



Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2016 – 02:28 PM EDT

PDB ID : 5HYN
Title : Structure of Human Polycomb Repressive Complex 2 (PRC2) with oncogenic histone H3K27M peptide
Authors : Zhang, Y.; Justin, N.; Wilson, J.R.; Gamblin, S.J.
Deposited on : 2016-02-01
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

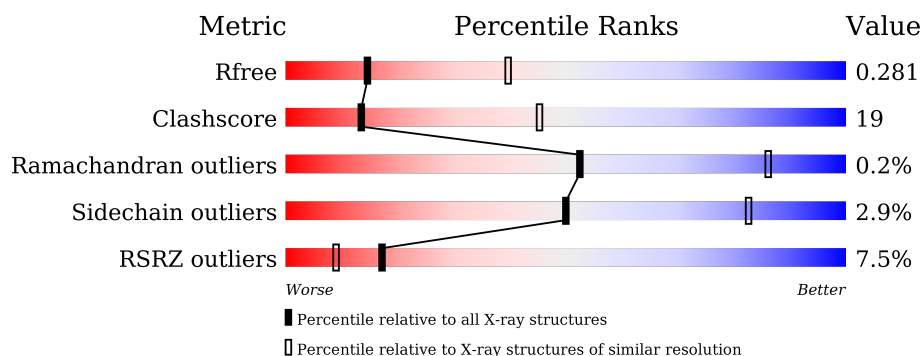
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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.





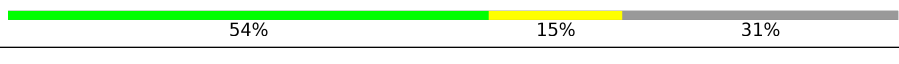

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	746	<div> <div>7%</div> <div> <div>47%</div> <div>28%</div> <div>•</div> <div>22%</div> </div> </div>
1	F	746	<div> <div>8%</div> <div> <div>48%</div> <div>25%</div> <div>•</div> <div>24%</div> </div> </div>
1	K	746	<div> <div>10%</div> <div> <div>50%</div> <div>23%</div> <div>•</div> <div>25%</div> </div> </div>
1	Q	746	<div> <div>8%</div> <div> <div>45%</div> <div>27%</div> <div>•</div> <div>24%</div> </div> </div>
2	B	367	<div> <div>3%</div> <div> <div>62%</div> <div>37%</div> <div>••</div> </div> </div>
2	G	367	<div> <div>4%</div> <div> <div>67%</div> <div>31%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	L	367	
2	R	367	
3	C	129	
3	H	129	
3	M	129	
3	S	129	
4	D	13	
4	I	13	
4	O	13	
4	T	13	
5	E	12	
5	J	12	
5	P	12	
5	U	12	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ZN	A	1004	-	-	-	X
6	ZN	F	1003	-	-	-	X
6	ZN	K	1004	-	-	-	X
6	ZN	K	1007	-	-	-	X
6	ZN	Q	1004	-	-	-	X
6	ZN	Q	1007	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 35028 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 Histone-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	581	Total	C	N	O	S	0	0	0
			4673	2932	825	874	42			
1	F	568	Total	C	N	O	S	0	0	0
			4567	2869	804	852	42			
1	K	562	Total	C	N	O	S	0	0	0
			4521	2836	799	844	42			
1	Q	565	Total	C	N	O	S	0	0	0
			4542	2850	801	849	42			

- Molecule 2 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	365	Total	C	N	O	S	0	0	0
			2959	1873	521	543	22			
2	G	365	Total	C	N	O	S	0	0	0
			2959	1873	521	543	22			
2	L	365	Total	C	N	O	S	0	0	0
			2959	1873	521	543	22			
2	R	365	Total	C	N	O	S	0	0	0
			2959	1873	521	543	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	75	GLY	-	expression tag	UNP O75530
B	76	SER	-	expression tag	UNP O75530
G	75	GLY	-	expression tag	UNP O75530
G	76	SER	-	expression tag	UNP O75530
L	75	GLY	-	expression tag	UNP O75530
L	76	SER	-	expression tag	UNP O75530
R	75	GLY	-	expression tag	UNP O75530
R	76	SER	-	expression tag	UNP O75530

- Molecule 3 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	125	Total	C	N	O	S	0	0	0
			1042	657	180	193	12			
3	H	124	Total	C	N	O	S	0	0	0
			1032	651	177	192	12			
3	M	125	Total	C	N	O	S	0	0	0
			1042	657	180	193	12			
3	S	125	Total	C	N	O	S	0	0	0
			1042	657	180	193	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	557	GLY	-	expression tag	UNP Q15022
H	557	GLY	-	expression tag	UNP Q15022
M	557	GLY	-	expression tag	UNP Q15022
S	557	GLY	-	expression tag	UNP Q15022

- Molecule 4 is a protein called H3K27M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	9	Total	C	N	O	S	0	0	0
			63	38	13	11	1			
4	I	9	Total	C	N	O	S	0	0	0
			63	38	13	11	1			
4	O	9	Total	C	N	O	S	0	0	0
			63	38	13	11	1			
4	T	9	Total	C	N	O	S	0	0	0
			63	38	13	11	1			

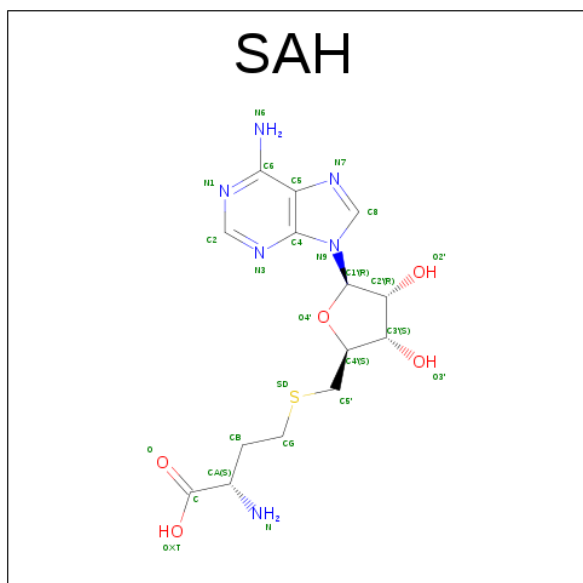
- Molecule 5 is a protein called JARID2 K116me3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	11	Total	C	N	O	0	0	0
			96	60	21	15			
5	J	10	Total	C	N	O	0	0	0
			85	54	17	14			
5	P	9	Total	C	N	O	0	0	0
			77	48	16	13			
5	U	10	Total	C	N	O	0	0	0
			85	54	17	14			

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Q	8	Total	Zn	0	0
			8	8		
6	A	8	Total	Zn	0	0
			8	8		
6	K	8	Total	Zn	0	0
			8	8		
6	F	8	Total	Zn	0	0
			8	8		

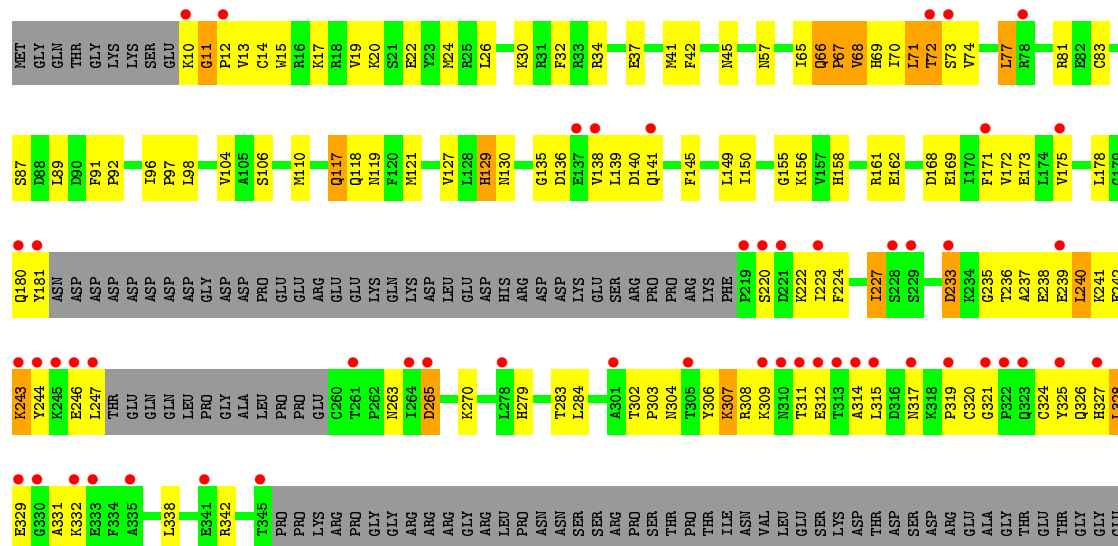
- Molecule 7 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).

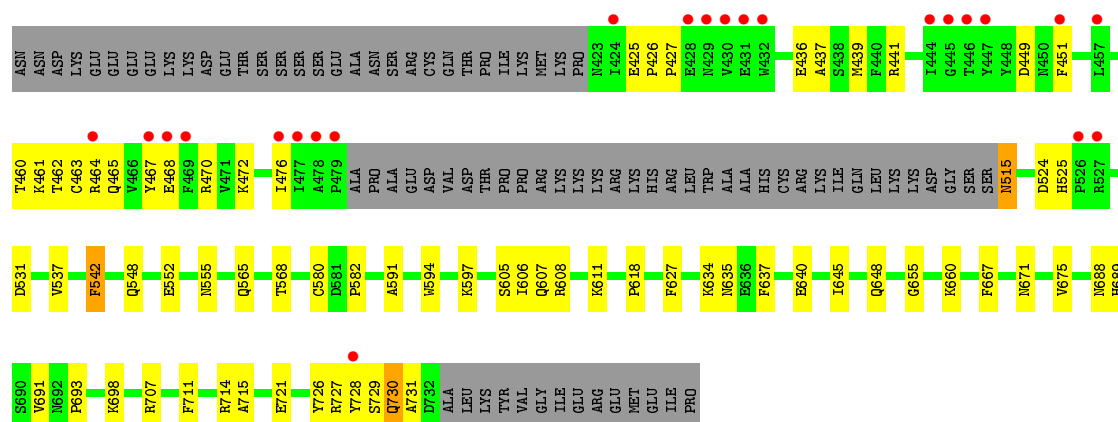


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
7	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
7	K	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
7	Q	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

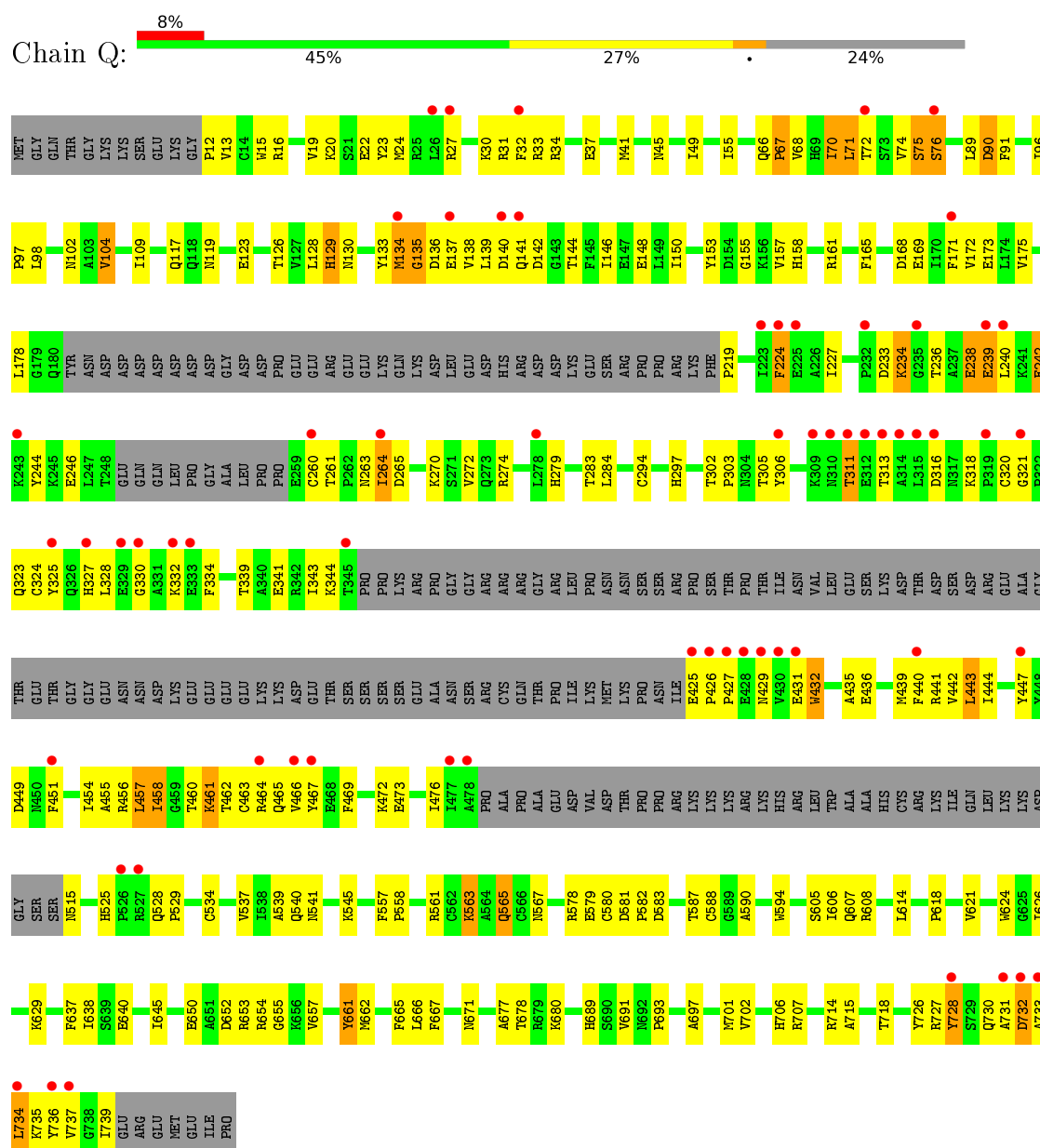
- Molecule 1: Histone-lysine N-methyltransferase EZH2



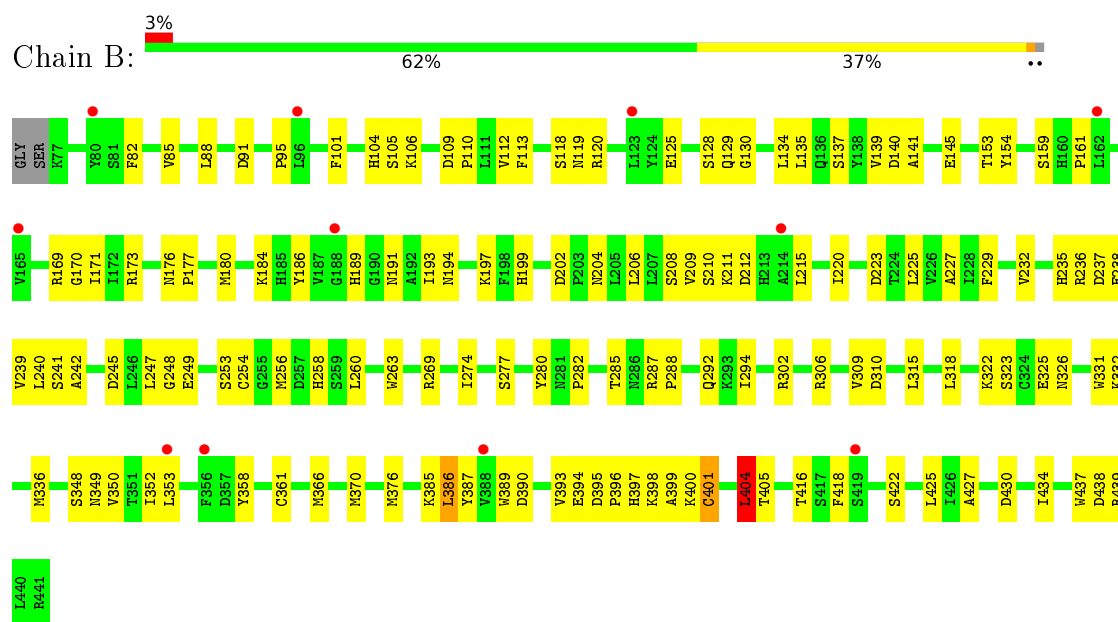




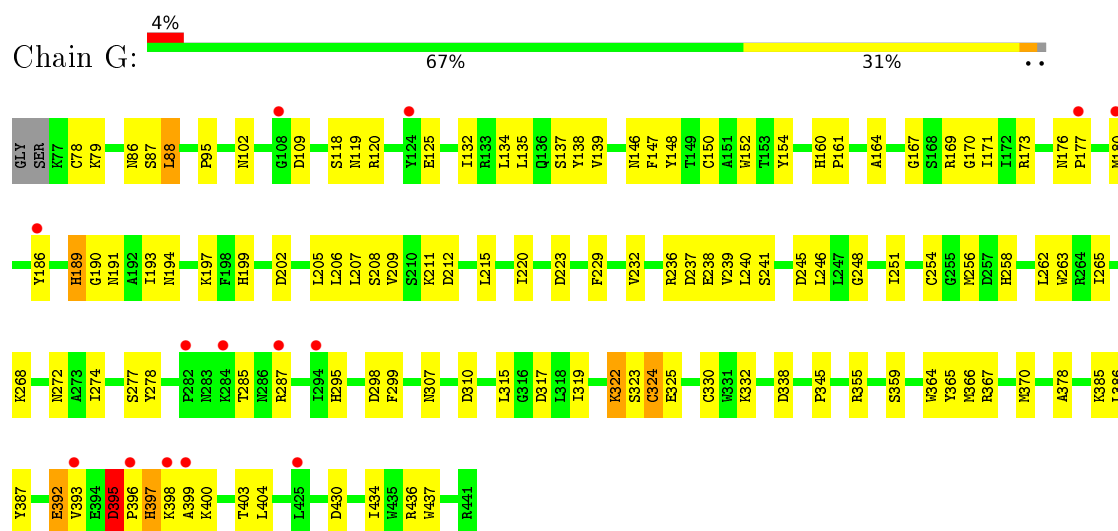
• Molecule 1: Histone-lysine N-methyltransferase EZH2



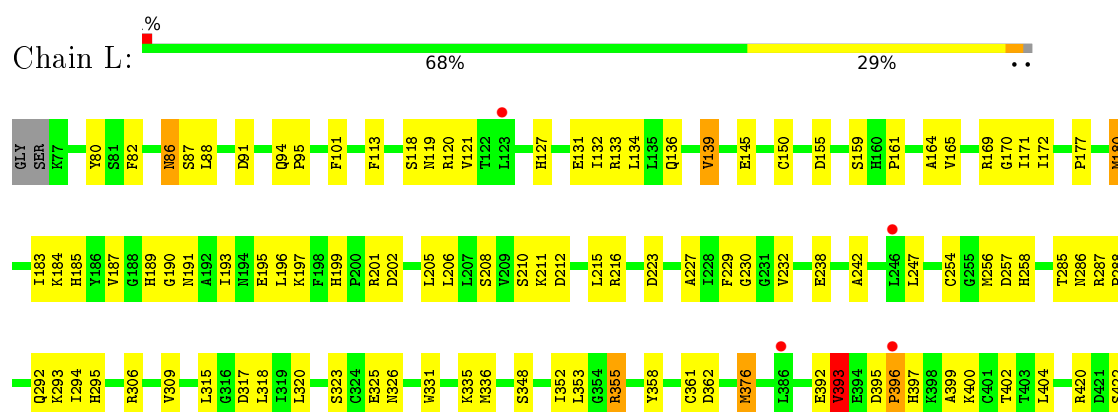
• Molecule 2: Polycomb protein EED

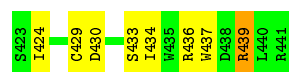


• Molecule 2: Polycomb protein EED

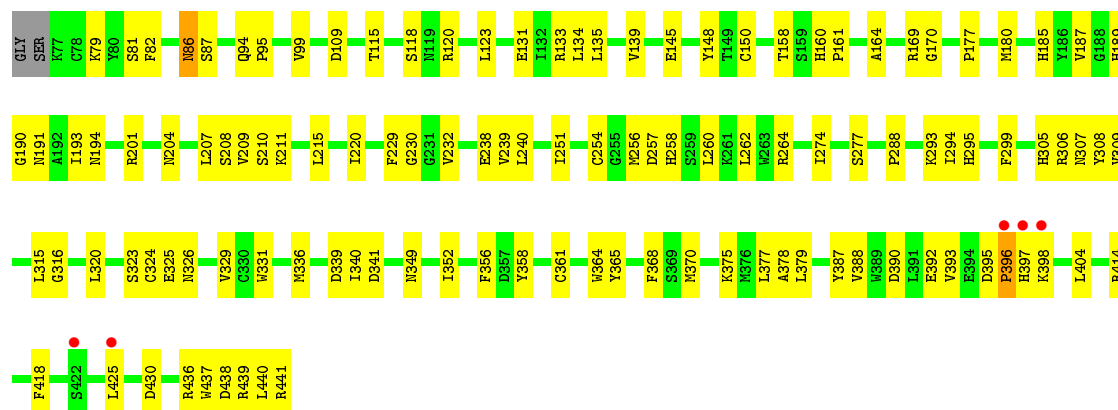


• Molecule 2: Polycomb protein EED

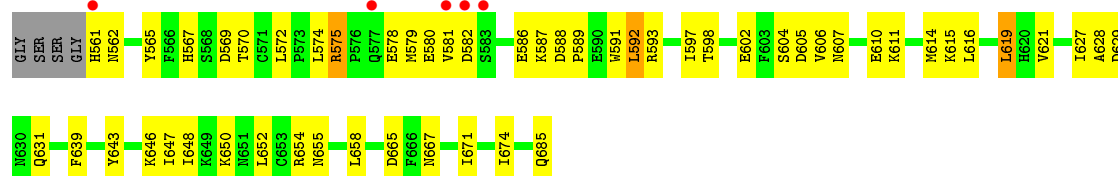




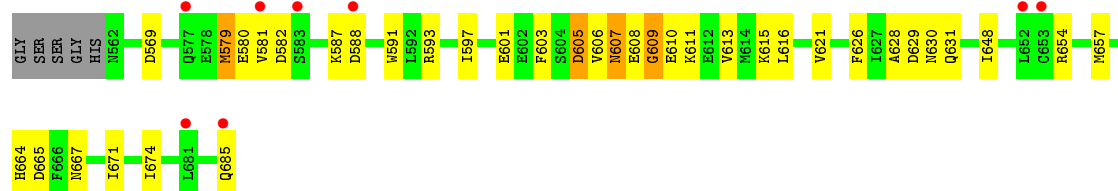
• Molecule 2: Polycomb protein EED



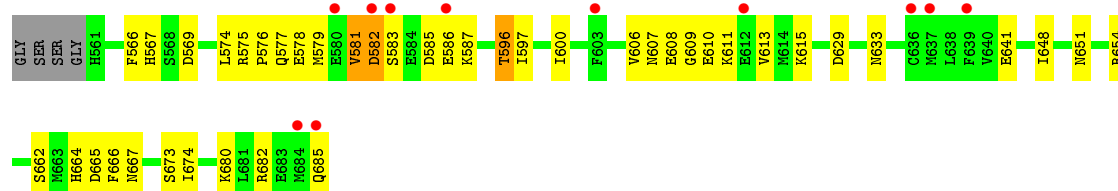
• Molecule 3: Polycomb protein SUZ12



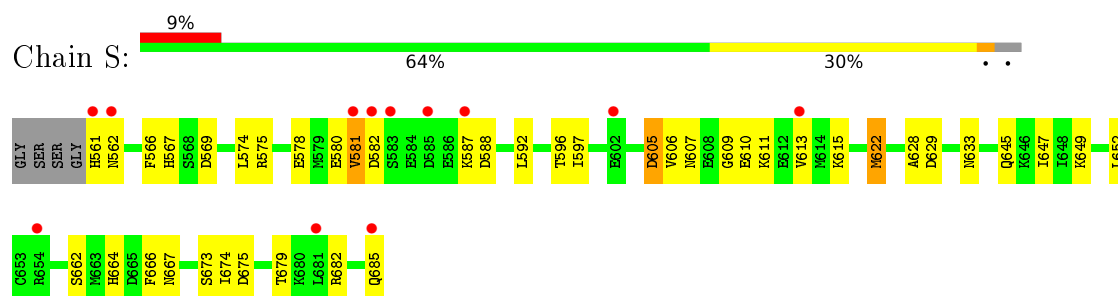
• Molecule 3: Polycomb protein SUZ12



• Molecule 3: Polycomb protein SUZ12



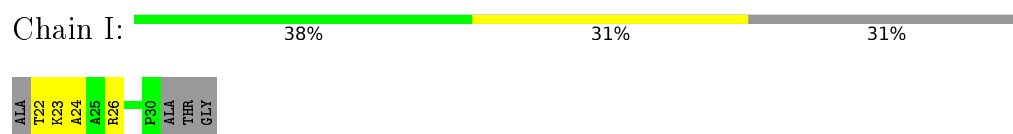
- Molecule 3: Polycomb protein SUZ12



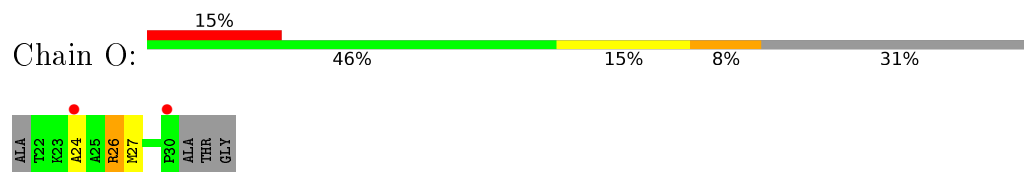
- Molecule 4: H3K27M



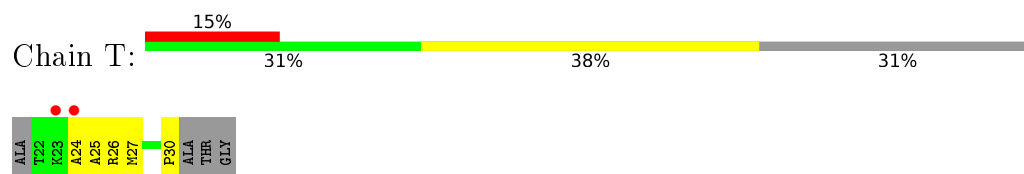
- Molecule 4: H3K27M



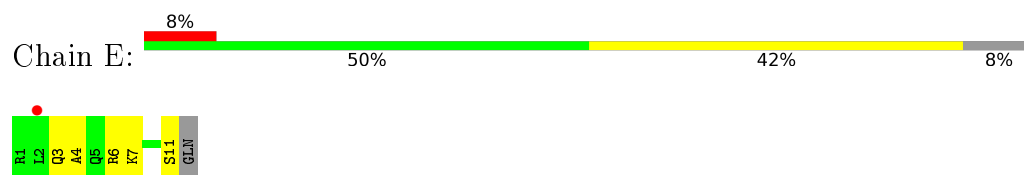
- Molecule 4: H3K27M



- Molecule 4: H3K27M



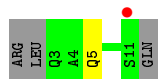
- Molecule 5: JARID2 K116me3



- Molecule 5: JARID2 K116me3



● Molecule 5: JARID2 K116me3



● Molecule 5: JARID2 K116me3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.64Å 171.51Å 274.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.01 – 2.95 104.43 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.01-2.95) 99.9 (104.43-2.94)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.219 , 0.273 0.235 , 0.281	Depositor DCC
R_{free} test set	12405 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	63.5	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35028	wwPDB-VP
Average B, all atoms (Å ²)	88.0	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 33.92 % 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 7.4013e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SAH, M3L

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	0.66	6/4777 (0.1%)	0.80	8/6443 (0.1%)
1	F	0.67	6/4667 (0.1%)	0.86	14/6293 (0.2%)
1	K	0.61	1/4621 (0.0%)	0.84	8/6232 (0.1%)
1	Q	0.72	6/4641 (0.1%)	0.93	13/6258 (0.2%)
2	B	0.50	0/3034	0.75	1/4107 (0.0%)
2	G	0.57	1/3034 (0.0%)	0.84	5/4107 (0.1%)
2	L	0.58	2/3034 (0.1%)	0.81	3/4107 (0.1%)
2	R	0.59	0/3034	0.82	1/4107 (0.0%)
3	C	0.54	0/1063	0.85	2/1427 (0.1%)
3	H	0.58	1/1052 (0.1%)	0.78	1/1412 (0.1%)
3	M	0.68	3/1063 (0.3%)	0.83	2/1427 (0.1%)
3	S	0.51	0/1063	0.74	2/1427 (0.1%)
4	D	0.50	0/63	0.86	0/83
4	I	0.50	0/63	0.72	0/83
4	O	0.57	0/63	1.07	1/83 (1.2%)
4	T	0.50	0/63	0.88	0/83
5	E	0.60	0/84	0.82	0/110
5	J	0.80	0/73	1.43	1/96 (1.0%)
5	P	0.56	0/65	0.62	0/85
5	U	0.95	1/73 (1.4%)	1.05	0/96
All	All	0.62	27/35630 (0.1%)	0.84	62/48066 (0.1%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	Q	0	4
2	G	0	2
2	L	0	3
2	R	0	1
3	H	0	1
All	All	0	15

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	ARG	NE-CZ	-12.29	1.17	1.33
1	F	181	TYR	CB-CG	-10.42	1.36	1.51
1	A	32	PHE	CE1-CZ	8.05	1.52	1.37
1	A	249	GLU	CD-OE1	7.87	1.34	1.25
2	G	396	PRO	N-CD	7.52	1.58	1.47
1	F	320	CYS	CB-SG	-7.50	1.69	1.82
1	A	249	GLU	CG-CD	7.36	1.62	1.51
1	Q	224	PHE	CB-CG	-7.34	1.38	1.51
3	M	583	SER	CB-OG	6.86	1.51	1.42
1	Q	661	TYR	CE2-CZ	6.59	1.47	1.38
1	F	181	TYR	CD1-CE1	-6.49	1.29	1.39
3	M	581	VAL	CB-CG2	6.47	1.66	1.52
1	K	11	GLY	CA-C	-6.21	1.42	1.51
1	F	463	CYS	CB-SG	-5.98	1.72	1.81
1	Q	91	PHE	CE1-CZ	5.95	1.48	1.37
3	H	588	ASP	CB-CG	5.80	1.64	1.51
1	Q	461	LYS	CE-NZ	-5.76	1.34	1.49
1	A	463	CYS	CB-SG	-5.65	1.72	1.81
2	L	139	VAL	CB-CG2	-5.56	1.41	1.52
2	L	393	VAL	CA-CB	5.43	1.66	1.54
1	F	661	TYR	CD2-CE2	5.36	1.47	1.39
1	Q	661	TYR	CG-CD2	5.31	1.46	1.39
1	F	181	TYR	CD2-CE2	-5.15	1.31	1.39
1	A	249	GLU	CD-OE2	5.11	1.31	1.25
5	U	5	GLN	CB-CG	-5.10	1.38	1.52
1	Q	91	PHE	CG-CD2	5.03	1.46	1.38
3	M	574	LEU	CG-CD1	5.00	1.70	1.51

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	443	LEU	CB-CG-CD1	-13.41	88.20	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	33	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	Q	70	ILE	CG1-CB-CG2	-10.19	88.99	111.40
5	J	6	ARG	NE-CZ-NH2	-9.21	115.69	120.30
2	G	324	CYS	CA-CB-SG	-8.72	98.31	114.00
1	F	161	ARG	NE-CZ-NH2	-8.36	116.12	120.30
2	R	324	CYS	CA-CB-SG	-7.88	99.82	114.00
1	F	181	TYR	CA-CB-CG	-7.79	98.60	113.40
1	F	71	LEU	CA-CB-CG	7.01	131.42	115.30
1	K	321	GLY	N-CA-C	-6.96	95.69	113.10
2	L	180	MET	CB-CG-SD	-6.84	91.88	112.40
1	Q	134	MET	CA-CB-CG	-6.76	101.81	113.30
4	O	26	ARG	NE-CZ-NH1	-6.67	116.97	120.30
3	C	575	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	K	68	VAL	CG1-CB-CG2	-6.44	100.59	110.90
1	A	315	LEU	CA-CB-CG	6.42	130.06	115.30
1	K	222	LYS	CD-CE-NZ	-6.35	97.10	111.70
1	Q	134	MET	N-CA-C	6.34	128.13	111.00
1	F	98	LEU	CB-CG-CD2	-6.17	100.51	111.00
1	Q	135	GLY	N-CA-C	-6.14	97.75	113.10
2	G	212	ASP	CB-CG-OD2	6.11	123.79	118.30
3	M	582	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	F	240	LEU	CB-CG-CD2	-6.02	100.77	111.00
3	M	582	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	33	ARG	CA-CB-CG	-6.00	100.19	113.40
1	Q	90	ASP	CB-CG-OD1	5.91	123.62	118.30
1	K	71	LEU	CA-CB-CG	5.85	128.76	115.30
3	S	622	MET	CG-SD-CE	-5.81	90.90	100.20
3	H	616	LEU	CB-CG-CD2	-5.80	101.13	111.00
1	Q	71	LEU	CA-CB-CG	5.79	128.60	115.30
1	A	161	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	G	245	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	77	LEU	CA-CB-CG	5.73	128.48	115.30
1	Q	458	ILE	CG1-CB-CG2	-5.72	98.82	111.40
1	F	284	LEU	CB-CG-CD2	-5.61	101.47	111.00
1	A	33	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	F	302	THR	N-CA-C	5.56	126.01	111.00
3	S	581	VAL	C-N-CA	5.54	135.55	121.70
2	B	404	LEU	CB-CG-CD1	-5.53	101.61	111.00
2	L	439	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	566	CYS	CA-CB-SG	5.51	123.92	114.00
2	G	212	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	A	284	LEU	CB-CG-CD2	-5.43	101.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	376	MET	CG-SD-CE	-5.39	91.57	100.20
2	G	322	LYS	CD-CE-NZ	-5.38	99.33	111.70
1	K	68	VAL	N-CA-C	-5.36	96.52	111.00
1	F	328	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	K	140	ASP	N-CA-C	5.34	125.42	111.00
1	F	321	GLY	N-CA-C	5.33	126.42	113.10
1	Q	728	TYR	CA-CB-CG	5.32	123.51	113.40
1	Q	457	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	K	542	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	Q	661	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	A	558	PRO	C-N-CA	-5.14	111.50	122.30
1	F	181	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	F	65	ILE	CA-CB-CG1	-5.12	101.28	111.00
1	K	67	PRO	C-N-CA	5.09	134.42	121.70
3	C	619	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	F	561	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	F	136	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	F	29	LEU	CA-CB-CG	5.01	126.83	115.30
1	Q	264	ILE	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ASN	Peptide
1	A	134	MET	Peptide
1	F	564	ALA	Peptide
2	G	392	GLU	Peptide
2	G	395	ASP	Peptide
3	H	608	GLU	Peptide
1	K	730	GLN	Peptide
2	L	355	ARG	Mainchain
2	L	393	VAL	Peptide
2	L	396	PRO	Peptide
1	Q	102	ASN	Peptide
1	Q	311	THR	Peptide
1	Q	327	HIS	Peptide
1	Q	76	SER	Peptide
2	R	396	PRO	Peptide

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	4673	0	4524	247	1
1	F	4567	0	4427	192	1
1	K	4521	0	4373	180	1
1	Q	4542	0	4400	233	1
2	B	2959	0	2881	148	0
2	G	2959	0	2881	98	0
2	L	2959	0	2881	94	0
2	R	2959	0	2881	98	0
3	C	1042	0	1021	56	0
3	H	1032	0	1014	37	0
3	M	1042	0	1021	49	0
3	S	1042	0	1021	35	0
4	D	63	0	68	3	0
4	I	63	0	68	4	0
4	O	63	0	68	4	0
4	T	63	0	68	12	0
5	E	96	0	106	3	0
5	J	85	0	90	5	0
5	P	77	0	79	1	0
5	U	85	0	90	8	0
6	A	8	0	0	0	0
6	F	8	0	0	0	0
6	K	8	0	0	0	0
6	Q	8	0	0	0	0
7	A	26	0	19	6	0
7	F	26	0	19	2	0
7	K	26	0	19	1	0
7	Q	26	0	19	1	0
All	All	35028	0	34038	1288	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 19.

All (1288) 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:Q:432:TRP:CH2	1:Q:461:LYS:HG3	1.65	1.32
1:Q:318:LYS:NZ	1:Q:324:CYS:SG	2.26	1.08
1:Q:432:TRP:HD1	1:Q:469:PHE:CD1	1.75	1.05
1:Q:432:TRP:HH2	1:Q:461:LYS:CG	1.70	1.04
1:A:430:VAL:HG21	1:A:465:GLN:HE21	1.19	1.03
1:Q:652:ASP:OD1	4:T:26:ARG:NH2	1.93	1.00
2:L:120:ARG:HG2	2:L:139:VAL:HG22	1.42	1.00
1:Q:71:LEU:HB3	1:Q:72:THR:HA	1.45	0.99
1:A:691:VAL:H	1:A:737:VAL:HG21	1.32	0.95
1:F:45:ASN:HD21	2:G:317:ASP:H	1.03	0.93
1:F:23:TYR:OH	1:F:165:PHE:O	1.87	0.93
1:K:117:GLN:HA	1:K:117:GLN:HE21	1.33	0.92
1:F:42:PHE:HB3	2:G:393:VAL:HB	1.52	0.90
1:K:320:CYS:O	1:K:324:CYS:HB2	1.72	0.90
1:A:330:GLY:HA2	1:A:334:PHE:H	1.35	0.89
2:R:305:HIS:ND1	2:R:325:GLU:OE1	2.05	0.89
1:K:427:PRO:HA	1:K:464:ARG:HH22	1.37	0.89
2:L:131:GLU:OE2	2:L:133:ARG:NH2	2.05	0.88
1:Q:128:LEU:HD21	1:Q:157:VAL:HG12	1.55	0.87
1:F:436:GLU:OE2	1:F:460:THR:OG1	1.92	0.87
1:A:10:LYS:HG3	1:A:15:TRP:HE1	1.37	0.87
1:A:68:VAL:HG21	2:B:110:PRO:HG2	1.56	0.87
1:Q:432:TRP:CE3	1:Q:432:TRP:HA	2.09	0.87
3:H:580:GLU:HB3	3:H:581:VAL:HA	1.54	0.87
1:F:688:ASN:OD1	7:F:1009:SAH:N	2.07	0.87
1:F:161:ARG:NH2	1:F:233:ASP:OD2	2.07	0.86
1:F:175:VAL:HG21	1:F:244:TYR:CE2	2.11	0.85
1:Q:432:TRP:CD1	1:Q:469:PHE:CD1	2.62	0.85
1:Q:727:ARG:HH21	4:T:30:PRO:HG3	1.41	0.85
1:K:72:THR:HA	1:K:73:SER:HB3	1.59	0.85
3:S:645:GLN:HE21	3:S:649:LYS:HE2	1.41	0.84
1:A:263:ASN:HD21	3:C:655:ASN:HD21	1.24	0.84
1:K:83:CYS:HB2	1:K:98:LEU:HD13	1.61	0.83
1:K:65:ILE:HB	1:K:67:PRO:HD3	1.57	0.83
1:Q:260:CYS:HB3	1:Q:261:THR:HA	1.61	0.82
1:K:729:SER:N	1:K:730:GLN:HB2	1.94	0.82
1:F:175:VAL:HG21	1:F:244:TYR:HE2	1.45	0.82
1:K:655:GLY:HA3	4:O:24:ALA:HB2	1.61	0.82
1:K:437:ALA:HB1	1:K:441:ARG:HH12	1.45	0.81
1:F:150:ILE:HG22	1:F:155:GLY:HA2	1.61	0.81
1:K:611:LYS:NZ	3:M:586:GLU:OE2	2.13	0.81
1:Q:136:ASP:OD2	5:U:7:M3L:N	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:460:THR:O	1:Q:461:LYS:HE3	1.81	0.81
1:Q:23:TYR:OH	1:Q:165:PHE:O	1.99	0.80
1:F:655:GLY:HA3	4:I:24:ALA:HB1	1.61	0.80
1:F:237:ALA:HA	1:F:240:LEU:HD12	1.64	0.79
1:Q:323:GLN:HG2	1:Q:462:THR:HB	1.64	0.79
1:A:161:ARG:HH11	1:A:164:GLY:N	1.82	0.77
1:F:234:LYS:HB3	1:F:240:LEU:HD21	1.65	0.77
2:B:197:LYS:NZ	2:B:242:ALA:O	2.17	0.77
2:G:324:CYS:SG	5:J:5:GLN:NE2	2.57	0.77
1:F:525:HIS:HB2	1:F:528:GLN:HG2	1.65	0.77
1:Q:440:PHE:CE2	1:Q:444:ILE:HD13	2.20	0.77
1:Q:655:GLY:HA3	4:T:24:ALA:CB	2.15	0.77
1:K:45:ASN:HD21	2:L:317:ASP:H	1.32	0.76
1:A:135:GLY:HA2	1:A:138:VAL:HB	1.66	0.76
1:F:430:VAL:HG21	1:F:465:GLN:HE21	1.50	0.76
1:F:655:GLY:HA3	4:I:24:ALA:CB	2.14	0.76
2:B:282:PRO:HB3	3:C:575:ARG:HH12	1.51	0.75
1:Q:175:VAL:HG21	1:Q:244:TYR:CE1	2.21	0.75
2:G:322:LYS:HE2	2:G:366:MET:O	1.87	0.75
1:Q:624:TRP:O	7:Q:1009:SAH:N	2.18	0.75
2:B:125:GLU:HB2	2:B:135:LEU:HD11	1.68	0.75
1:F:451:PHE:HD2	1:F:466:VAL:HG12	1.52	0.75
2:G:79:LYS:NZ	2:G:392:GLU:OE2	2.16	0.74
1:A:150:ILE:HG22	1:A:155:GLY:HA2	1.67	0.74
1:F:315:LEU:HD21	1:F:450:ASN:HB2	1.67	0.74
1:K:236:THR:O	1:K:240:LEU:HD22	1.87	0.74
1:A:130:ASN:ND2	2:B:237:ASP:OD2	2.20	0.74
1:F:714:ARG:NH2	1:F:720:GLU:OE1	2.20	0.74
1:K:689:HIS:HD2	1:K:726:TYR:H	1.34	0.74
1:A:476:ILE:HD13	1:Q:55:ILE:HG23	1.69	0.74
2:G:274:ILE:O	2:G:277:SER:OG	2.06	0.74
2:L:362:ASP:O	5:P:5:GLN:NE2	2.20	0.74
1:K:279:HIS:O	1:K:283:THR:HG22	1.88	0.74
1:Q:150:ILE:HG22	1:Q:155:GLY:HA2	1.69	0.73
2:R:396:PRO:HD2	2:R:397:HIS:HD2	1.51	0.73
1:Q:328:LEU:HG	1:Q:425:GLU:HG2	1.70	0.73
2:G:404:LEU:HB3	2:G:437:TRP:CZ3	2.23	0.73
1:F:731:ALA:C	1:F:733:ALA:HA	2.08	0.73
2:L:396:PRO:HD2	2:L:397:HIS:HD2	1.54	0.73
1:A:729:SER:N	1:A:730:GLN:HB2	2.04	0.73
1:A:284:LEU:HD21	1:A:293:ASP:HB2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:567:HIS:CE1	3:S:574:LEU:HD12	2.25	0.72
2:B:120:ARG:HB3	2:B:139:VAL:HG22	1.72	0.72
1:F:133:TYR:OH	1:F:136:ASP:HB2	1.87	0.72
1:K:15:TRP:HZ3	1:K:223:ILE:HG22	1.55	0.72
3:M:586:GLU:HB2	3:M:587:LYS:HB3	1.69	0.72
2:B:396:PRO:HB2	2:B:398:LYS:HG2	1.70	0.72
1:K:67:PRO:HB2	1:K:68:VAL:HG23	1.72	0.72
2:B:225:LEU:HD23	3:C:570:THR:HG23	1.71	0.72
1:A:597:LYS:HD3	1:A:608:ARG:HB3	1.72	0.72
1:F:153:TYR:O	1:F:156:LYS:HG2	1.88	0.71
1:F:233:ASP:N	1:F:233:ASP:OD1	2.22	0.71
1:A:233:ASP:N	1:A:233:ASP:OD1	2.23	0.71
2:G:125:GLU:HB2	2:G:135:LEU:HD11	1.72	0.71
1:A:167:ASN:ND2	2:B:350:VAL:O	2.24	0.71
2:L:358:TYR:CE1	2:L:361:CYS:HB3	2.25	0.71
1:Q:30:LYS:HE2	1:Q:34:ARG:HE	1.56	0.71
1:K:127:VAL:HG12	1:K:156:LYS:HB3	1.71	0.71
2:R:256:MET:O	2:R:258:HIS:HD2	1.74	0.71
1:A:302:THR:HG22	1:A:305:THR:HG22	1.72	0.71
1:A:691:VAL:HG23	1:A:737:VAL:HG11	1.71	0.70
3:S:561:HIS:N	3:S:562:ASN:HA	2.04	0.70
1:A:263:ASN:ND2	3:C:655:ASN:HD21	1.89	0.70
1:F:732:ASP:N	1:F:733:ALA:HA	2.06	0.70
1:K:135:GLY:O	1:K:141:GLN:HG3	1.91	0.70
1:F:652:ASP:OD1	4:I:26:ARG:NH2	2.23	0.70
1:Q:563:LYS:HB3	1:Q:587:THR:HG22	1.72	0.70
1:F:321:GLY:HA2	1:F:324:CYS:HB2	1.73	0.70
1:F:82:GLU:HG2	1:F:97:PRO:HA	1.72	0.70
1:A:328:LEU:HD23	1:A:424:ILE:HG23	1.73	0.70
1:Q:457:LEU:HD12	1:Q:458:ILE:N	2.06	0.70
1:K:263:ASN:CA	3:M:607:ASN:HD21	2.03	0.69
1:K:265:ASP:OD1	3:M:654:ARG:NH1	2.25	0.69
1:Q:134:MET:N	1:Q:135:GLY:HA3	2.05	0.69
1:Q:45:ASN:ND2	2:R:316:GLY:O	2.25	0.69
1:Q:334:PHE:HD2	1:Q:467:TYR:OH	1.76	0.69
2:R:307:ASN:HD21	5:U:5:GLN:HG3	1.58	0.69
1:Q:432:TRP:HE3	1:Q:432:TRP:HA	1.58	0.69
1:Q:441:ARG:NH2	1:Q:473:GLU:OE1	2.26	0.69
2:L:191:ASN:HB3	2:L:211:LYS:HB3	1.73	0.69
2:R:254:CYS:HB3	2:R:260:LEU:HD23	1.75	0.69
1:A:306:TYR:O	3:C:665:ASP:HB3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:GLY:HA2	1:A:334:PHE:N	2.06	0.69
1:K:451:PHE:HE2	1:K:467:TYR:HD1	1.40	0.69
1:K:308:ARG:HD2	3:M:664:HIS:CE1	2.26	0.69
2:L:355:ARG:O	2:L:397:HIS:HB2	1.94	0.68
1:Q:650:GLU:OE1	1:Q:653:ARG:NH1	2.26	0.68
3:H:587:LYS:HE2	3:H:593:ARG:HH12	1.58	0.68
1:K:77:LEU:H	1:K:77:LEU:HD12	1.59	0.68
1:Q:320:CYS:HB3	1:Q:321:GLY:HA2	1.75	0.68
1:A:68:VAL:HG23	2:B:112:VAL:HG22	1.76	0.68
1:K:22:GLU:OE2	1:K:181:TYR:OH	2.10	0.68
1:Q:142:ASP:OD1	1:Q:144:THR:OG1	2.12	0.68
1:Q:472:LYS:O	1:Q:476:ILE:HG12	1.94	0.68
1:K:91:PHE:N	1:K:92:PRO:HA	2.08	0.67
1:Q:71:LEU:CB	1:Q:72:THR:HA	2.23	0.67
1:A:615:LEU:HD21	3:C:581:VAL:HG11	1.75	0.67
1:F:61:LYS:O	1:F:64:ARG:NH1	2.24	0.67
3:H:601:GLU:HA	3:H:611:LYS:HD3	1.74	0.67
1:Q:691:VAL:O	1:Q:693:PRO:HD3	1.94	0.67
3:C:570:THR:HG22	3:C:572:LEU:HD13	1.77	0.67
1:A:234:LYS:HB3	1:A:240:LEU:HD21	1.76	0.67
2:B:269:ARG:NE	2:B:292:GLN:OE1	2.21	0.67
1:K:284:LEU:HD11	3:M:606:VAL:HG11	1.77	0.67
2:B:232:VAL:HG21	3:C:591:TRP:CE3	2.30	0.67
1:Q:140:ASP:N	1:Q:141:GLN:HA	2.08	0.67
1:A:19:VAL:HG11	1:A:227:ILE:HG22	1.77	0.67
2:B:88:LEU:HD11	2:B:434:ILE:HD12	1.75	0.67
1:Q:432:TRP:HD1	1:Q:469:PHE:CE1	2.13	0.67
1:Q:104:VAL:O	2:R:169:ARG:NH2	2.28	0.67
2:B:256:MET:O	2:B:258:HIS:HD2	1.78	0.67
1:Q:334:PHE:HD2	1:Q:467:TYR:HH	1.43	0.67
1:Q:655:GLY:HA3	4:T:24:ALA:HB2	1.76	0.67
2:B:399:ALA:HB1	2:B:400:LYS:HB2	1.77	0.66
1:A:212:SER:HB2	1:A:213:ARG:HG2	1.75	0.66
1:A:216:ARG:HH12	1:A:245:LYS:HE2	1.61	0.66
2:G:256:MET:O	2:G:258:HIS:HD2	1.78	0.66
2:L:396:PRO:HD2	2:L:397:HIS:CD2	2.30	0.66
2:R:315:LEU:HD13	2:R:370:MET:HE1	1.77	0.66
1:F:464:ARG:NH1	1:F:468:GLU:OE1	2.28	0.66
2:G:199:HIS:CE1	2:G:248:GLY:HA3	2.30	0.66
1:A:621:VAL:HG13	1:A:736:TYR:HD1	1.60	0.66
2:B:285:THR:OG1	2:B:287:ARG:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HG13	2:B:134:LEU:HG	1.76	0.66
3:H:628:ALA:HB3	3:H:631:GLN:HG3	1.77	0.66
2:L:127:HIS:HB2	2:L:131:GLU:HG3	1.78	0.66
3:S:581:VAL:HA	3:S:582:ASP:HB2	1.78	0.65
1:A:67:PRO:HG3	2:B:105:SER:CB	2.27	0.65
1:A:691:VAL:N	1:A:737:VAL:HG21	2.09	0.65
1:Q:129:HIS:H	1:Q:129:HIS:CD2	2.14	0.65
1:F:729:SER:N	1:F:730:GLN:HB2	2.11	0.65
1:Q:462:THR:N	1:Q:465:GLN:OE1	2.28	0.65
1:Q:71:LEU:HD13	2:R:180:MET:SD	2.37	0.65
1:K:688:ASN:OD1	7:K:1009:SAH:N	2.29	0.65
1:K:324:CYS:SG	1:K:325:TYR:N	2.70	0.65
1:A:655:GLY:HA3	4:D:24:ALA:CB	2.27	0.65
2:G:268:LYS:O	2:G:272:ASN:ND2	2.29	0.65
1:K:117:GLN:HA	1:K:117:GLN:NE2	2.09	0.65
1:K:328:LEU:HG	1:K:331:ALA:HB2	1.77	0.65
2:B:394:GLU:OE1	2:B:394:GLU:N	2.26	0.65
1:A:28:GLN:HB3	1:A:32:PHE:HE2	1.60	0.65
1:K:314:ALA:HB1	1:K:315:LEU:HB2	1.79	0.65
1:A:734:LEU:HA	1:A:735:LYS:HB3	1.80	0.64
1:K:265:ASP:OD2	3:M:654:ARG:N	2.24	0.64
1:K:42:PHE:CZ	2:L:396:PRO:HG3	2.31	0.64
1:Q:432:TRP:CD1	1:Q:469:PHE:CG	2.85	0.64
1:A:174:LEU:O	1:A:178:LEU:HG	1.98	0.64
1:A:303:PRO:HB2	1:A:306:TYR:CZ	2.32	0.64
2:B:125:GLU:HB2	2:B:135:LEU:HD21	1.78	0.64
3:C:598:THR:O	3:C:602:GLU:HG2	1.97	0.64
2:L:422:SER:HB2	2:L:439:ARG:NH1	2.13	0.64
1:K:303:PRO:HB2	1:K:306:TYR:CZ	2.32	0.64
1:A:220:SER:HB2	1:A:223:ILE:HG23	1.78	0.64
1:A:730:GLN:HG3	1:A:732:ASP:H	1.63	0.64
2:B:254:CYS:HB3	2:B:260:LEU:HD23	1.80	0.64
1:F:528:GLN:N	1:F:528:GLN:OE1	2.31	0.64
3:M:682:ARG:HA	3:M:685:GLN:HG3	1.79	0.64
1:K:71:LEU:HD11	1:K:97:PRO:HG2	1.79	0.63
1:Q:655:GLY:HA3	4:T:24:ALA:HB1	1.80	0.63
1:K:582:PRO:HB2	1:K:594:TRP:HH2	1.64	0.63
1:K:618:PRO:HD3	3:M:566:PHE:CE1	2.33	0.63
1:A:425:GLU:CD	1:A:426:PRO:HD2	2.18	0.63
1:A:731:ALA:C	1:A:733:ALA:HA	2.18	0.63
1:F:154:ASP:HB3	1:F:156:LYS:HE2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:118:SER:OG	2:G:119:ASN:N	2.31	0.63
1:A:324:CYS:SG	1:A:325:TYR:N	2.72	0.63
2:G:189:HIS:NE2	2:G:208:SER:OG	2.27	0.63
2:G:211:LYS:HG3	2:G:238:GLU:HG2	1.81	0.63
2:B:189:HIS:HD2	2:B:212:ASP:OD2	1.81	0.62
1:K:10:LYS:HG2	1:K:11:GLY:H	1.64	0.62
1:Q:456:ARG:NH2	3:S:679:THR:OG1	2.32	0.62
2:B:88:LEU:CD1	2:B:434:ILE:HD12	2.29	0.62
1:F:19:VAL:HG22	1:F:178:LEU:HD21	1.80	0.62
1:A:339:THR:OG1	1:A:449:ASP:OD2	2.17	0.62
1:F:128:LEU:HD21	1:F:157:VAL:HG12	1.80	0.62
1:K:104:VAL:O	2:L:169:ARG:NH2	2.32	0.62
1:Q:23:TYR:CZ	1:Q:27:ARG:HD2	2.34	0.62
1:Q:432:TRP:HH2	1:Q:461:LYS:HG3	0.74	0.62
2:B:104:HIS:NE2	2:B:153:THR:HA	2.14	0.62
1:K:436:GLU:OE2	1:K:460:THR:OG1	2.17	0.62
1:Q:726:TYR:CD1	4:T:27:MET:HG2	2.35	0.62
1:A:430:VAL:HG21	1:A:465:GLN:NE2	2.04	0.62
1:K:515:ASN:HA	1:K:671:ASN:HD21	1.65	0.62
2:R:189:HIS:NE2	2:R:208:SER:OG	2.33	0.62
1:A:318:LYS:NZ	1:A:325:TYR:O	2.25	0.62
1:F:430:VAL:HG21	1:F:465:GLN:NE2	2.14	0.62
2:R:86:ASN:HD22	2:R:87:SER:H	1.46	0.62
1:A:136:ASP:OD2	5:E:7:M3L:N	2.32	0.62
3:C:616:LEU:HD22	3:C:643:TYR:HD2	1.64	0.62
1:Q:150:ILE:CG2	1:Q:155:GLY:HA2	2.30	0.62
2:R:264:ARG:NH2	2:R:340:ILE:O	2.31	0.62
1:Q:139:LEU:HG	1:Q:140:ASP:HA	1.81	0.61
1:K:597:LYS:HD3	1:K:608:ARG:HB3	1.82	0.61
2:R:207:LEU:HD22	2:R:251:ILE:HD13	1.82	0.61
2:G:232:VAL:HG22	2:G:295:HIS:HB3	1.83	0.61
2:L:170:GLY:HA2	2:L:193:ILE:HG13	1.83	0.61
1:Q:128:LEU:H	1:Q:128:LEU:HD23	1.65	0.61
2:R:209:VAL:HG13	2:R:239:VAL:HB	1.81	0.61
3:H:607:ASN:O	3:H:611:LYS:N	2.28	0.61
1:A:291:LYS:HG2	3:C:621:VAL:HG21	1.81	0.61
2:G:118:SER:O	2:G:146:ASN:HA	2.01	0.61
1:K:20:LYS:HG2	1:K:24:MET:HE2	1.83	0.61
1:K:427:PRO:HA	1:K:464:ARG:NH2	2.14	0.61
1:Q:640:GLU:OE1	1:Q:707:ARG:HD3	2.01	0.61
1:F:16:ARG:HG3	1:F:17:LYS:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:730:GLN:HE21	1:F:731:ALA:H	1.46	0.61
1:K:220:SER:O	1:K:223:ILE:HG13	2.00	0.61
1:K:308:ARG:HG2	1:K:309:LYS:H	1.65	0.61
1:K:96:ILE:HG13	2:L:134:LEU:HG	1.83	0.61
1:Q:137:GLU:N	1:Q:139:LEU:HD13	2.16	0.61
2:G:207:LEU:HD22	2:G:251:ILE:HD13	1.83	0.61
1:K:161:ARG:HH21	1:K:233:ASP:CG	2.04	0.61
2:L:232:VAL:HG12	2:L:295:HIS:HB3	1.82	0.61
2:R:150:CYS:HA	2:R:164:ALA:O	2.01	0.61
3:S:580:GLU:OE1	3:S:580:GLU:N	2.34	0.61
3:C:579:MET:HG3	3:C:581:VAL:HG12	1.83	0.60
2:L:189:HIS:CE1	2:L:216:ARG:HG3	2.35	0.60
2:R:215:LEU:HB2	2:R:229:PHE:HB2	1.82	0.60
2:R:288:PRO:HB3	3:S:578:GLU:OE2	2.00	0.60
3:C:604:SER:O	3:C:605:ASP:OD1	2.19	0.60
1:K:437:ALA:HB1	1:K:441:ARG:NH1	2.17	0.60
1:K:308:ARG:HG3	3:M:667:ASN:ND2	2.16	0.60
1:A:330:GLY:CA	1:A:334:PHE:HB2	2.32	0.60
1:F:318:LYS:HG2	1:F:319:PRO:HA	1.84	0.60
1:Q:432:TRP:CH2	1:Q:461:LYS:CG	2.59	0.60
1:Q:515:ASN:HA	1:Q:671:ASN:HD21	1.67	0.60
1:A:330:GLY:HA2	1:A:334:PHE:HB2	1.83	0.60
1:Q:328:LEU:HD22	1:Q:330:GLY:H	1.66	0.60
1:A:128:LEU:HD21	1:A:157:VAL:HG22	1.82	0.60
1:A:23:TYR:OH	1:A:165:PHE:O	2.13	0.60
2:B:215:LEU:HB2	2:B:229:PHE:HB2	1.83	0.60
1:A:37:GLU:CD	2:B:336:MET:HG2	2.22	0.60
1:F:306:TYR:O	3:H:665:ASP:HB3	2.01	0.60
2:L:358:TYR:HE1	2:L:361:CYS:HB3	1.66	0.60
2:R:215:LEU:HD11	2:R:239:VAL:HG11	1.83	0.60
1:K:515:ASN:HA	1:K:671:ASN:ND2	2.17	0.60
2:R:161:PRO:O	2:R:177:PRO:HD2	2.01	0.60
1:A:161:ARG:NH2	1:A:231:PHE:CE2	2.70	0.59
2:B:386:LEU:HD11	2:B:427:ALA:HB2	1.84	0.59
2:L:306:ARG:N	2:L:325:GLU:OE2	2.33	0.59
2:B:125:GLU:CB	2:B:135:LEU:HD21	2.32	0.59
1:Q:270:LYS:O	1:Q:272:VAL:HG23	2.02	0.59
1:A:168:ASP:O	1:A:172:VAL:HG23	2.02	0.59
2:G:395:ASP:OD1	2:G:398:LYS:HG3	2.02	0.59
1:K:11:GLY:N	1:K:12:PRO:HD2	2.17	0.59
2:L:197:LYS:NZ	2:L:242:ALA:O	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:426:PRO:O	1:Q:464:ARG:NH2	2.35	0.59
1:Q:440:PHE:CZ	1:Q:444:ILE:HG21	2.38	0.59
1:Q:662:MET:HE3	1:Q:732:ASP:HB2	1.83	0.59
1:A:655:GLY:HA3	4:D:24:ALA:HB1	1.83	0.59
1:F:130:ASN:ND2	2:G:237:ASP:OD2	2.34	0.59
2:G:232:VAL:HG11	3:H:591:TRP:CE3	2.37	0.59
1:Q:728:TYR:HB3	1:Q:730:GLN:HB2	1.83	0.59
1:A:101:LEU:N	2:B:139:VAL:O	2.24	0.59
2:B:322:LYS:HD3	2:B:366:MET:O	2.02	0.59
1:Q:614:LEU:HB3	1:Q:626:ILE:HD11	1.84	0.59
3:C:628:ALA:HB3	3:C:631:GLN:HG3	1.84	0.59
1:F:140:ASP:N	1:F:141:GLN:HA	2.18	0.59
1:A:263:ASN:ND2	1:A:265:ASP:H	2.01	0.59
1:A:284:LEU:HD23	1:A:284:LEU:O	2.03	0.59
1:Q:236:THR:OG1	1:Q:239:GLU:HB3	2.02	0.59
1:K:67:PRO:HB3	2:L:161:PRO:HG2	1.85	0.59
1:Q:161:ARG:NH2	1:Q:233:ASP:OD2	2.35	0.59
1:Q:432:TRP:HZ3	1:Q:461:LYS:HZ3	1.50	0.59
2:B:400:LYS:HD2	2:B:401:CYS:H	1.68	0.59
3:C:588:ASP:OD2	3:C:593:ARG:NH1	2.35	0.59
1:Q:22:GLU:HG3	1:Q:178:LEU:HD23	1.85	0.59
1:A:33:ARG:O	1:A:33:ARG:HG2	2.03	0.59
2:B:170:GLY:HA2	2:B:193:ILE:HD12	1.85	0.59
1:Q:172:VAL:O	1:Q:175:VAL:HG22	2.03	0.59
1:K:171:PHE:O	1:K:175:VAL:HG22	2.03	0.58
1:K:67:PRO:CB	1:K:68:VAL:HG23	2.32	0.58
3:M:607:ASN:O	3:M:611:LYS:HG3	2.02	0.58
1:Q:590:ALA:O	1:Q:608:ARG:NH2	2.35	0.58
1:Q:701:MET:HE2	1:Q:706:HIS:CE1	2.38	0.58
1:A:272:VAL:HG12	1:A:276:GLN:HB2	1.85	0.58
1:F:22:GLU:OE2	1:F:177:ALA:HB1	2.03	0.58
1:F:629:LYS:O	1:F:718:THR:HG23	2.03	0.58
1:K:68:VAL:HG12	1:K:69:HIS:N	2.17	0.58
1:Q:563:LYS:HA	1:Q:588:CYS:HA	1.84	0.58
1:K:728:TYR:HB3	1:K:730:GLN:CB	2.34	0.58
2:R:396:PRO:HD2	2:R:397:HIS:CD2	2.36	0.58
1:F:128:LEU:CD2	1:F:157:VAL:HG12	2.33	0.58
1:F:144:THR:HG22	1:F:148:GLU:HG3	1.85	0.58
1:F:617:ALA:HB3	1:F:627:PHE:CE1	2.38	0.58
2:L:86:ASN:HD22	2:L:87:SER:H	1.50	0.58
1:Q:75:SER:OG	1:Q:76:SER:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:ASP:HB3	2:B:393:VAL:HG23	1.84	0.58
1:F:109:ILE:H	1:F:109:ILE:HD12	1.68	0.58
1:F:150:ILE:CG2	1:F:155:GLY:HA2	2.33	0.58
3:H:605:ASP:N	3:H:605:ASP:OD1	2.36	0.58
1:Q:665:PHE:HD2	1:Q:678:THR:HG22	1.67	0.58
1:A:68:VAL:HG23	2:B:112:VAL:CG2	2.34	0.58
1:A:101:LEU:HB2	2:B:140:ASP:HA	1.85	0.58
3:M:579:MET:O	3:M:581:VAL:HG12	2.03	0.58
1:Q:264:ILE:O	1:Q:435:ALA:HB2	2.03	0.58
1:F:265:ASP:OD1	3:H:654:ARG:HB2	2.03	0.58
1:K:13:VAL:O	1:K:17:LYS:HG2	2.04	0.58
1:A:320:CYS:HB3	1:A:321:GLY:HA2	1.85	0.58
1:A:91:PHE:CD1	1:A:92:PRO:HD2	2.39	0.58
1:A:63:ARG:NE	2:B:154:TYR:OH	2.32	0.58
1:F:77:LEU:O	1:F:78:ARG:HB3	2.03	0.58
3:M:577:GLN:OE1	3:M:577:GLN:N	2.27	0.58
2:B:199:HIS:CE1	2:B:248:GLY:HA3	2.39	0.57
1:F:302:THR:HG1	1:F:305:THR:H	1.52	0.57
2:B:145:GLU:OE2	2:B:169:ARG:HB2	2.04	0.57
3:C:561:HIS:HB2	3:C:562:ASN:HA	1.86	0.57
1:F:677:ALA:O	1:F:685:ARG:NH2	2.38	0.57
2:G:237:ASP:HB3	2:G:256:MET:HB2	1.86	0.57
2:B:318:LEU:HD13	2:B:353:LEU:HD12	1.86	0.57
1:F:324:CYS:HA	1:F:463:CYS:HB3	1.85	0.57
1:F:42:PHE:HB3	2:G:393:VAL:CB	2.31	0.57
1:F:304:ASN:HB2	1:F:524:ASP:OD2	2.04	0.57
2:L:136:GLN:NE2	2:L:180:MET:HG2	2.20	0.57
3:S:575:ARG:N	3:S:578:GLU:OE1	2.35	0.57
3:S:596:THR:HG21	3:S:622:MET:HE1	1.86	0.57
2:R:260:LEU:HD21	2:R:309:VAL:HG11	1.86	0.57
1:A:23:TYR:CZ	1:A:27:ARG:HD2	2.40	0.57
1:A:734:LEU:HB3	7:A:1009:SAH:N1	2.20	0.57
1:F:324:CYS:SG	1:F:325:TYR:N	2.78	0.57
2:L:288:PRO:HG3	3:M:567:HIS:HE1	1.69	0.57
1:Q:339:THR:O	1:Q:343:ILE:HG13	2.05	0.57
2:G:285:THR:OG1	2:G:287:ARG:HG2	2.03	0.57
1:F:128:LEU:HB3	1:F:153:TYR:CE2	2.39	0.57
1:A:732:ASP:N	1:A:733:ALA:HA	2.20	0.57
1:A:65:ILE:HG22	2:B:161:PRO:HG3	1.87	0.57
1:K:168:ASP:O	1:K:172:VAL:HG23	2.05	0.57
1:K:645:ILE:HG22	1:K:675:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:ASN:ND2	2:B:240:LEU:HD23	2.19	0.57
1:Q:629:LYS:O	1:Q:718:THR:HG23	2.05	0.57
1:A:629:LYS:O	1:A:718:THR:HG23	2.05	0.56
2:B:118:SER:OG	2:B:119:ASN:N	2.37	0.56
1:F:284:LEU:CD2	1:F:292:TYR:HB3	2.35	0.56
2:G:194:ASN:ND2	2:G:240:LEU:HD23	2.19	0.56
1:K:317:ASN:ND2	1:K:332:LYS:HD2	2.20	0.56
1:Q:728:TYR:CE1	4:T:25:ALA:HB1	2.39	0.56
3:S:645:GLN:NE2	3:S:649:LYS:HE2	2.16	0.56
1:A:161:ARG:HH11	1:A:164:GLY:C	2.08	0.56
2:L:80:TYR:O	2:L:402:THR:HG21	2.05	0.56
1:A:85:VAL:HG23	2:B:134:LEU:HD22	1.86	0.56
1:K:20:LYS:O	1:K:24:MET:HG2	2.05	0.56
3:M:585:ASP:CB	3:M:586:GLU:HB3	2.35	0.56
1:Q:303:PRO:HB2	1:Q:306:TYR:CZ	2.39	0.56
1:A:320:CYS:HB3	1:A:324:CYS:HB2	1.86	0.56
1:A:650:GLU:OE1	1:A:653:ARG:NH1	2.39	0.56
1:Q:582:PRO:CB	1:Q:594:TRP:HH2	2.18	0.56
3:H:580:GLU:CB	3:H:581:VAL:HA	2.31	0.56
1:K:319:PRO:HA	1:K:320:CYS:HB3	1.87	0.56
1:Q:279:HIS:O	1:Q:283:THR:HG22	2.05	0.56
1:Q:146:ILE:O	1:Q:150:ILE:HG12	2.06	0.56
2:R:230:GLY:O	2:R:293:LYS:HE2	2.05	0.56
1:F:104:VAL:O	2:G:169:ARG:NH2	2.37	0.56
1:F:339:THR:O	1:F:343:ILE:HG12	2.05	0.56
1:F:125:GLU:HG2	1:F:650:GLU:OE2	2.05	0.56
1:F:98:LEU:HB3	2:G:139:VAL:CG2	2.36	0.56
2:R:404:LEU:HB3	2:R:437:TRP:CZ3	2.41	0.56
1:K:26:LEU:HD22	1:K:173:GLU:OE2	2.06	0.56
1:K:263:ASN:HB3	3:M:607:ASN:HD21	1.70	0.56
1:Q:324:CYS:SG	1:Q:325:TYR:N	2.79	0.56
1:Q:545:LYS:HD3	1:Q:581:ASP:OD2	2.06	0.56
1:A:263:ASN:HD21	3:C:655:ASN:ND2	2.00	0.56
1:A:621:VAL:HG13	1:A:736:TYR:CD1	2.40	0.56
1:A:91:PHE:CG	1:A:92:PRO:HD2	2.41	0.55
2:B:331:TRP:HB3	2:B:352:ILE:HD13	1.87	0.55
2:L:95:PRO:HB3	2:L:430:ASP:HA	1.88	0.55
1:Q:219:PRO:HD2	1:Q:244:TYR:HE2	1.71	0.55
1:Q:665:PHE:HB2	1:Q:678:THR:HG23	1.89	0.55
1:A:579:GLU:HG3	1:A:702:VAL:HG22	1.87	0.55
1:A:689:HIS:HD2	1:A:726:TYR:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:10:LYS:C	1:K:12:PRO:HD2	2.26	0.55
1:K:312:GLU:N	1:K:312:GLU:OE1	2.38	0.55
2:R:260:LEU:HD13	2:R:331:TRP:CZ2	2.41	0.55
1:K:640:GLU:OE1	1:K:707:ARG:HD3	2.07	0.55
1:A:129:HIS:CD2	1:A:129:HIS:H	2.24	0.55
1:K:464:ARG:NH1	1:K:468:GLU:HB2	2.22	0.55
2:L:215:LEU:HB2	2:L:229:PHE:HB2	1.86	0.55
2:L:287:ARG:HG3	2:L:287:ARG:O	2.07	0.55
1:Q:316:ASP:HB3	1:Q:332:LYS:HE2	1.88	0.55
2:R:307:ASN:HD21	5:U:5:GLN:CG	2.19	0.55
1:A:624:TRP:N	7:A:1009:SAH:OXT	2.40	0.55
1:A:104:VAL:HG11	2:B:171:ILE:HG21	1.89	0.55
1:F:728:TYR:HB3	1:F:730:GLN:CB	2.36	0.55
1:Q:270:LYS:C	1:Q:272:VAL:HG23	2.26	0.55
1:Q:730:GLN:NE2	1:Q:732:ASP:H	2.05	0.55
3:S:597:ILE:HG23	3:S:615:LYS:HD2	1.89	0.55
1:Q:325:TYR:HE1	1:Q:463:CYS:SG	2.29	0.55
1:A:167:ASN:HD21	2:B:350:VAL:H	1.53	0.55
1:A:28:GLN:HB3	1:A:32:PHE:CE2	2.41	0.55
1:K:460:THR:O	1:K:461:LYS:HD2	2.07	0.55
3:M:651:ASN:ND2	3:M:651:ASN:O	2.40	0.55
1:Q:139:LEU:CD1	1:Q:140:ASP:HA	2.35	0.55
1:Q:168:ASP:HB2	2:R:349:ASN:ND2	2.21	0.55
1:Q:323:GLN:HG2	1:Q:462:THR:CB	2.37	0.55
2:B:280:TYR:OH	3:C:575:ARG:NH2	2.40	0.55
1:Q:606:ILE:CG2	1:Q:707:ARG:HD2	2.37	0.55
1:A:85:VAL:HG11	2:B:88:LEU:HD13	1.88	0.55
2:B:82:PHE:HA	2:B:438:ASP:O	2.06	0.55
1:F:82:GLU:HG2	1:F:97:PRO:CA	2.37	0.55
1:Q:339:THR:HG21	1:Q:449:ASP:OD2	2.06	0.55
1:A:728:TYR:HB3	1:A:730:GLN:CB	2.36	0.55
3:C:646:LYS:O	3:C:650:LYS:HG3	2.07	0.55
2:G:132:ILE:HD11	2:G:436:ARG:HB2	1.88	0.55
1:K:175:VAL:HG21	1:K:244:TYR:CD2	2.42	0.55
1:Q:130:ASN:OD1	2:R:257:ASP:HA	2.07	0.55
1:K:655:GLY:HA3	4:O:24:ALA:CB	2.36	0.54
1:K:648:GLN:HE22	4:O:26:ARG:NH1	2.05	0.54
1:Q:730:GLN:HG3	1:Q:731:ALA:N	2.22	0.54
2:R:307:ASN:ND2	2:R:308:TYR:H	2.05	0.54
2:R:148:TYR:HB3	2:R:365:TYR:OH	2.07	0.54
2:L:331:TRP:HB3	2:L:352:ILE:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:395:ASP:OD2	2:L:399:ALA:N	2.40	0.54
2:R:397:HIS:ND1	2:R:398:LYS:HG3	2.22	0.54
1:A:641:TYR:HB3	1:A:708:ILE:HB	1.90	0.54
2:G:125:GLU:HB2	2:G:135:LEU:HD21	1.89	0.54
1:Q:67:PRO:HG3	2:R:109:ASP:CG	2.28	0.54
1:A:263:ASN:HD22	1:A:264:ILE:N	2.06	0.54
2:G:186:TYR:HE2	2:G:220:ILE:HG22	1.71	0.54
1:K:548:GLN:HA	1:K:548:GLN:OE1	2.06	0.54
1:A:39:LYS:HE3	2:B:394:GLU:HB3	1.89	0.54
1:K:302:THR:N	1:K:303:PRO:HA	2.23	0.54
1:A:326:GLN:HB2	1:A:327:HIS:HB3	1.88	0.54
2:B:396:PRO:HA	2:B:397:HIS:CG	2.42	0.54
3:C:569:ASP:OD1	3:C:569:ASP:N	2.40	0.54
1:F:439:MET:HE1	3:H:657:MET:HB3	1.90	0.54
1:Q:431:GLU:O	1:Q:432:TRP:HE3	1.91	0.54
2:R:274:ILE:O	2:R:277:SER:OG	2.25	0.54
3:S:596:THR:HG21	3:S:622:MET:CE	2.38	0.54
1:Q:728:TYR:HE1	4:T:25:ALA:HB1	1.72	0.54
2:G:88:LEU:HD12	2:G:434:ILE:HB	1.88	0.54
1:Q:224:PHE:HZ	1:Q:244:TYR:CB	2.21	0.54
1:A:272:VAL:CG1	1:A:276:GLN:HB2	2.38	0.54
1:Q:582:PRO:HB3	1:Q:594:TRP:HH2	1.73	0.54
1:A:101:LEU:O	2:B:141:ALA:N	2.41	0.53
1:A:68:VAL:HG21	2:B:110:PRO:CG	2.35	0.53
1:F:67:PRO:HB3	2:G:109:ASP:OD2	2.07	0.53
2:L:230:GLY:O	2:L:293:LYS:HE2	2.08	0.53
2:L:326:ASN:HA	2:L:358:TYR:CE1	2.43	0.53
2:B:422:SER:HB2	2:B:439:ARG:HH11	1.74	0.53
1:A:427:PRO:HA	1:A:464:ARG:HH12	1.74	0.53
1:A:694:ASN:HB3	1:A:714:ARG:HH21	1.72	0.53
1:A:131:ILE:HG21	5:E:4:ALA:HB2	1.90	0.53
1:F:63:ARG:HD3	2:G:154:TYR:CZ	2.43	0.53
2:G:310:ASP:OD2	2:G:322:LYS:NZ	2.36	0.53
2:G:395:ASP:OD2	2:G:398:LYS:N	2.42	0.53
1:K:169:GLU:OE2	2:L:335:LYS:HG2	2.09	0.53
1:K:308:ARG:HG3	3:M:667:ASN:HD21	1.73	0.53
1:Q:119:ASN:HB3	1:Q:645:ILE:HG13	1.90	0.53
1:A:29:LEU:HA	1:A:32:PHE:HD2	1.73	0.53
2:B:140:ASP:OD2	2:B:173:ARG:NE	2.42	0.53
1:F:531:ASP:OD1	1:F:533:SER:N	2.37	0.53
1:K:263:ASN:CB	3:M:607:ASN:HD21	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:HD3	2:B:247:LEU:HG	1.91	0.53
2:B:211:LYS:HG3	2:B:238:GLU:HG2	1.91	0.53
1:K:580:CYS:O	1:K:607:GLN:NE2	2.41	0.53
1:K:689:HIS:CD2	1:K:726:TYR:H	2.20	0.53
1:K:96:ILE:HG22	1:K:97:PRO:O	2.08	0.53
1:Q:161:ARG:HG3	2:R:306:ARG:HH11	1.74	0.53
2:B:184:LYS:NZ	2:B:220:ILE:O	2.36	0.53
1:Q:728:TYR:CB	1:Q:730:GLN:HB2	2.39	0.53
1:A:562:CYS:SG	1:A:566:CYS:HB3	2.49	0.53
1:A:728:TYR:HB3	1:A:730:GLN:HB2	1.90	0.53
2:B:358:TYR:HE1	2:B:361:CYS:HB3	1.73	0.53
1:F:102:ASN:O	2:G:173:ARG:NH2	2.36	0.53
1:Q:515:ASN:HA	1:Q:671:ASN:ND2	2.22	0.53
2:R:339:ASP:OD1	2:R:341:ASP:N	2.42	0.53
1:K:338:LEU:O	1:K:342:ARG:HB2	2.09	0.53
1:Q:129:HIS:HD2	1:Q:129:HIS:H	1.55	0.53
1:Q:726:TYR:HD1	4:T:27:MET:HG2	1.74	0.53
1:A:460:THR:O	1:A:461:LYS:HD2	2.09	0.53
1:A:582:PRO:HB2	3:C:628:ALA:HB2	1.90	0.53
1:Q:171:PHE:O	1:Q:175:VAL:HG13	2.08	0.53
1:Q:161:ARG:HG3	2:R:306:ARG:NH1	2.24	0.53
1:F:728:TYR:HB3	1:F:730:GLN:HB2	1.91	0.53
1:K:728:TYR:HB3	1:K:730:GLN:HB2	1.91	0.53
1:A:35:ALA:HA	1:A:38:VAL:HG22	1.91	0.52
2:G:385:LYS:HE2	2:G:403:THR:HB	1.90	0.52
1:K:542:PHE:HB3	1:K:555:ASN:O	2.10	0.52
2:B:389:TRP:CD1	2:B:401:CYS:HB2	2.44	0.52
1:F:175:VAL:CG2	1:F:244:TYR:HE2	2.21	0.52
1:F:303:PRO:HB2	1:F:306:TYR:CZ	2.44	0.52
1:Q:171:PHE:HZ	1:Q:224:PHE:HE2	1.57	0.52
1:Q:451:PHE:HD2	1:Q:466:VAL:HG12	1.74	0.52
1:Q:98:LEU:HD22	2:R:139:VAL:HG23	1.91	0.52
1:A:688:ASN:OD1	7:A:1009:SAH:N	2.39	0.52
1:Q:67:PRO:HG3	2:R:109:ASP:OD2	2.09	0.52
1:A:304:ASN:HB2	1:A:524:ASP:OD2	2.09	0.52
1:A:617:ALA:HB3	1:A:627:PHE:CE1	2.45	0.52
2:G:148:TYR:HB3	2:G:365:TYR:OH	2.09	0.52
1:K:342:ARG:HD2	1:K:470:ARG:HH22	1.74	0.52
1:K:89:LEU:HD12	1:K:91:PHE:N	2.24	0.52
2:L:404:LEU:HB3	2:L:437:TRP:CZ3	2.43	0.52
2:R:191:ASN:HB3	2:R:211:LYS:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:730:GLN:HG3	1:F:731:ALA:N	2.25	0.52
1:Q:74:VAL:HB	1:Q:75:SER:O	2.10	0.52
2:R:145:GLU:OE1	2:R:169:ARG:HB2	2.09	0.52
2:R:204:ASN:O	2:R:220:ILE:HG12	2.10	0.52
2:B:197:LYS:O	2:B:206:LEU:HD12	2.09	0.52
3:M:585:ASP:HB3	3:M:586:GLU:HB3	1.92	0.52
2:R:94:GLN:HB2	2:R:118:SER:HB2	1.91	0.52
1:K:150:ILE:HG22	1:K:155:GLY:HA2	1.92	0.52
1:K:582:PRO:CB	1:K:594:TRP:HH2	2.22	0.52
2:R:414:ARG:NH1	5:U:8:PHE:CD1	2.78	0.52
1:A:231:PHE:HB3	1:A:234:LYS:HG2	1.92	0.51
1:A:322:PRO:HB2	1:F:58:GLN:HB3	1.91	0.51
1:K:175:VAL:HG21	1:K:244:TYR:HD2	1.75	0.51
2:L:88:LEU:O	2:L:434:ILE:N	2.39	0.51
1:Q:128:LEU:N	1:Q:128:LEU:HD23	2.22	0.51
1:F:531:ASP:C	1:F:531:ASP:OD1	2.49	0.51
1:K:119:ASN:HB3	1:K:645:ILE:HG23	1.93	0.51
2:B:106:LYS:O	2:B:109:ASP:HB2	2.09	0.51
2:B:211:LYS:HG3	2:B:238:GLU:CD	2.30	0.51
2:B:389:TRP:NE1	2:B:401:CYS:HB2	2.26	0.51
3:C:586:GLU:HB3	3:C:587:LYS:HB2	1.93	0.51
1:Q:462:THR:O	1:Q:466:VAL:HG23	2.10	0.51
5:U:6:ARG:HH11	5:U:10:GLN:NE2	2.07	0.51
2:G:262:LEU:HB3	2:G:299:PHE:HB3	1.92	0.51
1:F:629:LYS:NZ	3:H:581:VAL:O	2.43	0.51
1:K:306:TYR:O	3:M:665:ASP:HB3	2.10	0.51
1:Q:539:ALA:O	1:Q:540:GLN:HB2	2.09	0.51
3:C:570:THR:CG2	3:C:572:LEU:HD13	2.39	0.51
2:G:194:ASN:HD22	2:G:240:LEU:HA	1.74	0.51
1:Q:70:ILE:CG2	2:R:135:LEU:HD22	2.40	0.51
2:B:237:ASP:HB3	2:B:256:MET:HB2	1.92	0.51
1:F:117:GLN:NE2	1:F:117:GLN:HA	2.26	0.51
1:F:67:PRO:HG2	1:F:69:HIS:CE1	2.46	0.51
2:G:238:GLU:HB2	2:G:256:MET:HG3	1.92	0.51
1:Q:134:MET:H	1:Q:135:GLY:HA3	1.75	0.51
2:G:199:HIS:HB2	2:G:205:LEU:HB2	1.92	0.51
2:B:323:SER:C	2:B:325:GLU:H	2.14	0.51
2:B:225:LEU:HD23	3:C:570:THR:CG2	2.39	0.51
1:F:175:VAL:HG21	1:F:244:TYR:CD2	2.46	0.51
2:G:102:ASN:HB2	2:G:152:TRP:CE2	2.46	0.51
1:K:67:PRO:HB3	2:L:161:PRO:CG	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:691:VAL:O	1:K:693:PRO:HD3	2.11	0.51
1:A:528:GLN:N	1:A:528:GLN:OE1	2.38	0.51
1:K:71:LEU:HD12	1:K:73:SER:HB2	1.93	0.51
3:M:607:ASN:OD1	3:M:608:GLU:N	2.43	0.51
1:A:230:MET:HB2	1:A:231:PHE:CD1	2.46	0.51
1:A:615:LEU:HD21	3:C:581:VAL:CG1	2.42	0.51
1:F:129:HIS:HA	1:F:158:HIS:HB3	1.93	0.51
1:F:302:THR:HG1	1:F:305:THR:N	2.07	0.51
1:K:127:VAL:HG12	1:K:156:LYS:CB	2.41	0.51
1:Q:469:PHE:CE1	1:Q:473:GLU:OE2	2.64	0.51
1:Q:49:ILE:HG12	2:R:316:GLY:HA3	1.93	0.51
1:A:264:ILE:HD12	3:C:658:LEU:HD11	1.92	0.50
1:A:340:ALA:O	1:A:343:ILE:HG22	2.12	0.50
1:A:41:MET:HG3	2:B:336:MET:CE	2.41	0.50
1:F:125:GLU:OE1	2:G:236:ARG:NH2	2.44	0.50
2:G:186:TYR:CE2	2:G:220:ILE:HG22	2.46	0.50
1:K:130:ASN:OD1	2:L:257:ASP:HA	2.11	0.50
1:K:462:THR:OG1	1:K:465:GLN:OE1	2.11	0.50
3:M:576:PRO:HG2	3:M:577:GLN:OE1	2.12	0.50
1:Q:242:GLU:O	1:Q:246:GLU:HG3	2.10	0.50
1:A:241:LYS:O	1:A:245:LYS:HG3	2.11	0.50
1:A:694:ASN:HB3	1:A:714:ARG:NH2	2.25	0.50
1:K:618:PRO:HD3	3:M:566:PHE:HE1	1.74	0.50
1:Q:565:GLN:HG3	1:Q:567:ASN:OD1	2.10	0.50
1:Q:580:CYS:O	1:Q:607:GLN:NE2	2.44	0.50
2:R:145:GLU:HB2	2:R:169:ARG:HD3	1.93	0.50
1:A:161:ARG:NH1	1:A:165:PHE:N	2.59	0.50
1:A:665:PHE:HB3	1:A:677:ALA:HB3	1.94	0.50
1:K:129:HIS:H	1:K:129:HIS:CD2	2.29	0.50
2:L:127:HIS:HB2	2:L:131:GLU:CG	2.42	0.50
1:Q:224:PHE:CZ	1:Q:244:TYR:CB	2.94	0.50
1:Q:621:VAL:HG21	1:Q:737:VAL:HG22	1.94	0.50
1:Q:579:GLU:HG3	1:Q:702:VAL:HG22	1.93	0.50
1:Q:736:TYR:OH	1:Q:739:ILE:O	2.26	0.50
1:A:464:ARG:NH1	1:A:468:GLU:OE2	2.44	0.50
2:B:404:LEU:HB2	2:B:437:TRP:CZ3	2.46	0.50
1:F:302:THR:N	1:F:303:PRO:HA	2.26	0.50
1:K:121:MET:HA	1:K:645:ILE:HG13	1.93	0.50
1:K:138:VAL:HB	1:K:141:GLN:HG2	1.94	0.50
1:K:552:GLU:HG3	1:K:552:GLU:O	2.11	0.50
1:Q:20:LYS:O	1:Q:24:MET:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:219:PRO:HD2	1:Q:244:TYR:CE2	2.46	0.50
2:R:288:PRO:HD3	3:S:578:GLU:HG2	1.93	0.50
2:R:86:ASN:HD22	2:R:87:SER:N	2.09	0.50
1:Q:284:LEU:HD11	3:S:606:VAL:HG21	1.93	0.50
3:C:607:ASN:O	3:C:611:LYS:HG3	2.12	0.50
1:K:449:ASP:HA	1:K:451:PHE:CE1	2.46	0.50
3:M:569:ASP:OD1	3:M:569:ASP:N	2.45	0.50
3:M:607:ASN:HB3	3:M:610:GLU:HB2	1.94	0.50
2:G:211:LYS:HD2	2:G:238:GLU:CD	2.32	0.50
2:B:95:PRO:HB3	2:B:430:ASP:HA	1.92	0.50
1:F:303:PRO:HB2	1:F:306:TYR:CE2	2.46	0.50
1:F:592:ASP:HB3	1:F:593:HIS:ND1	2.26	0.50
1:F:691:VAL:O	1:F:693:PRO:HD3	2.12	0.50
2:G:120:ARG:HE	2:G:139:VAL:HG13	1.77	0.50
1:K:726:TYR:O	4:O:27:MET:HA	2.12	0.50
1:A:161:ARG:HH11	1:A:164:GLY:CA	2.23	0.50
1:A:19:VAL:HG22	1:A:178:LEU:CD2	2.42	0.50
1:F:640:GLU:OE1	1:F:707:ARG:HD2	2.11	0.50
2:G:120:ARG:HG2	2:G:139:VAL:HG13	1.93	0.50
2:G:229:PHE:HD2	2:G:263:TRP:CE3	2.30	0.50
3:H:621:VAL:HG12	3:H:626:PHE:HD2	1.76	0.50
1:A:212:SER:HB2	1:A:213:ARG:CG	2.42	0.50
1:A:70:ILE:HG13	2:B:135:LEU:HB3	1.93	0.50
1:F:314:ALA:H	1:F:315:LEU:HD12	1.77	0.50
2:L:94:GLN:HB2	2:L:118:SER:HB2	1.94	0.50
2:R:262:LEU:HB3	2:R:299:PHE:HB3	1.92	0.50
1:A:652:ASP:OD1	4:D:26:ARG:NH2	2.45	0.49
1:A:308:ARG:NH1	3:C:667:ASN:HA	2.27	0.49
1:F:89:LEU:HD11	1:F:91:PHE:CD1	2.47	0.49
2:G:150:CYS:HA	2:G:164:ALA:O	2.12	0.49
2:G:364:TRP:CE3	2:G:365:TYR:HB2	2.47	0.49
1:Q:12:PRO:O	1:Q:15:TRP:N	2.43	0.49
1:Q:23:TYR:CE1	1:Q:27:ARG:HD2	2.47	0.49
2:R:81:SER:HB2	2:R:440:LEU:HD11	1.93	0.49
1:A:11:GLY:HA3	1:A:14:CYS:SG	2.52	0.49
1:A:428:GLU:N	1:A:468:GLU:OE2	2.36	0.49
1:A:71:LEU:HD13	2:B:180:MET:HE3	1.94	0.49
3:C:586:GLU:CB	3:C:587:LYS:HB2	2.42	0.49
3:C:607:ASN:HB3	3:C:610:GLU:CG	2.41	0.49
1:F:432:TRP:CH2	1:F:461:LYS:HG2	2.47	0.49
3:H:603:PHE:O	3:H:611:LYS:NZ	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:OD2	2:B:348:SER:HB3	2.11	0.49
1:F:161:ARG:HB3	1:F:232:PRO:HD2	1.93	0.49
1:Q:303:PRO:HB2	1:Q:306:TYR:OH	2.12	0.49
1:Q:34:ARG:O	1:Q:37:GLU:N	2.44	0.49
2:R:158:THR:HB	2:R:160:HIS:CE1	2.47	0.49
2:R:257:ASP:N	2:R:257:ASP:OD1	2.44	0.49
3:S:605:ASP:OD1	3:S:605:ASP:N	2.36	0.49
1:A:148:GLU:HG3	1:A:656:LYS:HE2	1.94	0.49
3:C:627:ILE:H	3:C:631:GLN:NE2	2.10	0.49
1:F:319:PRO:HB2	1:F:321:GLY:HA3	1.94	0.49
1:Q:139:LEU:CG	1:Q:140:ASP:HA	2.41	0.49
1:Q:730:GLN:CG	1:Q:731:ALA:N	2.74	0.49
1:A:226:ALA:O	1:A:229:SER:OG	2.27	0.49
1:F:427:PRO:HA	1:F:464:ARG:HH22	1.77	0.49
5:J:6:ARG:HH11	5:J:10:GLN:NE2	2.10	0.49
2:L:121:VAL:HG21	2:L:165:VAL:HG11	1.94	0.49
2:L:256:MET:O	2:L:258:HIS:HD2	1.95	0.49
2:B:358:TYR:CE1	2:B:361:CYS:HB3	2.47	0.49
3:C:597:ILE:HG23	3:C:615:LYS:HD2	1.95	0.49
1:K:729:SER:H	1:K:730:GLN:HB2	1.71	0.49
1:Q:689:HIS:HD2	1:Q:726:TYR:H	1.60	0.49
1:A:135:GLY:O	1:A:139:LEU:N	2.45	0.49
2:G:355:ARG:O	2:G:397:HIS:HB2	2.11	0.49
2:L:199:HIS:HB3	2:L:202:ASP:O	2.13	0.49
1:A:528:GLN:HG3	1:K:81:ARG:HE	1.77	0.49
2:B:326:ASN:HA	2:B:358:TYR:CE1	2.47	0.49
1:F:137:GLU:N	1:F:138:VAL:HA	2.27	0.49
1:F:318:LYS:CG	1:F:319:PRO:HA	2.42	0.49
1:F:446:THR:HG23	1:F:447:TYR:CD1	2.47	0.49
2:R:120:ARG:HB3	2:R:139:VAL:HG22	1.95	0.49
2:R:329:VAL:HG11	2:R:352:ILE:HD12	1.95	0.49
3:S:569:ASP:OD1	3:S:569:ASP:N	2.44	0.49
1:A:677:ALA:O	1:A:685:ARG:NH2	2.42	0.49
1:F:224:PHE:CE1	1:F:241:LYS:HA	2.47	0.49
2:G:397:HIS:CD2	2:G:398:LYS:HG2	2.47	0.49
3:H:671:ILE:HA	3:H:674:ILE:HD12	1.95	0.49
1:K:634:LYS:HG2	1:K:635:ASN:ND2	2.27	0.49
1:Q:74:VAL:N	1:Q:75:SER:HA	2.28	0.49
1:A:67:PRO:HG3	2:B:105:SER:HA	1.95	0.49
1:A:730:GLN:HG3	1:A:732:ASP:N	2.28	0.49
1:A:733:ALA:H	1:A:734:LEU:HD13	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:HIS:HE2	2:B:153:THR:HA	1.78	0.49
2:B:186:TYR:HE2	2:B:220:ILE:HG22	1.76	0.49
1:A:125:GLU:OE1	2:B:236:ARG:NH2	2.46	0.49
2:B:386:LEU:HD21	2:B:416:THR:HG21	1.95	0.49
1:F:30:LYS:HE3	1:F:173:GLU:OE1	2.12	0.49
1:K:136:ASP:OD1	1:K:136:ASP:N	2.41	0.49
1:Q:234:LYS:N	1:Q:234:LYS:HD2	2.28	0.49
3:M:586:GLU:HB2	3:M:587:LYS:CB	2.41	0.48
1:Q:224:PHE:CZ	1:Q:244:TYR:HB3	2.49	0.48
1:A:133:TYR:CE1	1:A:136:ASP:HB2	2.48	0.48
1:F:594:TRP:HZ2	3:H:630:ASN:HD21	1.60	0.48
1:F:661:TYR:O	1:F:662:MET:HB2	2.13	0.48
1:K:236:THR:HG22	1:K:237:ALA:N	2.28	0.48
1:K:627:PHE:CE2	1:K:721:GLU:HB2	2.47	0.48
2:L:82:PHE:HZ	2:L:376:MET:HE1	1.77	0.48
1:Q:117:GLN:HA	1:Q:117:GLN:OE1	2.13	0.48
1:A:427:PRO:HA	1:A:464:ARG:HH22	1.79	0.48
1:K:317:ASN:HD21	1:K:332:LYS:HD2	1.78	0.48
1:A:322:PRO:HG3	1:F:59:GLU:HG2	1.95	0.48
2:G:332:LYS:NZ	2:G:338:ASP:O	2.26	0.48
1:Q:432:TRP:CE3	1:Q:432:TRP:CA	2.90	0.48
1:A:45:ASN:O	1:A:49:ILE:HG13	2.14	0.48
1:A:67:PRO:O	1:A:68:VAL:HG12	2.14	0.48
1:F:613:HIS:NE2	3:H:581:VAL:HB	2.29	0.48
1:K:451:PHE:CE2	1:K:467:TYR:HD1	2.28	0.48
3:M:664:HIS:HB2	3:M:674:ILE:HD11	1.94	0.48
1:Q:123:GLU:OE1	1:Q:123:GLU:N	2.32	0.48
2:B:282:PRO:HB3	3:C:575:ARG:NH1	2.23	0.48
2:G:241:SER:HB3	2:G:254:CYS:SG	2.54	0.48
2:G:319:ILE:O	2:G:330:CYS:HA	2.14	0.48
2:B:400:LYS:HE3	2:B:401:CYS:O	2.14	0.48
2:G:180:MET:O	2:G:180:MET:HG3	2.13	0.48
3:M:575:ARG:O	3:M:578:GLU:HG2	2.14	0.48
2:R:364:TRP:HD1	5:U:5:GLN:HB3	1.78	0.48
1:F:302:THR:OG1	1:F:305:THR:N	2.39	0.48
2:B:322:LYS:HE2	2:B:358:TYR:OH	2.13	0.48
1:F:83:CYS:HB2	1:F:98:LEU:HD21	1.95	0.48
1:K:236:THR:HG22	1:K:238:GLU:H	1.78	0.48
1:K:71:LEU:HB2	2:L:180:MET:SD	2.54	0.48
2:B:418:PHE:CE1	2:B:425:LEU:HD13	2.49	0.48
3:C:579:MET:HA	3:C:580:GLU:C	2.35	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:689:HIS:HD2	1:F:726:TYR:H	1.61	0.48
1:K:606:ILE:CG2	1:K:707:ARG:HD2	2.43	0.48
1:K:91:PHE:HE2	2:L:131:GLU:HB2	1.78	0.48
1:A:165:PHE:HE1	1:A:170:ILE:HD13	1.79	0.47
1:A:89:LEU:O	1:A:90:ASP:HB3	2.14	0.47
1:F:272:VAL:CG1	1:F:276:GLN:HB2	2.44	0.47
1:F:446:THR:HG23	1:F:447:TYR:HD1	1.79	0.47
1:Q:96:ILE:HG13	2:R:134:LEU:HG	1.95	0.47
1:A:330:GLY:H	1:A:333:GLU:HB2	1.78	0.47
1:A:594:TRP:O	1:A:597:LYS:HG2	2.14	0.47
1:K:10:LYS:HB3	1:K:12:PRO:HD2	1.96	0.47
1:Q:534:CYS:HB3	1:Q:537:VAL:HG22	1.96	0.47
2:R:95:PRO:HB3	2:R:430:ASP:HA	1.96	0.47
2:B:288:PRO:HB3	3:C:578:GLU:OE2	2.14	0.47
1:F:730:GLN:HG3	1:F:732:ASP:N	2.30	0.47
2:R:170:GLY:HA2	2:R:193:ILE:HG13	1.95	0.47
3:S:645:GLN:O	3:S:649:LYS:HD3	2.14	0.47
1:A:70:ILE:CD1	2:B:135:LEU:HD22	2.44	0.47
1:F:243:LYS:O	1:F:247:LEU:HG	2.14	0.47
1:F:619:SER:HB2	1:F:625:GLY:CA	2.45	0.47
2:G:148:TYR:CZ	5:J:7:M3L:HM11	2.49	0.47
3:H:597:ILE:HG23	3:H:615:LYS:HD2	1.96	0.47
3:H:606:VAL:O	3:H:611:LYS:HE3	2.14	0.47
2:R:210:SER:OG	2:R:211:LYS:N	2.47	0.47
1:F:619:SER:HB2	1:F:625:GLY:HA3	1.96	0.47
1:F:99:LYS:NZ	2:G:180:MET:O	2.47	0.47
1:K:106:SER:HB2	2:L:169:ARG:NH1	2.30	0.47
1:K:263:ASN:HA	3:M:607:ASN:HD21	1.76	0.47
3:M:633:ASN:ND2	3:M:673:SER:OG	2.48	0.47
1:Q:440:PHE:CD2	1:Q:469:PHE:HE2	2.33	0.47
1:A:302:THR:HG23	1:A:304:ASN:N	2.30	0.47
2:B:191:ASN:HD21	2:B:211:LYS:HE2	1.79	0.47
1:F:139:LEU:HB3	1:F:141:GLN:HA	1.97	0.47
2:G:161:PRO:O	2:G:177:PRO:HD2	2.14	0.47
2:G:232:VAL:HG11	3:H:591:TRP:CZ3	2.49	0.47
2:R:356:PHE:CZ	2:R:397:HIS:HB3	2.50	0.47
2:R:79:LYS:HE3	2:R:390:ASP:OD2	2.15	0.47
1:Q:456:ARG:NE	3:S:675:ASP:OD1	2.32	0.47
1:K:22:GLU:OE2	1:K:181:TYR:CZ	2.67	0.47
1:K:19:VAL:HG22	1:K:178:LEU:HD22	1.97	0.47
2:L:101:PHE:CD1	2:L:113:PHE:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:201:ARG:NH1	2:L:247:LEU:HD22	2.30	0.47
2:L:286:ASN:O	3:M:578:GLU:HB3	2.14	0.47
1:Q:68:VAL:HG11	2:R:123:LEU:HD23	1.96	0.47
1:A:19:VAL:HG22	1:A:178:LEU:HD21	1.97	0.47
1:A:129:HIS:HB3	2:B:302:ARG:HH21	1.78	0.47
1:F:121:MET:SD	1:F:645:ILE:HD11	2.54	0.47
3:S:606:VAL:O	3:S:611:LYS:HE3	2.15	0.47
3:C:650:LYS:HB2	3:C:652:LEU:HG	1.96	0.47
1:A:322:PRO:HG3	1:F:59:GLU:CG	2.44	0.47
1:K:162:GLU:OE1	1:K:162:GLU:N	2.48	0.47
1:Q:30:LYS:CE	1:Q:34:ARG:HH21	2.28	0.47
1:A:70:ILE:HD11	2:B:135:LEU:HD13	1.95	0.47
1:A:70:ILE:HD11	2:B:135:LEU:HD22	1.95	0.47
2:B:399:ALA:HA	2:B:400:LYS:HA	1.71	0.47
1:F:447:TYR:CB	1:F:454:ILE:HD11	2.45	0.47
1:F:730:GLN:HG3	1:F:732:ASP:H	1.80	0.47
3:H:581:VAL:HG12	3:H:582:ASP:OD1	2.15	0.47
1:K:324:CYS:HA	1:K:463:CYS:HB3	1.96	0.47
2:R:331:TRP:HB3	2:R:352:ILE:HD13	1.96	0.47
2:B:180:MET:HE2	2:B:180:MET:HB3	1.62	0.46
1:F:583:ASP:OD1	3:H:629:ASP:HB2	2.15	0.46
2:G:209:VAL:HG13	2:G:239:VAL:HB	1.97	0.46
1:K:150:ILE:CG2	1:K:155:GLY:HA2	2.45	0.46
2:L:189:HIS:NE2	2:L:208:SER:OG	2.38	0.46
1:Q:274:ARG:HG3	1:Q:442:VAL:HA	1.96	0.46
3:S:682:ARG:HA	3:S:685:GLN:HG3	1.97	0.46
1:A:145:PHE:CE2	1:A:660:LYS:HG2	2.51	0.46
1:F:96:ILE:HG22	1:F:97:PRO:HD2	1.95	0.46
3:H:569:ASP:OD1	3:H:569:ASP:N	2.49	0.46
1:K:65:ILE:O	1:K:66:GLN:HB3	2.15	0.46
1:A:161:ARG:NH1	1:A:164:GLY:C	2.68	0.46
2:B:189:HIS:HE1	2:B:208:SER:OG	1.98	0.46
3:H:587:LYS:HE2	3:H:593:ARG:NH1	2.28	0.46
1:K:265:ASP:HB3	3:M:651:ASN:O	2.15	0.46
1:F:129:HIS:H	1:F:129:HIS:CD2	2.34	0.46
1:F:291:LYS:HG2	3:H:621:VAL:HG21	1.98	0.46
3:H:648:ILE:HD13	3:H:685:GLN:HG2	1.97	0.46
2:G:86:ASN:ND2	2:G:87:SER:H	2.13	0.46
1:Q:528:GLN:CG	1:Q:529:PRO:HD2	2.45	0.46
1:A:566:CYS:HB2	1:A:571:CYS:HB2	1.96	0.46
2:B:274:ILE:O	2:B:277:SER:OG	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:539:ALA:O	1:F:540:GLN:HB2	2.15	0.46
3:H:664:HIS:HB2	3:H:674:ILE:HD11	1.98	0.46
1:A:734:LEU:HD13	1:A:734:LEU:N	2.31	0.46
1:F:308:ARG:HG3	3:H:667:ASN:OD1	2.15	0.46
1:Q:161:ARG:HD3	1:Q:233:ASP:OD2	2.16	0.46
1:Q:234:LYS:H	1:Q:234:LYS:HD2	1.81	0.46
1:Q:104:VAL:HG12	2:R:185:HIS:CG	2.50	0.46
2:R:256:MET:O	2:R:258:HIS:CD2	2.63	0.46
1:Q:666:LEU:O	4:T:27:MET:HG3	2.14	0.46
2:B:91:ASP:N	2:B:91:ASP:OD1	2.35	0.46
3:C:565:TYR:HB2	3:C:574:LEU:HD23	1.98	0.46
3:C:589:PRO:HG2	3:C:592:LEU:HB2	1.97	0.46
1:F:234:LYS:CB	1:F:240:LEU:HD21	2.42	0.46
1:F:440:PHE:O	1:F:444:ILE:HG23	2.15	0.46
1:F:65:ILE:HG22	2:G:161:PRO:HG3	1.97	0.46
1:F:45:ASN:ND2	2:G:317:ASP:H	1.88	0.46
1:K:180:GLN:HG2	1:K:181:TYR:HD2	1.80	0.46
2:L:171:ILE:HG23	2:L:187:VAL:HG22	1.98	0.46
3:M:608:GLU:HG3	3:M:609:GLY:N	2.31	0.46
1:Q:168:ASP:O	1:Q:172:VAL:HG23	2.16	0.46
2:R:99:VAL:HG23	2:R:115:THR:HG22	1.97	0.46
1:Q:98:LEU:HD13	2:R:139:VAL:HG21	1.98	0.46
1:A:734:LEU:HD12	7:A:1009:SAH:C4	2.46	0.46
1:A:137:GLU:OE1	1:A:137:GLU:N	2.49	0.46
1:A:64:ARG:O	2:B:159:SER:HB3	2.16	0.46
2:B:189:HIS:CD2	2:B:210:SER:CB	2.99	0.46
1:F:98:LEU:HB3	2:G:139:VAL:HG23	1.98	0.46
2:G:215:LEU:HB2	2:G:229:PHE:HB2	1.98	0.46
3:H:580:GLU:HB3	3:H:581:VAL:CA	2.35	0.46
2:B:176:ASN:HD22	2:B:177:PRO:HD2	1.81	0.46
2:B:229:PHE:HD2	2:B:263:TRP:CE3	2.34	0.46
2:B:260:LEU:HD13	2:B:331:TRP:CZ2	2.51	0.46
1:F:648:GLN:HE22	1:F:668:ASN:HD21	1.64	0.46
3:H:665:ASP:O	3:H:667:ASN:N	2.49	0.46
1:K:303:PRO:HB2	1:K:306:TYR:OH	2.16	0.46
2:R:392:GLU:HB3	2:R:393:VAL:HG22	1.97	0.46
1:A:531:ASP:OD1	1:K:81:ARG:NH2	2.48	0.45
3:H:579:MET:HA	3:H:580:GLU:HB2	1.97	0.45
1:K:263:ASN:N	3:M:607:ASN:HD21	2.14	0.45
3:M:641:GLU:OE2	3:M:680:LYS:NZ	2.49	0.45
1:Q:541:ASN:HD21	1:Q:701:MET:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:358:TYR:CE1	2:R:361:CYS:HB3	2.51	0.45
3:S:607:ASN:O	3:S:611:LYS:HG3	2.16	0.45
1:A:158:HIS:HA	1:A:159:GLY:HA2	1.56	0.45
2:B:128:SER:HA	2:B:129:GLN:HA	1.63	0.45
1:F:138:VAL:O	1:F:139:LEU:HB2	2.16	0.45
1:K:41:MET:HG3	2:L:336:MET:CE	2.46	0.45
5:E:3:GLN:HG2	5:E:4:ALA:H	1.82	0.45
1:F:70:ILE:HD13	1:F:70:ILE:HG21	1.74	0.45
1:K:34:ARG:O	1:K:37:GLU:N	2.49	0.45
1:Q:528:GLN:HG3	1:Q:529:PRO:HD2	1.98	0.45
1:Q:134:MET:CG	1:Q:661:TYR:HE1	2.29	0.45
1:A:531:ASP:OD2	1:K:81:ARG:NH2	2.49	0.45
1:A:263:ASN:CG	3:C:607:ASN:HD21	2.19	0.45
1:K:515:ASN:N	1:K:515:ASN:OD1	2.49	0.45
1:Q:109:ILE:HA	2:R:190:GLY:O	2.16	0.45
2:R:315:LEU:HD22	2:R:320:LEU:HD11	1.99	0.45
1:A:160:ASP:O	1:A:232:PRO:HD2	2.16	0.45
1:F:96:ILE:HD11	2:G:134:LEU:HG	1.98	0.45
1:F:96:ILE:CG2	1:F:97:PRO:HD2	2.47	0.45
2:G:170:GLY:HA2	2:G:193:ILE:HD12	1.99	0.45
1:F:104:VAL:HG21	2:G:171:ILE:HG21	1.99	0.45
1:K:235:GLY:O	1:K:239:GLU:HB2	2.16	0.45
3:M:597:ILE:HG23	3:M:615:LYS:HD2	1.97	0.45
2:R:326:ASN:HA	2:R:358:TYR:CE1	2.51	0.45
2:R:436:ARG:NE	2:R:438:ASP:OD1	2.48	0.45
3:S:647:ILE:HG23	3:S:652:LEU:HB2	1.99	0.45
1:A:59:GLU:O	1:A:63:ARG:HG3	2.17	0.45
1:K:531:ASP:O	1:K:537:VAL:HG21	2.16	0.45
2:L:288:PRO:HG3	3:M:567:HIS:CE1	2.51	0.45
1:Q:238:GLU:H	1:Q:238:GLU:HG3	1.31	0.45
1:Q:294:CYS:SG	1:Q:297:HIS:HB2	2.56	0.45
1:A:138:VAL:HG12	1:A:141:GLN:H	1.81	0.45
1:A:447:TYR:HB2	1:A:454:ILE:HD11	1.98	0.45
1:F:132:PRO:HB2	1:F:134:MET:HE1	1.99	0.45
1:F:619:SER:HB3	1:F:622:ALA:O	2.17	0.45
1:Q:175:VAL:HG21	1:Q:244:TYR:HE1	1.78	0.45
1:Q:334:PHE:CD2	1:Q:467:TYR:OH	2.60	0.45
1:A:128:LEU:HB3	1:A:153:TYR:CE2	2.52	0.45
1:K:698:LYS:HB2	1:K:711:PHE:HE2	1.81	0.45
2:L:150:CYS:HA	2:L:164:ALA:O	2.16	0.45
1:K:87:SER:HG	2:L:86:ASN:HD21	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:104:VAL:HG23	1:Q:104:VAL:O	2.16	0.45
1:Q:302:THR:HG1	1:Q:305:THR:H	1.65	0.45
1:Q:662:MET:CE	1:Q:732:ASP:HB2	2.46	0.45
2:B:306:ARG:N	2:B:325:GLU:OE2	2.48	0.45
1:F:154:ASP:CB	1:F:156:LYS:HE2	2.46	0.45
1:F:98:LEU:HD21	2:G:137:SER:HB3	1.97	0.45
1:K:57:ASN:HA	2:L:420:ARG:HH22	1.82	0.45
2:L:238:GLU:HB2	2:L:256:MET:HG3	1.98	0.45
2:L:315:LEU:HD22	2:L:320:LEU:HD11	1.99	0.45
1:A:245:LYS:O	1:A:248:THR:HG22	2.17	0.45
1:F:264:ILE:HG12	1:F:265:ASP:OD1	2.17	0.45
1:F:667:PHE:O	1:F:674:VAL:HG13	2.17	0.45
1:F:89:LEU:O	1:F:90:ASP:HB3	2.17	0.45
1:K:14:CYS:SG	1:K:15:TRP:HD1	2.40	0.45
1:Q:583:ASP:OD1	3:S:629:ASP:HB2	2.18	0.45
1:A:182:ASN:O	1:A:182:ASN:ND2	2.51	0.44
1:A:230:MET:HB2	1:A:231:PHE:HD1	1.82	0.44
3:M:648:ILE:CD1	3:M:685:GLN:HG2	2.46	0.44
1:Q:264:ILE:N	1:Q:265:ASP:HB2	2.31	0.44
1:Q:302:THR:N	1:Q:303:PRO:HA	2.32	0.44
2:R:232:VAL:HG22	2:R:295:HIS:HB3	1.99	0.44
2:B:211:LYS:HG3	2:B:238:GLU:CG	2.47	0.44
3:C:567:HIS:HB2	3:C:570:THR:O	2.17	0.44
1:K:19:VAL:HG11	1:K:227:ILE:HG22	2.00	0.44
3:M:596:THR:O	3:M:600:ILE:HG12	2.17	0.44
3:M:610:GLU:HA	3:M:613:VAL:HG12	2.00	0.44
1:Q:70:ILE:HG13	1:Q:70:ILE:O	2.16	0.44
2:R:131:GLU:OE1	2:R:133:ARG:NH2	2.39	0.44
2:R:418:PHE:CE1	2:R:425:LEU:HD13	2.52	0.44
1:A:330:GLY:CA	1:A:334:PHE:H	2.20	0.44
1:A:560:CYS:HB2	1:A:572:PRO:HD2	2.00	0.44
3:C:616:LEU:HD22	3:C:643:TYR:CD2	2.49	0.44
1:F:148:GLU:HA	1:F:151:LYS:HD2	1.97	0.44
1:Q:13:VAL:HA	1:Q:16:ARG:HG2	1.99	0.44
1:Q:15:TRP:O	1:Q:19:VAL:HG23	2.18	0.44
2:R:293:LYS:HG3	2:R:295:HIS:NE2	2.32	0.44
1:A:220:SER:O	1:A:223:ILE:HG13	2.17	0.44
1:A:668:ASN:HA	1:A:674:VAL:HG13	1.98	0.44
1:A:89:LEU:HA	1:A:89:LEU:HD23	1.78	0.44
2:B:189:HIS:CD2	2:B:210:SER:HB2	2.53	0.44
2:B:396:PRO:HA	2:B:397:HIS:ND1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:ILE:HD13	1:K:70:ILE:HG21	1.74	0.44
1:K:65:ILE:HG22	2:L:161:PRO:HG3	1.98	0.44
2:L:199:HIS:HB2	2:L:205:LEU:HB2	1.99	0.44
3:S:645:GLN:HG3	3:S:649:LYS:HE2	1.99	0.44
1:A:68:VAL:HG11	2:B:110:PRO:CG	2.48	0.44
1:F:99:LYS:O	2:G:138:TYR:HA	2.17	0.44
1:K:730:GLN:HG3	1:K:731:ALA:N	2.33	0.44
2:L:254:CYS:HB2	2:L:309:VAL:HB	1.99	0.44
2:L:395:ASP:HB3	2:L:396:PRO:C	2.37	0.44
1:Q:144:THR:O	1:Q:148:GLU:HG3	2.16	0.44
1:Q:728:TYR:CD2	1:Q:734:LEU:HD21	2.51	0.44
2:R:441:ARG:HB2	2:R:441:ARG:CZ	2.46	0.44
1:Q:697:ALA:O	4:T:30:PRO:HD2	2.17	0.44
1:A:158:HIS:O	2:B:258:HIS:CE1	2.70	0.44
2:B:325:GLU:O	2:B:326:ASN:HB2	2.18	0.44
3:C:639:PHE:CE2	3:C:647:ILE:HD11	2.52	0.44
1:K:129:HIS:H	1:K:129:HIS:HD2	1.66	0.44
1:Q:457:LEU:HD12	1:Q:458:ILE:H	1.78	0.44
1:A:231:PHE:N	1:A:231:PHE:CD1	2.85	0.44
1:A:443:LEU:HB3	1:A:454:ILE:HG13	2.00	0.44
1:A:83:CYS:HB2	1:A:98:LEU:HD13	2.00	0.44
2:B:227:ALA:HA	2:B:292:GLN:O	2.17	0.44
1:F:437:ALA:O	1:F:441:ARG:HG3	2.18	0.44
1:F:110:MET:O	2:G:190:GLY:HA3	2.18	0.44
1:K:11:GLY:N	1:K:12:PRO:CD	2.80	0.44
2:L:210:SER:HB3	2:L:212:ASP:OD1	2.16	0.44
2:L:392:GLU:HA	2:L:393:VAL:HA	1.70	0.44
3:M:577:GLN:CD	3:M:577:GLN:H	2.14	0.44
3:M:662:SER:O	3:M:666:PHE:HD1	2.01	0.44
1:Q:264:ILE:HB	1:Q:265:ASP:HB2	1.99	0.44
1:Q:443:LEU:HD13	1:Q:457:LEU:HD11	2.00	0.44
1:Q:662:MET:HE3	1:Q:733:ALA:HB2	1.99	0.44
2:R:194:ASN:ND2	2:R:240:LEU:HD23	2.31	0.44
1:A:223:ILE:O	1:A:226:ALA:N	2.51	0.44
1:A:318:LYS:HZ3	1:A:326:GLN:HB3	1.82	0.44
1:A:583:ASP:OD1	3:C:629:ASP:HB2	2.18	0.44
1:F:98:LEU:CD2	2:G:137:SER:HB3	2.48	0.44
2:L:145:GLU:OE1	2:L:169:ARG:HB2	2.18	0.44
2:L:210:SER:OG	2:L:211:LYS:N	2.50	0.44
1:Q:436:GLU:OE2	1:Q:461:LYS:NZ	2.51	0.44
1:A:10:LYS:HE3	1:A:222:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:PRO:HB2	1:A:306:TYR:OH	2.18	0.44
2:B:253:SER:O	2:B:260:LEU:HA	2.18	0.44
2:B:361:CYS:SG	2:B:366:MET:HG3	2.58	0.44
1:Q:168:ASP:N	1:Q:168:ASP:OD1	2.51	0.44
1:Q:89:LEU:O	1:Q:90:ASP:HB3	2.17	0.44
2:R:395:ASP:N	2:R:396:PRO:HA	2.32	0.44
1:A:263:ASN:HD22	1:A:265:ASP:H	1.66	0.43
2:B:294:ILE:N	2:B:294:ILE:HD12	2.32	0.43
3:C:581:VAL:HA	3:C:582:ASP:HA	1.60	0.43
1:F:125:GLU:HG3	1:F:125:GLU:O	2.18	0.43
1:F:172:VAL:O	1:F:175:VAL:HG22	2.17	0.43
2:L:227:ALA:HA	2:L:292:GLN:O	2.17	0.43
1:Q:171:PHE:CZ	1:Q:224:PHE:HE2	2.35	0.43
1:Q:607:GLN:HG2	1:Q:702:VAL:CG1	2.48	0.43
2:R:323:SER:HB3	2:R:325:GLU:HG3	1.99	0.43
3:C:561:HIS:N	3:C:562:ASN:HB3	2.33	0.43
1:F:175:VAL:HG23	1:F:176:ASN:N	2.32	0.43
1:F:223:ILE:HG13	1:F:224:PHE:N	2.34	0.43
1:F:650:GLU:HA	1:F:653:ARG:NH1	2.33	0.43
1:F:98:LEU:HA	1:F:98:LEU:HD23	1.43	0.43
2:L:86:ASN:HD22	2:L:87:SER:N	2.16	0.43
1:A:67:PRO:HG3	2:B:105:SER:HB3	1.97	0.43
1:A:41:MET:HG3	2:B:336:MET:HE1	1.99	0.43
1:F:660:LYS:HD2	1:F:660:LYS:HA	1.83	0.43
1:K:19:VAL:HG22	1:K:178:LEU:CD2	2.48	0.43
1:A:566:CYS:HB2	1:A:571:CYS:CB	2.49	0.43
2:L:82:PHE:HZ	2:L:376:MET:CE	2.30	0.43
2:G:378:ALA:HA	2:G:387:TYR:O	2.18	0.43
1:K:72:THR:HG22	1:K:74:VAL:N	2.34	0.43
2:L:323:SER:C	2:L:325:GLU:H	2.21	0.43
1:Q:169:GLU:O	1:Q:173:GLU:HG2	2.18	0.43
1:Q:654:ARG:O	1:Q:657:VAL:HG12	2.19	0.43
1:A:141:GLN:HA	1:A:142:ASP:HA	1.67	0.43
1:A:128:LEU:CD2	1:A:157:VAL:HG22	2.47	0.43
2:B:397:HIS:HA	2:B:398:LYS:C	2.39	0.43
1:A:428:GLU:OE2	1:F:51:GLU:OE2	2.35	0.43
2:G:160:HIS:HB3	2:G:176:ASN:HD21	1.83	0.43
1:Q:129:HIS:HA	1:Q:158:HIS:HB2	2.00	0.43
2:R:258:HIS:CE1	2:R:307:ASN:HA	2.53	0.43
3:S:664:HIS:HB2	3:S:674:ILE:HD11	2.01	0.43
1:F:244:TYR:CD1	1:F:244:TYR:C	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:22:GLU:OE1	1:K:178:LEU:HD23	2.18	0.43
1:K:304:ASN:HA	1:K:307:LYS:HD3	2.00	0.43
1:K:326:GLN:HB2	1:K:327:HIS:HB2	2.00	0.43
1:K:425:GLU:OE2	1:K:426:PRO:HD2	2.19	0.43
1:K:472:LYS:O	1:K:476:ILE:HG12	2.18	0.43
1:Q:139:LEU:HD12	1:Q:140:ASP:HA	2.00	0.43
1:Q:440:PHE:CD2	1:Q:469:PHE:CE2	3.07	0.43
1:A:257:PRO:N	1:A:258:PRO:HD3	2.34	0.43
1:A:337:ALA:O	1:A:341:GLU:HG3	2.19	0.43
1:Q:557:PHE:CG	1:Q:558:PRO:HD2	2.54	0.43
1:Q:563:LYS:CB	1:Q:587:THR:HG22	2.45	0.43
1:Q:96:ILE:HG22	1:Q:97:PRO:O	2.18	0.43
2:R:414:ARG:HD3	2:R:414:ARG:HA	1.81	0.43
2:B:101:PHE:CD1	2:B:113:PHE:HB3	2.54	0.43
1:F:168:ASP:O	1:F:172:VAL:HG23	2.19	0.43
1:F:261:THR:HG22	1:F:262:PRO:O	2.19	0.43
1:F:644:GLU:O	1:F:675:VAL:HA	2.18	0.43
2:G:322:LYS:HB3	2:G:322:LYS:HE3	1.42	0.43
1:F:263:ASN:N	3:H:607:ASN:OD1	2.52	0.43
1:K:224:PHE:CE1	1:K:241:LYS:HA	2.54	0.43
1:K:714:ARG:HG3	1:K:715:ALA:O	2.19	0.43
2:R:414:ARG:NH1	5:U:8:PHE:HD1	2.17	0.43
2:B:199:HIS:HB3	2:B:202:ASP:O	2.19	0.43
2:B:204:ASN:O	2:B:220:ILE:HG12	2.19	0.43
2:B:186:TYR:CE2	2:B:220:ILE:HG22	2.53	0.43
1:F:131:ILE:HG21	1:F:131:ILE:HD13	1.80	0.43
1:F:272:VAL:HG12	1:F:276:GLN:HB2	1.99	0.43
2:G:397:HIS:NE2	2:G:398:LYS:HG2	2.34	0.43
3:H:610:GLU:HA	3:H:613:VAL:HG12	2.01	0.43
3:M:666:PHE:O	3:M:667:ASN:HB2	2.19	0.43
1:Q:270:LYS:HE3	1:Q:270:LYS:HB3	1.75	0.43
1:Q:461:LYS:HD3	1:Q:461:LYS:HA	1.69	0.43
1:Q:665:PHE:CD2	1:Q:678:THR:HG22	2.49	0.43
1:Q:263:ASN:OD1	3:S:609:GLY:HA3	2.19	0.43
1:A:245:LYS:HA	1:A:248:THR:HG22	2.00	0.42
1:A:438:SER:O	1:A:442:VAL:HG23	2.18	0.42
1:A:516:HIS:HB3	1:A:671:ASN:ND2	2.34	0.42
2:B:241:SER:HB3	2:B:254:CYS:SG	2.59	0.42
1:F:22:GLU:O	1:F:26:LEU:HD12	2.18	0.42
1:F:612:LYS:HA	1:F:612:LYS:HD3	1.84	0.42
1:K:243:LYS:HE3	1:K:243:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:591:ALA:O	1:K:594:TRP:CZ2	2.72	0.42
1:Q:460:THR:O	1:Q:461:LYS:CE	2.61	0.42
1:Q:541:ASN:HD21	1:Q:701:MET:CE	2.32	0.42
3:S:633:ASN:ND2	3:S:673:SER:OG	2.51	0.42
1:A:533:SER:HB3	1:K:81:ARG:HB3	2.00	0.42
1:F:141:GLN:CD	1:F:141:GLN:H	2.21	0.42
1:F:141:GLN:H	1:F:141:GLN:NE2	2.16	0.42
1:F:45:ASN:HD21	2:G:317:ASP:N	1.88	0.42
2:G:197:LYS:O	2:G:206:LEU:HD12	2.18	0.42
1:K:238:GLU:H	1:K:238:GLU:HG3	1.63	0.42
1:K:242:GLU:O	1:K:246:GLU:HG3	2.19	0.42
2:L:88:LEU:HD11	2:L:132:ILE:HG21	2.01	0.42
2:L:161:PRO:O	2:L:177:PRO:HD2	2.19	0.42
1:Q:138:VAL:HB	1:Q:139:LEU:HA	2.01	0.42
1:Q:41:MET:HG3	2:R:336:MET:CE	2.49	0.42
2:R:211:LYS:HG3	2:R:238:GLU:CD	2.39	0.42
1:A:68:VAL:HG13	1:A:68:VAL:O	2.19	0.42
1:A:68:VAL:CG2	2:B:110:PRO:HG2	2.37	0.42
2:B:254:CYS:HB3	2:B:260:LEU:CD2	2.47	0.42
1:F:634:LYS:HG3	1:F:713:LYS:O	2.19	0.42
1:F:96:ILE:CD1	2:G:134:LEU:HG	2.48	0.42
2:G:307:ASN:OD1	5:J:5:GLN:HG3	2.18	0.42
1:K:451:PHE:HE2	1:K:467:TYR:CD1	2.29	0.42
3:M:579:MET:O	3:M:581:VAL:N	2.53	0.42
1:Q:582:PRO:HB2	3:S:628:ALA:HB2	2.00	0.42
2:R:294:ILE:HD12	2:R:294:ILE:N	2.34	0.42
2:R:375:LYS:HG2	2:R:392:GLU:OE1	2.19	0.42
1:A:516:HIS:HB3	1:A:671:ASN:HD21	1.84	0.42
2:B:332:LYS:HD3	2:B:336:MET:HE3	2.02	0.42
2:G:399:ALA:HB1	2:G:400:LYS:HB2	2.01	0.42
1:K:168:ASP:OD2	2:L:348:SER:HB3	2.20	0.42
1:Q:168:ASP:O	1:Q:171:PHE:HB3	2.20	0.42
2:R:308:TYR:CE2	5:U:5:GLN:HB2	2.54	0.42
1:A:129:HIS:CE1	2:B:236:ARG:HG3	2.54	0.42
1:A:241:LYS:HG2	1:A:245:LYS:HE3	2.00	0.42
1:A:66:GLN:HG3	1:A:66:GLN:O	2.20	0.42
1:A:67:PRO:HG3	2:B:105:SER:CA	2.49	0.42
3:C:570:THR:O	3:C:572:LEU:N	2.53	0.42
1:F:431:GLU:H	1:F:431:GLU:HG3	1.64	0.42
2:G:191:ASN:HD22	2:G:211:LYS:HG2	1.84	0.42
2:G:323:SER:C	2:G:325:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLY:HA2	1:A:233:ASP:OD2	2.19	0.42
2:G:248:GLY:O	2:G:265:ILE:HD11	2.20	0.42
1:K:145:PHE:CE1	1:K:660:LYS:HD3	2.55	0.42
1:K:726:TYR:O	1:K:727:ARG:HB2	2.20	0.42
1:Q:128:LEU:HD22	1:Q:153:TYR:CG	2.54	0.42
1:A:737:VAL:HA	1:A:738:GLY:HA2	1.58	0.42
1:A:129:HIS:CB	2:B:302:ARG:HH21	2.33	0.42
2:L:155:ASP:O	2:L:159:SER:N	2.49	0.42
2:L:399:ALA:HA	2:L:400:LYS:HA	1.77	0.42
1:Q:328:LEU:CG	1:Q:425:GLU:HG2	2.44	0.42
1:Q:638:ILE:HD13	1:Q:638:ILE:HG21	1.84	0.42
3:S:587:LYS:HB2	3:S:588:ASP:HA	2.02	0.42
1:A:557:PHE:CD2	1:A:558:PRO:O	2.72	0.42
1:A:599:VAL:HG22	1:A:600:SER:N	2.35	0.42
2:B:210:SER:OG	2:B:211:LYS:N	2.53	0.42
1:F:129:HIS:HE1	2:G:236:ARG:HG3	1.84	0.42
1:K:158:HIS:O	2:L:258:HIS:CE1	2.72	0.42
1:K:263:ASN:HB3	3:M:607:ASN:ND2	2.34	0.42
1:Q:727:ARG:NH2	4:T:30:PRO:HG3	2.22	0.42
1:A:169:GLU:O	1:A:173:GLU:HG3	2.20	0.42
1:A:599:VAL:HG22	1:A:600:SER:H	1.85	0.42
1:A:731:ALA:O	1:A:733:ALA:HA	2.20	0.42
2:G:95:PRO:HB3	2:G:430:ASP:HA	2.01	0.42
1:K:302:THR:HB	1:K:524:ASP:OD2	2.19	0.42
2:L:183:ILE:HG13	2:L:184:LYS:HG3	2.02	0.42
2:R:187:VAL:O	2:R:187:VAL:HG12	2.19	0.42
1:A:726:TYR:O	1:A:727:ARG:HB2	2.20	0.42
2:B:385:LYS:HG3	2:B:405:THR:HG22	2.01	0.42
1:F:121:MET:HB2	1:F:295:PHE:O	2.20	0.42
1:F:571:CYS:SG	1:F:573:CYS:HB2	2.59	0.42
2:G:319:ILE:HG23	2:G:319:ILE:HD12	1.78	0.42
2:L:118:SER:OG	2:L:119:ASN:N	2.53	0.42
1:Q:714:ARG:HG3	1:Q:715:ALA:O	2.20	0.42
2:R:392:GLU:HB3	2:R:393:VAL:CG2	2.50	0.42
1:F:18:ARG:NH1	1:F:18:ARG:HG3	2.35	0.41
1:F:227:ILE:CD1	1:F:240:LEU:HD13	2.50	0.41
3:H:597:ILE:HA	3:H:615:LYS:HD2	2.02	0.41
1:K:308:ARG:HG2	1:K:309:LYS:N	2.31	0.41
2:L:429:CYS:HB2	2:L:433:SER:OG	2.20	0.41
1:Q:311:THR:OG1	1:Q:313:THR:HG23	2.20	0.41
1:Q:31:ARG:HB2	1:Q:31:ARG:HE	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:582:PRO:HB2	1:Q:594:TRP:HH2	1.84	0.41
1:A:70:ILE:HG12	2:B:135:LEU:HD22	2.01	0.41
2:B:254:CYS:HB2	2:B:309:VAL:HB	2.02	0.41
2:B:404:LEU:HD22	2:B:437:TRP:CE3	2.55	0.41
3:C:610:GLU:O	3:C:614:MET:HG3	2.20	0.41
1:F:443:LEU:HA	1:F:446:THR:HG22	2.01	0.41
1:F:99:LYS:NZ	2:G:180:MET:HG3	2.35	0.41
3:H:609:GLY:O	3:H:613:VAL:HG12	2.19	0.41
2:R:86:ASN:ND2	2:R:87:SER:H	2.15	0.41
1:A:320:CYS:HB2	1:A:324:CYS:SG	2.60	0.41
1:F:13:VAL:O	1:F:17:LYS:HG2	2.20	0.41
1:F:302:THR:HB	1:F:524:ASP:OD2	2.20	0.41
2:G:298:ASP:HA	2:G:345:PRO:HG3	2.03	0.41
1:K:180:GLN:CG	1:K:181:TYR:HD2	2.34	0.41
2:L:195:GLU:HG3	2:L:196:LEU:N	2.36	0.41
3:S:662:SER:O	3:S:666:PHE:HD2	2.03	0.41
1:A:340:ALA:O	1:A:344:LYS:HG3	2.21	0.41
2:B:235:HIS:CD2	2:B:239:VAL:HG22	2.55	0.41
1:A:38:VAL:HG12	2:B:353:LEU:HD22	2.02	0.41
2:B:396:PRO:C	2:B:398:LYS:HB2	2.40	0.41
1:A:613:HIS:CE1	3:C:582:ASP:HB3	2.56	0.41
3:C:606:VAL:HG12	3:C:611:LYS:HG3	2.01	0.41
2:G:258:HIS:CE1	2:G:307:ASN:HA	2.55	0.41
2:L:132:ILE:HD11	2:L:436:ARG:HB2	2.02	0.41
1:Q:341:GLU:O	1:Q:344:LYS:HB2	2.20	0.41
2:R:378:ALA:HA	2:R:387:TYR:O	2.20	0.41
1:A:117:GLN:OE1	1:A:117:GLN:HA	2.20	0.41
1:A:258:PRO:HA	1:A:259:GLU:HA	1.79	0.41
2:B:315:LEU:HD13	2:B:370:MET:HE1	2.02	0.41
3:C:579:MET:HG3	3:C:581:VAL:CG1	2.48	0.41
1:K:180:GLN:HG2	1:K:181:TYR:CD2	2.56	0.41
1:K:270:LYS:HB3	1:K:270:LYS:HE3	1.88	0.41
2:L:180:MET:HE2	2:L:180:MET:HB3	1.78	0.41
2:R:258:HIS:N	2:R:258:HIS:CD2	2.89	0.41
2:B:376:MET:HG3	2:B:418:PHE:CZ	2.54	0.41
3:C:593:ARG:HD2	3:C:619:LEU:CD2	2.50	0.41
1:K:30:LYS:HA	1:K:30:LYS:HD2	1.85	0.41
1:K:515:ASN:CA	1:K:671:ASN:HD21	2.31	0.41
2:L:196:LEU:HD22	2:L:206:LEU:HD11	2.01	0.41
2:L:285:THR:OG1	2:L:287:ARG:HG2	2.21	0.41
3:S:607:ASN:OD1	3:S:610:GLU:N	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLN:HG3	1:A:731:ALA:N	2.36	0.41
1:A:98:LEU:HD12	2:B:137:SER:O	2.20	0.41
3:C:671:ILE:HA	3:C:674:ILE:HD12	2.01	0.41
1:F:265:ASP:HA	3:H:654:ARG:NH1	2.36	0.41
1:F:582:PRO:HB2	1:F:594:TRP:HH2	1.85	0.41
2:L:294:ILE:HD12	2:L:294:ILE:N	2.36	0.41
1:Q:161:ARG:HE	2:R:306:ARG:HD2	1.85	0.41
1:A:166:ILE:HG21	1:A:234:LYS:HE3	2.01	0.41
1:A:691:VAL:O	1:A:693:PRO:HD3	2.21	0.41
2:B:422:SER:HB2	2:B:439:ARG:NH1	2.36	0.41
1:F:344:LYS:O	1:F:345:THR:HB	2.21	0.41
2:G:202:ASP:OD2	2:G:278:TYR:OH	2.32	0.41
1:K:605:SER:HB3	1:K:637:PHE:CD2	2.56	0.41
1:K:68:VAL:CG1	1:K:69:HIS:N	2.83	0.41
1:K:71:LEU:HD11	1:K:97:PRO:CG	2.47	0.41
2:R:377:LEU:O	2:R:388:VAL:HA	2.21	0.41
2:R:82:PHE:CE2	2:R:439:ARG:HB2	2.56	0.41
1:A:320:CYS:CB	1:A:324:CYS:HB2	2.50	0.41
1:F:454:ILE:HD12	1:F:454:ILE:N	2.36	0.41
1:F:621:VAL:HG13	1:F:736:TYR:HB3	2.02	0.41
2:G:148:TYR:CE2	5:J:7:M3L:HM11	2.55	0.41
1:F:594:TRP:CH2	3:H:628:ALA:HB2	2.55	0.41
1:K:41:MET:HG3	2:L:336:MET:HE2	2.03	0.41
2:L:136:GLN:HE22	2:L:180:MET:HG2	1.86	0.41
3:M:585:ASP:CG	3:M:586:GLU:HB3	2.41	0.41
1:Q:227:ILE:HG13	1:Q:240:LEU:HD13	2.02	0.41
1:Q:460:THR:C	1:Q:461:LYS:HG2	2.41	0.41
1:A:475:SER:O	2:R:201:ARG:NH2	2.53	0.41
2:B:85:VAL:CG2	2:B:130:GLY:HA2	2.51	0.41
2:B:395:ASP:O	2:B:397:HIS:ND1	2.53	0.41
1:F:132:PRO:HB2	1:F:134:MET:CE	2.51	0.41
1:F:545:LYS:NZ	1:F:583:ASP:OD2	2.50	0.41
2:L:86:ASN:ND2	2:L:87:SER:H	2.16	0.41
1:Q:12:PRO:HD2	1:Q:15:TRP:HD1	1.85	0.41
1:Q:30:LYS:HE2	1:Q:34:ARG:NE	2.30	0.41
1:Q:455:ALA:HB2	1:Q:466:VAL:HG21	2.02	0.41
1:Q:618:PRO:HD3	3:S:566:PHE:CE1	2.56	0.41
1:Q:732:ASP:HA	1:Q:733:ALA:HA	1.53	0.41
3:S:592:LEU:HA	3:S:592:LEU:HD12	1.89	0.41
1:A:265:ASP:OD1	3:C:654:ARG:HB2	2.21	0.41
1:A:71:LEU:HB3	2:B:180:MET:HE1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:ASP:OD1	2:B:249:GLU:N	2.54	0.41
1:F:442:VAL:O	1:F:446:THR:HG22	2.21	0.41
2:G:315:LEU:HD13	2:G:370:MET:HE1	2.03	0.41
1:A:161:ARG:NH1	1:A:164:GLY:N	2.61	0.40
1:A:565:GLN:HG2	1:A:565:GLN:H	1.38	0.40
1:A:714:ARG:HG2	1:A:715:ALA:O	2.21	0.40
1:A:689:HIS:CD2	1:A:726:TYR:H	2.37	0.40
2:G:211:LYS:HG3	2:G:238:GLU:CG	2.50	0.40
3:M:586:GLU:CB	3:M:587:LYS:HB3	2.46	0.40
1:Q:133:TYR:CE2	1:Q:136:ASP:HB2	2.55	0.40
2:R:368:PHE:HB3	2:R:379:LEU:HB2	2.03	0.40
1:A:168:ASP:HB2	2:B:349:ASN:ND2	2.36	0.40
1:A:224:PHE:HB3	1:A:237:ALA:HB1	2.02	0.40
1:A:436:GLU:OE2	1:A:460:THR:HG23	2.21	0.40
1:A:129:HIS:HE1	2:B:236:ARG:HG3	1.86	0.40
2:B:397:HIS:CD2	2:B:397:HIS:O	2.74	0.40
1:A:89:LEU:HD21	2:B:85:VAL:O	2.21	0.40
7:F:1009:SAH:O4'	7:F:1009:SAH:HA	2.21	0.40
2:G:147:PHE:HA	2:G:167:GLY:HA3	2.04	0.40
1:Q:447:TYR:HB3	1:Q:454:ILE:HD11	2.03	0.40
1:Q:432:TRP:CD1	1:Q:469:PHE:CE1	2.99	0.40
3:S:610:GLU:HA	3:S:613:VAL:HG12	2.02	0.40
1:A:302:THR:HG22	1:A:305:THR:CG2	2.46	0.40
1:A:302:THR:N	1:A:303:PRO:HA	2.36	0.40
3:C:607:ASN:HB3	3:C:610:GLU:H	1.86	0.40
3:C:648:ILE:HD13	3:C:685:GLN:HG2	2.03	0.40
1:F:314:ALA:N	1:F:315:LEU:HD12	2.36	0.40
1:F:454:ILE:HD12	1:F:454:ILE:H	1.87	0.40
1:F:56:LEU:HD11	2:G:246:LEU:O	2.22	0.40
1:F:644:GLU:HG3	1:F:680:LYS:HG2	2.03	0.40
4:I:22:THR:HA	4:I:23:LYS:HA	1.65	0.40
1:K:110:MET:O	2:L:190:GLY:HA3	2.20	0.40
2:L:424:ILE:HG21	2:L:424:ILE:HD13	1.91	0.40
2:L:286:ASN:ND2	3:M:577:GLN:HB2	2.36	0.40
1:Q:578:ARG:HB3	1:Q:578:ARG:HE	1.55	0.40
1:Q:605:SER:HB3	1:Q:637:PHE:CD2	2.56	0.40
7:A:1009:SAH:H5'2	7:A:1009:SAH:H8	2.03	0.40
1:A:15:TRP:O	1:A:19:VAL:HG23	2.21	0.40
1:A:270:LYS:O	1:A:272:VAL:HG23	2.20	0.40
1:A:734:LEU:HB3	7:A:1009:SAH:C6	2.51	0.40
2:B:387:TYR:HD2	2:B:401:CYS:SG	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:PRO:CB	3:C:575:ARG:HH12	2.26	0.40
1:F:22:GLU:OE2	1:F:177:ALA:CB	2.68	0.40
1:F:119:ASN:HB3	1:F:645:ILE:HG23	2.04	0.40
2:G:285:THR:HG21	2:G:287:ARG:HE	1.86	0.40
1:K:427:PRO:HB3	1:K:468:GLU:HG3	2.03	0.40
1:K:606:ILE:HG21	1:K:707:ARG:HD2	2.04	0.40
2:L:91:ASP:CG	2:L:120:ARG:HH12	2.24	0.40
2:L:318:LEU:HD13	2:L:353:LEU:HD12	2.03	0.40
1:Q:426:PRO:HA	1:Q:427:PRO:HD3	1.97	0.40
1:Q:677:ALA:HA	1:Q:680:LYS:O	2.21	0.40
3:S:666:PHE:O	3:S:667:ASN:HB2	2.21	0.40
1:A:145:PHE:CZ	1:A:660:LYS:HG2	2.56	0.40
2:L:172:ILE:O	2:L:185:HIS:HA	2.22	0.40
1:Q:224:PHE:HZ	1:Q:244:TYR:CG	2.40	0.40
1:Q:440:PHE:C	1:Q:440:PHE:CD2	2.95	0.40
1:Q:606:ILE:HG22	1:Q:707:ARG:HD2	2.03	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)
1:A:568:THR:OG1	1:Q:561:ARG:NH1[3_644]	2.11	0.09
1:F:561:ARG:NH1	1:K:568:THR:OG1[2_545]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	569/746 (76%)	534 (94%)	34 (6%)	1 (0%)	52	86
1	F	558/746 (75%)	526 (94%)	31 (6%)	1 (0%)	52	86
1	K	552/746 (74%)	527 (96%)	23 (4%)	2 (0%)	39	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	555/746 (74%)	527 (95%)	27 (5%)	1 (0%)	52	86
2	B	363/367 (99%)	348 (96%)	15 (4%)	0	100	100
2	G	363/367 (99%)	355 (98%)	8 (2%)	0	100	100
2	L	363/367 (99%)	354 (98%)	9 (2%)	0	100	100
2	R	363/367 (99%)	352 (97%)	11 (3%)	0	100	100
3	C	123/129 (95%)	120 (98%)	3 (2%)	0	100	100
3	H	122/129 (95%)	119 (98%)	2 (2%)	1 (1%)	24	64
3	M	123/129 (95%)	118 (96%)	4 (3%)	1 (1%)	24	64
3	S	123/129 (95%)	121 (98%)	2 (2%)	0	100	100
4	D	7/13 (54%)	7 (100%)	0	0	100	100
4	I	7/13 (54%)	7 (100%)	0	0	100	100
4	O	7/13 (54%)	7 (100%)	0	0	100	100
4	T	7/13 (54%)	7 (100%)	0	0	100	100
5	E	8/12 (67%)	8 (100%)	0	0	100	100
5	J	7/12 (58%)	7 (100%)	0	0	100	100
5	P	6/12 (50%)	6 (100%)	0	0	100	100
5	U	7/12 (58%)	6 (86%)	1 (14%)	0	100	100
All	All	4233/5068 (84%)	4056 (96%)	170 (4%)	7 (0%)	52	86

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	K	66	GLN
1	F	139	LEU
3	M	582	ASP
1	K	265	ASP
1	Q	104	VAL
3	H	609	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	520/667 (78%)	496 (95%)	24 (5%)	33	71
1	F	507/667 (76%)	486 (96%)	21 (4%)	37	74
1	K	503/667 (75%)	481 (96%)	22 (4%)	35	72
1	Q	505/667 (76%)	485 (96%)	20 (4%)	38	75
2	B	328/329 (100%)	322 (98%)	6 (2%)	66	89
2	G	328/329 (100%)	319 (97%)	9 (3%)	52	84
2	L	328/329 (100%)	326 (99%)	2 (1%)	90	97
2	R	328/329 (100%)	327 (100%)	1 (0%)	94	98
3	C	119/121 (98%)	118 (99%)	1 (1%)	86	95
3	H	118/121 (98%)	115 (98%)	3 (2%)	55	85
3	M	119/121 (98%)	117 (98%)	2 (2%)	68	90
3	S	119/121 (98%)	118 (99%)	1 (1%)	86	95
4	D	6/7 (86%)	6 (100%)	0	100	100
4	I	6/7 (86%)	6 (100%)	0	100	100
4	O	6/7 (86%)	6 (100%)	0	100	100
4	T	6/7 (86%)	6 (100%)	0	100	100
5	E	8/9 (89%)	6 (75%)	2 (25%)	1	3
5	J	7/9 (78%)	7 (100%)	0	100	100
5	P	6/9 (67%)	6 (100%)	0	100	100
5	U	7/9 (78%)	7 (100%)	0	100	100
All	All	3874/4532 (86%)	3760 (97%)	114 (3%)	50	82

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	77	LEU
1	A	98	LEU
1	A	129	HIS
1	A	134	MET
1	A	137	GLU
1	A	161	ARG
1	A	231	PHE

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Mol	Chain	Res	Type
1	A	233	ASP
1	A	263	ASN
1	A	284	LEU
1	A	311	THR
1	A	312	GLU
1	A	424	ILE
1	A	527	ARG
1	A	565	GLN
1	A	587	THR
1	A	593	HIS
1	A	626	ILE
1	A	663	CYS
1	A	667	PHE
1	A	708	ILE
1	A	714	ARG
1	A	734	LEU
2	B	209	VAL
2	B	223	ASP
2	B	310	ASP
2	B	386	LEU
2	B	401	CYS
2	B	404	LEU
3	C	592	LEU
5	E	6	ARG
5	E	11	SER
1	F	26	LEU
1	F	32	PHE
1	F	71	LEU
1	F	89	LEU
1	F	129	HIS
1	F	134	MET
1	F	141	GLN
1	F	169	GLU
1	F	233	ASP
1	F	260	CYS
1	F	264	ILE
1	F	265	ASP
1	F	270	LYS
1	F	339	THR
1	F	342	ARG
1	F	439	MET
1	F	460	THR

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Mol	Chain	Res	Type
1	F	528	GLN
1	F	663	CYS
1	F	667	PHE
1	F	668	ASN
2	G	78	CYS
2	G	88	LEU
2	G	189	HIS
2	G	223	ASP
2	G	359	SER
2	G	367	ARG
2	G	386	LEU
2	G	395	ASP
2	G	397	HIS
3	H	579	MET
3	H	605	ASP
3	H	607	ASN
1	K	32	PHE
1	K	72	THR
1	K	77	LEU
1	K	117	GLN
1	K	118	GLN
1	K	129	HIS
1	K	139	LEU
1	K	149	LEU
1	K	227	ILE
1	K	233	ASP
1	K	240	LEU
1	K	243	LYS
1	K	247	LEU
1	K	307	LYS
1	K	311	THR
1	K	328	LEU
1	K	329	GLU
1	K	439	MET
1	K	515	ASN
1	K	525	HIS
1	K	565	GLN
1	K	667	PHE
2	L	86	ASN
2	L	223	ASP
3	M	596	THR
3	M	629	ASP

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Mol	Chain	Res	Type
1	Q	32	PHE
1	Q	66	GLN
1	Q	67	PRO
1	Q	75	SER
1	Q	126	THR
1	Q	129	HIS
1	Q	234	LYS
1	Q	238	GLU
1	Q	239	GLU
1	Q	242	GLU
1	Q	429	ASN
1	Q	432	TRP
1	Q	439	MET
1	Q	525	HIS
1	Q	563	LYS
1	Q	565	GLN
1	Q	667	PHE
1	Q	732	ASP
1	Q	734	LEU
1	Q	735	LYS
2	R	86	ASN
3	S	605	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	69	HIS
1	A	129	HIS
1	A	182	ASN
1	A	263	ASN
1	A	282	HIS
1	A	429	ASN
1	A	689	HIS
2	B	94	GLN
2	B	136	GLN
2	B	160	HIS
2	B	176	ASN
2	B	189	HIS
2	B	258	HIS
2	B	286	ASN
2	B	349	ASN

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Mol	Chain	Res	Type
3	C	562	ASN
3	C	599	GLN
3	C	607	ASN
3	C	631	GLN
3	C	633	ASN
3	C	642	ASN
3	C	667	ASN
1	F	45	ASN
1	F	69	HIS
1	F	117	GLN
1	F	129	HIS
1	F	141	GLN
1	F	176	ASN
1	F	180	GLN
1	F	263	ASN
1	F	268	ASN
1	F	297	HIS
1	F	326	GLN
1	F	429	ASN
1	F	570	GLN
1	F	598	ASN
1	F	668	ASN
1	F	730	GLN
2	G	86	ASN
2	G	136	GLN
2	G	160	HIS
2	G	176	ASN
2	G	191	ASN
2	G	194	ASN
2	G	258	HIS
2	G	286	ASN
2	G	349	ASN
3	H	633	ASN
3	H	642	ASN
5	J	5	GLN
5	J	10	GLN
1	K	45	ASN
1	K	117	GLN
1	K	129	HIS
1	K	273	GLN
1	K	317	ASN
1	K	326	GLN

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Mol	Chain	Res	Type
1	K	429	ASN
1	K	515	ASN
1	K	648	GLN
1	K	668	ASN
1	K	671	ASN
1	K	689	HIS
1	K	730	GLN
2	L	86	ASN
2	L	185	HIS
2	L	213	HIS
2	L	258	HIS
2	L	286	ASN
2	L	349	ASN
2	L	397	HIS
3	M	567	HIS
3	M	599	GLN
3	M	631	GLN
3	M	633	ASN
3	M	645	GLN
3	M	651	ASN
3	M	655	ASN
3	M	667	ASN
5	P	5	GLN
1	Q	129	HIS
1	Q	152	ASN
1	Q	158	HIS
1	Q	268	ASN
1	Q	521	GLN
1	Q	525	HIS
1	Q	671	ASN
1	Q	689	HIS
1	Q	706	HIS
2	R	86	ASN
2	R	94	GLN
2	R	213	HIS
2	R	258	HIS
2	R	286	ASN
2	R	307	ASN
2	R	349	ASN
3	S	631	GLN
3	S	633	ASN
3	S	642	ASN

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Mol	Chain	Res	Type
3	S	645	GLN
5	U	10	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
5	M3L	E	7	5	9,11,12	0.48	0	12,14,16	1.31	2 (16%)
5	M3L	J	7	5	9,11,12	0.52	0	12,14,16	1.29	1 (8%)
5	M3L	P	7	5	9,11,12	0.45	0	12,14,16	0.84	0
5	M3L	U	7	5	9,11,12	0.49	0	12,14,16	1.50	1 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	M3L	E	7	5	-	0/8/10/12	0/0/0/0
5	M3L	J	7	5	-	0/8/10/12	0/0/0/0
5	M3L	P	7	5	-	0/8/10/12	0/0/0/0
5	M3L	U	7	5	-	0/8/10/12	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	U	7	M3L	CM3-NZ-CM1	-3.36	100.27	108.96
5	E	7	M3L	CM3-NZ-CM1	-3.27	100.49	108.96
5	J	7	M3L	CM2-NZ-CM1	-3.25	100.56	108.96
5	E	7	M3L	CM2-NZ-CM1	2.00	114.14	108.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	7	M3L	1	0
5	J	7	M3L	2	0
5	U	7	M3L	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 32 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
7	SAH	A	1009	-	22,28,28	1.04	2 (9%)	18,40,40	2.87	5 (27%)
7	SAH	F	1009	-	22,28,28	1.12	2 (9%)	18,40,40	2.81	5 (27%)
7	SAH	K	1009	-	22,28,28	1.07	2 (9%)	18,40,40	3.03	4 (22%)
7	SAH	Q	1009	-	22,28,28	1.06	2 (9%)	18,40,40	2.79	4 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SAH	A	1009	-	-	0/7/31/31	0/3/3/3
7	SAH	F	1009	-	-	0/7/31/31	0/3/3/3
7	SAH	K	1009	-	-	0/7/31/31	0/3/3/3
7	SAH	Q	1009	-	-	0/7/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1009	SAH	C2-N1	2.10	1.38	1.33
7	Q	1009	SAH	C2-N1	2.15	1.38	1.33
7	K	1009	SAH	C2-N1	2.22	1.38	1.33
7	F	1009	SAH	C2-N1	2.67	1.39	1.33
7	A	1009	SAH	C2-N3	3.22	1.37	1.32
7	F	1009	SAH	C2-N3	3.23	1.37	1.32
7	Q	1009	SAH	C2-N3	3.32	1.38	1.32
7	K	1009	SAH	C2-N3	3.81	1.38	1.32

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1009	SAH	N3-C2-N1	-10.58	120.56	128.87
7	K	1009	SAH	N3-C2-N1	-10.57	120.57	128.87
7	Q	1009	SAH	N3-C2-N1	-9.53	121.38	128.87
7	F	1009	SAH	N3-C2-N1	-9.16	121.67	128.87
7	K	1009	SAH	C5'-SD-CG	-5.60	85.42	102.42
7	Q	1009	SAH	C5'-SD-CG	-5.08	86.98	102.42
7	F	1009	SAH	C5'-SD-CG	-4.95	87.40	102.42
7	F	1009	SAH	C2'-C1'-N9	-3.31	104.59	113.47
7	Q	1009	SAH	C2'-C1'-N9	-2.92	105.64	113.47
7	A	1009	SAH	C2'-C1'-N9	-2.74	106.13	113.47
7	A	1009	SAH	C5'-SD-CG	-2.53	94.73	102.42
7	A	1009	SAH	O2'-C2'-C1'	-2.44	103.97	111.61
7	K	1009	SAH	C2'-C1'-N9	-2.05	107.97	113.47
7	Q	1009	SAH	C4'-O4'-C1'	2.18	111.95	109.64
7	F	1009	SAH	N6-C6-N1	2.68	123.02	118.52
7	A	1009	SAH	C4'-O4'-C1'	2.87	112.69	109.64
7	F	1009	SAH	C4'-O4'-C1'	3.20	113.03	109.64
7	K	1009	SAH	C4'-O4'-C1'	3.37	113.22	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1009	SAH	6	0
7	F	1009	SAH	2	0
7	K	1009	SAH	1	0
7	Q	1009	SAH	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	581/746 (77%)	0.60	52 (8%) 12 6	40, 84, 159, 196	0
1	F	568/746 (76%)	0.67	58 (10%) 9 5	40, 92, 162, 224	0
1	K	562/746 (75%)	0.79	75 (13%) 4 2	43, 92, 165, 189	0
1	Q	565/746 (75%)	0.70	63 (11%) 7 4	45, 86, 165, 202	0
2	B	365/367 (99%)	0.40	11 (3%) 54 33	51, 79, 121, 171	0
2	G	365/367 (99%)	0.37	14 (3%) 44 26	49, 76, 115, 177	0
2	L	365/367 (99%)	0.29	4 (1%) 82 65	41, 65, 103, 140	0
2	R	365/367 (99%)	0.28	5 (1%) 78 59	35, 61, 92, 147	0
3	C	125/129 (96%)	0.47	5 (4%) 42 25	48, 72, 148, 172	0
3	H	124/129 (96%)	0.51	8 (6%) 22 12	58, 89, 143, 187	0
3	M	125/129 (96%)	0.74	11 (8%) 12 6	56, 92, 135, 158	0
3	S	125/129 (96%)	0.66	12 (9%) 10 5	54, 91, 139, 159	0
4	D	9/13 (69%)	0.16	0 100 100	67, 86, 111, 118	0
4	I	9/13 (69%)	0.16	0 100 100	62, 81, 103, 113	0
4	O	9/13 (69%)	1.70	2 (22%) 1 1	68, 76, 88, 93	9 (100%)
4	T	9/13 (69%)	1.72	2 (22%) 1 1	70, 73, 81, 94	9 (100%)
5	E	10/12 (83%)	0.34	1 (10%) 9 5	67, 89, 139, 140	0
5	J	9/12 (75%)	0.03	0 100 100	63, 82, 127, 133	0
5	P	8/12 (66%)	0.52	1 (12%) 5 2	69, 84, 117, 140	0
5	U	9/12 (75%)	0.87	0 100 100	71, 95, 133, 134	0
All	All	4307/5068 (84%)	0.56	324 (7%) 17 9	35, 79, 155, 224	18 (0%)

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	311	THR	13.6
1	Q	314	ALA	12.5
1	Q	235	GLY	11.8
1	F	74	VAL	10.5
1	F	75	SER	10.5
1	Q	430	VAL	10.5
1	A	330	GLY	9.6
1	F	73	SER	9.4
1	A	79	GLY	8.4
1	F	478	ALA	8.2
1	F	426	PRO	8.1
1	K	479	PRO	7.6
1	K	327	HIS	7.1
1	F	315	LEU	7.1
1	K	329	GLU	7.0
1	Q	310	ASN	7.0
1	F	424	ILE	6.9
1	K	314	ALA	6.9
1	A	249	GLU	6.9
3	C	583	SER	6.8
3	S	583	SER	6.7
1	K	312	GLU	6.7
1	K	313	THR	6.5
1	Q	429	ASN	6.5
3	S	582	ASP	6.5
1	A	75	SER	6.3
1	F	427	PRO	6.3
1	Q	329	GLU	6.2
1	A	327	HIS	6.2
1	K	477	ILE	6.1
1	Q	478	ALA	5.9
1	K	345	THR	5.6
1	K	73	SER	5.6
1	F	76	SER	5.5
1	F	78	ARG	5.5
1	Q	313	THR	5.5
1	K	424	ILE	5.4
1	A	423	ASN	5.2
1	K	310	ASN	5.2
1	Q	315	LEU	5.1
1	K	446	THR	5.1
1	F	475	SER	4.9
1	K	478	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	Q	477	ILE	4.8
2	G	393	VAL	4.8
1	A	214	PRO	4.8
1	Q	330	GLY	4.8
1	Q	734	LEU	4.7
1	A	74	VAL	4.7
1	A	15	TRP	4.6
1	A	239	GLU	4.5
1	K	10	LYS	4.4
3	S	685	GLN	4.4
1	Q	427	PRO	4.4
1	K	527	ARG	4.4
1	F	738	GLY	4.4
1	K	322	PRO	4.4
1	A	314	ALA	4.4
1	F	138	VAL	4.4
1	A	78	ARG	4.4
1	Q	141	GLN	4.2
1	Q	736	TYR	4.2
1	A	68	VAL	4.2
3	M	685	GLN	4.1
1	Q	325	TYR	4.1
1	Q	732	ASP	4.1
1	K	319	PRO	4.1
1	A	597	LYS	4.1
1	F	178	LEU	4.0
1	Q	426	PRO	4.0
2	G	124	TYR	3.9
4	O	30	PRO	3.9
1	F	79	GLY	3.9
1	Q	733	ALA	3.9
1	K	78	ARG	3.9
1	K	315	LEU	3.8
1	K	457	LEU	3.7
1	K	432	TRP	3.7
1	K	171	PHE	3.7
1	A	72	THR	3.7
1	F	736	TYR	3.7
1	F	12	PRO	3.7
1	F	595	ASP	3.7
1	F	739	ILE	3.7
2	B	188	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	313	THR	3.7
1	K	428	GLU	3.6
3	C	577	GLN	3.6
1	A	258	PRO	3.6
2	B	80	TYR	3.6
3	C	581	VAL	3.6
2	G	108	GLY	3.6
1	Q	345	THR	3.6
3	H	583	SER	3.6
1	F	330	GLY	3.6
1	A	247	LEU	3.6
3	C	561	HIS	3.6
1	K	301	ALA	3.6
1	F	329	GLU	3.6
1	A	76	SER	3.6
1	K	467	TYR	3.6
1	A	221	ASP	3.6
1	F	429	ASN	3.6
1	K	429	ASN	3.5
1	F	11	GLY	3.5
1	A	737	VAL	3.5
1	K	309	LYS	3.5
1	K	219	PRO	3.4
1	F	477	ILE	3.4
1	F	170	ILE	3.4
1	A	227	ILE	3.4
1	A	328	LEU	3.4
4	T	24	ALA	3.4
1	Q	243	LYS	3.3
1	A	331	ALA	3.3
1	F	18	ARG	3.3
1	Q	428	GLU	3.3
1	K	335	ALA	3.3
1	Q	311	THR	3.3
1	F	235	GLY	3.3
1	Q	464	ARG	3.3
1	Q	447	TYR	3.3
1	F	458	ILE	3.3
1	K	451	PHE	3.3
1	A	317	ASN	3.3
1	K	444	ILE	3.3
1	A	735	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	G	399	ALA	3.2
3	S	562	ASN	3.2
1	A	230	MET	3.2
1	Q	171	PHE	3.2
3	S	585	ASP	3.2
1	K	12	PRO	3.1
1	A	69	HIS	3.1
1	F	327	HIS	3.1
1	Q	737	VAL	3.1
2	B	162	LEU	3.1
1	Q	319	PRO	3.1
1	Q	440	PHE	3.1
1	K	341	GLU	3.1
1	Q	239	GLU	3.1
1	K	321	GLY	3.0
1	Q	134	MET	3.0
1	Q	232	PRO	3.0
1	F	142	ASP	3.0
1	Q	264	ILE	3.0
1	Q	467	TYR	3.0
1	A	34	ARG	3.0
1	F	345	THR	3.0
1	K	332	LYS	3.0
1	A	180	GLN	3.0
1	F	82	GLU	3.0
1	K	181	TYR	3.0
1	A	101	LEU	3.0
1	F	316	ASP	3.0
2	B	214	ALA	2.9
1	Q	425	GLU	2.9
1	A	141	GLN	2.9
1	K	305	THR	2.9
1	K	330	GLY	2.9
1	A	312	GLU	2.9
4	O	24	ALA	2.9
1	K	243	LYS	2.9
1	K	244	TYR	2.9
1	A	216	ARG	2.9
1	Q	527	ARG	2.9
3	C	582	ASP	2.9
1	Q	332	LYS	2.9
1	K	264	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	Q	137	GLU	2.9
1	A	248	THR	2.8
1	F	23	TYR	2.8
1	F	431	GLU	2.8
4	T	23	LYS	2.8
1	F	224	PHE	2.8
1	K	221	ASP	2.8
3	S	613	VAL	2.8
1	F	141	GLN	2.8
1	F	91	PHE	2.8
1	K	728	TYR	2.8
1	Q	312	GLU	2.8
1	F	72	THR	2.8
1	F	101	LEU	2.8
1	K	476	ILE	2.8
1	Q	27	ARG	2.7
2	G	284	LYS	2.7
1	K	333	GLU	2.7
1	K	323	GLN	2.7
1	K	317	ASN	2.7
1	F	71	LEU	2.7
3	M	582	ASP	2.7
1	F	181	TYR	2.7
1	K	223	ILE	2.7
1	F	430	VAL	2.7
1	K	278	LEU	2.7
1	Q	26	LEU	2.7
1	Q	466	VAL	2.7
1	K	175	VAL	2.7
1	A	329	GLU	2.7
2	G	398	LYS	2.7
1	K	325	TYR	2.7
3	H	652	LEU	2.7
1	Q	316	ASP	2.7
1	F	428	GLU	2.6
1	Q	278	LEU	2.6
1	Q	451	PHE	2.6
1	F	17	LYS	2.6
1	A	67	PRO	2.6
1	Q	731	ALA	2.6
2	G	287	ARG	2.6
1	K	247	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	H	653	CYS	2.6
1	Q	333	GLU	2.6
1	A	213	ARG	2.6
1	F	137	GLU	2.6
3	M	612	GLU	2.6
1	Q	223	ILE	2.6
1	A	240	LEU	2.6
1	Q	309	LYS	2.5
2	G	180	MET	2.5
1	K	138	VAL	2.5
1	A	181	TYR	2.5
3	M	583	SER	2.5
5	E	2	LEU	2.5
1	Q	76	SER	2.5
2	B	123	LEU	2.5
1	A	736	TYR	2.5
2	R	398	LYS	2.5
2	L	386	LEU	2.5
1	Q	260	CYS	2.5
2	L	396	PRO	2.4
3	H	581	VAL	2.4
1	K	229	SER	2.4
1	K	447	TYR	2.4
1	Q	32	PHE	2.4
1	A	235	GLY	2.4
1	F	179	GLY	2.4
1	K	526	PRO	2.4
1	K	265	ASP	2.4
1	K	246	GLU	2.4
1	K	431	GLU	2.4
1	Q	327	HIS	2.4
3	S	587	LYS	2.4
3	M	637	MET	2.4
3	M	684	MET	2.4
1	Q	321	GLY	2.3
1	Q	526	PRO	2.3
1	F	174	LEU	2.3
1	A	103	ALA	2.3
1	A	245	LYS	2.3
3	H	577	GLN	2.3
1	K	469	PHE	2.3
3	M	639	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	R	422	SER	2.3
3	S	581	VAL	2.3
5	P	11	SER	2.3
1	A	231	PHE	2.3
1	A	73	SER	2.3
1	A	479	PRO	2.3
1	K	445	GLY	2.3
1	F	716	ILE	2.2
1	K	228	SER	2.2
2	R	396	PRO	2.2
1	F	32	PHE	2.2
1	K	233	ASP	2.2
3	S	561	HIS	2.2
1	F	597	LYS	2.2
1	F	166	ILE	2.2
1	K	261	THR	2.2
2	R	397	HIS	2.2
1	Q	306	TYR	2.2
1	A	142	ASP	2.2
1	K	220	SER	2.2
3	M	603	PHE	2.2
1	Q	728	TYR	2.2
1	Q	140	ASP	2.2
1	A	169	GLU	2.2
3	M	586	GLU	2.2
1	Q	240	LEU	2.2
1	Q	72	THR	2.2
1	F	425	GLU	2.2
1	K	464	ARG	2.2
1	Q	225	GLU	2.2
3	S	602	GLU	2.2
2	B	419	SER	2.1
2	L	246	LEU	2.1
2	R	425	LEU	2.1
1	K	468	GLU	2.1
2	B	388	VAL	2.1
3	M	636	CYS	2.1
2	G	294	ILE	2.1
1	F	691	VAL	2.1
1	K	430	VAL	2.1
1	K	239	GLU	2.1
1	Q	224	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	356	PHE	2.1
2	L	123	LEU	2.1
3	H	681	LEU	2.1
3	H	588	ASP	2.1
1	K	245	LYS	2.1
1	K	72	THR	2.1
1	K	141	GLN	2.1
1	F	10	LYS	2.1
2	B	165	VAL	2.1
3	S	681	LEU	2.1
1	Q	431	GLU	2.1
2	G	282	PRO	2.1
3	M	580	GLU	2.1
2	B	96	LEU	2.1
1	K	180	GLN	2.1
1	F	180	GLN	2.0
1	F	222	LYS	2.0
2	G	425	LEU	2.0
1	K	137	GLU	2.0
2	G	186	TYR	2.0
1	A	172	VAL	2.0
2	B	353	LEU	2.0
1	A	236	THR	2.0
2	G	396	PRO	2.0
1	F	314	ALA	2.0
1	A	19	VAL	2.0
3	S	654	ARG	2.0
2	G	177	PRO	2.0
3	H	685	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	M3L	P	7	12/13	0.95	0.26	-	39,57,65,71	0
5	M3L	E	7	12/13	0.97	0.26	-	40,58,78,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	M3L	U	7	12/13	0.97	0.24	-	34,59,68,68	0
5	M3L	J	7	12/13	0.98	0.22	-	41,52,63,65	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	ZN	K	1004	1/1	0.98	0.19	2.68	70,70,70,70	0
6	ZN	F	1003	1/1	0.98	0.21	2.57	65,65,65,65	0
6	ZN	A	1004	1/1	0.98	0.24	2.32	63,63,63,63	0
6	ZN	Q	1007	1/1	0.99	0.22	2.29	54,54,54,54	0
6	ZN	K	1007	1/1	0.98	0.21	2.17	54,54,54,54	0
6	ZN	Q	1004	1/1	0.99	0.18	2.10	77,77,77,77	0
6	ZN	F	1004	1/1	0.99	0.21	1.68	65,65,65,65	0
6	ZN	Q	1003	1/1	0.98	0.18	1.42	69,69,69,69	0
6	ZN	Q	1008	1/1	0.99	0.21	1.34	50,50,50,50	0
6	ZN	F	1008	1/1	0.98	0.21	1.18	54,54,54,54	0
6	ZN	A	1008	1/1	0.99	0.21	1.16	58,58,58,58	0
6	ZN	F	1001	1/1	0.99	0.20	0.89	63,63,63,63	0
6	ZN	F	1007	1/1	0.99	0.21	0.81	54,54,54,54	0
6	ZN	A	1003	1/1	0.99	0.22	0.74	51,51,51,51	0
6	ZN	K	1006	1/1	0.98	0.21	0.74	63,63,63,63	0
6	ZN	K	1001	1/1	0.97	0.22	0.73	69,69,69,69	0
6	ZN	K	1003	1/1	0.98	0.17	0.57	66,66,66,66	0
6	ZN	A	1007	1/1	0.98	0.21	0.57	52,52,52,52	0
6	ZN	K	1008	1/1	0.98	0.21	0.44	59,59,59,59	0
6	ZN	F	1005	1/1	0.99	0.20	0.41	67,67,67,67	0
6	ZN	A	1005	1/1	0.99	0.21	0.38	56,56,56,56	0
6	ZN	Q	1006	1/1	0.98	0.22	0.38	66,66,66,66	0
6	ZN	Q	1005	1/1	0.99	0.19	0.20	72,72,72,72	0
6	ZN	F	1006	1/1	0.99	0.20	0.08	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	ZN	A	1006	1/1	0.99	0.20	0.07	58,58,58,58	0
6	ZN	Q	1001	1/1	0.99	0.21	0.04	60,60,60,60	0
6	ZN	K	1005	1/1	0.99	0.17	-0.00	74,74,74,74	0
6	ZN	A	1001	1/1	0.99	0.20	-0.08	54,54,54,54	0
7	SAH	Q	1009	26/26	0.88	0.21	-0.34	55,77,177,321	0
7	SAH	F	1009	26/26	0.92	0.20	-0.38	40,75,86,146	0
7	SAH	A	1009	26/26	0.94	0.21	-0.39	58,77,90,93	0
7	SAH	K	1009	26/26	0.89	0.21	-0.40	60,74,184,324	0
6	ZN	Q	1002	1/1	0.99	0.15	-0.55	128,128,128,128	0
6	ZN	F	1002	1/1	0.98	0.16	-0.94	110,110,110,110	0
6	ZN	A	1002	1/1	0.98	0.16	-1.13	64,64,64,64	0
6	ZN	K	1002	1/1	0.92	0.12	-1.33	122,122,122,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.