:192:PHE:CZ	2.35	0.52
2:L:154:LEU:HD23	2:L:159:ILE:HB	1.91	0.52
1:O:52:GLN:HE22	1:O:207:LYS:HA	1.74	0.52
1:O:465:ILE:HD11	1:O:525:PHE:HD2	1.73	0.52
2:L:306:LEU:HB2	2:L:309:ASP:HB2	1.90	0.52
1:O:325:ARG:HD2	2:P:88:PHE:CD1	2.45	0.52
1:A:421:ASP:O	1:A:424:LYS:N	2.34	0.52
1:A:202:LEU:HD13	1:A:217:TYR:CD1	2.45	0.52
1:A:490:LEU:HA	1:A:493:LEU:CD1	2.39	0.52
1:E:35:ARG:HE	1:E:80:ARG:NE	2.07	0.52
2:F:407:VAL:HB	2:F:424:LEU:HD11	1.92	0.52
1:K:462:MET:SD	1:K:465:ILE:HD12	2.50	0.52
1:O:443:LYS:HD2	2:P:480:THR:HB	1.90	0.52
1:O:467:GLU:OE1	5:T:204:THR:HG21	2.10	0.52
1:A:226:ASP:HB2	2:B:436:SER:HB3	1.92	0.52
1:E:78:SER:OG	1:E:81:ASP:OD1	2.17	0.52
1:K:340:PHE:HB2	1:K:407:PRO:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:63:GLY:O	2:P:76:ASN:HA	2.09	0.52
2:P:188:HIS:HB2	2:P:519:PRO:HG3	1.92	0.52
1:A:294:GLU:HG3	2:B:297:LEU:HD11	1.92	0.52
2:L:188:HIS:HB2	2:L:519:PRO:HG3	1.92	0.52
1:E:247:ARG:HB3	1:E:484:GLN:HE22	1.74	0.52
3:G:9:DG:N2	4:H:20:DC:N3	2.57	0.52
2:L:252:THR:HG22	2:L:258:SER:OG	2.09	0.52
2:P:529:PRO:HA	2:P:532:LYS:NZ	2.25	0.52
1:E:343:PRO:HG3	1:E:403:ARG:HA	1.92	0.51
5:J:185:LEU:HD13	5:J:192:SER:HB3	1.91	0.51
1:K:352:PRO:HD2	1:K:355:LEU:HD12	1.92	0.51
2:L:177:ASP:HB2	2:L:194:LEU:HD21	1.91	0.51
2:L:253:ILE:HB	2:L:257:LEU:HD23	1.91	0.51
1:E:40:PHE:HZ	1:E:70:VAL:HG11	1.75	0.51
1:K:343:PRO:HA	1:K:401:THR:O	2.10	0.51
1:O:321:ILE:HG13	1:O:326:GLN:HG3	1.93	0.51
2:P:477:PHE:HD1	2:P:519:PRO:HD3	1.76	0.51
1:A:63:SER:O	1:A:67:ILE:HG12	2.11	0.51
1:O:302:THR:CG2	2:P:291:LYS:HE3	2.41	0.51
2:P:250:ARG:HD3	2:P:258:SER:HB3	1.91	0.51
1:A:170:THR:HG21	1:A:217:TYR:OH	2.11	0.51
1:E:45:SER:HA	1:E:138:GLY:HA2	1.92	0.51
1:E:457:GLU:N	1:E:457:GLU:OE1	2.41	0.51
2:F:253:ILE:HG12	2:F:342:VAL:HG11	1.92	0.51
1:K:165:ARG:HD3	1:K:201:ASP:OD2	2.11	0.51
1:K:392:LYS:HZ1	2:L:455:ASP:CG	2.14	0.51
2:B:411:HIS:CD2	2:B:416:TYR:CE2	2.98	0.51
1:E:488:ARG:HD3	1:E:501:GLU:HG3	1.93	0.51
1:O:462:MET:SD	1:O:465:ILE:HD12	2.51	0.51
1:A:267:ILE:HA	2:B:539:LEU:HD11	1.93	0.51
2:B:115:MET:HE2	2:B:150:ILE:HG23	1.92	0.51
1:E:69:SER:O	1:E:72:ILE:HG13	2.11	0.51
2:F:154:LEU:HD23	2:F:159:ILE:HB	1.93	0.51
2:F:431:ARG:NH1	3:G:4:DT:OP1	2.41	0.51
2:F:528:ILE:HD12	2:F:528:ILE:H	1.74	0.51
1:K:170:THR:HG21	1:K:217:TYR:OH	2.11	0.51
1:K:322:TYR:OH	2:L:274:LYS:HG3	2.11	0.51
2:L:337:GLY:HA2	2:L:399:LYS:CG	2.37	0.51
1:O:328:ILE:HD12	2:P:284:LEU:HD22	1.92	0.51
1:O:369:TYR:CG	1:O:370:PRO:HD2	2.45	0.51
2:F:253:ILE:HA	2:F:342:VAL:CG1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:15:DC:H2"	4:H:16:DG:OP2	2.10	0.51
1:O:57:LEU:HB3	1:O:61:ASP:HB3	1.92	0.51
1:A:115:ARG:O	1:A:119:LEU:HD13	2.10	0.51
1:E:518:LEU:HD22	1:E:521:LEU:HD22	1.92	0.51
2:F:6:ASN:OD1	2:F:129:LYS:NZ	2.42	0.51
1:O:99:PHE:CE2	1:O:148:TRP:HE3	2.29	0.51
3:C:9:DG:H2'	3:C:10:DG:C8	2.46	0.51
1:O:525:PHE:O	1:O:529:VAL:HG22	2.10	0.51
2:P:295:TYR:CE2	2:P:307:LYS:HG3	2.46	0.51
1:A:297:LYS:HB2	2:B:298:ASN:HA	1.93	0.50
2:B:188:HIS:HB2	2:B:519:PRO:HG3	1.93	0.50
1:K:97:VAL:HG21	1:K:148:TRP:HZ3	1.76	0.50
2:L:23:SER:HB2	2:L:29:SER:HB3	1.92	0.50
2:P:528:ILE:HD12	2:P:528:ILE:H	1.76	0.50
1:A:458:GLN:HG2	1:A:529:VAL:HG12	1.93	0.50
1:A:474:ARG:HB2	1:A:477:SER:OG	2.10	0.50
1:A:69:SER:HB2	1:A:243:LEU:HD21	1.92	0.50
1:A:72:ILE:HG13	1:A:73:SER:N	2.27	0.50
1:E:247:ARG:HH12	1:E:488:ARG:HG3	1.75	0.50
1:K:69:SER:HB2	1:K:243:LEU:HD21	1.92	0.50
2:L:477:PHE:HD1	2:L:519:PRO:HD3	1.75	0.50
1:O:69:SER:O	1:O:72:ILE:HG13	2.10	0.50
1:O:246:VAL:HG12	1:O:246:VAL:O	2.11	0.50
1:O:488:ARG:HH11	1:O:501:GLU:CG	2.20	0.50
1:E:474:ARG:HH12	5:J:194:LYS:HB3	1.75	0.50
1:K:202:LEU:HD13	1:K:217:TYR:CD1	2.46	0.50
2:P:124:GLY:O	2:P:126:LYS:N	2.44	0.50
2:P:146:GLN:HG2	2:P:149:ILE:HD13	1.93	0.50
2:F:70:GLY:CA	1:K:148:TRP:HZ2	2.24	0.50
1:A:52:GLN:NE2	1:A:52:GLN:HA	2.27	0.50
1:K:171:ASN:O	1:K:207:LYS:HD3	2.11	0.50
1:A:369:TYR:CG	1:A:370:PRO:HD2	2.46	0.50
1:O:159:PHE:CZ	1:O:160:LYS:HE2	2.47	0.50
1:E:213:ILE:HG12	1:E:230:ARG:HA	1.93	0.50
2:F:250:ARG:CD	2:F:258:SER:HB3	2.26	0.50
2:P:132:ILE:HB	2:P:161:LEU:HD23	1.93	0.50
2:B:12:LEU:HD23	2:B:133:GLU:HB2	1.94	0.50
2:B:28:GLU:HB2	2:B:185:LEU:HD11	1.93	0.50
1:E:63:SER:O	1:E:67:ILE:HG12	2.11	0.50
2:P:199:GLU:HA	2:P:202:LYS:HE3	1.93	0.50
1:A:495:LEU:CB	1:A:498:MET:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ASP:HB2	2:B:59:PHE:CZ	2.46	0.49
1:K:40:PHE:CD1	1:K:67:ILE:HD12	2.47	0.49
2:P:64:THR:C	2:P:66:ASN:H	2.15	0.49
1:A:462:MET:HG2	2:B:380:LEU:HA	1.94	0.49
1:E:297:LYS:HB2	2:F:298:ASN:HA	1.94	0.49
1:K:369:TYR:CG	1:K:370:PRO:HD2	2.47	0.49
2:P:41:PHE:HA	2:P:237:PHE:CZ	2.47	0.49
2:P:412:ILE:HG23	2:P:417:GLU:HG3	1.93	0.49
2:P:477:PHE:CE1	2:P:518:PRO:HA	2.46	0.49
1:A:257:SER:HA	4:D:29:DG:H5"	1.94	0.49
2:B:6:ASN:CB	2:B:242:ARG:HG2	2.38	0.49
2:B:397:TYR:CE2	4:D:19:DC:H4'	2.48	0.49
2:L:477:PHE:CE1	2:L:518:PRO:HA	2.47	0.49
2:P:28:GLU:HB2	2:P:185:LEU:HD11	1.92	0.49
1:E:488:ARG:HA	1:E:491:GLU:HG2	1.94	0.49
1:A:128:GLN:O	1:A:132:GLN:HG3	2.12	0.49
1:E:75:ILE:CG1	1:E:111:PRO:HB2	2.43	0.49
1:K:63:SER:O	1:K:67:ILE:HG12	2.13	0.49
3:M:18:DT:H2"	4:R:15:DC:H5"	1.95	0.49
1:A:216:PHE:O	1:A:217:TYR:HB2	2.12	0.49
1:E:33:SER:OG	4:H:29:DG:O3'	2.25	0.49
1:O:45:SER:HA	1:O:138:GLY:HA2	1.93	0.49
1:O:322:TYR:CE1	2:P:274:LYS:HG3	2.47	0.49
1:O:322:TYR:OH	2:P:274:LYS:HG3	2.11	0.49
1:O:490:LEU:HA	1:O:493:LEU:HG	1.94	0.49
1:O:524:GLU:HG2	1:O:525:PHE:CD1	2.47	0.49
1:E:204:HIS:CD2	1:E:232:HIS:HB3	2.48	0.49
1:E:352:PRO:HG2	2:F:473:LEU:HD21	1.94	0.49
1:E:448:PHE:CG	1:E:448:PHE:O	2.65	0.49
2:P:18:PHE:HB2	2:P:102:SER:HA	1.93	0.49
2:P:253:ILE:HA	2:P:342:VAL:CG1	2.40	0.49
2:B:407:VAL:HB	2:B:424:LEU:HD11	1.95	0.49
1:E:216:PHE:O	1:E:217:TYR:HB2	2.12	0.49
2:L:15:ASP:HB2	2:L:59:PHE:CZ	2.47	0.49
1:O:235:GLU:HG3	1:O:239:LEU:HD23	1.94	0.49
1:O:267:ILE:HD13	2:P:530:LEU:HD22	1.95	0.49
1:E:35:ARG:NE	1:E:80:ARG:HB3	2.27	0.49
1:E:72:ILE:HD11	1:E:245:LYS:CG	2.38	0.49
2:P:271:ARG:HG2	2:P:272:VAL:H	1.77	0.49
2:P:466:LYS:HA	2:P:473:LEU:HA	1.95	0.49
2:B:390:VAL:HG21	2:B:407:VAL:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:369:TYR:CG	1:E:370:PRO:HD2	2.48	0.49
2:L:457:LEU:HD12	2:L:529:PRO:HB2	1.94	0.49
1:E:147:LEU:HB3	1:E:193:LEU:HD11	1.94	0.48
1:K:266:ASP:HB3	2:L:534:LYS:NZ	2.28	0.48
1:O:54:GLU:HG2	1:O:55:ASP:OD1	2.13	0.48
1:O:63:SER:O	1:O:67:ILE:HG12	2.11	0.48
1:O:366:LEU:HD12	1:O:434:LEU:HD22	1.95	0.48
1:K:329:LEU:HD12	2:L:276:TRP:CH2	2.49	0.48
1:O:171:ASN:O	1:O:207:LYS:HD3	2.12	0.48
1:E:403:ARG:HD2	4:H:27:DC:OP1	2.13	0.48
1:E:530:TYR:CD1	2:F:372:ALA:HB1	2.48	0.48
2:F:271:ARG:HG2	2:F:272:VAL:H	1.78	0.48
1:O:40:PHE:CD1	1:O:67:ILE:HD12	2.48	0.48
1:O:325:ARG:HD2	2:P:88:PHE:CG	2.49	0.48
1:E:143:LEU:H	1:E:176:HIS:HE1	1.61	0.48
1:A:507:THR:O	2:B:343:LEU:HD21	2.14	0.48
3:C:14:DG:H1	3:G:18:DT:H72	1.77	0.48
2:F:165:LEU:HD23	2:F:167:PHE:CZ	2.49	0.48
1:K:262:LYS:CE	1:K:265:LYS:HA	2.42	0.48
2:L:71:GLY:C	2:L:73:GLN:H	2.16	0.48
2:P:69:SER:HA	2:P:73:GLN:O	2.13	0.48
1:A:471:PHE:CE1	2:B:344:GLY:HA3	2.49	0.48
2:B:390:VAL:HG22	2:B:391:ALA:H	1.79	0.48
4:H:15:DC:H4'	4:H:16:DG:C5'	2.44	0.48
1:K:72:ILE:HG13	1:K:73:SER:N	2.29	0.48
1:K:489:ASN:O	1:K:493:LEU:HG	2.14	0.48
2:L:111:LEU:HD13	2:L:134:ILE:HD11	1.95	0.48
2:L:407:VAL:HB	2:L:424:LEU:HD11	1.95	0.48
1:O:334:THR:O	1:O:338:LYS:HD2	2.13	0.48
1:O:414:VAL:HG23	1:O:433:GLN:HB3	1.96	0.48
2:B:297:LEU:HG	2:B:299:ASP:OD2	2.14	0.48
2:F:171:LYS:H	2:F:171:LYS:HD2	1.79	0.48
2:F:477:PHE:CE1	2:F:518:PRO:HA	2.49	0.48
1:A:41:LEU:HA	1:A:86:VAL:HG23	1.95	0.48
1:E:426:GLN:HE21	1:E:430:PRO:HD3	1.79	0.48
2:F:11:VAL:CG1	2:F:132:ILE:HG12	2.44	0.48
2:L:412:ILE:HG23	2:L:417:GLU:HG3	1.94	0.48
2:P:111:LEU:HD13	2:P:134:ILE:HD11	1.95	0.48
1:E:352:PRO:HD2	1:E:355:LEU:HD12	1.96	0.47
1:K:99:PHE:CE2	1:K:145:GLU:CG	2.94	0.47
2:P:253:ILE:HG12	2:P:342:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:9:DG:H2'	3:Q:10:DG:C8	2.49	0.47
1:A:297:LYS:HE3	1:A:299:LYS:HE3	1.96	0.47
1:K:455:THR:OG1	1:K:456:PRO:HD2	2.14	0.47
1:O:418:GLU:HG3	1:O:430:PRO:HD3	1.95	0.47
2:P:390:VAL:HG23	2:P:409:PHE:HB3	1.96	0.47
1:E:53:SER:HB2	1:E:56:GLU:HB3	1.96	0.47
1:E:281:LEU:HD11	4:H:21:DC:OP2	2.14	0.47
1:E:366:LEU:HD12	1:E:434:LEU:HD22	1.96	0.47
2:F:8:ALA:HB2	2:F:129:LYS:HB2	1.96	0.47
2:F:70:GLY:HA2	1:K:148:TRP:CZ2	2.49	0.47
1:K:249:LYS:HD2	1:K:249:LYS:HA	1.72	0.47
1:O:355:LEU:HD21	2:P:473:LEU:HG	1.97	0.47
2:P:180:ASP:HA	2:P:194:LEU:HD13	1.96	0.47
2:P:432:GLN:NE2	5:T:193:LYS:HE3	2.29	0.47
2:B:251:LEU:HD23	2:B:253:ILE:HG13	1.96	0.47
1:K:99:PHE:HD1	1:K:99:PHE:HA	1.60	0.47
1:K:283:PRO:HD2	1:K:486:HIS:CE1	2.50	0.47
2:L:509:GLN:HG2	2:L:511:HIS:CE1	2.49	0.47
3:M:14:DG:H1	3:Q:18:DT:H73	1.79	0.47
1:O:75:ILE:HG12	1:O:111:PRO:HB2	1.97	0.47
1:O:90:THR:HG21	1:O:103:TYR:HB2	1.96	0.47
1:E:90:THR:HG21	1:E:103:TYR:HB2	1.96	0.47
1:K:189:LYS:HD2	1:K:189:LYS:HA	1.67	0.47
2:L:479:THR:HA	2:L:482:ILE:HD12	1.96	0.47
1:O:104:VAL:HG13	1:O:104:VAL:O	2.13	0.47
1:O:489:ASN:O	1:O:493:LEU:HG	2.14	0.47
1:E:204:HIS:HD2	1:E:232:HIS:HB3	1.80	0.47
2:F:70:GLY:CA	1:K:148:TRP:CZ2	2.97	0.47
1:O:99:PHE:HE2	1:O:148:TRP:HE3	1.62	0.47
2:P:7:LYS:HA	2:P:52:ASP:OD1	2.15	0.47
2:P:76:ASN:OD1	2:P:103:GLN:HG3	2.15	0.47
1:A:148:TRP:HD1	1:A:189:LYS:NZ	2.13	0.47
1:A:189:LYS:HD2	1:A:189:LYS:HA	1.70	0.47
1:A:352:PRO:HD2	1:A:355:LEU:HD12	1.96	0.47
1:A:403:ARG:NE	4:D:28:DC:H4'	2.30	0.47
1:A:485:GLN:OE1	1:A:503:ALA:N	2.38	0.47
3:G:9:DG:H2'	3:G:10:DG:C8	2.49	0.47
1:K:174:ASN:HB2	1:K:215:LEU:HB3	1.97	0.47
1:K:493:LEU:HD13	2:L:321:VAL:CG1	2.30	0.47
1:O:159:PHE:CE1	1:O:160:LYS:HE2	2.50	0.47
1:O:488:ARG:HA	1:O:491:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:115:MET:HE2	2:P:150:ILE:HG23	1.95	0.47
2:P:312:GLN:HG2	2:P:325:LYS:HG3	1.97	0.47
1:K:340:PHE:HB3	1:K:408:PRO:HD3	1.96	0.47
1:K:488:ARG:HD3	1:K:501:GLU:CG	2.45	0.47
1:O:53:SER:HB2	1:O:56:GLU:HG3	1.96	0.47
2:B:252:THR:HB	2:B:341:SER:HA	1.96	0.47
1:E:490:LEU:HA	1:E:493:LEU:HG	1.95	0.47
2:F:6:ASN:HB2	2:F:242:ARG:HG2	1.97	0.47
2:F:19:THR:H	2:F:104:GLN:HE22	1.62	0.47
1:K:525:PHE:O	1:K:529:VAL:HG22	2.15	0.47
2:P:390:VAL:HG22	2:P:391:ALA:H	1.80	0.47
1:A:204:HIS:CD2	1:A:235:GLU:HA	2.50	0.47
2:B:529:PRO:HA	2:B:532:LYS:NZ	2.29	0.47
1:E:340:PHE:HB2	1:E:407:PRO:HA	1.96	0.47
2:F:104:GLN:OE1	2:F:140:SER:OG	2.20	0.47
1:K:282:LYS:HE3	1:K:486:HIS:HD2	1.78	0.47
2:L:133:GLU:HG2	2:L:162:GLN:HB2	1.96	0.47
2:L:295:TYR:CE1	2:L:307:LYS:HE2	2.48	0.47
1:O:75:ILE:CG1	1:O:111:PRO:HB2	2.45	0.47
1:O:392:LYS:HZ1	2:P:455:ASP:CG	2.18	0.47
2:P:16:VAL:HG12	2:P:100:PRO:HA	1.96	0.47
2:B:129:LYS:HD3	2:B:239:LYS:O	2.15	0.46
1:E:173:ASP:O	1:E:216:PHE:HB3	2.16	0.46
2:F:295:TYR:CE2	2:F:307:LYS:HG3	2.50	0.46
1:K:216:PHE:O	1:K:217:TYR:HB2	2.15	0.46
1:A:220:ILE:HG13	1:A:221:ILE:N	2.31	0.46
2:B:23:SER:HB2	2:B:29:SER:HB3	1.97	0.46
2:B:400:ARG:HE	3:C:10:DG:H4'	1.80	0.46
1:E:444:ARG:HB2	2:F:266:SER:O	2.14	0.46
2:F:352:GLN:HB2	2:F:355:PHE:CD2	2.50	0.46
2:L:5:GLY:HA2	2:L:129:LYS:NZ	2.29	0.46
2:L:186:GLY:H	2:L:228:SER:HB2	1.80	0.46
1:O:189:LYS:HA	1:O:189:LYS:HD2	1.63	0.46
1:O:216:PHE:O	1:O:217:TYR:HB2	2.15	0.46
2:P:236:VAL:HG23	2:P:237:PHE:CD1	2.50	0.46
2:B:132:ILE:HB	2:B:161:LEU:HD23	1.98	0.46
2:F:497:ARG:HH11	2:F:497:ARG:HA	1.80	0.46
1:K:56:GLU:HG2	1:K:237:SER:O	2.15	0.46
2:L:252:THR:HA	2:L:258:SER:HA	1.98	0.46
1:O:418:GLU:HB2	1:O:430:PRO:HB3	1.97	0.46
2:P:400:ARG:CD	3:Q:12:DC:H4'	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:HIS:CE1	1:A:182:LYS:HD2	2.51	0.46
1:E:171:ASN:O	1:E:207:LYS:HD3	2.16	0.46
5:J:185:LEU:HD22	5:J:192:SER:OG	2.15	0.46
5:J:186:ILE:HG13	5:J:187:ASN:N	2.30	0.46
3:C:14:DG:H1	3:G:18:DT:H73	1.79	0.46
1:O:283:PRO:HD2	1:O:486:HIS:CE1	2.51	0.46
2:L:529:PRO:HA	2:L:532:LYS:NZ	2.31	0.46
1:O:173:ASP:O	1:O:216:PHE:HB3	2.16	0.46
2:P:132:ILE:HB	2:P:161:LEU:CD2	2.45	0.46
2:P:431:ARG:HD3	2:P:433:TYR:OH	2.16	0.46
2:P:509:GLN:HG2	2:P:511:HIS:CE1	2.51	0.46
1:A:261:LEU:HD12	1:A:345:LEU:HD23	1.97	0.46
2:B:479:THR:HA	2:B:482:ILE:HD12	1.98	0.46
1:K:461:LYS:HD2	1:K:525:PHE:CE1	2.51	0.46
1:O:66:CYS:SG	1:O:242:LEU:HB3	2.56	0.46
2:P:407:VAL:HB	2:P:424:LEU:HD11	1.98	0.46
1:A:317:LYS:HD2	2:B:281:ALA:HA	1.97	0.46
1:A:455:THR:OG1	1:A:456:PRO:HD2	2.15	0.46
2:B:112:ILE:HD11	2:B:150:ILE:HD11	1.98	0.46
2:B:450:GLN:HA	2:B:536:LEU:HD23	1.98	0.46
1:E:67:ILE:HD11	1:E:169:PHE:CE1	2.50	0.46
1:E:259:LEU:HD22	1:E:344:GLY:N	2.30	0.46
2:F:94:ILE:HA	2:F:98:ILE:HD12	1.98	0.46
1:K:259:LEU:HD22	1:K:344:GLY:N	2.31	0.46
1:K:321:ILE:HG13	1:K:326:GLN:HG3	1.97	0.46
2:P:104:GLN:OE1	2:P:140:SER:OG	2.25	0.46
1:A:99:PHE:CE2	1:A:148:TRP:CE3	3.04	0.46
2:F:250:ARG:HD3	2:F:258:SER:CB	2.27	0.46
1:O:280:ALA:O	1:O:483:LEU:HD11	2.16	0.46
1:O:515:ASN:HD21	2:P:255:SER:HB3	1.81	0.46
3:Q:11:DC:N4	4:R:17:DG:O6	2.48	0.46
1:A:392:LYS:HD2	2:B:458:ILE:CD1	2.39	0.46
2:F:16:VAL:HG12	2:F:100:PRO:HA	1.97	0.46
2:F:467:ASP:OD2	2:F:470:THR:HG22	2.16	0.46
1:O:455:THR:OG1	1:O:456:PRO:HD2	2.16	0.46
2:P:465:LYS:O	2:P:474:GLU:N	2.39	0.46
1:A:300:THR:HG23	2:B:293:THR:HG22	1.97	0.45
2:B:19:THR:HA	2:B:22:ASN:ND2	2.31	0.45
2:F:111:LEU:HD13	2:F:134:ILE:HD11	1.98	0.45
1:K:458:GLN:NE2	1:K:529:VAL:HG12	2.31	0.45
2:L:296:CYS:SG	2:L:304:GLU:HG2	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:91:GLU:HG2	1:O:136:GLY:H	1.80	0.45
1:O:261:LEU:HG	1:O:345:LEU:HB3	1.99	0.45
1:A:99:PHE:HB3	1:A:102:ILE:HD12	1.98	0.45
1:E:358:LYS:HG2	2:F:353:ARG:NE	2.31	0.45
1:O:35:ARG:HG3	1:O:159:PHE:CE1	2.52	0.45
2:P:68:LEU:HD21	2:P:116:ASP:CG	2.36	0.45
1:A:40:PHE:CD1	1:A:67:ILE:HD12	2.51	0.45
2:F:411:HIS:CE1	2:F:413:LYS:HE3	2.51	0.45
1:K:468:LYS:HB2	1:K:518:LEU:HD21	1.99	0.45
1:A:297:LYS:N	2:B:296:CYS:O	2.49	0.45
1:E:54:GLU:HG2	1:E:55:ASP:OD1	2.17	0.45
1:E:99:PHE:CE2	1:E:148:TRP:CE3	3.02	0.45
1:E:322:TYR:CE1	2:F:274:LYS:HG3	2.51	0.45
2:F:477:PHE:HD1	2:F:519:PRO:HD3	1.81	0.45
1:K:343:PRO:HG3	1:K:403:ARG:CA	2.46	0.45
1:K:414:VAL:HG22	1:K:433:GLN:HB3	1.98	0.45
1:A:143:LEU:HD12	1:A:176:HIS:CD2	2.52	0.45
2:F:120:HIS:HE1	1:K:188:THR:OG1	2.00	0.45
1:K:244:ARG:NH1	1:K:421:ASP:OD2	2.49	0.45
2:L:307:LYS:HA	2:L:310:ILE:HD12	1.97	0.45
2:B:465:LYS:HD3	2:B:474:GLU:OE1	2.15	0.45
2:F:12:LEU:HD23	2:F:133:GLU:HB2	1.98	0.45
2:F:271:ARG:HD3	3:G:7:DA:OP2	2.17	0.45
5:J:184:SER:CB	5:J:188:PRO:HA	2.46	0.45
1:K:486:HIS:CE1	1:K:490:LEU:HD11	2.51	0.45
1:O:40:PHE:CG	1:O:67:ILE:HD12	2.52	0.45
2:B:247:TRP:HA	2:B:248:PRO:HD3	1.90	0.45
1:E:252:ARG:HA	1:E:252:ARG:HD2	1.75	0.45
1:E:264:ASN:HB3	1:E:267:ILE:HD12	1.99	0.45
1:E:438:PRO:HB2	1:E:442:ASP:HB2	1.99	0.45
2:F:431:ARG:HD3	2:F:433:TYR:OH	2.17	0.45
2:F:509:GLN:HG2	2:F:511:HIS:CE1	2.51	0.45
1:K:204:HIS:CE1	1:K:233:PHE:CE1	3.04	0.45
1:K:462:MET:HB3	2:L:383:ALA:HB2	1.97	0.45
1:A:91:GLU:HG2	1:A:136:GLY:CA	2.45	0.45
2:B:413:LYS:HB2	2:B:416:TYR:CE1	2.51	0.45
1:K:217:TYR:O	1:K:221:ILE:HG12	2.16	0.45
1:K:345:LEU:HD21	1:K:413:LEU:HD11	1.98	0.45
1:A:217:TYR:O	1:A:221:ILE:HG12	2.16	0.45
1:A:244:ARG:HE	1:A:425:ILE:HD12	1.82	0.45
1:A:530:TYR:CD1	2:B:372:ALA:HB1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:462:MET:HG2	2:F:380:LEU:HA	1.98	0.45
2:F:15:ASP:HB2	2:F:59:PHE:CZ	2.52	0.45
1:K:280:ALA:O	1:K:483:LEU:HD11	2.17	0.45
1:O:247:ARG:NH1	1:O:488:ARG:HH21	2.14	0.45
2:P:23:SER:HB2	2:P:29:SER:HB3	1.99	0.45
1:E:280:ALA:O	1:E:483:LEU:HD11	2.17	0.45
1:E:525:PHE:O	1:E:529:VAL:HG22	2.17	0.45
1:K:204:HIS:HE1	1:K:233:PHE:CE1	2.34	0.45
1:O:463:LYS:HE2	2:P:386:ASP:HB2	1.99	0.45
1:A:448:PHE:CG	1:A:448:PHE:O	2.69	0.44
2:B:277:THR:HG23	2:B:286:LYS:HD2	1.98	0.44
1:K:268:VAL:O	2:L:539:LEU:HD13	2.17	0.44
1:K:488:ARG:HD2	1:K:503:ALA:HB2	1.99	0.44
1:O:91:GLU:HG2	1:O:136:GLY:CA	2.45	0.44
1:O:91:GLU:HG2	1:O:136:GLY:N	2.32	0.44
1:O:423:GLN:HB2	1:O:425:ILE:HG13	1.97	0.44
2:P:154:LEU:HD23	2:P:159:ILE:HB	1.99	0.44
1:A:99:PHE:HD1	1:A:99:PHE:HA	1.70	0.44
1:E:99:PHE:HE2	1:E:148:TRP:HE3	1.63	0.44
2:L:340:PHE:CE1	2:L:395:TYR:CD1	3.05	0.44
1:A:51:SER:CA	1:A:58:THR:HG22	2.48	0.44
1:E:40:PHE:CD1	1:E:67:ILE:HD12	2.53	0.44
1:E:462:MET:HA	1:E:465:ILE:HD12	1.98	0.44
2:L:68:LEU:O	2:L:70:GLY:N	2.50	0.44
1:O:34:GLY:HA2	1:O:160:LYS:CD	2.46	0.44
2:P:270:GLU:HG3	2:P:487:PHE:CZ	2.53	0.44
1:K:244:ARG:HH11	1:K:425:ILE:HD12	1.82	0.44
3:M:14:DG:H1	3:Q:18:DT:H72	1.82	0.44
1:O:322:TYR:CZ	2:P:274:LYS:HG3	2.53	0.44
2:P:44:ARG:HB3	2:P:237:PHE:CZ	2.52	0.44
2:B:169:LEU:O	2:B:172:GLU:HB3	2.17	0.44
1:E:72:ILE:HG22	1:E:116:ILE:HD13	2.00	0.44
1:E:258:ARG:HD2	1:E:374:LEU:CD1	2.44	0.44
2:F:115:MET:HE1	2:F:150:ILE:HG23	1.98	0.44
1:K:304:ASN:ND2	1:K:311:LEU:HD13	2.31	0.44
1:K:481:PRO:HG3	1:K:505:ASP:OD1	2.18	0.44
1:O:438:PRO:HB2	1:O:442:ASP:HB2	2.00	0.44
1:E:296:VAL:HG21	2:F:305:VAL:HG11	1.99	0.44
2:L:427:MET:HA	2:L:430:LEU:HD12	2.00	0.44
1:O:72:ILE:HD11	1:O:245:LYS:CG	2.30	0.44
1:O:281:LEU:HG	1:O:282:LYS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:340:PHE:HE1	2:P:485:PRO:HB2	1.82	0.44
1:A:481:PRO:HG3	1:A:505:ASP:OD1	2.18	0.44
1:K:220:ILE:HG13	1:K:221:ILE:N	2.33	0.44
1:K:518:LEU:HD22	1:K:521:LEU:HD22	2.00	0.44
2:L:5:GLY:N	2:L:243:HIS:HD2	2.15	0.44
1:O:530:TYR:CD1	2:P:372:ALA:HB1	2.53	0.44
1:A:252:ARG:HD2	1:A:252:ARG:HA	1.59	0.44
2:B:160:SER:HA	2:B:215:LEU:HD21	2.00	0.44
1:E:66:CYS:SG	1:E:242:LEU:HB3	2.58	0.44
1:E:322:TYR:CZ	2:F:274:LYS:HG3	2.52	0.44
2:F:466:LYS:HE2	2:F:471:ASP:CG	2.37	0.44
1:K:173:ASP:OD2	1:K:215:LEU:HD12	2.17	0.44
1:O:72:ILE:HG22	1:O:116:ILE:HD13	2.00	0.44
2:P:106:ASP:HB3	2:P:109:ASP:HB2	1.98	0.44
1:A:99:PHE:CE2	1:A:145:GLU:HG2	2.52	0.44
1:E:54:GLU:C	1:E:56:GLU:H	2.21	0.44
1:E:268:VAL:O	2:F:539:LEU:HD13	2.18	0.44
2:F:270:GLU:HG3	2:F:487:PHE:CZ	2.53	0.44
2:F:530:LEU:O	2:F:533:ILE:HG13	2.18	0.44
1:K:171:ASN:HB3	1:K:205:LEU:HB2	1.99	0.44
1:K:296:VAL:HG21	2:L:305:VAL:HG11	1.99	0.44
1:K:35:ARG:HG2	1:K:80:ARG:CB	2.47	0.43
1:K:328:ILE:HD12	2:L:284:LEU:HD22	2.00	0.43
2:B:146:GLN:HG2	2:B:149:ILE:HD13	2.01	0.43
2:B:195:LYS:H	2:B:195:LYS:HG2	1.42	0.43
1:E:220:ILE:HG13	1:E:221:ILE:N	2.33	0.43
2:L:390:VAL:HG21	2:L:407:VAL:CG2	2.48	0.43
2:L:530:LEU:O	2:L:533:ILE:HG13	2.18	0.43
1:O:446:MET:HA	1:O:447:PRO:HD3	1.86	0.43
1:O:448:PHE:O	1:O:448:PHE:CG	2.70	0.43
2:P:19:THR:H	2:P:104:GLN:HE22	1.63	0.43
2:P:56:LEU:HD21	2:P:58:LEU:HD21	2.00	0.43
1:A:322:TYR:CE1	2:B:274:LYS:HE2	2.53	0.43
2:B:465:LYS:HB2	2:B:476:LEU:HD21	2.00	0.43
1:E:467:GLU:OE1	5:J:204:THR:HG21	2.18	0.43
1:K:206:LYS:HG2	1:K:237:SER:HA	2.00	0.43
2:L:184:ARG:HD3	2:L:514:ASN:HD22	1.83	0.43
1:O:281:LEU:HD11	4:R:21:DC:OP2	2.18	0.43
2:P:12:LEU:HD23	2:P:133:GLU:HB2	2.00	0.43
1:A:245:LYS:HD3	1:A:425:ILE:HG12	2.00	0.43
1:E:189:LYS:HZ3	1:E:193:LEU:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:366:LEU:HD12	1:K:434:LEU:HD22	2.01	0.43
3:M:10:DG:N2	3:M:11:DC:C2	2.86	0.43
2:L:400:ARG:NH1	3:M:10:DG:H4'	2.33	0.43
1:O:220:ILE:HG13	1:O:221:ILE:N	2.33	0.43
2:P:497:ARG:HH11	2:P:497:ARG:HA	1.83	0.43
1:E:281:LEU:HG	1:E:282:LYS:N	2.32	0.43
2:F:33:GLN:O	2:F:37:VAL:HG23	2.19	0.43
1:K:121:GLN:O	1:K:130:ARG:HD2	2.18	0.43
1:K:229:LEU:H	1:K:229:LEU:HG	1.71	0.43
1:K:448:PHE:CG	1:K:448:PHE:O	2.71	0.43
1:K:530:TYR:HA	1:K:531:PRO:HD3	1.90	0.43
2:L:112:ILE:HD11	2:L:150:ILE:HD11	2.00	0.43
1:O:411:VAL:HG11	1:O:434:LEU:HD21	1.99	0.43
1:O:438:PRO:O	2:P:480:THR:HA	2.19	0.43
1:A:50:GLU:C	1:A:52:GLN:H	2.20	0.43
1:A:321:ILE:HG13	1:A:326:GLN:HG3	2.01	0.43
1:A:531:PRO:HD2	1:A:532:PRO:CD	2.48	0.43
2:B:198:THR:HG23	2:B:201:GLN:OE1	2.18	0.43
2:F:8:ALA:N	2:F:52:ASP:OD1	2.50	0.43
1:K:446:MET:HA	1:K:447:PRO:HD3	1.86	0.43
1:O:128:GLN:O	1:O:132:GLN:HG3	2.19	0.43
1:O:303:PHE:HB3	1:O:310:LEU:HA	2.01	0.43
2:P:530:LEU:O	2:P:533:ILE:HG13	2.18	0.43
1:A:289:TYR:HD1	2:B:305:VAL:HG13	1.84	0.43
1:A:304:ASN:ND2	1:A:311:LEU:HD13	2.30	0.43
1:A:366:LEU:HB2	1:A:434:LEU:HB3	1.99	0.43
2:B:509:GLN:HG2	2:B:511:HIS:CE1	2.54	0.43
2:B:530:LEU:O	2:B:533:ILE:HG13	2.19	0.43
1:E:41:LEU:HD23	1:E:168:LEU:HD13	2.00	0.43
1:K:113:ALA:HB2	2:L:316:TYR:CE2	2.54	0.43
1:K:525:PHE:N	1:K:525:PHE:HD1	2.12	0.43
2:L:72:ASP:O	2:L:75:GLN:HG3	2.19	0.43
1:O:143:LEU:O	1:O:147:LEU:HD13	2.19	0.43
1:O:165:ARG:HD3	1:O:201:ASP:OD2	2.19	0.43
2:P:15:ASP:HB2	2:P:59:PHE:CZ	2.52	0.43
2:P:165:LEU:O	2:P:226:SER:HA	2.19	0.43
2:P:297:LEU:HB3	2:P:301:ASP:O	2.18	0.43
1:A:345:LEU:HD21	1:A:413:LEU:HD11	2.01	0.43
1:A:525:PHE:N	1:A:525:PHE:CD1	2.85	0.43
1:K:443:LYS:HD2	2:L:480:THR:HB	1.99	0.43
2:P:337:GLY:HA2	2:P:399:LYS:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ILE:HG22	1:A:116:ILE:HD13	2.00	0.43
1:A:249:LYS:HD2	1:A:249:LYS:HA	1.65	0.43
1:A:295:PRO:HD2	2:B:299:ASP:OD1	2.19	0.43
1:E:35:ARG:HE	1:E:80:ARG:HE	1.65	0.43
1:E:340:PHE:HB3	1:E:408:PRO:HD3	1.99	0.43
1:K:485:GLN:NE2	1:K:501:GLU:O	2.51	0.43
2:P:296:CYS:HB3	2:P:302:GLU:HB3	2.01	0.43
3:Q:9:DG:N2	4:R:20:DC:N3	2.59	0.43
1:A:91:GLU:HG2	1:A:136:GLY:H	1.84	0.42
3:C:3:DA:N1	4:D:25:DA:N1	2.67	0.42
1:E:126:GLN:O	1:E:130:ARG:HG3	2.19	0.42
1:K:495:LEU:O	1:K:497:LEU:N	2.52	0.42
1:K:508:LEU:HA	1:K:509:PRO:HD3	1.89	0.42
1:A:465:ILE:HD11	1:A:525:PHE:CD2	2.46	0.42
3:C:9:DG:H2'	3:C:10:DG:H8	1.82	0.42
1:E:403:ARG:NE	4:H:27:DC:H4'	2.34	0.42
2:F:6:ASN:HB2	2:F:242:ARG:HE	1.84	0.42
3:G:9:DG:H2'	3:G:10:DG:H8	1.84	0.42
1:O:91:GLU:HG3	1:O:92:LYS:N	2.34	0.42
1:O:245:LYS:HB2	1:O:245:LYS:HE2	1.71	0.42
2:F:467:ASP:HB3	2:F:470:THR:HG22	2.01	0.42
1:K:489:ASN:HD22	1:K:500:PRO:HB2	1.84	0.42
1:O:67:ILE:HD11	1:O:169:PHE:CE1	2.54	0.42
1:O:268:VAL:O	2:P:539:LEU:HD13	2.19	0.42
1:O:525:PHE:N	1:O:525:PHE:HD1	2.14	0.42
2:P:342:VAL:HA	2:P:393:VAL:HG22	2.01	0.42
2:P:467:ASP:O	2:P:471:ASP:HB2	2.19	0.42
1:A:74:LYS:HD3	1:A:79:ASP:OD2	2.20	0.42
1:E:488:ARG:HH11	1:E:501:GLU:CG	2.28	0.42
2:L:38:ILE:O	2:L:42:VAL:HG23	2.19	0.42
1:O:340:PHE:HZ	2:P:486:ARG:HA	1.80	0.42
1:O:515:ASN:HD21	2:P:255:SER:CB	2.33	0.42
2:P:81:ARG:HH22	2:P:87:ASP:CG	2.22	0.42
2:P:91:LEU:HD13	2:P:495:LEU:HD13	2.01	0.42
1:A:178:ASN:OD1	1:A:179:ASP:N	2.53	0.42
1:A:356:LEU:CD2	1:A:437:LEU:HD21	2.49	0.42
2:B:416:TYR:CD2	2:B:416:TYR:C	2.92	0.42
1:E:41:LEU:HA	1:E:86:VAL:HG23	2.01	0.42
1:E:256:LEU:HB3	1:E:273:ILE:O	2.20	0.42
1:E:345:LEU:HD12	1:E:345:LEU:HA	1.84	0.42
3:M:3:DA:N1	4:N:25:DA:N1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:390:VAL:HG21	2:P:407:VAL:CG2	2.49	0.42
2:F:197:ILE:HG13	2:F:201:GLN:HB2	2.02	0.42
1:K:252:ARG:HD2	1:K:252:ARG:HA	1.60	0.42
1:O:345:LEU:HD12	1:O:345:LEU:HA	1.79	0.42
1:O:518:LEU:HD23	1:O:518:LEU:HA	1.80	0.42
2:P:407:VAL:O	2:P:421:TYR:HA	2.19	0.42
1:K:35:ARG:HE	1:K:80:ARG:NE	2.18	0.42
2:L:18:PHE:HB2	2:L:102:SER:HA	2.01	0.42
1:E:305:THR:HG22	2:F:288:ASP:HA	2.00	0.42
2:F:66:ASN:OD1	2:F:67:PRO:HD2	2.20	0.42
1:K:173:ASP:HA	1:K:211:PHE:CZ	2.55	0.42
1:K:322:TYR:CE1	2:L:274:LYS:HE2	2.55	0.42
2:L:115:MET:SD	2:L:154:LEU:HG	2.60	0.42
2:L:132:ILE:HB	2:L:161:LEU:HD23	2.01	0.42
3:M:17:DA:C8	3:M:18:DT:H72	2.54	0.42
1:O:465:ILE:HD11	1:O:525:PHE:CD2	2.53	0.42
2:P:27:ILE:HD11	2:P:183:PHE:CD2	2.54	0.42
2:P:479:THR:HA	2:P:482:ILE:HD12	2.02	0.42
2:B:477:PHE:CE1	2:B:518:PRO:HA	2.54	0.42
2:F:77:ILE:HG21	2:F:113:VAL:HG21	2.02	0.42
1:K:172:GLU:O	1:K:217:TYR:HE2	2.03	0.42
1:O:517:ARG:O	1:O:518:LEU:HD23	2.20	0.42
1:A:51:SER:N	1:A:58:THR:HG22	2.35	0.42
2:B:138:LEU:HD13	2:B:165:LEU:HG	2.02	0.42
1:E:303:PHE:HB3	1:E:310:LEU:HA	2.02	0.42
2:F:120:HIS:CG	1:K:185:ARG:HG3	2.55	0.42
2:F:404:GLN:HB3	2:F:423:GLN:HG3	2.01	0.42
2:F:445:ALA:HA	2:F:446:PRO:HD3	1.89	0.42
1:K:91:GLU:HG2	1:K:136:GLY:CA	2.49	0.42
1:O:474:ARG:HH12	5:T:194:LYS:HB3	1.85	0.42
2:P:45:GLN:HG3	2:P:54:ILE:HD11	2.02	0.42
1:A:232:HIS:CE1	1:A:233:PHE:CE2	3.08	0.41
1:A:518:LEU:HD22	1:A:521:LEU:HD22	2.02	0.41
2:B:11:VAL:HG11	2:B:114:SER:HB3	2.00	0.41
2:B:70:GLY:O	2:B:73:GLN:HG2	2.20	0.41
2:B:81:ARG:HH22	2:B:87:ASP:CG	2.23	0.41
1:K:216:PHE:CE2	1:K:220:ILE:HD13	2.55	0.41
1:K:233:PHE:CD2	1:K:233:PHE:N	2.88	0.41
2:L:390:VAL:HG22	2:L:391:ALA:H	1.84	0.41
1:O:524:GLU:HG2	1:O:525:PHE:CE1	2.55	0.41
2:P:400:ARG:CZ	3:Q:12:DC:H5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:537:PHE:HA	2:P:538:PRO:HD3	1.88	0.41
1:A:465:ILE:HG21	2:B:257:LEU:HD21	2.02	0.41
2:B:9:ALA:HB2	2:B:127:PHE:CD1	2.55	0.41
2:B:184:ARG:HD3	2:B:514:ASN:HD22	1.85	0.41
1:E:91:GLU:HG2	1:E:136:GLY:CA	2.48	0.41
2:F:18:PHE:HB2	2:F:102:SER:HA	2.02	0.41
2:F:171:LYS:HD2	2:F:171:LYS:N	2.35	0.41
1:K:356:LEU:CD2	1:K:437:LEU:HD21	2.50	0.41
2:L:250:ARG:HD2	2:L:258:SER:HB3	2.02	0.41
1:A:91:GLU:HG3	1:A:92:LYS:N	2.35	0.41
1:A:143:LEU:O	1:A:147:LEU:HD13	2.20	0.41
2:B:33:GLN:O	2:B:37:VAL:HG23	2.19	0.41
1:E:334:THR:O	1:E:337:LEU:HG	2.21	0.41
1:E:517:ARG:HH22	5:J:203:GLU:HA	1.86	0.41
1:O:515:ASN:OD1	2:P:255:SER:HB3	2.20	0.41
2:P:165:LEU:HD23	2:P:167:PHE:CZ	2.55	0.41
1:A:121:GLN:O	1:A:130:ARG:HD2	2.19	0.41
1:A:329:LEU:HD12	2:B:276:TRP:CH2	2.56	0.41
1:E:257:SER:CB	1:E:403:ARG:HH22	2.33	0.41
1:E:302:THR:CG2	2:F:291:LYS:HG3	2.43	0.41
1:E:325:ARG:HD2	2:F:88:PHE:CD1	2.55	0.41
2:F:123:ILE:HD11	1:K:184:SER:CB	2.45	0.41
2:L:482:ILE:HA	2:L:483:PRO:HD3	1.97	0.41
1:O:488:ARG:CD	1:O:503:ALA:HB2	2.49	0.41
1:A:91:GLU:HG2	1:A:136:GLY:N	2.35	0.41
2:L:65:ASP:O	2:L:78:THR:HA	2.20	0.41
1:O:444:ARG:HB2	2:P:266:SER:O	2.21	0.41
2:B:13:CYS:SG	2:B:110:ALA:HB1	2.61	0.41
2:B:537:PHE:HA	2:B:538:PRO:HD3	1.85	0.41
3:C:1:DG:N2	4:D:28:DC:O2	2.54	0.41
1:K:143:LEU:O	1:K:147:LEU:HD13	2.19	0.41
1:O:90:THR:O	1:O:101:ASN:HA	2.19	0.41
1:O:99:PHE:HD1	1:O:99:PHE:HA	1.78	0.41
1:O:264:ASN:HB3	1:O:267:ILE:HD12	2.01	0.41
2:P:38:ILE:O	2:P:42:VAL:HG23	2.20	0.41
2:P:299:ASP:HB3	2:P:301:ASP:OD1	2.20	0.41
5:T:187:ASN:HB3	5:T:190:PHE:CD2	2.55	0.41
5:T:202:ASP:N	5:T:202:ASP:OD1	2.54	0.41
1:A:90:THR:HG21	1:A:103:TYR:HB2	2.02	0.41
1:A:259:LEU:HB3	1:A:344:GLY:HA2	2.02	0.41
1:A:418:GLU:HA	1:A:428:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:LEU:CD2	2:B:253:ILE:HG13	2.49	0.41
1:E:468:LYS:CB	1:E:518:LEU:HD21	2.50	0.41
1:K:189:LYS:O	1:K:193:LEU:HG	2.21	0.41
1:K:285:PRO:HB3	2:L:314:PHE:CZ	2.55	0.41
1:K:297:LYS:HE3	1:K:299:LYS:HE3	2.03	0.41
2:L:312:GLN:HG2	2:L:325:LYS:HG3	2.01	0.41
1:O:35:ARG:NE	1:O:80:ARG:HB3	2.36	0.41
1:O:276:LEU:HD13	1:O:367:PHE:HB3	2.03	0.41
2:P:352:GLN:HB2	2:P:355:PHE:CD2	2.55	0.41
2:B:270:GLU:HG3	2:B:487:PHE:CZ	2.56	0.41
1:E:418:GLU:HB2	1:E:430:PRO:HB3	2.03	0.41
2:F:253:ILE:HB	2:F:257:LEU:HD23	2.02	0.41
2:F:311:ILE:HD13	2:F:311:ILE:HA	1.94	0.41
2:F:431:ARG:HH22	3:G:4:DT:P	2.43	0.41
2:L:445:ALA:HA	2:L:446:PRO:HD3	1.96	0.41
3:M:3:DA:H61	4:N:25:DA:H61	1.68	0.41
1:A:507:THR:HB	2:B:394:ARG:HG3	2.02	0.41
2:B:53:GLU:HB2	2:B:127:PHE:CZ	2.56	0.41
2:F:44:ARG:HB3	2:F:237:PHE:CZ	2.56	0.41
2:F:295:TYR:CE2	2:F:307:LYS:HE2	2.54	0.41
2:F:537:PHE:HA	2:F:538:PRO:HD3	1.90	0.41
1:K:488:ARG:HD3	1:K:501:GLU:HG2	2.02	0.41
1:K:495:LEU:C	1:K:497:LEU:H	2.23	0.41
2:L:407:VAL:O	2:L:421:TYR:HA	2.20	0.41
1:O:52:GLN:NE2	1:O:208:PRO:HD3	2.36	0.41
1:O:210:GLY:HA2	1:O:233:PHE:CB	2.51	0.41
1:A:333:GLU:OE2	2:B:497:ARG:NH2	2.53	0.41
2:B:197:ILE:HG13	2:B:201:GLN:HB2	2.02	0.41
3:C:10:DG:N2	3:C:11:DC:C2	2.89	0.41
1:E:247:ARG:NH2	1:E:488:ARG:HG3	2.36	0.41
1:E:343:PRO:HA	1:E:401:THR:O	2.20	0.41
2:F:93:ASP:HA	2:F:97:LYS:HB2	2.03	0.41
1:K:515:ASN:OD1	2:L:255:SER:HB3	2.21	0.41
1:O:356:LEU:CD2	1:O:437:LEU:HD21	2.51	0.41
1:O:488:ARG:O	1:O:491:GLU:HG2	2.21	0.41
1:A:40:PHE:CG	1:A:67:ILE:HD12	2.55	0.40
2:B:247:TRP:HZ3	2:B:249:CYS:HB2	1.86	0.40
2:B:251:LEU:HA	2:B:340:PHE:HB2	2.03	0.40
2:B:252:THR:HG23	2:B:258:SER:OG	2.21	0.40
1:E:267:ILE:HD13	2:F:530:LEU:HD22	2.03	0.40
2:F:132:ILE:HB	2:F:161:LEU:HD23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:165:ARG:HG3	1:K:199:PHE:HB2	2.02	0.40
2:L:165:LEU:HD23	2:L:167:PHE:CZ	2.56	0.40
1:O:530:TYR:HA	1:O:531:PRO:HD3	1.94	0.40
4:R:15:DC:H2"	4:R:16:DG:OP2	2.21	0.40
1:A:531:PRO:HD2	1:A:532:PRO:HD2	2.03	0.40
2:B:38:ILE:O	2:B:42:VAL:HG23	2.21	0.40
1:E:356:LEU:CD2	1:E:437:LEU:HD21	2.51	0.40
2:F:341:SER:N	2:F:394:ARG:O	2.54	0.40
2:F:368:ARG:HG2	2:F:369:ASP:OD1	2.21	0.40
2:L:463:LEU:HD22	2:L:477:PHE:HB2	2.03	0.40
1:A:179:ASP:OD2	1:A:182:LYS:NZ	2.38	0.40
1:E:189:LYS:HD2	1:E:189:LYS:HA	1.54	0.40
2:F:27:ILE:HD11	2:F:183:PHE:CD2	2.57	0.40
2:F:351:VAL:O	2:F:351:VAL:HG23	2.21	0.40
1:K:485:GLN:HE22	1:K:502:GLN:HA	1.86	0.40
1:O:322:TYR:CE1	2:P:274:LYS:HE2	2.57	0.40
1:O:522:VAL:HG13	2:P:257:LEU:HB2	2.04	0.40
1:A:233:PHE:CG	1:A:245:LYS:HE2	2.56	0.40
2:B:407:VAL:O	2:B:421:TYR:HA	2.22	0.40
2:L:457:LEU:HD11	2:L:530:LEU:HG	2.03	0.40
1:E:125:GLN:HB2	1:E:126:GLN:OE1	2.20	0.40
2:F:198:THR:O	2:F:201:GLN:N	2.53	0.40
1:K:41:LEU:HD23	1:K:168:LEU:HD13	2.03	0.40
1:K:485:GLN:NE2	1:K:502:GLN:HA	2.36	0.40
1:K:489:ASN:ND2	1:K:500:PRO:HB2	2.36	0.40
4:N:18:DG:C2	4:N:19:DC:C2	3.10	0.40
1:O:204:HIS:HD1	1:O:204:HIS:H	1.70	0.40
1:O:241:ASP:HA	1:O:244:ARG:NH1	2.36	0.40
1:O:403:ARG:HD2	4:R:27:DC:OP1	2.22	0.40
2:P:64:THR:HG22	2:P:66:ASN:H	1.86	0.40
2:P:311:ILE:HD13	2:P:311:ILE:HA	1.93	0.40
5:T:194:LYS:HA	5:T:195:PRO:HD3	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/544 (91%)	478 (97%)	15 (3%)	2 (0%)	34	69
1	E	493/544 (91%)	474 (96%)	16 (3%)	3 (1%)	25	60
1	K	498/544 (92%)	484 (97%)	13 (3%)	1 (0%)	47	79
1	O	494/544 (91%)	472 (96%)	21 (4%)	1 (0%)	47	79
2	B	525/572 (92%)	513 (98%)	11 (2%)	1 (0%)	47	79
2	F	533/572 (93%)	517 (97%)	14 (3%)	2 (0%)	34	69
2	L	524/572 (92%)	507 (97%)	15 (3%)	2 (0%)	34	69
2	P	527/572 (92%)	506 (96%)	18 (3%)	3 (1%)	25	60
5	J	26/28 (93%)	24 (92%)	2 (8%)	0	100	100
5	T	26/28 (93%)	23 (88%)	3 (12%)	0	100	100
All	All	4141/4520 (92%)	3998 (96%)	128 (3%)	15 (0%)	34	69

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	530	TYR
1	E	55	ASP
2	L	302	GLU
2	P	69	SER
2	P	125	LYS
2	B	299	ASP
1	E	52	GLN
2	F	174	GLY
2	L	299	ASP
2	F	340	PHE
1	O	175	PRO
1	A	52	GLN
1	K	496	ASP
2	P	471	ASP
1	E	175	PRO

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	453/492 (92%)	451 (100%)	2 (0%)	91 96
1	E	452/492 (92%)	446 (99%)	6 (1%)	69 87
1	K	456/492 (93%)	452 (99%)	4 (1%)	78 91
1	O	453/492 (92%)	449 (99%)	4 (1%)	78 91
2	B	478/513 (93%)	476 (100%)	2 (0%)	91 96
2	F	481/513 (94%)	478 (99%)	3 (1%)	86 94
2	L	476/513 (93%)	474 (100%)	2 (0%)	91 96
2	P	477/513 (93%)	474 (99%)	3 (1%)	86 94
5	J	23/23 (100%)	23 (100%)	0	100 100
5	T	23/23 (100%)	23 (100%)	0	100 100
All	All	3772/4066 (93%)	3746 (99%)	26 (1%)	84 93

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	PHE
1	A	139	SER
2	B	441	SER
2	B	509	GLN
1	E	36	ASP
1	E	79	ASP
1	E	99	PHE
1	E	139	SER
1	E	245	LYS
1	E	247	ARG
2	F	441	SER
2	F	502	ARG
2	F	539	LEU
1	K	99	PHE
1	K	139	SER
1	K	229	LEU
1	K	525	PHE
2	L	441	SER
2	L	539	LEU
1	O	50	GLU

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Mol	Chain	Res	Type
1	O	99	PHE
1	O	139	SER
1	O	518	LEU
2	P	236	VAL
2	P	441	SER
2	P	539	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	HIS
1	A	360	HIS
1	A	489	ASN
2	B	22	ASN
2	B	45	GLN
2	B	509	GLN
2	B	514	ASN
2	F	120	HIS
1	K	52	GLN
1	K	176	HIS
1	K	204	HIS
1	K	360	HIS
1	K	433	GLN
1	K	486	HIS
2	L	75	GLN
2	L	119	GLN
2	L	243	HIS
2	L	514	ASN
1	O	486	HIS
2	P	22	ASN
2	P	80	HIS
2	P	243	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	SO4	F	601	-	4,4,4	0.13	0	6,6,6	0.07	0
6	SO4	P	601	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	K	601	-	4,4,4	0.15	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	499/544 (91%)	0.19	36 (7%) 15 8	51, 105, 175, 256	0
1	E	497/544 (91%)	-0.16	7 (1%) 75 59	46, 80, 134, 187	0
1	K	502/544 (92%)	0.32	43 (8%) 10 6	43, 112, 181, 235	0
1	O	498/544 (91%)	-0.12	9 (1%) 68 51	44, 81, 136, 204	0
2	B	531/572 (92%)	0.01	27 (5%) 28 17	44, 92, 161, 227	0
2	F	537/572 (93%)	-0.12	13 (2%) 59 42	47, 84, 145, 208	0
2	L	530/572 (92%)	0.18	43 (8%) 12 6	33, 93, 159, 257	0
2	P	531/572 (92%)	-0.10	16 (3%) 50 34	45, 83, 137, 194	0
3	C	19/30 (63%)	-0.89	0 100 100	105, 146, 174, 176	0
3	G	20/30 (66%)	-0.90	0 100 100	106, 143, 164, 174	0
3	M	19/30 (63%)	-0.83	0 100 100	102, 148, 184, 186	0
3	Q	20/30 (66%)	-1.00	0 100 100	108, 145, 172, 187	0
4	D	14/15 (93%)	-0.96	0 100 100	130, 154, 191, 201	0
4	H	15/15 (100%)	-0.75	0 100 100	106, 123, 176, 193	0
4	N	14/15 (93%)	-0.72	0 100 100	134, 143, 180, 223	0
4	R	15/15 (100%)	-0.87	0 100 100	114, 131, 185, 213	0
5	J	28/28 (100%)	-0.32	0 100 100	83, 104, 141, 161	0
5	T	28/28 (100%)	-0.37	1 (3%) 42 28	77, 107, 149, 165	0
All	All	4317/4700 (91%)	-0.01	195 (4%) 33 21	33, 92, 163, 257	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	322	PRO	24.4
2	L	321	VAL	12.2
1	K	459	VAL	9.6

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Mol	Chain	Res	Type	RSRZ
1	K	131	PHE	9.6
2	L	257	LEU	8.3
2	L	340	PHE	6.8
1	A	529	VAL	6.8
1	A	298	THR	6.7
1	K	133	ASP	6.1
2	F	298	ASN	6.1
2	L	331	MET	6.0
2	L	323	PHE	6.0
1	A	122	PHE	5.9
2	L	320	ILE	5.9
1	K	108	LEU	5.9
2	L	197	ILE	5.8
2	B	257	LEU	5.8
2	L	256	ASN	5.7
2	B	322	PRO	5.5
2	B	318	SER	5.4
2	L	253	ILE	5.4
1	K	522	VAL	5.3
2	F	469	LYS	5.2
1	K	122	PHE	5.2
2	L	314	PHE	5.0
2	L	251	LEU	5.0
1	A	496	ASP	4.9
2	P	197	ILE	4.9
2	L	376	ALA	4.9
1	A	313	PRO	4.8
1	E	456	PRO	4.6
1	K	288	LEU	4.6
2	L	315	ARG	4.5
1	A	158	GLN	4.5
1	K	298	THR	4.5
2	B	315	ARG	4.4
1	A	137	HIS	4.4
1	K	283	PRO	4.4
2	L	88	PHE	4.3
1	A	328	ILE	4.3
1	A	291	GLU	4.3
1	A	459	VAL	4.3
2	L	345	PHE	4.2
1	A	435	VAL	4.2
2	B	314	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	327	ILE	4.2
2	B	253	ILE	4.2
2	F	468	GLU	4.1
1	A	312	LEU	4.1
1	K	309	GLY	4.1
1	A	516	LYS	4.1
1	K	279	LYS	4.1
2	L	381	ILE	4.0
2	B	259	ILE	4.0
2	B	287	GLU	4.0
2	B	542	ALA	4.0
2	B	251	LEU	4.0
1	A	46	LYS	4.0
1	K	143	LEU	4.0
1	K	305	THR	4.0
1	A	63	SER	3.9
1	A	530	TYR	3.9
2	L	286	LYS	3.9
2	L	255	SER	3.8
2	P	488	GLN	3.8
1	K	137	HIS	3.8
2	B	320	ILE	3.8
2	L	342	VAL	3.8
2	F	297	LEU	3.8
2	B	331	MET	3.7
1	A	103	TYR	3.6
1	A	356	LEU	3.6
1	K	295	PRO	3.6
1	K	306	SER	3.6
2	L	341	SER	3.6
1	K	157	VAL	3.6
2	P	165	LEU	3.6
1	A	305	THR	3.6
1	E	248	ALA	3.5
1	A	60	PHE	3.5
2	L	380	LEU	3.5
1	K	60	PHE	3.4
1	A	131	PHE	3.4
2	P	291	LYS	3.4
2	L	367	ALA	3.3
2	L	287	GLU	3.3
2	F	244	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	330	GLN	3.3
1	O	168	LEU	3.2
1	A	87	PHE	3.2
1	K	327	ILE	3.2
1	A	108	LEU	3.2
1	K	455	THR	3.1
2	F	281	ALA	3.1
1	K	89	GLY	3.1
1	K	125	GLN	3.1
1	A	65	GLN	3.1
1	O	200	LEU	3.0
2	P	258	SER	3.0
1	K	85	VAL	3.0
2	P	243	HIS	2.9
2	B	422	VAL	2.9
2	L	364	VAL	2.9
2	L	192	PHE	2.9
2	L	365	PHE	2.9
1	A	50	GLU	2.9
1	K	47	ALA	2.9
2	L	259	ILE	2.9
5	T	204	THR	2.9
1	A	240	GLU	2.8
1	K	290	ARG	2.8
2	L	473	LEU	2.8
1	K	328	ILE	2.8
2	B	47	PHE	2.8
1	K	63	SER	2.8
2	L	318	SER	2.8
1	K	105	LEU	2.8
1	E	340	PHE	2.8
1	A	105	LEU	2.7
1	K	310	LEU	2.7
2	L	466	LYS	2.7
1	K	303	PHE	2.7
2	P	257	LEU	2.7
2	B	258	SER	2.7
2	B	323	PHE	2.7
1	A	49	PHE	2.7
1	O	55	ASP	2.6
1	E	495	LEU	2.6
1	K	466	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	L	47	PHE	2.6
2	P	290	GLN	2.6
2	B	18	PHE	2.6
2	F	488	GLN	2.6
2	L	343	LEU	2.6
2	F	165	LEU	2.6
1	K	499	GLU	2.6
1	O	165	ARG	2.5
1	K	282	LYS	2.5
1	O	41	LEU	2.5
2	B	46	VAL	2.5
2	B	469	LYS	2.5
1	A	302	THR	2.5
2	P	300	ASP	2.5
1	O	72	ILE	2.5
2	L	258	SER	2.4
2	L	252	THR	2.4
2	F	294	VAL	2.4
1	A	299	LYS	2.4
1	K	124	GLY	2.4
1	K	123	LYS	2.4
2	B	118	ILE	2.4
2	L	274	LYS	2.4
1	K	168	LEU	2.4
1	K	286	ILE	2.4
1	K	462	MET	2.3
1	A	242	LEU	2.3
2	L	379	SER	2.3
2	B	74	TYR	2.3
1	A	460	GLY	2.3
2	P	241	GLU	2.3
2	L	167	PHE	2.3
1	K	244	ARG	2.3
2	F	183	PHE	2.3
2	L	491	PHE	2.3
1	A	489	ASN	2.3
2	L	377	LEU	2.3
1	A	321	ILE	2.3
1	K	41	LEU	2.2
2	B	210	MET	2.2
2	L	123	ILE	2.2
1	A	82	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	P	536	LEU	2.2
1	O	340	PHE	2.2
2	P	167	PHE	2.2
2	L	422	VAL	2.2
1	K	62	MET	2.2
2	B	88	PHE	2.2
2	B	340	PHE	2.1
2	B	337	GLY	2.1
2	B	197	ILE	2.1
2	F	181	GLY	2.1
1	E	487	PHE	2.1
1	K	242	LEU	2.1
2	F	537	PHE	2.1
2	F	320	ILE	2.1
1	O	460	GLY	2.1
1	O	119	LEU	2.1
2	B	380	LEU	2.1
1	E	445	LYS	2.1
1	K	291	GLU	2.1
2	P	392	ILE	2.1
2	P	234	LEU	2.1
2	P	299	ASP	2.0
1	E	291	GLU	2.0
2	P	253	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SO4	K	601	5/5	0.95	0.15	81,82,87,90	0
6	SO4	A	601	5/5	0.97	0.13	98,103,110,110	0
6	SO4	F	601	5/5	0.98	0.13	70,72,77,77	0
6	SO4	P	601	5/5	0.98	0.12	79,80,84,96	0

6.5 Other polymers (i)

There are no such residues in this entry.