Full wwPDB X-ray Structure Validation Report

Jan 24, 2017 – 02:03 PM EST

PDB ID	:	5JXT
Title	:	Crystal structure of MtISWI bound with histone H4 tail
Authors	:	Chen, Z.; Yan, L.
Deposited on	:	2016-05-13
Resolution	:	3.01 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

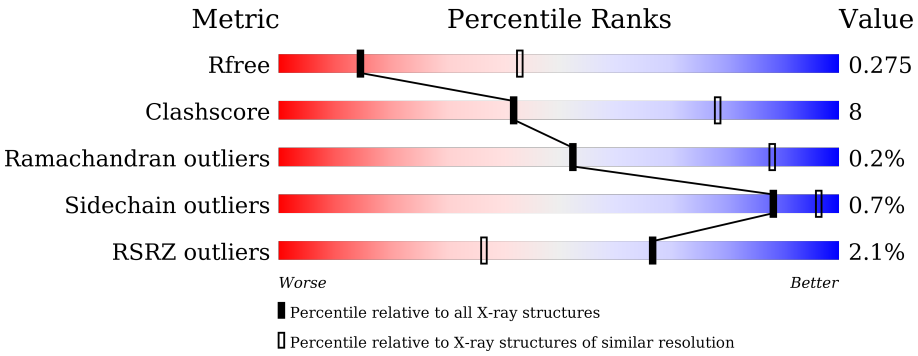
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.01 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 <=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	349	71% 21% 6%
1	B	349	3% 74% 20% 6%
1	C	349	71% 21% 7%
1	D	349	3% 64% 19% 16%
1	E	349	74% 16% 10%
1	F	349	5% 71% 22% 7%

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Mol	Chain	Length	Quality of chain
1	G	349	2% 72% 16% 12%
1	H	349	% 71% 21% 8%
1	I	349	% 70% 16% 14%
1	J	349	% 72% 18% 9%
1	K	349	% 68% 19% 12%
1	L	349	3% 68% 21% 11%
1	M	349	% 76% 16% 7%
1	N	349	% 75% 16% 9%
1	O	349	% 71% 21% 8%
1	P	349	4% 74% 17% 9%
2	Q	21	19% 5% 76%
2	R	21	19% 5% 76%
2	S	21	5% 19% 5% 76%
2	T	21	24% 76%
2	U	21	5% 19% 5% 76%
2	V	21	19% 5% 76%
2	W	21	5% 14% 5% 81%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40399 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 Chromatin-remodeling complex ATPase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	328	Total	C	N	O	S	0	0	0
			2599	1636	454	497	12			
1	E	313	Total	C	N	O	S	0	0	0
			2484	1566	437	469	12			
1	F	324	Total	C	N	O	S	0	0	0
			2578	1623	450	493	12			
1	G	308	Total	C	N	O	S	0	0	0
			2439	1536	430	461	12			
1	J	317	Total	C	N	O	S	0	0	0
			2515	1583	439	481	12			
1	N	319	Total	C	N	O	S	0	0	0
			2536	1596	442	486	12			
1	O	322	Total	C	N	O	S	0	0	0
			2563	1613	447	491	12			
1	P	316	Total	C	N	O	S	0	0	0
			2517	1585	439	481	12			
1	C	324	Total	C	N	O	S	0	0	0
			2574	1623	446	493	12			
1	H	321	Total	C	N	O	S	0	0	0
			2549	1602	446	489	12			
1	K	306	Total	C	N	O	S	0	0	0
			2427	1529	426	460	12			
1	L	311	Total	C	N	O	S	0	0	0
			2464	1551	434	467	12			
1	A	327	Total	C	N	O	S	0	0	0
			2597	1636	453	496	12			
1	I	301	Total	C	N	O	S	0	0	0
			2388	1506	420	450	12			
1	D	292	Total	C	N	O	S	0	0	0
			2326	1467	411	437	11			
1	M	324	Total	C	N	O	S	0	0	0
			2574	1622	448	492	12			

- Molecule 2 is a protein called Histone H4.

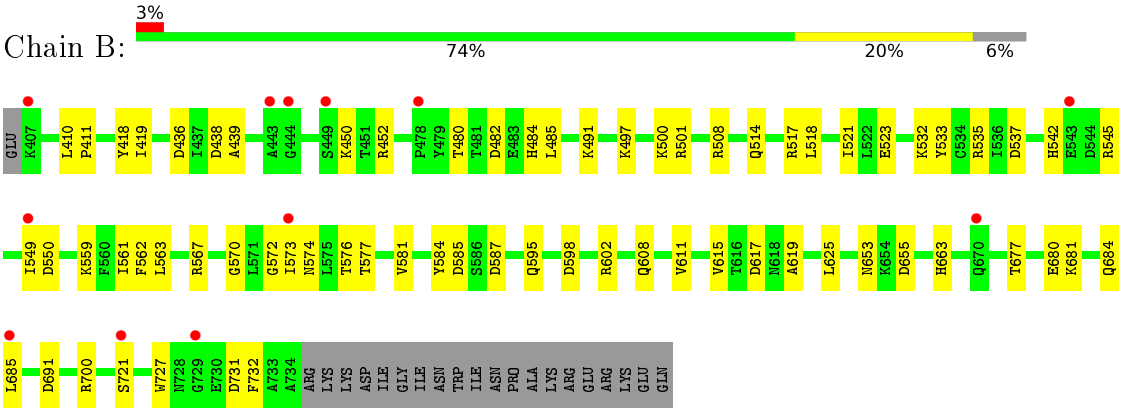
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	R	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	S	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	U	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	Q	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	T	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	V	5	Total	C	N	O	0	0	0
			39	23	11	5			
2	W	4	Total	C	N	O	0	0	0
			35	21	10	4			

3 Residue-property plots (i)

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

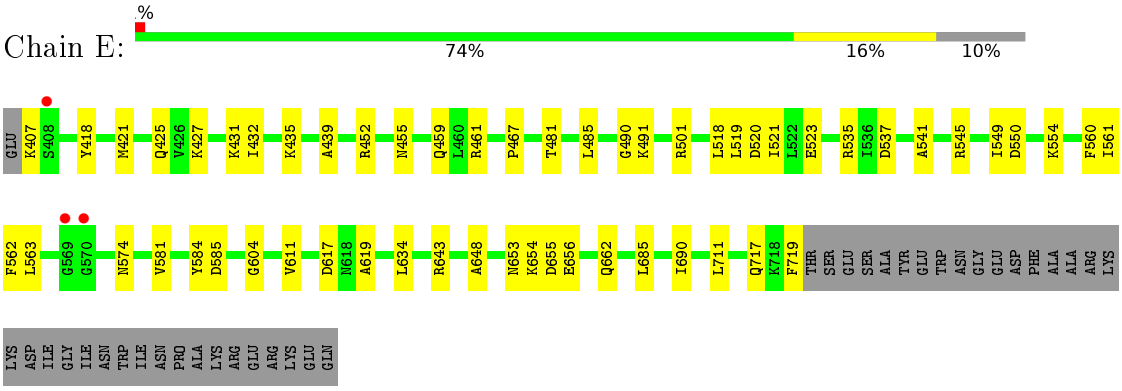
- Molecule 1: Chromatin-remodeling complex ATPase-like protein

Chain B:



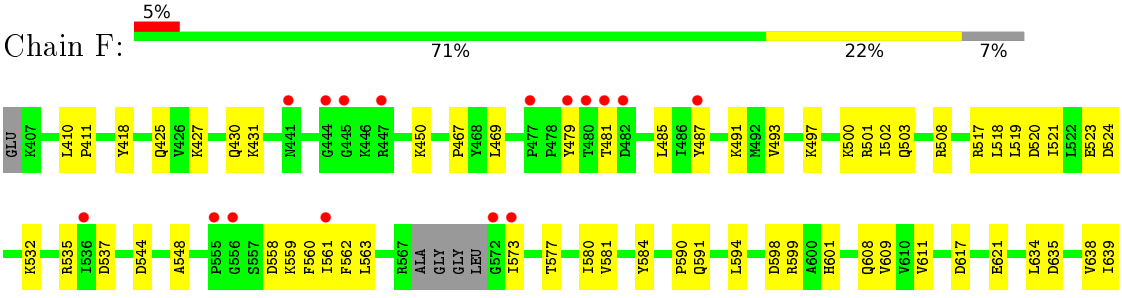
- Molecule 1: Chromatin-remodeling complex ATPase-like protein

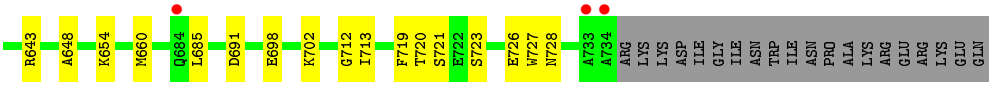
Chain E:



- Molecule 1: Chromatin-remodeling complex ATPase-like protein

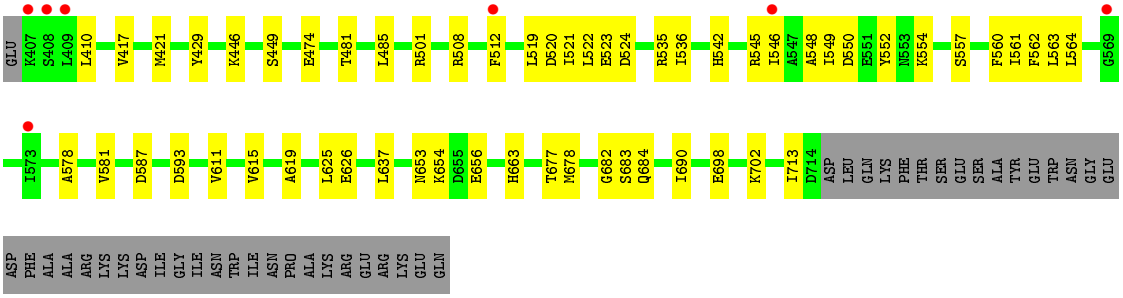
Chain F:





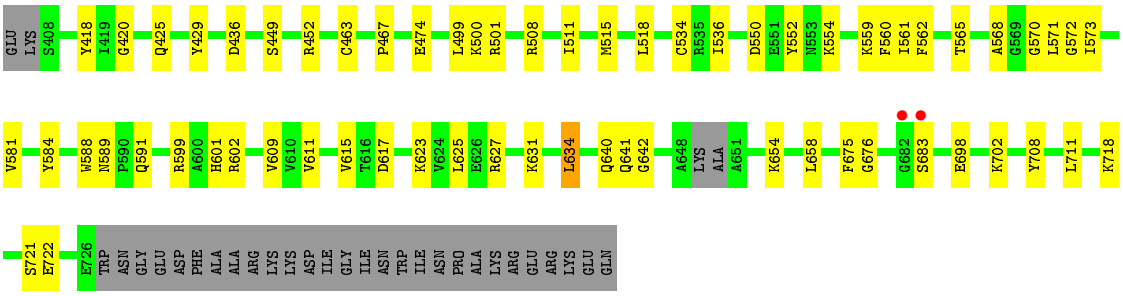
• Molecule 1: Chromatin-remodeling complex ATPase-like protein

Chain G:



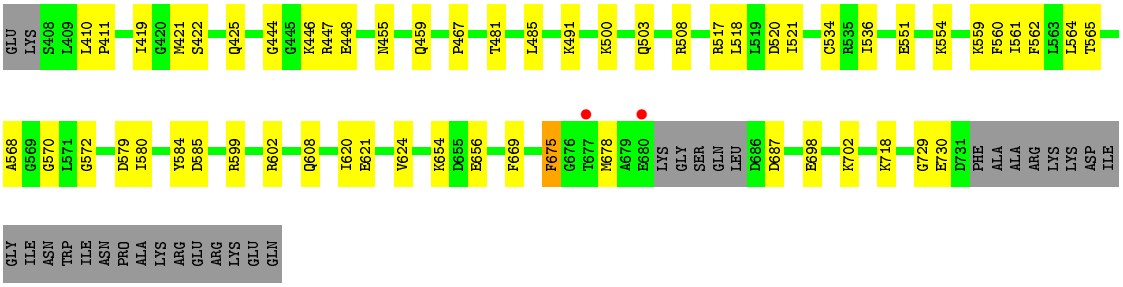
• Molecule 1: Chromatin-remodeling complex ATPase-like protein

Chain J:



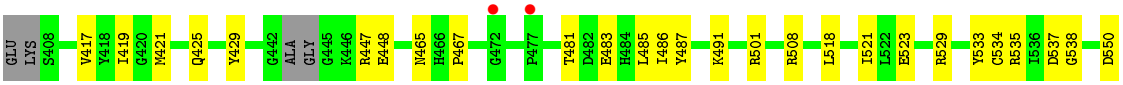
• Molecule 1: Chromatin-remodeling complex ATPase-like protein

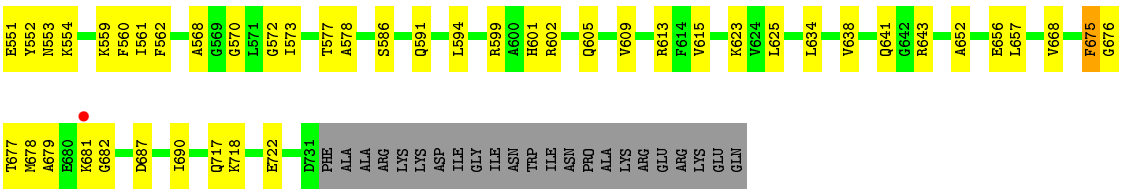
Chain N:



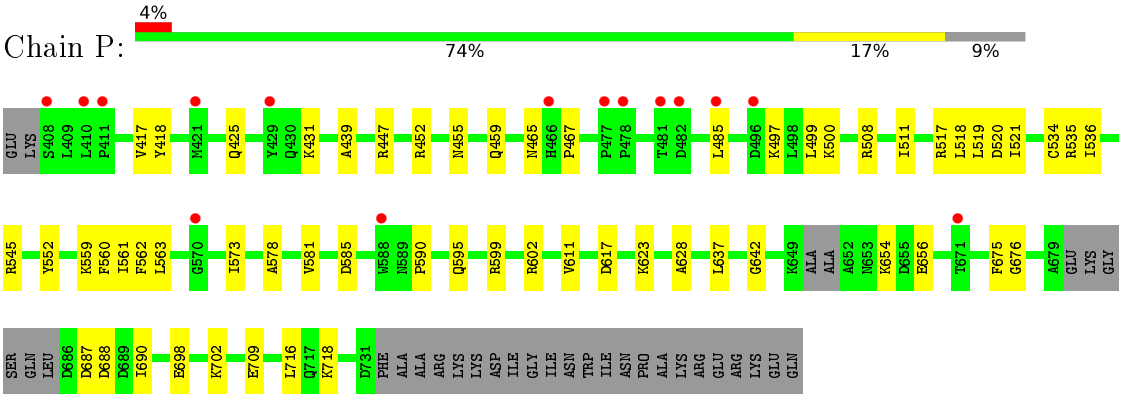
• Molecule 1: Chromatin-remodeling complex ATPase-like protein

Chain O:

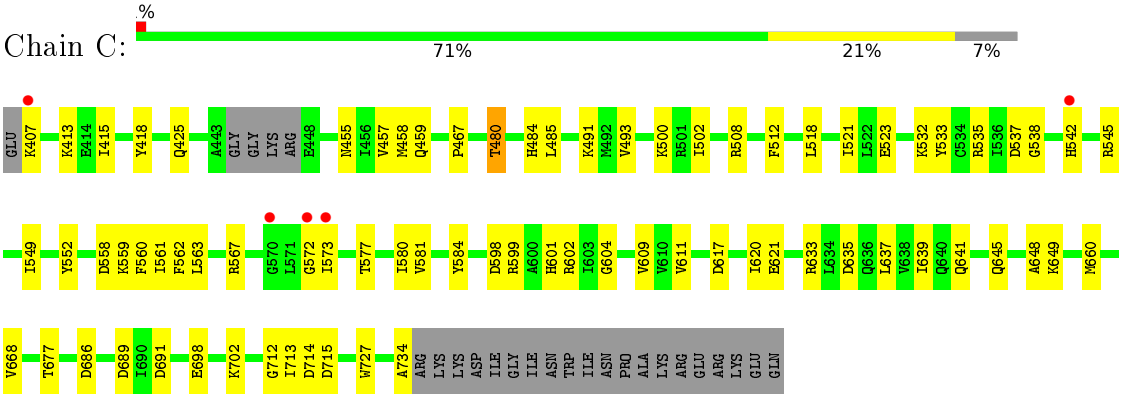




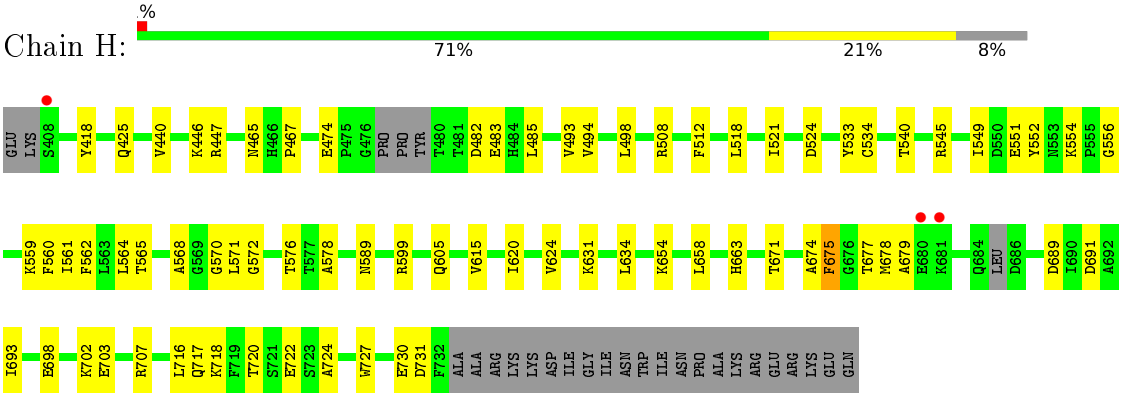
• Molecule 1: Chromatin-remodeling complex ATPase-like protein



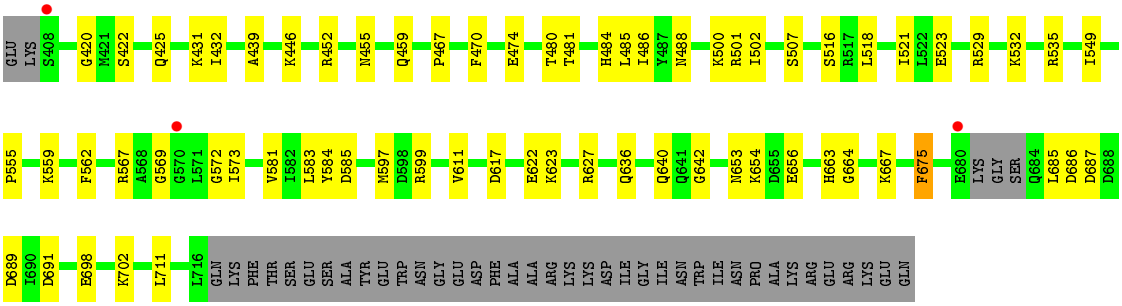
• Molecule 1: Chromatin-remodeling complex ATPase-like protein



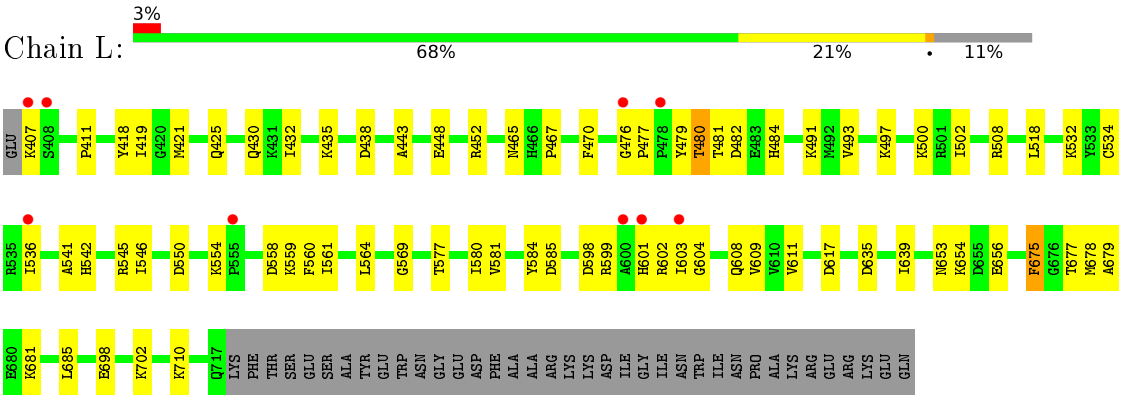
• Molecule 1: Chromatin-remodeling complex ATPase-like protein



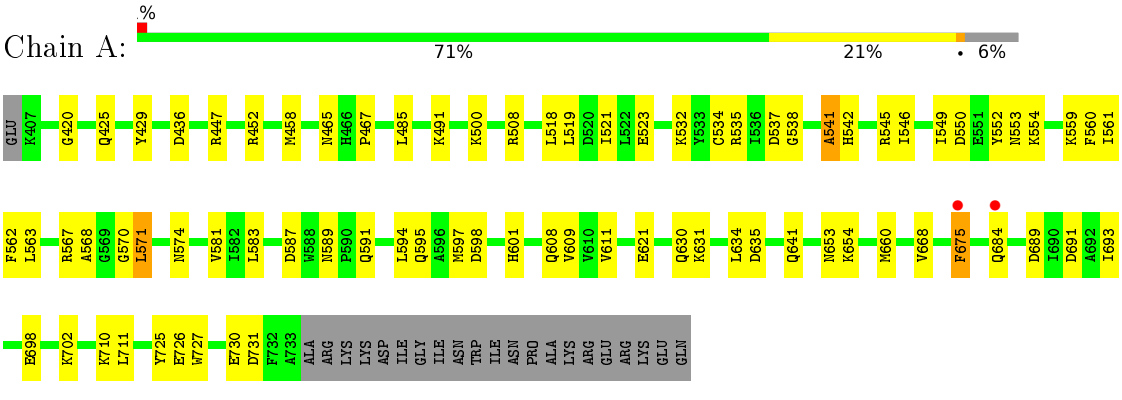
• Molecule 1: Chromatin-remodeling complex ATPase-like protein



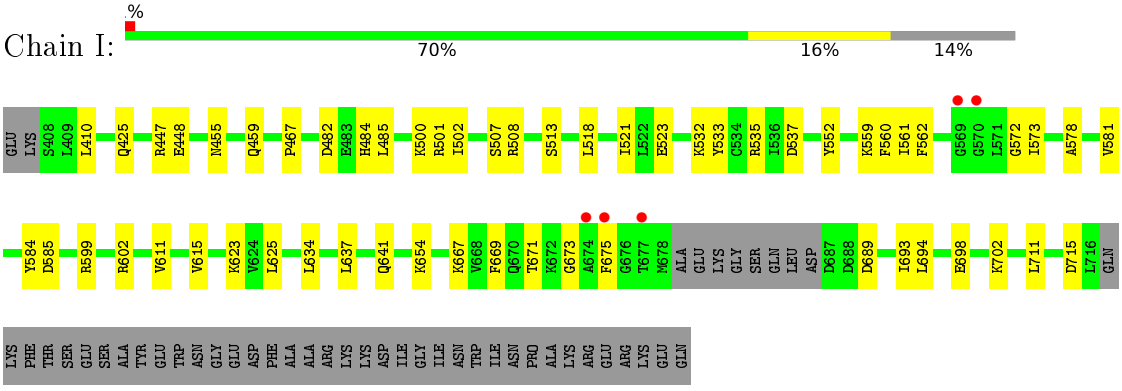
• Molecule 1: Chromatin-remodeling complex ATPase-like protein



• Molecule 1: Chromatin-remodeling complex ATPase-like protein

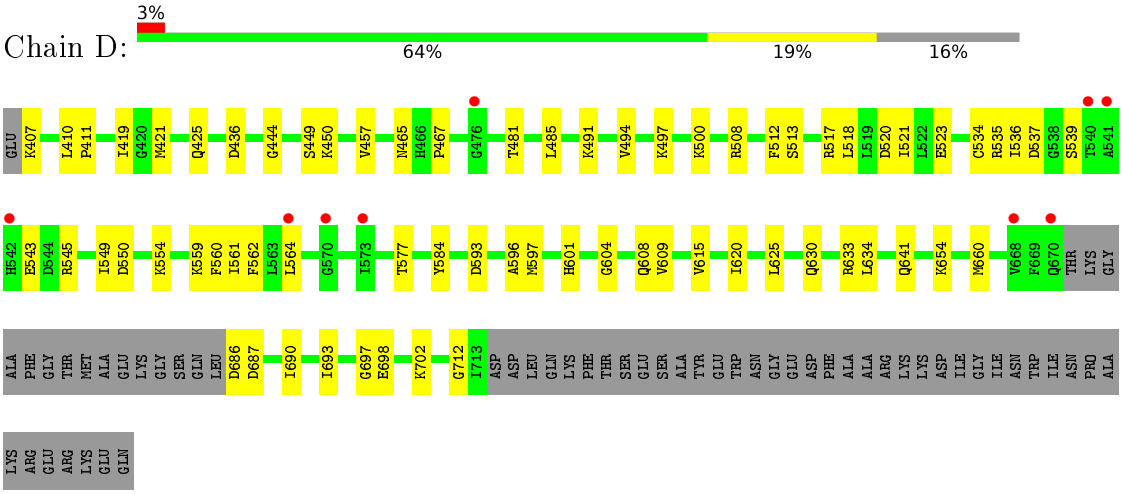


• Molecule 1: Chromatin-remodeling complex ATPase-like protein



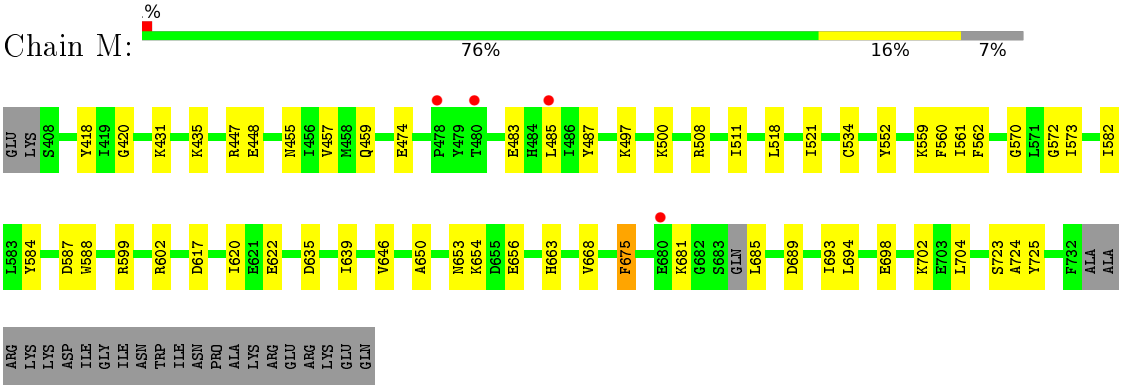
• Molecule 1: Chromatin-remodeling complex ATPase-like protein

Chain D:



• Molecule 1: Chromatin-remodeling complex ATPase-like protein

Chain M:



• Molecule 2: Histone H4

Chain R:

• Molecule 2: Histone H4

Chain S:

• Molecule 2: Histone H4

Chain U:

• Molecule 2: Histone H4

Chain Q:

- Molecule 2: Histone H4

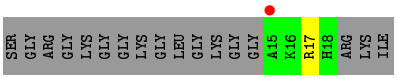
Chain T:

- Molecule 2: Histone H4

Chain V:

- Molecule 2: Histone H4

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	102.24Å 119.32Å 132.50Å 89.59° 105.96° 93.08°	Depositor
Resolution (Å)	42.00 – 3.01 45.37 – 3.01	Depositor EDS
% Data completeness (in resolution range)	94.2 (42.00-3.01) 94.3 (45.37-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.218 , 0.276 0.217 , 0.275	Depositor DCC
R_{free} test set	5659 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	71.6	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	40399	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.26	0/2637	0.48	1/3549 (0.0%)
1	B	0.26	0/2639	0.43	0/3552
1	C	0.25	0/2613	0.44	0/3518
1	D	0.27	0/2359	0.48	1/3174 (0.0%)
1	E	0.25	0/2520	0.44	0/3389
1	F	0.25	0/2617	0.42	0/3521
1	G	0.25	0/2474	0.43	0/3328
1	H	0.26	0/2584	0.42	0/3472
1	I	0.24	0/2422	0.39	0/3259
1	J	0.24	0/2551	0.39	0/3432
1	K	0.24	0/2461	0.40	0/3312
1	L	0.25	0/2499	0.45	0/3362
1	M	0.24	0/2613	0.40	0/3516
1	N	0.24	0/2574	0.40	0/3465
1	O	0.24	0/2601	0.40	0/3500
1	P	0.23	0/2554	0.39	0/3436
2	Q	0.21	0/39	0.46	0/49
2	R	0.21	0/39	0.32	0/49
2	S	0.21	0/39	0.40	0/49
2	T	0.20	0/39	0.48	0/49
2	U	0.22	0/39	0.40	0/49
2	V	0.22	0/39	0.47	0/49
2	W	0.17	0/35	0.36	0/44
All	All	0.25	0/40987	0.42	2/55123 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	571	LEU	CA-CB-CG	-5.89	101.75	115.30
1	D	436	ASP	CB-CG-OD2	5.30	123.07	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	570	GLY	Peptide
1	H	675	PHE	Peptide
1	O	681	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2597	0	2607	66	0
1	B	2599	0	2603	55	0
1	C	2574	0	2579	54	0
1	D	2326	0	2364	49	0
1	E	2484	0	2521	45	0
1	F	2578	0	2580	61	0
1	G	2439	0	2476	54	0
1	H	2549	0	2553	57	0
1	I	2388	0	2422	40	0
1	J	2515	0	2532	44	0
1	K	2427	0	2456	54	0
1	L	2464	0	2499	54	0
1	M	2574	0	2580	42	0
1	N	2536	0	2539	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2563	0	2571	56	0
1	P	2517	0	2522	43	0
2	Q	39	0	40	4	0
2	R	39	0	40	2	0
2	S	39	0	40	1	0
2	T	39	0	40	0	0
2	U	39	0	40	1	0
2	V	39	0	40	1	0
2	W	35	0	37	4	0
All	All	40399	0	40681	684	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (684) 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:F:532:LYS:NZ	1:F:558:ASP:OD2	1.84	1.10
1:D:481:THR:HG22	1:M:447:ARG:HH12	1.19	1.04
1:M:681:LYS:NZ	1:M:689:ASP:OD2	1.91	1.03
1:N:481:THR:HG22	2:R:17:ARG:HH12	1.21	1.02
1:E:523:GLU:OE1	1:E:535:ARG:NH1	1.92	1.02
1:A:508:ARG:NH1	1:A:559:LYS:O	1.93	1.00
1:E:654:LYS:NZ	1:H:446:LYS:O	1.98	0.97
1:B:567:ARG:NH1	1:B:587:ASP:OD2	2.00	0.95
1:A:538:GLY:HA2	1:A:545:ARG:HH11	1.29	0.93
1:E:461:ARG:HH12	1:E:585:ASP:HB2	1.31	0.93
1:B:501:ARG:NH1	1:K:691:ASP:OD1	2.02	0.92
1:E:481:THR:HG22	1:N:447:ARG:HH12	1.33	0.91
1:J:570:GLY:O	1:J:599:ARG:NH1	2.06	0.88
1:C:535:ARG:NH2	1:C:537:ASP:OD2	2.06	0.87
1:B:598:ASP:OD2	1:B:727:TRP:HB2	1.75	0.87
1:F:481:THR:HG22	1:O:447:ARG:HH12	1.38	0.86
1:O:551:GLU:OE2	1:O:554:LYS:NZ	2.11	0.84
1:M:681:LYS:HD3	1:M:685:LEU:HD11	1.59	0.83
1:B:691:ASP:OD1	1:K:501:ARG:NH1	2.11	0.82
1:G:481:THR:HG22	1:P:447:ARG:HH12	1.44	0.81
1:D:497:LYS:NZ	1:D:500:LYS:HD2	1.96	0.81
1:E:432:ILE:HA	1:E:435:LYS:HE2	1.63	0.80
1:H:718:LYS:NZ	1:H:722:GLU:OE1	2.12	0.80
1:D:523:GLU:OE1	1:D:535:ARG:NH1	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:572:GLY:HA2	1:N:602:ARG:HH12	1.47	0.78
1:G:523:GLU:OE1	1:G:535:ARG:NH1	2.15	0.78
1:H:474:GLU:OE2	2:W:17:ARG:NH1	2.15	0.77
1:I:671:THR:HG22	1:I:673:GLY:H	1.50	0.77
1:A:538:GLY:HA2	1:A:545:ARG:NH1	2.00	0.76
1:B:535:ARG:NE	1:B:537:ASP:OD1	2.18	0.75
1:H:551:GLU:OE2	1:H:554:LYS:NZ	2.14	0.74
1:G:481:THR:HG22	1:P:447:ARG:NH1	2.01	0.74
1:A:542:HIS:CE1	1:A:546:ILE:HD11	2.23	0.74
1:L:681:LYS:HD2	1:L:685:LEU:HD23	1.69	0.73
1:B:523:GLU:OE1	1:B:535:ARG:NH1	2.19	0.73
1:O:538:GLY:HA3	1:O:568:ALA:HB1	1.70	0.73
1:H:570:GLY:O	1:H:599:ARG:NH1	2.20	0.73
1:J:425:GLN:HG2	1:J:467:PRO:HG3	1.70	0.73
1:O:675:PHE:O	1:O:679:ALA:N	2.19	0.73
1:L:480:THR:O	1:L:484:HIS:NE2	2.18	0.73
1:A:598:ASP:OD2	1:A:727:TRP:HB2	1.90	0.72
1:A:571:LEU:HD12	1:A:595:GLN:HE21	1.55	0.71
1:D:497:LYS:HZ2	1:D:500:LYS:HD2	1.55	0.71
1:N:446:LYS:O	1:L:654:LYS:NZ	2.23	0.70
1:G:562:PHE:CE2	1:G:564:LEU:HD21	2.26	0.70
1:A:535:ARG:NE	1:A:537:ASP:OD1	2.24	0.70
1:E:427:LYS:HE2	1:E:431:LYS:NZ	2.07	0.70
1:F:712:GLY:HA2	1:I:637:LEU:HD21	1.74	0.69
1:O:508:ARG:NH2	1:O:552:TYR:O	2.21	0.69
1:F:591:GLN:NE2	1:F:726:GLU:O	2.26	0.69
1:F:598:ASP:OD2	1:F:727:TRP:HB2	1.93	0.68
1:C:598:ASP:OD2	1:C:727:TRP:HB2	1.93	0.68
1:F:481:THR:HG22	1:O:447:ARG:NH1	2.09	0.68
1:K:481:THR:CG2	2:Q:17:ARG:HH12	2.07	0.67
1:P:675:PHE:HB3	1:D:421:MET:H	1.59	0.67
1:H:465:ASN:HB3	1:H:518:LEU:HD13	1.75	0.67
1:K:572:GLY:H	1:K:599:ARG:HH12	1.42	0.67
1:D:485:LEU:HD11	1:D:521:ILE:HG23	1.76	0.66
1:B:485:LEU:HD11	1:B:521:ILE:HG23	1.77	0.66
1:F:523:GLU:OE1	1:F:535:ARG:NH1	2.27	0.66
1:B:418:TYR:HB3	1:B:617:ASP:HB2	1.78	0.66
1:M:508:ARG:NH2	1:M:552:TYR:O	2.20	0.66
1:B:439:ALA:HB2	1:B:452:ARG:NH1	2.11	0.65
1:E:501:ARG:NH1	1:H:691:ASP:OD1	2.30	0.65
1:O:465:ASN:HB3	1:O:518:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:698:GLU:HG2	1:P:702:LYS:HE3	1.78	0.64
1:H:698:GLU:HG2	1:H:702:LYS:HE3	1.78	0.64
1:K:686:ASP:N	1:K:689:ASP:OD2	2.30	0.64
1:L:438:ASP:OD2	1:L:452:ARG:NH2	2.30	0.64
1:B:615:VAL:HG21	1:B:625:LEU:HD22	1.80	0.64
1:H:524:ASP:OD2	2:W:17:ARG:HG3	1.97	0.64
1:K:523:GLU:OE1	1:K:535:ARG:NH1	2.31	0.64
1:F:524:ASP:OD2	1:O:447:ARG:HG3	1.98	0.63
1:I:572:GLY:H	1:I:599:ARG:HH12	1.46	0.63
1:F:508:ARG:NH2	1:F:577:THR:OG1	2.32	0.63
1:N:481:THR:HG22	2:R:17:ARG:NH1	2.04	0.63
1:A:550:ASP:HB3	1:A:554:LYS:HE3	1.81	0.63
1:B:574:ASN:OD1	1:B:576:THR:HG23	1.99	0.63
1:N:698:GLU:HG2	1:N:702:LYS:HE3	1.80	0.63
1:A:508:ARG:NH2	1:A:552:TYR:O	2.30	0.62
1:B:572:GLY:HA2	1:B:602:ARG:HH12	1.64	0.62
1:G:474:GLU:OE1	1:P:447:ARG:NH2	2.33	0.62
1:G:536:ILE:HD11	1:G:548:ALA:HB3	1.81	0.62
1:G:653:ASN:OD1	1:G:654:LYS:N	2.33	0.62
1:C:485:LEU:HD11	1:C:521:ILE:HG23	1.82	0.62
1:L:432:ILE:HA	1:L:435:LYS:HE3	1.82	0.62
1:B:542:HIS:HA	1:B:545:ARG:HB2	1.81	0.61
1:J:722:GLU:OE1	1:H:589:ASN:ND2	2.32	0.61
1:F:532:LYS:HB3	1:F:559:LYS:HD3	1.82	0.61
1:C:572:GLY:HA2	1:C:602:ARG:HH12	1.63	0.61
1:H:508:ARG:NH2	1:H:552:TYR:O	2.26	0.61
1:K:572:GLY:H	1:K:599:ARG:NH1	1.98	0.61
1:N:551:GLU:OE2	1:N:554:LYS:NZ	2.32	0.61
1:B:581:VAL:HB	1:B:611:VAL:HG22	1.83	0.61
1:A:591:GLN:NE2	1:A:726:GLU:O	2.26	0.61
1:L:536:ILE:HB	1:L:564:LEU:HD23	1.82	0.61
1:B:411:PRO:O	1:B:608:GLN:NE2	2.26	0.60
1:N:508:ARG:NH1	1:N:559:LYS:O	2.33	0.60
1:F:501:ARG:HH12	1:I:694:LEU:HD12	1.65	0.60
1:B:532:LYS:HB3	1:B:559:LYS:HD3	1.84	0.60
1:I:535:ARG:NE	1:I:537:ASP:OD1	2.31	0.60
1:A:485:LEU:HD11	1:A:521:ILE:HG23	1.83	0.60
1:G:550:ASP:O	1:G:554:LYS:HG3	2.02	0.60
1:O:487:TYR:HE1	1:A:684:GLN:HB2	1.66	0.60
1:G:690:ILE:HG13	1:M:497:LYS:HG2	1.82	0.60
1:N:421:MET:H	1:L:675:PHE:HB3	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:GLY:HA3	1:A:568:ALA:HB1	1.84	0.59
1:P:573:ILE:O	1:P:602:ARG:NH1	2.35	0.59
1:A:571:LEU:HD13	1:A:595:GLN:HG2	1.83	0.59
1:K:481:THR:HG22	2:Q:17:ARG:HH12	1.66	0.59
1:A:436:ASP:OD2	1:A:452:ARG:NE	2.36	0.59
1:F:450:LYS:HB3	1:I:654:LYS:HG2	1.84	0.59
1:N:675:PHE:HB2	1:L:421:MET:H	1.67	0.59
1:O:535:ARG:NE	1:O:537:ASP:OD1	2.31	0.59
1:I:425:GLN:HG2	1:I:467:PRO:HG3	1.85	0.59
1:E:490:GLY:HA2	1:H:678:MET:SD	2.42	0.59
1:L:675:PHE:O	1:L:679:ALA:N	2.32	0.59
1:E:535:ARG:NE	1:E:537:ASP:OD1	2.36	0.59
1:G:449:SER:HB2	1:M:654:LYS:NZ	2.18	0.58
1:K:581:VAL:HB	1:K:611:VAL:HG22	1.85	0.58
1:K:653:ASN:OD1	1:K:654:LYS:N	2.37	0.58
1:P:656:GLU:OE2	1:P:718:LYS:HE3	2.03	0.58
1:E:685:LEU:HD11	1:H:494:VAL:HA	1.84	0.58
1:N:729:GLY:H	1:K:567:ARG:HH21	1.50	0.58
1:O:578:ALA:O	1:O:605:GLN:NE2	2.35	0.58
1:E:481:THR:HG22	1:N:447:ARG:NH1	2.12	0.58
1:J:698:GLU:HG2	1:J:702:LYS:HE3	1.85	0.58
1:C:413:LYS:HE2	1:C:415:ILE:HD11	1.85	0.58
1:C:698:GLU:HG2	1:C:702:LYS:HE3	1.85	0.58
1:H:485:LEU:HD11	1:H:521:ILE:HG23	1.84	0.58
1:J:425:GLN:NE2	1:J:463:CYS:O	2.37	0.58
1:C:458:MET:HE1	1:L:448:GLU:HA	1.86	0.58
1:K:480:THR:O	1:K:484:HIS:NE2	2.30	0.58
1:E:427:LYS:HE2	1:E:431:LYS:HZ3	1.67	0.58
1:F:719:PHE:HD1	1:A:541:ALA:HA	1.69	0.58
1:K:572:GLY:N	1:K:599:ARG:HH12	2.02	0.58
1:L:482:ASP:HB2	1:L:484:HIS:HD2	1.69	0.58
1:K:685:LEU:HB3	1:K:689:ASP:OD2	2.04	0.58
1:N:425:GLN:HG2	1:N:467:PRO:HG3	1.86	0.58
1:B:497:LYS:HE2	1:K:687:ASP:HB3	1.86	0.57
1:L:518:LEU:HD11	1:L:584:TYR:CE1	2.39	0.57
1:P:465:ASN:HB3	1:P:518:LEU:HD13	1.85	0.57
1:P:687:ASP:O	1:P:690:ILE:HG22	2.04	0.57
1:D:518:LEU:HD21	1:D:584:TYR:CD1	2.38	0.57
1:O:687:ASP:HA	1:O:690:ILE:HG22	1.85	0.57
1:F:591:GLN:HG2	1:F:728:ASN:HB2	1.85	0.57
1:N:570:GLY:O	1:N:599:ARG:NH2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:698:GLU:HG2	1:K:702:LYS:HE3	1.87	0.57
1:H:534:CYS:HB2	1:H:562:PHE:CD1	2.39	0.57
1:J:436:ASP:OD1	1:J:452:ARG:NH2	2.38	0.57
1:D:534:CYS:HB2	1:D:562:PHE:CD1	2.40	0.56
1:I:523:GLU:OE2	1:I:533:TYR:OH	2.12	0.56
1:L:508:ARG:NH2	1:L:577:THR:OG1	2.37	0.56
1:G:536:ILE:HB	1:G:564:LEU:HD22	1.86	0.56
1:B:438:ASP:HB2	1:B:452:ARG:HH22	1.70	0.56
1:F:501:ARG:NH1	1:I:694:LEU:HD12	2.20	0.56
1:F:485:LEU:HD11	1:F:521:ILE:HG23	1.87	0.56
1:I:581:VAL:HB	1:I:611:VAL:HG22	1.88	0.56
1:K:664:GLY:HA2	1:K:667:LYS:HE2	1.87	0.56
1:P:623:LYS:HG2	1:D:660:MET:HA	1.87	0.56
1:F:427:LYS:HE2	1:F:431:LYS:NZ	2.21	0.56
1:F:427:LYS:HE2	1:F:431:LYS:HZ3	1.71	0.56
1:N:565:THR:OG1	1:N:568:ALA:HB2	2.05	0.55
1:B:721:SER:HB3	1:C:542:HIS:CE1	2.41	0.55
1:A:581:VAL:HB	1:A:611:VAL:HG22	1.88	0.55
1:L:550:ASP:O	1:L:554:LYS:HG3	2.07	0.55
1:P:439:ALA:HB2	1:P:452:ARG:HE	1.71	0.55
1:G:615:VAL:HG21	1:G:625:LEU:HD22	1.88	0.55
1:G:663:HIS:HE1	1:M:622:GLU:OE2	1.89	0.55
1:H:534:CYS:SG	1:H:559:LYS:HG3	2.47	0.55
1:A:436:ASP:OD2	1:A:452:ARG:NH2	2.38	0.55
1:C:538:GLY:HA2	1:C:545:ARG:NH1	2.21	0.55
1:D:411:PRO:O	1:D:608:GLN:NE2	2.35	0.55
1:H:576:THR:O	1:H:605:GLN:NE2	2.39	0.55
1:D:444:GLY:C	1:D:449:SER:HB2	2.26	0.55
1:G:542:HIS:CE1	1:G:546:ILE:HD11	2.41	0.55
1:N:517:ARG:HA	1:N:520:ASP:OD2	2.07	0.55
1:F:418:TYR:HB3	1:F:617:ASP:HB2	1.89	0.55
1:G:519:LEU:HD22	1:G:563:LEU:HB3	1.89	0.55
1:C:645:GLN:HG3	1:H:720:THR:HG21	1.88	0.55
1:C:523:GLU:OE1	1:C:535:ARG:NH1	2.36	0.55
1:F:535:ARG:NE	1:F:537:ASP:OD1	2.27	0.54
1:G:677:THR:HB	1:M:420:GLY:H	1.72	0.54
1:E:550:ASP:O	1:E:554:LYS:HG3	2.08	0.54
1:H:565:THR:OG1	1:H:568:ALA:HB2	2.08	0.54
1:O:501:ARG:NH1	1:A:691:ASP:OD1	2.41	0.54
1:P:687:ASP:HB3	1:D:497:LYS:HE2	1.90	0.54
1:O:421:MET:H	1:A:675:PHE:HB3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:536:ILE:HD12	1:G:545:ARG:HA	1.89	0.54
1:A:552:TYR:HD1	1:A:559:LYS:HB2	1.72	0.54
1:C:545:ARG:O	1:C:549:ILE:HG12	2.07	0.54
1:C:538:GLY:HA2	1:C:545:ARG:HH11	1.73	0.54
1:E:461:ARG:NH1	1:E:585:ASP:HB2	2.12	0.54
1:G:698:GLU:HG2	1:G:702:LYS:HE3	1.90	0.54
1:L:698:GLU:HG2	1:L:702:LYS:HE3	1.89	0.54
1:N:421:MET:HB3	1:N:425:GLN:HB2	1.89	0.54
1:A:553:ASN:ND2	1:A:574:ASN:O	2.40	0.53
1:C:508:ARG:NH2	1:C:552:TYR:O	2.30	0.53
1:C:518:LEU:HD11	1:C:584:TYR:CE1	2.43	0.53
1:E:653:ASN:OD1	1:E:656:GLU:HB2	2.08	0.53
1:O:623:LYS:HG2	1:A:660:MET:HA	1.91	0.53
1:L:542:HIS:CE1	1:L:546:ILE:HD11	2.43	0.53
1:O:485:LEU:HD11	1:O:521:ILE:HG23	1.91	0.53
1:P:709:GLU:HA	1:D:633:ARG:HD3	1.89	0.53
1:A:567:ARG:NE	1:A:587:ASP:OD2	2.42	0.53
1:O:417:VAL:HG23	1:A:693:ILE:HG22	1.91	0.53
1:H:425:GLN:HG2	1:H:467:PRO:HG3	1.90	0.53
1:M:483:GLU:HB3	1:M:487:TYR:CE2	2.44	0.53
1:M:572:GLY:C	1:M:602:ARG:HH12	2.12	0.53
1:O:487:TYR:CE1	1:A:684:GLN:HB2	2.44	0.53
1:H:474:GLU:CD	2:W:17:ARG:HH12	2.11	0.53
1:D:550:ASP:O	1:D:554:LYS:HG3	2.08	0.53
1:J:508:ARG:NH2	1:J:552:TYR:O	2.34	0.53
1:B:450:LYS:HD2	1:K:654:LYS:HE2	1.91	0.53
1:M:431:LYS:HG2	1:M:435:LYS:HE3	1.90	0.53
1:G:521:ILE:HA	1:P:447:ARG:HG2	1.91	0.53
1:J:615:VAL:HG21	1:J:625:LEU:HD22	1.91	0.53
1:K:572:GLY:CA	1:K:599:ARG:HH12	2.22	0.53
1:N:654:LYS:NZ	1:L:443:ALA:HB1	2.24	0.53
1:N:485:LEU:HD11	1:N:521:ILE:HG23	1.90	0.53
1:O:570:GLY:O	1:O:599:ARG:NH2	2.42	0.53
1:I:615:VAL:HG21	1:I:625:LEU:HD22	1.90	0.52
1:B:700:ARG:NH1	1:K:617:ASP:OD2	2.32	0.52
1:P:418:TYR:HB3	1:P:617:ASP:HB2	1.92	0.52
1:G:563:LEU:O	1:G:564:LEU:HD23	2.09	0.52
1:M:518:LEU:HD21	1:M:584:TYR:CD1	2.44	0.52
1:N:572:GLY:HA3	1:K:711:LEU:HD21	1.91	0.52
1:E:634:LEU:HD11	1:H:716:LEU:HB3	1.90	0.52
1:H:689:ASP:O	1:H:693:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:595:GLN:O	1:P:599:ARG:NE	2.43	0.52
1:O:481:THR:HG22	2:S:17:ARG:HH12	1.74	0.52
1:D:481:THR:HG22	1:M:447:ARG:NH1	2.04	0.52
1:D:686:ASP:O	1:D:690:ILE:N	2.39	0.52
1:O:419:ILE:HD12	1:O:491:LYS:HG2	1.92	0.52
1:O:643:ARG:HH21	1:O:717:GLN:HG2	1.74	0.52
1:B:535:ARG:HA	1:B:563:LEU:O	2.09	0.52
1:C:645:GLN:O	1:C:649:LYS:HG2	2.10	0.52
1:D:698:GLU:HG2	1:D:702:LYS:HE3	1.92	0.52
1:H:521:ILE:HA	2:W:17:ARG:HG2	1.92	0.52
1:B:482:ASP:H	1:B:484:HIS:CE1	2.28	0.52
1:C:455:ASN:O	1:C:459:GLN:HG2	2.10	0.52
1:G:508:ARG:NH1	1:G:557:SER:HB3	2.24	0.52
1:J:420:GLY:H	1:C:677:THR:HB	1.74	0.52
1:O:656:GLU:OE2	1:O:718:LYS:HD2	2.09	0.52
1:P:508:ARG:HB2	1:P:578:ALA:HA	1.92	0.52
1:I:502:ILE:HG23	1:I:507:SER:HB2	1.91	0.52
1:P:508:ARG:NH2	1:P:552:TYR:O	2.25	0.52
1:C:567:ARG:HH11	1:C:734:ALA:HB2	1.73	0.51
1:E:425:GLN:OE1	1:E:490:GLY:N	2.41	0.51
1:E:439:ALA:HB2	1:E:452:ARG:NH1	2.26	0.51
1:E:485:LEU:HD11	1:E:521:ILE:HG23	1.92	0.51
1:O:601:HIS:HB2	1:O:609:VAL:HG11	1.91	0.51
1:N:654:LYS:HZ1	1:L:443:ALA:HB1	1.74	0.51
1:F:581:VAL:HB	1:F:611:VAL:HG22	1.91	0.51
1:I:508:ARG:NH2	1:I:552:TYR:O	2.23	0.51
1:I:572:GLY:H	1:I:599:ARG:NH1	2.09	0.51
1:O:586:SER:OG	1:O:613:ARG:NH1	2.36	0.51
1:C:532:LYS:NZ	1:C:558:ASP:OD2	2.43	0.51
1:E:545:ARG:O	1:E:549:ILE:HG12	2.10	0.51
1:F:532:LYS:HB2	1:F:559:LYS:HA	1.91	0.51
1:J:515:MET:HA	1:H:730:GLU:HG2	1.93	0.51
1:D:508:ARG:NH2	1:D:577:THR:OG1	2.42	0.51
1:O:508:ARG:NH1	1:O:559:LYS:O	2.42	0.51
1:P:485:LEU:HD11	1:P:521:ILE:HG23	1.93	0.51
1:A:601:HIS:HB2	1:A:609:VAL:HG11	1.92	0.51
1:C:532:LYS:HB3	1:C:559:LYS:HD3	1.92	0.51
1:D:536:ILE:HG12	1:D:562:PHE:CZ	2.46	0.51
1:F:648:ALA:HB2	1:I:634:LEU:HB3	1.93	0.51
1:I:523:GLU:OE1	1:I:535:ARG:NH1	2.38	0.51
1:O:641:GLN:HB2	1:A:641:GLN:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:ARG:NH2	1:E:585:ASP:OD2	2.40	0.51
1:F:713:ILE:HG13	1:I:641:GLN:HG3	1.93	0.51
1:M:418:TYR:HB3	1:M:617:ASP:HB2	1.93	0.51
1:C:660:MET:HE1	1:H:727:TRP:CH2	2.46	0.50
1:E:574:ASN:HD22	1:L:603:ILE:HD12	1.76	0.50
1:H:512:PHE:CE2	1:H:564:LEU:HD13	2.45	0.50
1:B:677:THR:HB	1:K:420:GLY:H	1.76	0.50
1:L:411:PRO:O	1:L:608:GLN:NE2	2.38	0.50
1:L:710:LYS:HA	1:L:710:LYS:NZ	2.26	0.50
1:P:455:ASN:O	1:P:459:GLN:HG2	2.11	0.50
1:A:534:CYS:SG	1:A:559:LYS:HG3	2.51	0.50
1:C:601:HIS:HB2	1:C:609:VAL:HG11	1.92	0.50
1:F:591:GLN:HE21	1:F:728:ASN:N	2.08	0.50
1:J:627:ARG:O	1:J:631:LYS:HG2	2.11	0.50
1:A:730:GLU:HG2	1:A:731:ASP:H	1.77	0.50
1:C:637:LEU:HD22	1:C:713:ILE:HD12	1.93	0.50
1:F:573:ILE:HG13	1:F:599:ARG:HD3	1.93	0.50
1:J:711:LEU:HD21	1:H:572:GLY:HA3	1.92	0.50
1:H:671:THR:HG21	1:H:674:ALA:O	2.11	0.50
1:O:573:ILE:CD1	1:O:599:ARG:HH11	2.25	0.50
1:P:417:VAL:HG13	1:D:693:ILE:HG21	1.94	0.50
1:E:711:LEU:HD13	1:E:719:PHE:CD2	2.47	0.50
1:F:497:LYS:NZ	1:F:500:LYS:HD2	2.26	0.50
1:H:674:ALA:HB3	1:H:679:ALA:HB2	1.93	0.50
1:I:455:ASN:O	1:I:459:GLN:HG2	2.11	0.50
1:H:703:GLU:OE1	1:H:707:ARG:NH2	2.45	0.50
1:A:594:LEU:HD21	1:A:725:TYR:C	2.32	0.50
1:F:601:HIS:HB2	1:F:609:VAL:HG11	1.94	0.50
1:K:425:GLN:HG2	1:K:467:PRO:HG3	1.92	0.50
1:D:497:LYS:HZ3	1:D:500:LYS:HD2	1.72	0.50
1:H:534:CYS:HB2	1:H:562:PHE:CE1	2.47	0.50
1:I:532:LYS:HB3	1:I:559:LYS:HD3	1.93	0.50
1:L:542:HIS:O	1:L:546:ILE:HG13	2.11	0.50
1:E:541:ALA:O	1:E:545:ARG:HG3	2.11	0.49
1:I:698:GLU:HG2	1:I:702:LYS:HE3	1.94	0.49
1:I:572:GLY:N	1:I:599:ARG:HH12	2.09	0.49
1:N:411:PRO:O	1:N:608:GLN:NE2	2.37	0.49
1:O:572:GLY:HA2	1:O:602:ARG:HH12	1.77	0.49
1:I:518:LEU:HD21	1:I:584:TYR:CD1	2.47	0.49
1:L:534:CYS:SG	1:L:559:LYS:HG3	2.52	0.49
1:P:497:LYS:NZ	1:P:500:LYS:HD2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:633:ARG:HH12	1:C:714:ASP:CG	2.15	0.49
1:K:555:PRO:HG2	1:A:608:GLN:HB2	1.94	0.49
1:G:542:HIS:HA	1:G:545:ARG:HE	1.78	0.49
1:E:662:GLN:NE2	1:H:440:VAL:O	2.36	0.49
1:K:549:ILE:HD11	1:K:573:ILE:HD12	1.93	0.49
1:O:652:ALA:HB1	1:O:657:LEU:HG	1.93	0.49
1:L:407:LYS:HE3	1:L:603:ILE:HG23	1.95	0.49
1:P:425:GLN:HG2	1:P:467:PRO:HG3	1.93	0.49
1:F:719:PHE:CD1	1:A:541:ALA:HA	2.46	0.49
1:C:581:VAL:HB	1:C:611:VAL:HG22	1.95	0.49
1:F:430:GLN:HG2	1:I:669:PHE:HD1	1.78	0.49
1:J:474:GLU:OE1	2:U:17:ARG:NH2	2.41	0.49
1:G:446:LYS:NZ	1:M:724:ALA:HA	2.27	0.49
1:I:410:LEU:HD12	1:I:410:LEU:H	1.77	0.49
1:M:485:LEU:HD11	1:M:521:ILE:HG23	1.93	0.49
1:M:570:GLY:O	1:M:599:ARG:NH2	2.24	0.49
1:N:455:ASN:O	1:N:459:GLN:HG2	2.13	0.49
1:F:487:TYR:HD1	1:F:493:VAL:HG22	1.78	0.48
1:O:534:CYS:SG	1:O:559:LYS:HG3	2.52	0.48
1:A:630:GLN:O	1:A:634:LEU:HG	2.13	0.48
1:D:630:GLN:O	1:D:634:LEU:HG	2.13	0.48
1:D:693:ILE:O	1:D:697:GLY:N	2.30	0.48
1:G:512:PHE:CE2	1:G:564:LEU:HD12	2.48	0.48
1:G:581:VAL:HB	1:G:611:VAL:HG22	1.95	0.48
1:O:643:ARG:HE	1:O:717:GLN:HG2	1.78	0.48
1:G:508:ARG:HH12	1:G:557:SER:HB3	1.76	0.48
1:M:560:PHE:CD2	1:M:561:ILE:HG13	2.48	0.48
1:F:479:TYR:CD2	1:O:448:GLU:HB3	2.48	0.48
1:O:678:MET:O	1:O:682:GLY:HA3	2.13	0.48
1:G:519:LEU:HD23	1:G:522:LEU:HD12	1.94	0.48
1:G:637:LEU:HD22	1:G:713:ILE:HD12	1.94	0.48
1:E:581:VAL:HB	1:E:611:VAL:HG22	1.95	0.48
1:K:636:GLN:O	1:K:640:GLN:HB2	2.12	0.48
1:C:480:THR:O	1:C:484:HIS:NE2	2.43	0.48
1:M:573:ILE:HG12	1:M:599:ARG:HD2	1.94	0.48
1:O:483:GLU:HB3	1:O:487:TYR:HE2	1.79	0.48
1:B:700:ARG:HH12	1:K:617:ASP:CG	2.16	0.48
1:F:698:GLU:HG2	1:F:702:LYS:HE3	1.96	0.48
1:G:653:ASN:HB3	1:G:656:GLU:HG3	1.94	0.48
1:P:517:ARG:HA	1:P:520:ASP:OD2	2.14	0.48
1:B:436:ASP:OD2	1:B:452:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLN:HG2	1:A:467:PRO:HG3	1.95	0.48
1:M:653:ASN:HB2	1:M:656:GLU:HG3	1.96	0.48
1:N:421:MET:H	1:L:675:PHE:CB	2.27	0.48
1:O:668:VAL:HG11	1:A:429:TYR:CD1	2.49	0.47
1:G:545:ARG:O	1:G:549:ILE:HG12	2.14	0.47
1:J:571:LEU:O	1:H:707:ARG:HD3	2.14	0.47
1:J:718:LYS:HZ3	1:J:722:GLU:HG2	1.79	0.47
1:K:474:GLU:OE1	2:Q:17:ARG:NH2	2.39	0.47
1:P:581:VAL:HB	1:P:611:VAL:HG22	1.96	0.47
1:B:533:TYR:HA	1:B:561:ILE:O	2.14	0.47
1:B:514:GLN:HB2	1:B:585:ASP:OD2	2.15	0.47
1:C:573:ILE:HB	1:C:599:ARG:HH11	1.79	0.47
1:E:518:LEU:HD21	1:E:584:TYR:CD1	2.49	0.47
1:J:641:GLN:HG3	1:C:713:ILE:HG21	1.96	0.47
1:G:501:ARG:HH12	1:M:694:LEU:HD12	1.78	0.47
1:F:654:LYS:NZ	1:I:448:GLU:HB3	2.29	0.47
1:N:730:GLU:OE1	1:K:516:SER:N	2.44	0.47
1:E:685:LEU:HG	1:H:493:VAL:HG12	1.96	0.47
1:F:721:SER:HB3	1:A:542:HIS:CE1	2.49	0.47
1:L:598:ASP:O	1:L:602:ARG:HD2	2.14	0.47
1:O:615:VAL:HG21	1:O:625:LEU:HD22	1.95	0.47
1:A:523:GLU:OE1	1:A:535:ARG:NH1	2.33	0.47
1:J:634:LEU:HB3	1:C:648:ALA:HB2	1.97	0.47
1:J:565:THR:OG1	1:J:568:ALA:HB2	2.13	0.47
1:J:718:LYS:NZ	1:J:722:GLU:HG2	2.30	0.47
1:G:654:LYS:HE2	1:M:448:GLU:O	2.15	0.47
1:J:518:LEU:HD21	1:J:584:TYR:CD1	2.50	0.47
1:G:626:GLU:HG2	1:M:704:LEU:HD11	1.97	0.47
1:N:656:GLU:OE2	1:N:718:LYS:HE3	2.15	0.47
1:A:595:GLN:NE2	1:A:730:GLU:O	2.48	0.47
1:O:483:GLU:OE1	1:O:529:ARG:NH2	2.48	0.47
1:G:421:MET:H	1:M:675:PHE:HB3	1.79	0.47
1:N:491:LYS:HZ1	1:N:621:GLU:CD	2.19	0.47
1:E:634:LEU:HD12	1:H:716:LEU:HD13	1.96	0.46
1:H:447:ARG:HH12	1:L:481:THR:CG2	2.28	0.46
1:E:491:LYS:HD2	1:E:584:TYR:CE1	2.50	0.46
1:L:425:GLN:HG2	1:L:467:PRO:HG3	1.97	0.46
1:E:418:TYR:HB3	1:E:617:ASP:HB2	1.96	0.46
1:G:485:LEU:HD11	1:G:521:ILE:HG23	1.97	0.46
1:G:536:ILE:HG23	1:G:545:ARG:HG2	1.98	0.46
1:I:560:PHE:CD2	1:I:561:ILE:HG13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:448:GLU:HG2	1:O:448:GLU:H	1.53	0.46
1:O:573:ILE:HG12	1:O:599:ARG:HH11	1.80	0.46
1:K:518:LEU:HD11	1:K:584:TYR:CE1	2.51	0.46
1:O:483:GLU:HB3	1:O:487:TYR:CE2	2.51	0.46
1:A:491:LYS:NZ	1:A:621:GLU:OE2	2.45	0.46
1:B:410:LEU:H	1:B:410:LEU:HD12	1.81	0.46
1:H:545:ARG:O	1:H:549:ILE:HG12	2.15	0.46
1:K:486:ILE:HD12	1:K:529:ARG:HH21	1.81	0.46
1:L:560:PHE:CD2	1:L:561:ILE:HG13	2.51	0.46
1:A:500:LYS:HE3	1:A:500:LYS:HB2	1.71	0.46
1:C:686:ASP:OD2	1:C:689:ASP:N	2.47	0.46
1:D:593:ASP:O	1:D:597:MET:HG3	2.15	0.46
1:E:425:GLN:HG2	1:E:467:PRO:HG3	1.97	0.46
1:J:573:ILE:HG12	1:J:599:ARG:HH11	1.80	0.46
1:L:419:ILE:HD13	1:L:491:LYS:HA	1.97	0.46
1:F:485:LEU:HD22	1:O:447:ARG:NH1	2.31	0.46
1:G:542:HIS:HA	1:G:545:ARG:HH11	1.81	0.46
1:O:429:TYR:CD1	1:A:668:VAL:HG11	2.50	0.46
1:J:581:VAL:HB	1:J:611:VAL:HG22	1.98	0.46
1:G:619:ALA:O	1:M:663:HIS:HD2	1.99	0.46
1:A:549:ILE:HG22	1:A:553:ASN:ND2	2.32	0.46
1:D:410:LEU:H	1:D:410:LEU:HD12	1.81	0.46
1:D:535:ARG:NE	1:D:537:ASP:OD1	2.41	0.46
1:L:581:VAL:HB	1:L:611:VAL:HG22	1.97	0.46
1:N:444:GLY:HA3	1:N:448:GLU:OE1	2.17	0.45
1:N:422:SER:HA	1:L:678:MET:HE2	1.98	0.45
1:P:590:PRO:HG3	1:P:628:ALA:HB1	1.97	0.45
1:P:536:ILE:HD13	1:P:545:ARG:HB2	1.98	0.45
1:G:536:ILE:CD1	1:G:545:ARG:HA	2.47	0.45
1:J:500:LYS:HE3	1:J:500:LYS:HB2	1.72	0.45
1:J:721:SER:HB2	1:H:631:LYS:HD3	1.98	0.45
1:N:500:LYS:HE3	1:N:500:LYS:HB2	1.75	0.45
1:D:513:SER:OG	1:D:518:LEU:HD23	2.17	0.45
1:L:432:ILE:HD11	1:L:470:PHE:CZ	2.51	0.45
1:M:587:ASP:OD1	1:M:588:TRP:N	2.50	0.45
1:P:688:ASP:HB3	1:H:556:GLY:HA2	1.99	0.45
1:N:410:LEU:HD12	1:N:410:LEU:H	1.82	0.45
1:C:533:TYR:HA	1:C:561:ILE:O	2.17	0.45
1:D:465:ASN:HB3	1:D:518:LEU:HD13	1.99	0.45
1:G:449:SER:HB2	1:M:654:LYS:HZ2	1.81	0.45
1:H:560:PHE:CD2	1:H:561:ILE:HG13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ILE:HG12	1:I:447:ARG:HB2	1.99	0.45
1:F:691:ASP:OD1	1:I:501:ARG:NH1	2.50	0.45
1:J:534:CYS:SG	1:J:559:LYS:HG3	2.57	0.45
1:L:532:LYS:NZ	1:L:558:ASP:OD2	2.40	0.45
1:O:553:ASN:HA	1:O:577:THR:HG21	1.98	0.45
1:B:549:ILE:HG13	1:B:550:ASP:H	1.81	0.45
1:G:410:LEU:H	1:G:410:LEU:HD12	1.82	0.45
1:M:646:VAL:O	1:M:650:ALA:N	2.50	0.45
1:P:642:GLY:HA2	1:D:641:GLN:NE2	2.32	0.45
1:E:520:ASP:OD1	1:E:535:ARG:NH2	2.47	0.45
1:G:520:ASP:OD1	1:G:535:ARG:NH1	2.46	0.45
1:M:698:GLU:HG2	1:M:702:LYS:HE3	1.99	0.45
1:N:572:GLY:CA	1:N:602:ARG:HH12	2.24	0.45
1:D:407:LYS:NZ	1:D:604:GLY:H	2.14	0.44
1:F:654:LYS:HZ1	1:I:448:GLU:HB3	1.80	0.44
1:C:418:TYR:HB3	1:C:617:ASP:HB2	1.99	0.44
1:B:518:LEU:HD21	1:B:584:TYR:CD1	2.52	0.44
1:D:687:ASP:HA	1:D:690:ILE:HG22	1.98	0.44
1:H:508:ARG:HB2	1:H:578:ALA:HA	1.98	0.44
1:J:588:TRP:CZ3	1:J:589:ASN:HB3	2.52	0.44
1:G:524:ASP:OD2	1:P:447:ARG:HG3	2.17	0.44
1:A:698:GLU:HG2	1:A:702:LYS:HE3	2.00	0.44
1:B:436:ASP:OD2	1:B:452:ARG:CZ	2.65	0.44
1:F:502:ILE:HG23	1:F:580:ILE:HD12	2.00	0.44
1:L:653:ASN:HB2	1:L:656:GLU:H	1.82	0.44
1:N:534:CYS:SG	1:N:559:LYS:HG3	2.58	0.44
1:A:583:LEU:HD11	1:A:597:MET:HE3	1.99	0.44
1:D:534:CYS:HB2	1:D:562:PHE:HD1	1.82	0.44
1:D:560:PHE:CD2	1:D:561:ILE:HG13	2.52	0.44
1:D:562:PHE:CD2	1:D:564:LEU:HD11	2.53	0.44
1:F:635:ASP:O	1:F:639:ILE:HG13	2.17	0.44
1:A:532:LYS:HB3	1:A:559:LYS:HD3	1.99	0.44
1:K:585:ASP:N	1:K:585:ASP:OD1	2.51	0.44
1:B:653:ASN:ND2	1:B:655:ASP:HB2	2.32	0.44
1:G:417:VAL:HG23	1:M:693:ILE:HG22	2.00	0.44
1:G:560:PHE:CD2	1:G:561:ILE:HG13	2.53	0.44
1:O:425:GLN:HG2	1:O:467:PRO:HG3	2.00	0.44
1:J:591:GLN:NE2	1:H:717:GLN:O	2.41	0.44
1:M:500:LYS:HB2	1:M:500:LYS:HE3	1.83	0.44
1:O:550:ASP:O	1:O:554:LYS:HG3	2.18	0.44
1:B:595:GLN:HE22	1:B:731:ASP:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:TYR:OH	1:K:446:LYS:NZ	2.50	0.44
1:D:419:ILE:HD13	1:D:491:LYS:HA	2.00	0.44
1:D:539:SER:O	1:D:543:GLU:HB3	2.18	0.44
1:F:518:LEU:HD21	1:F:584:TYR:CD1	2.53	0.44
1:N:536:ILE:HB	1:N:564:LEU:CD2	2.47	0.44
1:A:567:ARG:NH2	1:A:589:ASN:HB3	2.34	0.43
1:B:419:ILE:HD13	1:B:491:LYS:HA	2.00	0.43
1:B:508:ARG:NH2	1:B:577:THR:OG1	2.51	0.43
1:F:411:PRO:O	1:F:608:GLN:NE2	2.37	0.43
1:G:683:SER:OG	1:G:684:GLN:N	2.50	0.43
1:E:421:MET:O	1:H:674:ALA:HB1	2.18	0.43
1:B:497:LYS:CE	1:K:687:ASP:HB3	2.46	0.43
1:O:677:THR:HB	1:A:420:GLY:H	1.83	0.43
1:I:585:ASP:N	1:I:585:ASP:OD1	2.51	0.43
1:K:502:ILE:HG23	1:K:507:SER:HB2	2.01	0.43
1:P:690:ILE:CD1	1:D:494:VAL:HG13	2.47	0.43
1:E:560:PHE:CD2	1:E:561:ILE:HG13	2.53	0.43
1:F:491:LYS:NZ	1:F:621:GLU:OE2	2.48	0.43
1:F:634:LEU:O	1:F:638:VAL:HG23	2.18	0.43
1:N:678:MET:HE1	1:L:493:VAL:HG21	2.01	0.43
1:O:486:ILE:HD12	1:O:529:ARG:HH21	1.84	0.43
1:P:637:LEU:HD21	1:D:712:GLY:HA2	2.00	0.43
1:A:710:LYS:HA	1:A:710:LYS:HD3	1.83	0.43
1:I:689:ASP:O	1:I:693:ILE:HG13	2.18	0.43
1:G:446:LYS:NZ	1:M:723:SER:O	2.37	0.43
1:B:595:GLN:NE2	1:B:731:ASP:HA	2.34	0.43
1:B:663:HIS:HE1	1:K:622:GLU:OE2	2.02	0.43
1:L:418:TYR:HB3	1:L:617:ASP:HB2	2.01	0.43
1:O:523:GLU:HG2	1:O:533:TYR:CE1	2.54	0.43
1:E:519:LEU:HD22	1:E:563:LEU:HB3	2.00	0.43
1:F:520:ASP:OD1	1:F:535:ARG:NH1	2.37	0.43
1:G:446:LYS:HE2	1:M:725:TYR:HB3	2.01	0.43
1:H:654:LYS:O	1:H:658:LEU:HB2	2.17	0.43
1:H:674:ALA:C	1:H:679:ALA:HB2	2.39	0.43
1:I:711:LEU:HD22	1:I:715:ASP:OD2	2.18	0.43
1:K:675:PHE:HD1	1:K:675:PHE:HA	1.71	0.43
1:J:560:PHE:CD2	1:J:561:ILE:HG13	2.54	0.43
1:J:501:ARG:NH1	1:C:691:ASP:OD1	2.46	0.43
1:E:643:ARG:HD3	1:E:717:GLN:HE22	1.84	0.43
1:J:429:TYR:CD1	1:C:668:VAL:HG11	2.53	0.43
1:A:545:ARG:O	1:A:549:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:681:LYS:HG3	1:B:685:LEU:HD22	2.01	0.43
1:C:491:LYS:HZ1	1:C:621:GLU:CD	2.23	0.43
1:E:407:LYS:NZ	1:E:604:GLY:H	2.17	0.43
1:L:479:TYR:O	1:L:480:THR:HG23	2.18	0.43
1:A:465:ASN:HB3	1:A:518:LEU:HD13	1.99	0.43
1:F:410:LEU:HD22	1:F:608:GLN:HB2	2.01	0.43
1:F:469:LEU:HA	1:F:517:ARG:HH21	1.84	0.43
1:M:511:ILE:HG12	1:M:582:ILE:HB	2.00	0.43
1:O:718:LYS:HD3	1:O:722:GLU:OE1	2.19	0.43
1:P:534:CYS:SG	1:P:559:LYS:HG3	2.58	0.43
1:K:455:ASN:O	1:K:459:GLN:HG2	2.19	0.42
1:N:669:PHE:HD2	1:L:430:GLN:HG2	1.84	0.42
1:N:419:ILE:HA	1:L:677:THR:HG21	2.01	0.42
1:F:560:PHE:CD2	1:F:561:ILE:HG13	2.54	0.42
1:J:499:LEU:HD21	1:J:511:ILE:HD11	2.01	0.42
1:J:418:TYR:HB3	1:J:617:ASP:HB2	1.99	0.42
1:B:549:ILE:HD13	1:B:573:ILE:HD13	2.00	0.42
1:K:481:THR:HG22	2:Q:17:ARG:NH1	2.33	0.42
1:K:485:LEU:HD11	1:K:521:ILE:HG23	2.01	0.42
1:A:571:LEU:HA	1:A:571:LEU:HD23	1.63	0.42
1:B:500:LYS:HB2	1:B:500:LYS:HE3	1.82	0.42
1:B:532:LYS:HB2	1:B:559:LYS:HA	2.00	0.42
1:J:642:GLY:HA2	1:C:641:GLN:HE22	1.85	0.42
1:H:482:ASP:CG	1:H:483:GLU:H	2.21	0.42
1:J:572:GLY:HA2	1:J:602:ARG:HH12	1.85	0.42
1:K:583:LEU:HD11	1:K:597:MET:HE2	2.02	0.42
1:L:585:ASP:N	1:L:585:ASP:OD1	2.52	0.42
1:P:654:LYS:HE2	1:D:450:LYS:HE3	2.00	0.42
1:D:512:PHE:CE2	1:D:596:ALA:HB1	2.54	0.42
1:F:723:SER:HB2	1:F:726:GLU:HG3	2.02	0.42
1:H:620:ILE:O	1:H:624:VAL:HG23	2.19	0.42
1:I:500:LYS:HE3	1:I:500:LYS:HB2	1.78	0.42
1:K:623:LYS:O	1:K:627:ARG:HG2	2.18	0.42
1:C:637:LEU:HD22	1:C:713:ILE:CD1	2.50	0.42
1:C:649:LYS:HA	1:H:724:ALA:HB2	2.01	0.42
1:J:623:LYS:HG2	1:C:660:MET:HA	2.01	0.42
1:D:517:ARG:HA	1:D:520:ASP:OD2	2.19	0.42
1:H:552:TYR:CE1	1:H:562:PHE:HB2	2.55	0.42
1:F:660:MET:HA	1:I:623:LYS:HG2	2.00	0.42
1:J:601:HIS:HB2	1:J:609:VAL:HG11	2.01	0.42
1:L:541:ALA:O	1:L:545:ARG:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:585:ASP:N	1:N:585:ASP:OD1	2.51	0.42
1:N:687:ASP:HB3	1:L:497:LYS:HE2	2.01	0.42
1:C:635:ASP:O	1:C:639:ILE:HG12	2.19	0.42
1:E:535:ARG:HA	1:E:563:LEU:O	2.19	0.42
1:E:648:ALA:HB2	1:H:634:LEU:HB3	2.01	0.42
1:G:587:ASP:N	1:G:593:ASP:OD2	2.41	0.42
1:A:571:LEU:CD1	1:A:595:GLN:HG2	2.48	0.42
1:O:638:VAL:HG13	1:A:641:GLN:HE21	1.85	0.42
1:A:653:ASN:OD1	1:A:654:LYS:N	2.51	0.42
1:I:485:LEU:HD11	1:I:521:ILE:HG23	2.01	0.42
1:L:601:HIS:HB2	1:L:609:VAL:HG11	2.02	0.42
1:M:534:CYS:SG	1:M:559:LYS:HG3	2.59	0.42
1:B:480:THR:O	1:B:484:HIS:CE1	2.73	0.42
1:D:545:ARG:O	1:D:549:ILE:HG12	2.20	0.42
1:D:601:HIS:HB2	1:D:609:VAL:HG11	2.02	0.42
1:E:455:ASN:O	1:E:459:GLN:HG2	2.20	0.42
1:F:535:ARG:HA	1:F:563:LEU:O	2.19	0.42
1:B:684:GLN:NE2	1:K:486:ILE:HG21	2.35	0.42
1:B:450:LYS:HB3	1:K:654:LYS:HE2	2.01	0.42
1:P:716:LEU:HB3	1:D:634:LEU:HD23	2.02	0.42
1:G:690:ILE:HG13	1:M:497:LYS:CG	2.48	0.42
1:K:432:ILE:HD11	1:K:470:PHE:CZ	2.55	0.42
1:N:503:GLN:HB2	1:N:560:PHE:CZ	2.55	0.42
1:O:572:GLY:C	1:O:602:ARG:HH12	2.23	0.42
1:E:427:LYS:HE2	1:E:431:LYS:HZ1	1.84	0.41
1:I:482:ASP:HB2	1:I:484:HIS:HD2	1.85	0.41
1:M:483:GLU:HB3	1:M:487:TYR:HE2	1.82	0.41
1:P:520:ASP:OD1	1:P:535:ARG:NH2	2.47	0.41
1:C:425:GLN:HG2	1:C:467:PRO:HG3	2.01	0.41
1:F:497:LYS:HZ2	1:F:500:LYS:HD2	1.85	0.41
1:F:719:PHE:O	1:A:545:ARG:HD2	2.20	0.41
1:H:533:TYR:HA	1:H:561:ILE:O	2.20	0.41
1:I:667:LYS:O	1:I:671:THR:OG1	2.31	0.41
1:L:407:LYS:NZ	1:L:604:GLY:H	2.18	0.41
1:A:595:GLN:CD	1:A:727:TRP:HE1	2.23	0.41
1:B:570:GLY:HA3	1:B:573:ILE:HD12	2.01	0.41
1:E:690:ILE:HD11	1:H:498:LEU:HD13	2.02	0.41
1:G:678:MET:O	1:G:682:GLY:HA3	2.19	0.41
1:K:431:LYS:NZ	1:K:431:LYS:HB2	2.35	0.41
1:K:569:GLY:O	1:K:599:ARG:HD2	2.20	0.41
1:N:620:ILE:O	1:N:624:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:GLU:O	1:B:681:LYS:HD2	2.20	0.41
1:C:535:ARG:HA	1:C:563:LEU:O	2.20	0.41
1:H:418:TYR:HA	1:H:615:VAL:O	2.20	0.41
1:L:502:ILE:HG23	1:L:580:ILE:HD12	2.01	0.41
1:M:474:GLU:OE1	2:V:17:ARG:NH2	2.34	0.41
1:N:518:LEU:HD21	1:N:584:TYR:CD1	2.55	0.41
1:F:503:GLN:HB2	1:F:560:PHE:CZ	2.56	0.41
1:F:643:ARG:NH2	1:F:720:THR:O	2.45	0.41
1:G:429:TYR:CD1	1:M:668:VAL:HG11	2.56	0.41
1:J:536:ILE:HG22	1:J:568:ALA:HB1	2.02	0.41
1:J:654:LYS:HZ2	1:J:658:LEU:HD22	1.85	0.41
1:M:455:ASN:O	1:M:459:GLN:HG2	2.21	0.41
1:O:560:PHE:CD2	1:O:561:ILE:HG13	2.55	0.41
1:P:431:LYS:HB2	1:P:431:LYS:NZ	2.35	0.41
1:A:458:MET:HE3	1:A:458:MET:HB3	1.79	0.41
1:A:519:LEU:HD22	1:A:563:LEU:HB3	2.02	0.41
1:I:552:TYR:HE2	1:I:578:ALA:HB2	1.86	0.41
1:N:560:PHE:CD2	1:N:561:ILE:HG13	2.56	0.41
1:C:500:LYS:HE3	1:C:500:LYS:HB2	1.78	0.41
1:D:457:VAL:HG13	1:D:620:ILE:HD11	2.01	0.41
1:E:653:ASN:ND2	1:E:655:ASP:HB2	2.35	0.41
1:L:635:ASP:O	1:L:639:ILE:HG12	2.21	0.41
1:A:447:ARG:HG3	1:A:447:ARG:H	1.65	0.41
1:A:560:PHE:CD2	1:A:561:ILE:HG13	2.55	0.41
1:C:660:MET:HE1	1:H:727:TRP:HH2	1.84	0.41
1:A:631:LYS:O	1:A:635:ASP:HB2	2.21	0.41
1:C:508:ARG:NH2	1:C:577:THR:OG1	2.49	0.41
1:F:544:ASP:O	1:F:548:ALA:N	2.52	0.41
1:J:708:TYR:CE1	1:H:571:LEU:HB2	2.56	0.41
1:J:573:ILE:HG12	1:J:599:ARG:NH1	2.36	0.41
1:L:500:LYS:HE3	1:L:500:LYS:HB2	1.88	0.41
1:P:499:LEU:HD21	1:P:511:ILE:HD11	2.02	0.41
1:A:689:ASP:O	1:A:693:ILE:HG13	2.21	0.41
1:B:450:LYS:HB3	1:K:654:LYS:HG2	2.02	0.41
1:C:560:PHE:CD2	1:C:561:ILE:HG13	2.55	0.41
1:D:534:CYS:SG	1:D:559:LYS:HE2	2.61	0.41
1:E:619:ALA:O	1:H:663:HIS:HD2	2.04	0.41
1:F:590:PRO:O	1:F:594:LEU:HD13	2.21	0.41
1:G:542:HIS:CA	1:G:545:ARG:HH11	2.34	0.41
1:K:653:ASN:HB3	1:K:656:GLU:HG3	2.03	0.41
1:L:569:GLY:O	1:L:599:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ARG:HA	1:A:563:LEU:O	2.21	0.41
1:C:512:PHE:HZ	1:C:599:ARG:HD2	1.86	0.41
1:D:425:GLN:HG2	1:D:467:PRO:HG3	2.02	0.41
1:D:654:LYS:H	1:D:654:LYS:HG2	1.56	0.41
1:I:573:ILE:O	1:I:602:ARG:NH1	2.54	0.41
1:J:550:ASP:O	1:J:554:LYS:HG3	2.21	0.41
1:K:422:SER:OG	1:K:488:ASN:O	2.36	0.41
1:P:519:LEU:HD22	1:P:563:LEU:HB3	2.03	0.41
1:F:521:ILE:HA	1:O:447:ARG:HG2	2.03	0.40
1:N:551:GLU:HA	1:N:554:LYS:HD2	2.03	0.40
1:B:595:GLN:HE22	1:B:732:PHE:H	1.69	0.40
1:G:552:TYR:HE2	1:G:578:ALA:HB2	1.87	0.40
1:J:623:LYS:HA	1:J:623:LYS:HD2	1.97	0.40
1:J:683:SER:HA	1:C:493:VAL:HG11	2.02	0.40
1:K:532:LYS:HB2	1:K:559:LYS:HA	2.03	0.40
1:L:685:LEU:HA	1:L:685:LEU:HD12	1.87	0.40
1:O:591:GLN:HA	1:O:594:LEU:HB2	2.02	0.40
1:B:595:GLN:HE22	1:B:732:PHE:N	2.19	0.40
1:C:457:VAL:HG13	1:C:620:ILE:HD11	2.04	0.40
1:C:712:GLY:O	1:C:715:ASP:OD2	2.39	0.40
1:F:519:LEU:O	1:F:523:GLU:N	2.52	0.40
1:L:432:ILE:O	1:L:435:LYS:HG2	2.21	0.40
1:M:457:VAL:HG13	1:M:620:ILE:HD11	2.02	0.40
1:N:579:ASP:OD2	1:N:580:ILE:HG13	2.21	0.40
1:P:654:LYS:HE3	1:P:654:LYS:HB2	1.89	0.40
1:B:497:LYS:HD2	1:B:497:LYS:HA	1.85	0.40
1:D:615:VAL:HG21	1:D:625:LEU:HD22	2.03	0.40
1:P:585:ASP:N	1:P:585:ASP:OD1	2.55	0.40
1:B:567:ARG:NE	1:B:732:PHE:HB3	2.37	0.40
1:B:619:ALA:O	1:K:663:HIS:HD2	2.05	0.40
1:C:502:ILE:HG23	1:C:580:ILE:HD12	2.04	0.40
1:C:407:LYS:NZ	1:C:604:GLY:H	2.20	0.40
1:F:425:GLN:HG2	1:F:467:PRO:HG3	2.03	0.40
1:F:532:LYS:HG3	1:F:558:ASP:CG	2.42	0.40
1:I:513:SER:OG	1:I:518:LEU:HD23	2.22	0.40
1:B:517:ARG:NH1	1:J:449:SER:HA	2.37	0.40
1:K:439:ALA:HB2	1:K:452:ARG:CZ	2.52	0.40
1:K:500:LYS:HB2	1:K:500:LYS:HE3	1.81	0.40
1:L:465:ASN:HB3	1:L:518:LEU:HD12	2.04	0.40
1:L:476:GLY:HA2	1:L:477:PRO:HD3	1.88	0.40
1:M:635:ASP:O	1:M:639:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:669:PHE:CD2	1:L:430:GLN:HG2	2.56	0.40
1:O:668:VAL:HG11	1:A:429:TYR:HD1	1.86	0.40
1:P:560:PHE:CD2	1:P:561:ILE:HG13	2.57	0.40
1:P:535:ARG:HA	1:P:563:LEU:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	325/349 (93%)	309 (95%)	14 (4%)	2 (1%)	30 72
1	B	326/349 (93%)	309 (95%)	17 (5%)	0	100 100
1	C	320/349 (92%)	307 (96%)	13 (4%)	0	100 100
1	D	288/349 (82%)	279 (97%)	9 (3%)	0	100 100
1	E	311/349 (89%)	294 (94%)	17 (6%)	0	100 100
1	F	320/349 (92%)	310 (97%)	10 (3%)	0	100 100
1	G	306/349 (88%)	297 (97%)	9 (3%)	0	100 100
1	H	315/349 (90%)	307 (98%)	6 (2%)	2 (1%)	30 72
1	I	297/349 (85%)	287 (97%)	10 (3%)	0	100 100
1	J	313/349 (90%)	302 (96%)	10 (3%)	1 (0%)	46 84
1	K	302/349 (86%)	293 (97%)	8 (3%)	1 (0%)	46 84
1	L	309/349 (88%)	297 (96%)	12 (4%)	0	100 100
1	M	320/349 (92%)	311 (97%)	9 (3%)	0	100 100
1	N	315/349 (90%)	307 (98%)	8 (2%)	0	100 100
1	O	318/349 (91%)	307 (96%)	10 (3%)	1 (0%)	46 84
1	P	310/349 (89%)	298 (96%)	11 (4%)	1 (0%)	46 84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	Q	3/21 (14%)	2 (67%)	1 (33%)	0	100 100
2	R	3/21 (14%)	2 (67%)	1 (33%)	0	100 100
2	S	3/21 (14%)	2 (67%)	1 (33%)	0	100 100
2	T	3/21 (14%)	2 (67%)	1 (33%)	0	100 100
2	U	3/21 (14%)	2 (67%)	1 (33%)	0	100 100
2	V	3/21 (14%)	2 (67%)	1 (33%)	0	100 100
2	W	2/21 (10%)	2 (100%)	0	0	100 100
All	All	5015/5731 (88%)	4828 (96%)	179 (4%)	8 (0%)	52 88

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	731	ASP
1	O	676	GLY
1	J	676	GLY
1	A	541	ALA
1	H	540	THR
1	K	642	GLY
1	A	711	LEU
1	P	676	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	275/294 (94%)	273 (99%)	2 (1%)	88 96
1	B	274/294 (93%)	273 (100%)	1 (0%)	93 98
1	C	273/294 (93%)	271 (99%)	2 (1%)	88 96
1	D	248/294 (84%)	248 (100%)	0	100 100
1	E	264/294 (90%)	263 (100%)	1 (0%)	93 98
1	F	273/294 (93%)	271 (99%)	2 (1%)	88 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	259/294 (88%)	259 (100%)	0	100 100
1	H	270/294 (92%)	268 (99%)	2 (1%)	88 96
1	I	254/294 (86%)	252 (99%)	2 (1%)	86 96
1	J	268/294 (91%)	264 (98%)	4 (2%)	72 92
1	K	258/294 (88%)	256 (99%)	2 (1%)	86 96
1	L	262/294 (89%)	260 (99%)	2 (1%)	86 96
1	M	273/294 (93%)	271 (99%)	2 (1%)	88 96
1	N	269/294 (92%)	267 (99%)	2 (1%)	88 96
1	O	273/294 (93%)	270 (99%)	3 (1%)	80 94
1	P	268/294 (91%)	267 (100%)	1 (0%)	93 98
2	Q	3/12 (25%)	3 (100%)	0	100 100
2	R	3/12 (25%)	3 (100%)	0	100 100
2	S	3/12 (25%)	3 (100%)	0	100 100
2	T	3/12 (25%)	3 (100%)	0	100 100
2	U	3/12 (25%)	3 (100%)	0	100 100
2	V	3/12 (25%)	3 (100%)	0	100 100
2	W	3/12 (25%)	3 (100%)	0	100 100
All	All	4282/4788 (89%)	4254 (99%)	28 (1%)	88 96

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	562	PHE
1	E	562	PHE
1	F	562	PHE
1	F	685	LEU
1	J	562	PHE
1	J	634	LEU
1	J	640	GLN
1	J	675	PHE
1	N	562	PHE
1	N	675	PHE
1	O	562	PHE
1	O	634	LEU
1	O	675	PHE
1	P	562	PHE

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Mol	Chain	Res	Type
1	C	480	THR
1	C	562	PHE
1	H	675	PHE
1	H	677	THR
1	K	562	PHE
1	K	675	PHE
1	L	480	THR
1	L	675	PHE
1	A	562	PHE
1	A	675	PHE
1	I	562	PHE
1	I	675	PHE
1	M	562	PHE
1	M	675	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	484	HIS
1	B	595	GLN
1	B	640	GLN
1	E	455	ASN
1	F	591	GLN
1	G	542	HIS
1	O	589	ASN
2	U	18	HIS
1	H	484	HIS
1	L	641	GLN
1	A	542	HIS
1	A	595	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	327/349 (93%)	-0.07	2 (0%) 90 73	40, 74, 108, 133	0
1	B	328/349 (93%)	0.03	12 (3%) 45 19	38, 68, 111, 145	0
1	C	324/349 (92%)	-0.20	5 (1%) 76 49	38, 61, 90, 139	0
1	D	292/349 (83%)	0.12	9 (3%) 52 24	38, 76, 125, 169	0
1	E	313/349 (89%)	-0.11	3 (0%) 84 60	40, 71, 104, 132	0
1	F	324/349 (92%)	0.25	19 (5%) 26 10	42, 80, 128, 177	0
1	G	308/349 (88%)	-0.03	7 (2%) 64 33	45, 75, 107, 142	0
1	H	321/349 (91%)	-0.10	3 (0%) 85 64	41, 64, 97, 121	0
1	I	301/349 (86%)	-0.18	5 (1%) 73 45	35, 58, 109, 145	0
1	J	317/349 (90%)	-0.28	2 (0%) 90 73	36, 55, 91, 124	0
1	K	306/349 (87%)	-0.15	3 (0%) 84 60	42, 63, 99, 137	0
1	L	311/349 (89%)	-0.00	9 (2%) 55 26	46, 69, 105, 139	0
1	M	324/349 (92%)	-0.13	4 (1%) 81 55	38, 65, 98, 132	0
1	N	319/349 (91%)	-0.25	2 (0%) 90 73	39, 63, 92, 132	0
1	O	322/349 (92%)	-0.04	3 (0%) 85 64	45, 75, 101, 128	0
1	P	316/349 (90%)	0.23	15 (4%) 35 14	46, 92, 125, 151	0
2	Q	5/21 (23%)	-0.12	0 100 100	58, 66, 78, 80	0
2	R	5/21 (23%)	0.44	0 100 100	63, 71, 74, 88	0
2	S	5/21 (23%)	0.57	1 (20%) 1 1	76, 77, 81, 113	0
2	T	5/21 (23%)	0.47	0 100 100	53, 56, 85, 87	0
2	U	5/21 (23%)	-0.05	1 (20%) 1 1	58, 65, 72, 91	0
2	V	5/21 (23%)	0.47	0 100 100	64, 66, 79, 79	0
2	W	4/21 (19%)	1.59	1 (25%) 1 1	79, 81, 81, 85	0
All	All	5087/5731 (88%)	-0.05	106 (2%) 67 36	35, 69, 109, 177	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	444	GLY	15.3
1	F	445	GLY	11.9
1	P	478	PRO	6.9
1	K	680	GLU	6.4
1	D	542	HIS	6.3
1	F	479	TYR	6.2
1	B	444	GLY	5.9
1	K	570	GLY	5.7
1	P	485	LEU	5.7
1	D	541	ALA	5.3
1	D	540	THR	5.1
1	P	408	SER	5.1
1	B	721	SER	4.9
1	K	408	SER	4.7
1	F	481	THR	4.5
1	F	734	ALA	4.4
1	P	477	PRO	4.4
1	N	680	GLU	4.1
1	L	600	ALA	4.0
1	B	549	ILE	3.8
1	F	684	GLN	3.8
1	I	570	GLY	3.8
1	F	441	ASN	3.8
1	P	466	HIS	3.7
1	G	407	LYS	3.6
1	P	588	TRP	3.6
1	H	680	GLU	3.5
2	W	15	ALA	3.5
1	F	561	ILE	3.5
1	F	572	GLY	3.4
1	P	570	GLY	3.4
1	E	569	GLY	3.3
1	G	546	ILE	3.3
1	F	487	TYR	3.2
1	G	408	SER	3.1
1	L	408	SER	3.1
1	B	685	LEU	3.1
1	G	573	ILE	3.1
1	F	573	ILE	3.1
1	P	410	LEU	3.0
1	P	482	ASP	3.0
1	A	684	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	675	PHE	2.9
1	O	681	LYS	2.9
1	M	480	THR	2.9
1	P	421	MET	2.9
1	N	677	THR	2.9
1	J	682	GLY	2.8
1	F	447	ARG	2.8
1	P	429	TYR	2.8
1	B	543	GLU	2.7
1	H	681	LYS	2.7
1	D	570	GLY	2.7
1	M	478	PRO	2.7
1	M	485	LEU	2.7
1	G	569	GLY	2.6
1	B	729	GLY	2.6
1	P	671	THR	2.6
1	C	407	LYS	2.6
1	L	603	ILE	2.6
2	U	14	GLY	2.6
1	P	481	THR	2.5
1	F	555	PRO	2.5
1	F	482	ASP	2.5
1	D	668	VAL	2.4
1	L	478	PRO	2.4
1	H	408	SER	2.4
1	L	555	PRO	2.4
1	L	407	LYS	2.4
1	D	573	ILE	2.4
1	C	570	GLY	2.4
1	L	536	ILE	2.4
1	C	542	HIS	2.4
1	D	670	GLN	2.4
1	I	677	THR	2.4
1	D	476	GLY	2.4
1	O	477	PRO	2.3
1	B	407	LYS	2.3
1	C	573	ILE	2.3
1	B	478	PRO	2.3
1	O	472	GLY	2.3
1	D	564	LEU	2.3
1	J	683	SER	2.3
1	M	680	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	569	GLY	2.2
1	F	477	PRO	2.2
1	F	556	GLY	2.2
1	P	411	PRO	2.2
1	C	572	GLY	2.2
1	B	443	ALA	2.2
1	F	733	ALA	2.2
1	B	573	ILE	2.1
1	G	512	PHE	2.1
1	G	409	LEU	2.1
2	S	14	GLY	2.1
1	P	496	ASP	2.1
1	A	675	PHE	2.1
1	E	570	GLY	2.1
1	F	480	THR	2.1
1	B	449	SER	2.1
1	E	408	SER	2.1
1	F	536	ILE	2.1
1	B	670	GLN	2.1
1	L	476	GLY	2.0
1	L	601	HIS	2.0
1	I	674	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.