Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 06:13 PM JST

PDB ID	:	8H58
Title	:	Crystal structure of YhaJ effector binding domain
Authors	:	Kim, M.; Ryu, S.E.
Deposited on	:	2022-10-12
Resolution	:	2.64 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

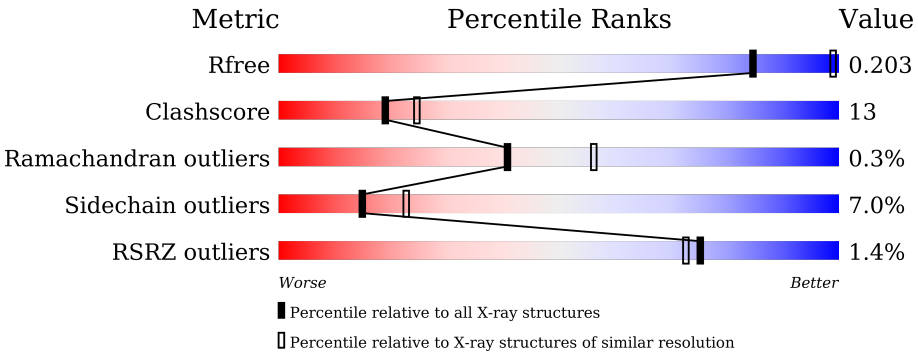
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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

Mol	Chain	Length	Quality of chain
1	A	207	76% 15% 5%
1	B	207	2% 71% 26%
1	C	207	69% 24% 5%
1	D	207	3% 72% 23%
1	E	207	% 71% 23%
1	F	207	2% 74% 22%

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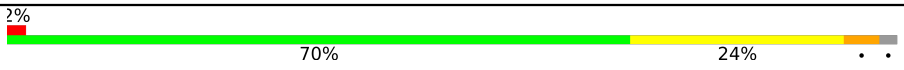
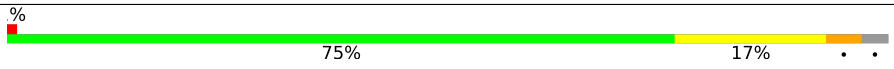
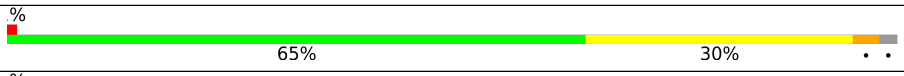
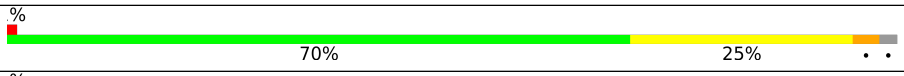
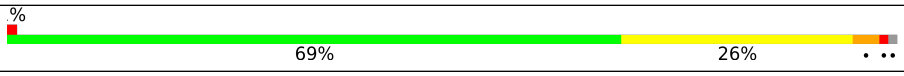
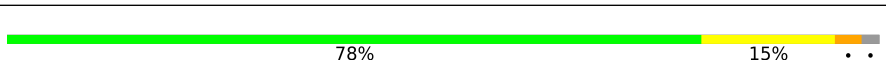
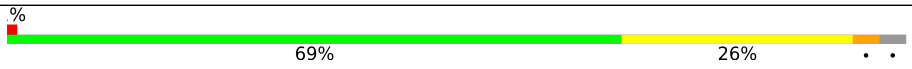
Mol	Chain	Length	Quality of chain
1	G	207	
1	H	207	
1	I	207	
1	J	207	
1	K	207	
1	L	207	
1	M	207	
1	N	207	
1	O	207	
1	P	207	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25530 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 HTH-type transcriptional regulator YhaJ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	B	204	Total	C	N	O	S	0	0	0
			1593	1011	279	295	8			
1	C	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	D	204	Total	C	N	O	S	0	0	0
			1593	1010	278	297	8			
1	E	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	F	205	Total	C	N	O	S	0	0	0
			1606	1019	281	298	8			
1	G	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	H	203	Total	C	N	O	S	0	0	0
			1593	1011	278	296	8			
1	I	201	Total	C	N	O	S	0	0	0
			1575	1000	276	292	7			
1	J	204	Total	C	N	O	S	0	0	0
			1593	1011	279	295	8			
1	K	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	L	203	Total	C	N	O	S	0	0	0
			1592	1010	278	296	8			
1	M	203	Total	C	N	O	S	0	0	0
			1593	1011	279	296	7			
1	N	205	Total	C	N	O	S	0	0	0
			1606	1019	281	298	8			
1	O	202	Total	C	N	O	S	0	0	0
			1584	1006	278	293	7			
1	P	201	Total	C	N	O	S	0	0	0
			1573	1000	273	292	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	GLY	-	expression tag	UNP P67661
A	93	SER	-	expression tag	UNP P67661
A	94	HIS	-	expression tag	UNP P67661
A	95	MET	-	expression tag	UNP P67661
B	92	GLY	-	expression tag	UNP P67661
B	93	SER	-	expression tag	UNP P67661
B	94	HIS	-	expression tag	UNP P67661
B	95	MET	-	expression tag	UNP P67661
C	92	GLY	-	expression tag	UNP P67661
C	93	SER	-	expression tag	UNP P67661
C	94	HIS	-	expression tag	UNP P67661
C	95	MET	-	expression tag	UNP P67661
D	92	GLY	-	expression tag	UNP P67661
D	93	SER	-	expression tag	UNP P67661
D	94	HIS	-	expression tag	UNP P67661
D	95	MET	-	expression tag	UNP P67661
E	92	GLY	-	expression tag	UNP P67661
E	93	SER	-	expression tag	UNP P67661
E	94	HIS	-	expression tag	UNP P67661
E	95	MET	-	expression tag	UNP P67661
F	92	GLY	-	expression tag	UNP P67661
F	93	SER	-	expression tag	UNP P67661
F	94	HIS	-	expression tag	UNP P67661
F	95	MET	-	expression tag	UNP P67661
G	92	GLY	-	expression tag	UNP P67661
G	93	SER	-	expression tag	UNP P67661
G	94	HIS	-	expression tag	UNP P67661
G	95	MET	-	expression tag	UNP P67661
H	92	GLY	-	expression tag	UNP P67661
H	93	SER	-	expression tag	UNP P67661
H	94	HIS	-	expression tag	UNP P67661
H	95	MET	-	expression tag	UNP P67661
I	92	GLY	-	expression tag	UNP P67661
I	93	SER	-	expression tag	UNP P67661
I	94	HIS	-	expression tag	UNP P67661
I	95	MET	-	expression tag	UNP P67661
J	92	GLY	-	expression tag	UNP P67661
J	93	SER	-	expression tag	UNP P67661
J	94	HIS	-	expression tag	UNP P67661
J	95	MET	-	expression tag	UNP P67661
K	92	GLY	-	expression tag	UNP P67661
K	93	SER	-	expression tag	UNP P67661

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Chain	Residue	Modelled	Actual	Comment	Reference
K	94	HIS	-	expression tag	UNP P67661
K	95	MET	-	expression tag	UNP P67661
L	92	GLY	-	expression tag	UNP P67661
L	93	SER	-	expression tag	UNP P67661
L	94	HIS	-	expression tag	UNP P67661
L	95	MET	-	expression tag	UNP P67661
M	92	GLY	-	expression tag	UNP P67661
M	93	SER	-	expression tag	UNP P67661
M	94	HIS	-	expression tag	UNP P67661
M	95	MET	-	expression tag	UNP P67661
N	92	GLY	-	expression tag	UNP P67661
N	93	SER	-	expression tag	UNP P67661
N	94	HIS	-	expression tag	UNP P67661
N	95	MET	-	expression tag	UNP P67661
O	92	GLY	-	expression tag	UNP P67661
O	93	SER	-	expression tag	UNP P67661
O	94	HIS	-	expression tag	UNP P67661
O	95	MET	-	expression tag	UNP P67661
P	92	GLY	-	expression tag	UNP P67661
P	93	SER	-	expression tag	UNP P67661
P	94	HIS	-	expression tag	UNP P67661
P	95	MET	-	expression tag	UNP P67661

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Na 2 2	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0
2	I	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	2	Total Na 2 2	0	0
2	M	1	Total Na 1 1	0	0
2	N	1	Total Na 1 1	0	0
2	O	1	Total Na 1 1	0	0
2	P	1	Total Na 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	6	Total O 6 6	0	0
3	C	4	Total O 4 4	0	0
3	D	6	Total O 6 6	0	0
3	E	5	Total O 5 5	0	0
3	F	4	Total O 4 4	0	0
3	G	8	Total O 8 8	0	0
3	H	6	Total O 6 6	0	0
3	I	7	Total O 7 7	0	0
3	J	3	Total O 3 3	0	0
3	K	5	Total O 5 5	0	0
3	L	8	Total O 8 8	0	0
3	M	5	Total O 5 5	0	0
3	N	4	Total O 4 4	0	0

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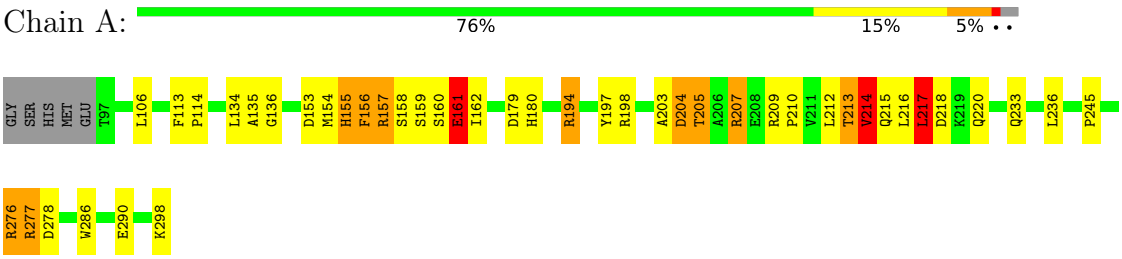
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	O	8	Total O 8 8	0	0
3	P	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

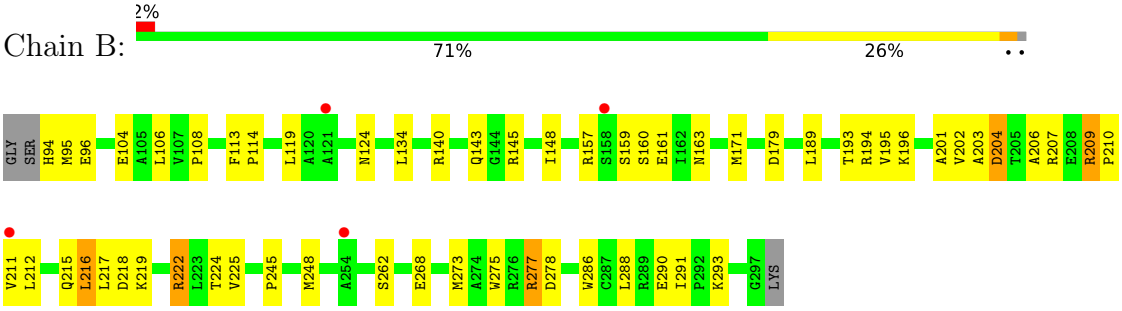
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain A:



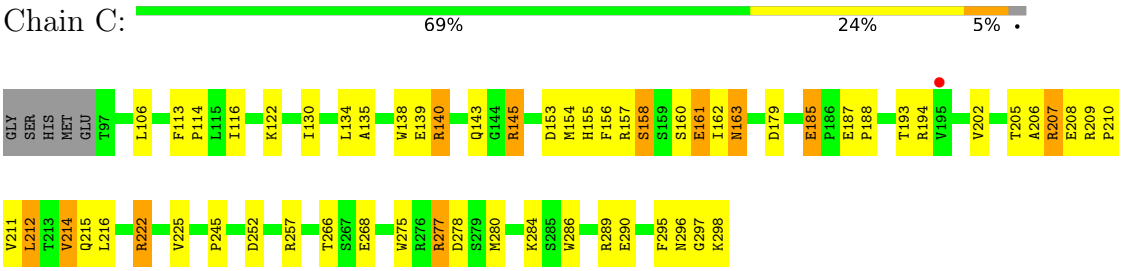
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain B:



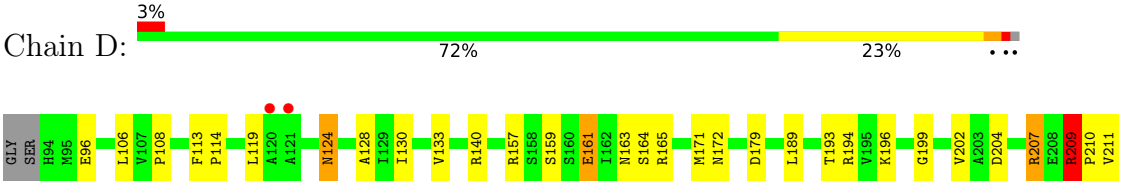
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain C:

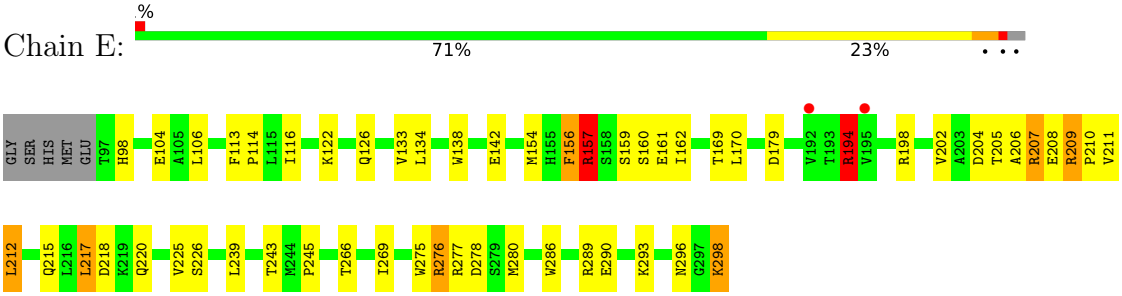


• Molecule 1: HTH-type transcriptional regulator YhaJ

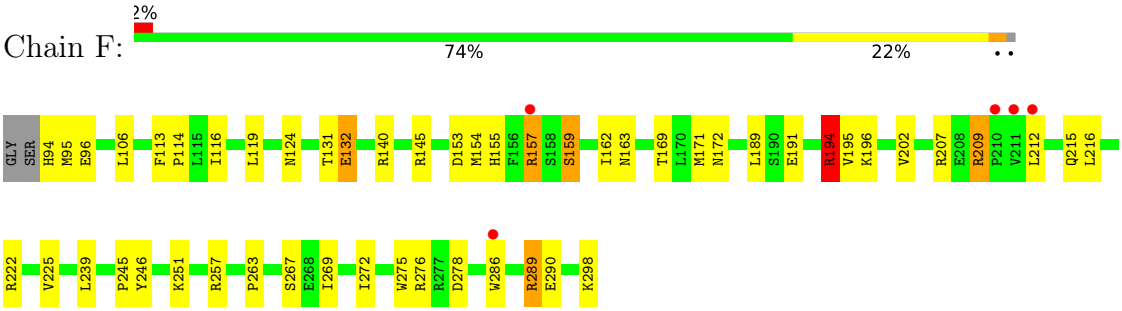
Chain D:



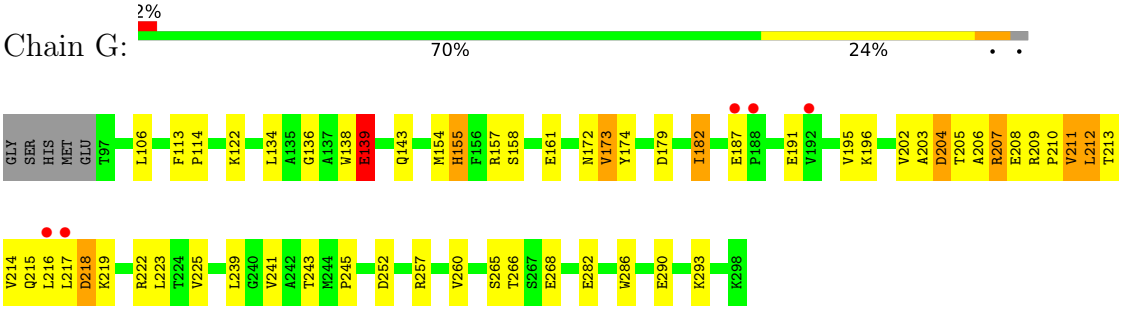
• Molecule 1: HTH-type transcriptional regulator YhaJ



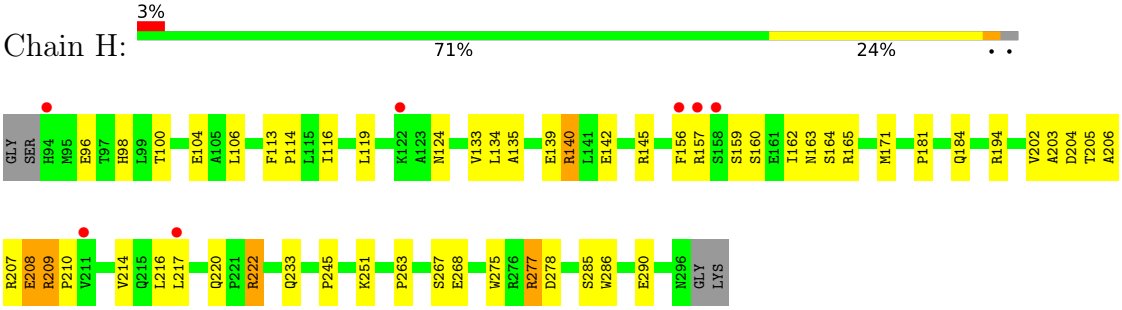
• Molecule 1: HTH-type transcriptional regulator YhaJ



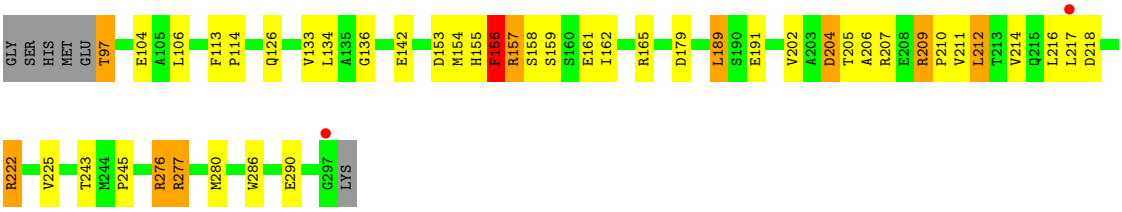
• Molecule 1: HTH-type transcriptional regulator YhaJ



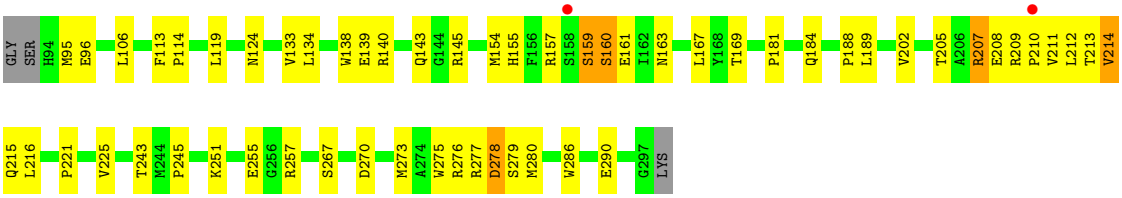
• Molecule 1: HTH-type transcriptional regulator YhaJ



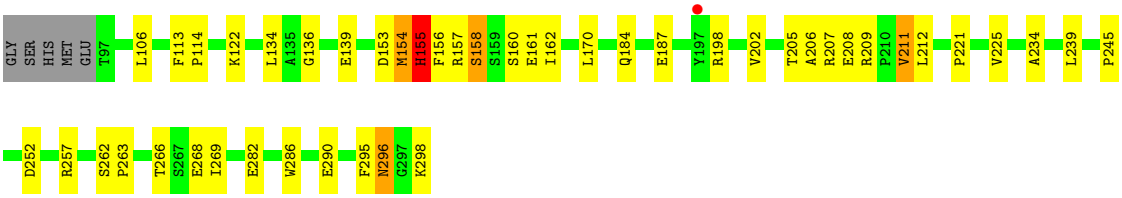
• Molecule 1: HTH-type transcriptional regulator YhaJ



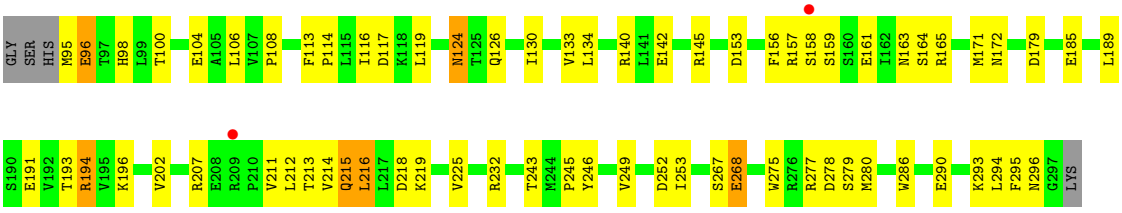
• Molecule 1: HTH-type transcriptional regulator YhaJ



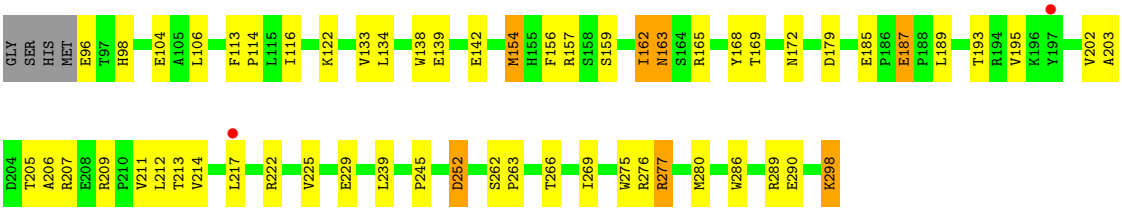
• Molecule 1: HTH-type transcriptional regulator YhaJ



• Molecule 1: HTH-type transcriptional regulator YhaJ

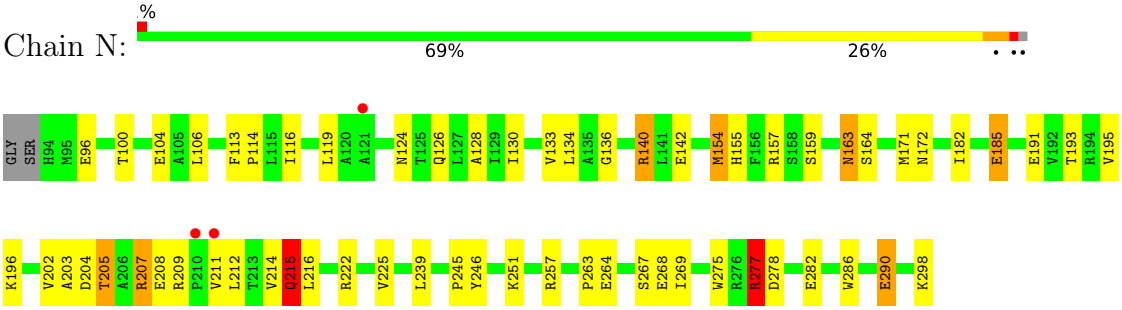


• Molecule 1: HTH-type transcriptional regulator YhaJ



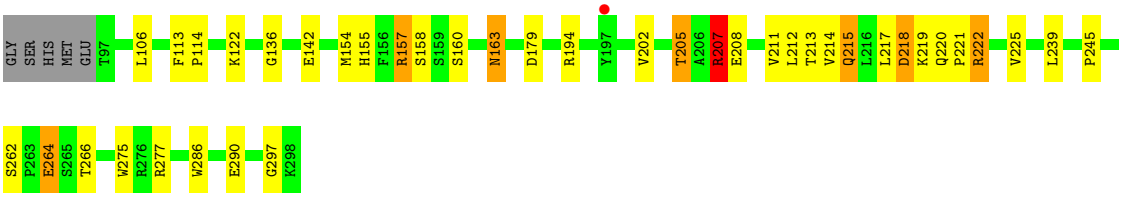
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain N:



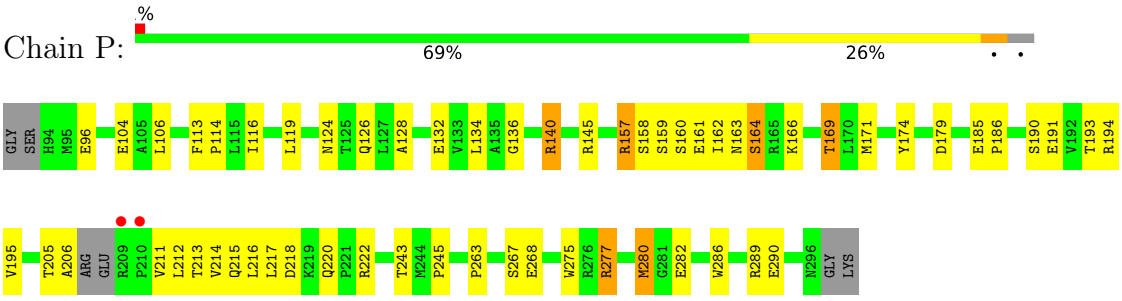
• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain O:



• Molecule 1: HTH-type transcriptional regulator YhaJ

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	215.19Å 215.19Å 263.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.91 – 2.64 36.90 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.0 (36.91-2.64) 99.9 (36.90-2.64)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.177 , 0.236 0.158 , 0.203	Depositor DCC
R_{free} test set	6573 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	54.2	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.220 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.220 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.227 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.227 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.227 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.227 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.256 for h,-h-k,-l	Xtriage

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[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.

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Property	Value	Source
Reported twinning fraction	0.139 for H, K, L 0.135 for K, H, -L 0.124 for -2/3H-1/3K+2/3L, -1/3H-2/3K-2/3L, 2/3H-2/3K+1/3L 0.124 for -1/3H-2/3K-2/3L, -2/3H-1/3K+2/3L, -2/3H+2/3K-1/3L 0.117 for -1/3H+1/3K-2/3L, -K, -4/3H-2/3K+1/3L 0.119 for -K, -1/3H+1/3K-2/3L, 4/3H+2/3K-1/3L 0.120 for 1/3H-1/3K+2/3L, -H, -2/3H-4/3K-1/3L 0.122 for -H, 1/3H-1/3K+2/3L, 2/3H+4/3K+1/3L	Depositor
Outliers	0 of 133605 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25530	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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

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	0.52	1/1615 (0.1%)	0.91	3/2196 (0.1%)
1	B	0.49	0/1624	0.83	3/2209 (0.1%)
1	C	0.56	1/1615 (0.1%)	0.86	4/2196 (0.2%)
1	D	0.53	0/1624	0.86	5/2210 (0.2%)
1	E	0.55	0/1615	0.86	5/2196 (0.2%)
1	F	0.57	1/1637 (0.1%)	0.90	4/2225 (0.2%)
1	G	0.57	3/1615 (0.2%)	0.84	2/2196 (0.1%)
1	H	0.56	1/1624 (0.1%)	0.82	1/2209 (0.0%)
1	I	0.52	0/1606	0.81	1/2185 (0.0%)
1	J	0.52	0/1624	0.82	2/2209 (0.1%)
1	K	0.61	1/1615 (0.1%)	0.85	1/2196 (0.0%)
1	L	0.56	1/1623 (0.1%)	0.84	6/2207 (0.3%)
1	M	0.54	0/1624	0.84	0/2208
1	N	0.61	4/1637 (0.2%)	0.87	6/2225 (0.3%)
1	O	0.51	0/1615	0.89	5/2196 (0.2%)
1	P	0.59	2/1603 (0.1%)	0.88	1/2180 (0.0%)
All	All	0.55	15/25916 (0.1%)	0.86	49/35243 (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	1
1	D	0	1
1	F	0	1
1	I	0	1
All	All	0	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	268	GLU	CD-OE2	8.52	1.35	1.25
1	H	142	GLU	CD-OE2	7.96	1.34	1.25
1	K	187	GLU	CD-OE2	7.52	1.33	1.25
1	N	185	GLU	CD-OE2	7.22	1.33	1.25
1	C	185	GLU	CD-OE2	6.82	1.33	1.25
1	N	142	GLU	CD-OE2	6.72	1.33	1.25
1	N	282	GLU	CD-OE1	6.51	1.32	1.25
1	G	187	GLU	CD-OE2	6.26	1.32	1.25
1	A	161	GLU	CD-OE2	-6.18	1.18	1.25
1	N	290	GLU	CD-OE2	5.87	1.32	1.25
1	P	282	GLU	CD-OE1	5.80	1.32	1.25
1	F	132	GLU	CD-OE1	5.24	1.31	1.25
1	G	139	GLU	CD-OE2	5.10	1.31	1.25
1	G	265	SER	CB-OG	-5.04	1.35	1.42
1	P	161	GLU	CD-OE2	-5.01	1.20	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	157	ARG	CG-CD-NE	8.36	129.34	111.80
1	O	207	ARG	CG-CD-NE	8.21	129.04	111.80
1	D	218	ASP	CB-CG-OD1	7.23	124.81	118.30
1	F	94	HIS	CB-CA-C	6.96	124.33	110.40
1	O	222	ARG	CB-CG-CD	6.93	129.62	111.60
1	C	278	ASP	CB-CG-OD1	-6.75	112.23	118.30
1	H	140	ARG	CG-CD-NE	6.58	125.62	111.80
1	O	264	GLU	CB-CA-C	-6.58	97.24	110.40
1	N	277	ARG	CG-CD-NE	6.44	125.32	111.80
1	C	145	ARG	CG-CD-NE	6.02	124.44	111.80
1	F	194	ARG	CG-CD-NE	5.94	124.28	111.80
1	E	276	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	N	290	GLU	OE1-CD-OE2	-5.80	116.34	123.30
1	L	140	ARG	CG-CD-NE	5.79	123.95	111.80
1	G	174	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	E	157	ARG	CB-CG-CD	5.74	126.53	111.60
1	D	218	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	D	140	ARG	CG-CD-NE	5.67	123.70	111.80
1	L	96	GLU	CB-CA-C	5.62	121.64	110.40
1	P	289	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	L	117	ASP	CB-CG-OD1	5.50	123.25	118.30
1	N	140	ARG	CG-CD-NE	5.49	123.33	111.80
1	B	157	ARG	CB-CG-CD	5.46	125.79	111.60
1	O	194	ARG	CG-CD-NE	5.43	123.20	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	298	LYS	CB-CA-C	5.42	121.24	110.40
1	A	217	LEU	CB-CG-CD1	5.41	120.20	111.00
1	C	140	ARG	CB-CG-CD	-5.39	97.58	111.60
1	K	155	HIS	CB-CA-C	-5.39	99.63	110.40
1	F	145	ARG	CG-CD-NE	-5.35	100.57	111.80
1	N	185	GLU	CA-CB-CG	5.34	125.15	113.40
1	C	194	ARG	CG-CD-NE	5.33	123.00	111.80
1	F	153	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	214	VAL	CA-CB-CG1	5.30	118.85	110.90
1	G	173	VAL	CA-CB-CG1	5.29	118.83	110.90
1	D	194	ARG	CG-CD-NE	5.21	122.75	111.80
1	E	293	LYS	CG-CD-CE	5.21	127.54	111.90
1	L	194	ARG	CB-CG-CD	-5.21	98.06	111.60
1	E	194	ARG	CG-CD-NE	5.15	122.62	111.80
1	D	276	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	J	278	ASP	CB-CG-OD2	5.15	122.93	118.30
1	L	153	ASP	CB-CG-OD1	-5.14	113.68	118.30
1	B	140	ARG	CG-CD-NE	5.13	122.57	111.80
1	J	140	ARG	CG-CD-NE	5.11	122.52	111.80
1	I	204	ASP	CB-CA-C	5.10	120.61	110.40
1	L	145	ARG	CG-CD-NE	-5.10	101.09	111.80
1	N	215	GLN	CA-CB-CG	5.07	124.56	113.40
1	B	195	VAL	CA-CB-CG1	5.05	118.48	110.90
1	A	194	ARG	CG-CD-NE	5.05	122.40	111.80
1	N	207	ARG	CB-CG-CD	5.05	124.72	111.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	HIS	Peptide
1	D	209	ARG	Mainchain
1	F	132	GLU	Sidechain
1	I	156	PHE	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	1584	0	1628	48	0
1	B	1593	0	1630	63	0
1	C	1584	0	1630	68	0
1	D	1593	0	1622	37	1
1	E	1584	0	1630	60	1
1	F	1606	0	1647	47	0
1	G	1584	0	1629	47	1
1	H	1593	0	1630	33	1
1	I	1575	0	1617	49	0
1	J	1593	0	1628	46	0
1	K	1584	0	1630	54	0
1	L	1592	0	1631	64	3
1	M	1593	0	1636	47	2
1	N	1606	0	1647	51	0
1	O	1584	0	1629	32	2
1	P	1573	0	1610	58	3
2	A	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	L	2	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	10	0	0	2	0
3	B	6	0	0	2	0
3	C	4	0	0	1	0
3	D	6	0	0	1	0
3	E	5	0	0	2	0
3	F	4	0	0	0	0
3	G	8	0	0	0	0
3	H	6	0	0	0	0
3	I	7	0	0	4	0
3	J	3	0	0	0	0
3	K	5	0	0	0	0
3	L	8	0	0	5	0
3	M	5	0	0	2	0
3	N	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	8	0	0	0	0
3	P	5	0	0	1	0
All	All	25530	0	26074	669	7

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 13.

All (669) 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:E:98:HIS:HB3	1:F:207:ARG:NH2	1.57	1.20
1:L:296:ASN:OD1	3:L:401:HOH:O	1.61	1.18
1:E:98:HIS:HB3	1:F:207:ARG:CZ	1.76	1.16
1:B:209:ARG:CG	1:B:216:LEU:HD22	1.79	1.13
1:C:185:GLU:OE1	1:C:187:GLU:N	1.85	1.09
1:I:211:VAL:HG22	1:K:207:ARG:HG3	1.35	1.08
1:B:209:ARG:HG3	1:B:216:LEU:HD22	1.08	1.08
1:I:156:PHE:HA	1:K:154:MET:HG3	1.35	1.07
1:P:216:LEU:O	1:P:217:LEU:HG	1.52	1.07
1:C:143:GLN:OE1	1:C:145:ARG:NH1	1.88	1.06
1:J:138:TRP:NE1	1:J:154:MET:SD	2.27	1.05
1:G:207:ARG:NH1	1:H:100:THR:OG1	1.91	1.04
1:B:95:MET:SD	1:D:276:ARG:NH1	2.30	1.03
1:B:216:LEU:HD23	1:B:222:ARG:HD3	1.40	1.02
1:B:273:MET:HE2	1:B:288:LEU:HD23	1.41	1.02
1:B:209:ARG:HG3	1:B:216:LEU:CD2	1.91	0.99
1:A:212:LEU:HB3	1:C:139:GLU:OE2	1.61	0.98
1:P:159:SER:HB3	1:P:162:ILE:HG12	1.46	0.97
1:O:262:SER:OG	1:O:264:GLU:HG3	1.65	0.95
1:B:216:LEU:CD2	1:B:222:ARG:HD3	1.97	0.95
1:P:194:ARG:HB2	1:P:217:LEU:CD1	1.96	0.95
1:L:249:VAL:O	1:L:253:ILE:HD12	1.67	0.93
1:M:134:LEU:HA	1:M:154:MET:HE1	1.51	0.93
1:O:221:PRO:HA	1:P:126:GLN:NE2	1.84	0.92
1:I:206:ALA:HB2	1:J:145:ARG:HH12	1.34	0.91
1:M:139:GLU:OE1	3:M:401:HOH:O	1.88	0.90
1:I:211:VAL:HG22	1:K:207:ARG:CG	2.01	0.90
1:D:199:GLY:HA3	1:D:216:LEU:HD21	1.54	0.89
1:L:185:GLU:HG2	1:L:193:THR:HG21	1.54	0.89
1:E:208:GLU:OE2	1:E:209:ARG:NH1	2.06	0.89
1:J:138:TRP:CD1	1:J:154:MET:SD	2.66	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:280:MET:HA	3:P:401:HOH:O	1.74	0.87
1:K:157:ARG:NH2	1:K:162:ILE:O	2.08	0.87
1:J:214:VAL:HG22	1:J:243:THR:HB	1.57	0.87
1:B:203:ALA:HA	3:B:304:HOH:O	1.74	0.86
1:P:157:ARG:HA	1:P:162:ILE:HD11	1.57	0.86
1:J:251:LYS:HD3	1:J:257:ARG:HH22	1.40	0.86
1:B:94:HIS:HA	1:D:161:GLU:OE2	1.76	0.86
1:B:193:THR:HA	1:B:196:LYS:NZ	1.91	0.85
1:K:136:GLY:HA3	1:K:205:THR:HB	1.58	0.85
1:M:168:TYR:HB2	1:M:298:LYS:HD2	1.59	0.85
1:P:194:ARG:HB2	1:P:217:LEU:HD11	1.61	0.82
1:D:161:GLU:HB2	1:D:276:ARG:NH2	1.94	0.82
1:B:209:ARG:CD	1:B:216:LEU:HD22	2.10	0.82
1:A:156:PHE:HD1	1:C:154:MET:SD	2.03	0.82
1:G:155:HIS:O	1:G:157:ARG:NH1	2.13	0.81
1:I:153:ASP:O	1:K:158:SER:HB3	1.80	0.81
1:I:156:PHE:CZ	1:K:211:VAL:HG12	2.14	0.81
1:E:156:PHE:HB3	1:E:157:ARG:NH2	1.96	0.81
1:K:239:LEU:HD11	1:L:113:PHE:HB3	1.61	0.81
1:I:156:PHE:CA	1:K:154:MET:HG3	2.10	0.81
1:F:246:TYR:CD1	1:N:263:PRO:HG2	2.16	0.80
1:C:185:GLU:OE1	1:C:187:GLU:C	2.19	0.80
1:E:156:PHE:HD1	1:E:157:ARG:HE	1.26	0.80
1:C:185:GLU:HG3	1:C:193:THR:HG21	1.64	0.80
1:K:252:ASP:OD1	1:K:257:ARG:NH1	2.15	0.80
1:O:239:LEU:HD13	1:P:116:ILE:HD12	1.64	0.80
1:M:159:SER:O	1:M:162:ILE:HG22	1.81	0.79
1:G:211:VAL:HG22	1:G:216:LEU:HD22	1.65	0.79
1:G:211:VAL:CG2	1:G:216:LEU:HD22	2.13	0.78
1:P:195:VAL:HA	1:P:220:GLN:HG3	1.63	0.78
1:B:273:MET:HE3	1:B:291:ILE:HD12	1.63	0.78
1:M:185:GLU:HG2	1:M:193:THR:HG21	1.65	0.78
1:C:135:ALA:HB3	1:C:206:ALA:HB3	1.64	0.78
1:C:139:GLU:HG3	1:C:207:ARG:HH21	1.47	0.78
1:G:134:LEU:HD12	1:G:204:ASP:OD1	1.84	0.77
1:I:191:GLU:OE2	3:I:401:HOH:O	2.02	0.77
1:K:139:GLU:OE1	1:K:206:ALA:HB3	1.85	0.77
1:F:246:TYR:CE1	1:N:263:PRO:HG3	2.20	0.77
1:A:212:LEU:HD13	1:C:139:GLU:OE2	1.85	0.77
1:E:206:ALA:O	1:F:140:ARG:NH1	2.17	0.77
1:K:221:PRO:HA	1:L:126:GLN:NE2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASP:OD1	1:C:257:ARG:NH1	2.19	0.76
1:G:252:ASP:OD1	1:G:257:ARG:NH1	2.18	0.76
1:N:133:VAL:HG21	1:N:203:ALA:O	1.85	0.76
1:E:98:HIS:CB	1:F:207:ARG:CZ	2.62	0.76
1:O:221:PRO:HA	1:P:126:GLN:HE22	1.51	0.76
1:P:194:ARG:HB2	1:P:217:LEU:HD12	1.66	0.75
1:M:138:TRP:HB3	1:M:156:PHE:CD1	2.21	0.75
1:P:216:LEU:O	1:P:217:LEU:CG	2.33	0.75
1:A:277:ARG:HG3	1:A:277:ARG:O	1.86	0.75
1:C:185:GLU:CD	1:C:187:GLU:H	1.90	0.75
1:K:221:PRO:HA	1:L:126:GLN:HE22	1.52	0.75
1:F:251:LYS:HE2	1:F:257:ARG:HH22	1.52	0.75
1:B:193:THR:HA	1:B:196:LYS:HZ3	1.53	0.73
1:M:133:VAL:HG12	1:M:134:LEU:HG	1.70	0.73
1:B:201:ALA:HB2	1:B:216:LEU:HD21	1.70	0.73
1:D:108:PRO:HD3	3:D:404:HOH:O	1.89	0.73
1:L:185:GLU:HG2	1:L:193:THR:CG2	2.19	0.73
1:J:143:GLN:HG2	1:L:96:GLU:OE2	1.88	0.73
1:C:208:GLU:HB3	1:C:211:VAL:HG22	1.70	0.73
1:B:273:MET:CE	1:B:291:ILE:HD12	2.19	0.72
1:C:140:ARG:HH12	1:D:207:ARG:HH21	1.38	0.72
1:L:213:THR:HG21	1:L:243:THR:CB	2.19	0.72
1:E:207:ARG:HA	1:F:140:ARG:HH22	1.55	0.72
1:C:157:ARG:HB3	1:C:160:SER:HA	1.71	0.72
1:M:211:VAL:HG12	1:M:212:LEU:H	1.55	0.72
1:A:214:VAL:HG13	1:A:215:GLN:HG3	1.71	0.71
1:M:195:VAL:HB	1:M:217:LEU:HD23	1.72	0.71
1:O:222:ARG:HH12	1:P:128:ALA:HB2	1.55	0.71
1:F:209:ARG:HD2	1:F:216:LEU:HD13	1.72	0.70
1:O:218:ASP:OD1	1:O:219:LYS:N	2.24	0.70
1:I:243:THR:HG22	3:I:405:HOH:O	1.90	0.70
1:B:290:GLU:HA	1:B:293:LYS:HD2	1.73	0.69
1:I:155:HIS:CD2	1:K:156:PHE:O	2.45	0.69
1:J:167:LEU:HD21	1:J:273:MET:HE1	1.74	0.69
1:A:154:MET:SD	1:C:209:ARG:NH2	2.66	0.69
1:B:194:ARG:NH2	1:B:217:LEU:HD21	2.07	0.69
1:I:210:PRO:HG3	1:I:222:ARG:NH2	2.07	0.69
1:F:246:TYR:CD1	1:N:263:PRO:CG	2.74	0.69
1:G:173:VAL:HG21	1:G:260:VAL:HG22	1.73	0.69
1:L:172:ASN:HD22	1:L:243:THR:HG22	1.57	0.69
1:B:209:ARG:HD2	1:B:222:ARG:NH1	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLY:HA2	1:A:205:THR:HG23	1.75	0.68
1:L:133:VAL:HB	3:L:403:HOH:O	1.92	0.68
1:O:205:THR:O	1:O:207:ARG:NH1	2.27	0.68
1:L:213:THR:HG21	1:L:243:THR:HB	1.74	0.68
1:B:273:MET:CE	1:B:288:LEU:HD23	2.22	0.67
1:D:96:GLU:HA	1:D:124:ASN:HB3	1.76	0.67
1:K:157:ARG:HB3	1:K:160:SER:HA	1.74	0.67
1:B:161:GLU:HA	1:B:277:ARG:HE	1.58	0.67
1:M:185:GLU:HG3	1:M:187:GLU:H	1.59	0.67
1:A:203:ALA:HB1	1:A:207:ARG:O	1.95	0.67
1:G:172:ASN:HD22	1:G:243:THR:HG22	1.58	0.67
1:E:298:LYS:HE3	1:G:293:LYS:NZ	2.10	0.67
1:F:157:ARG:HD3	1:F:272:ILE:CD1	2.25	0.67
1:I:97:THR:HG21	3:I:403:HOH:O	1.94	0.67
1:K:239:LEU:HD13	1:L:116:ILE:HD12	1.76	0.67
1:E:156:PHE:HB3	1:E:157:ARG:HH21	1.60	0.66
1:F:157:ARG:HD3	1:F:272:ILE:HD12	1.76	0.66
1:A:212:LEU:HD13	1:C:139:GLU:OE1	1.95	0.66
1:I:154:MET:O	1:K:156:PHE:HB3	1.95	0.66
1:I:142:GLU:OE2	1:I:162:ILE:HD11	1.94	0.66
1:A:212:LEU:HD13	1:C:139:GLU:CD	2.16	0.66
1:N:193:THR:HA	1:N:196:LYS:HD2	1.77	0.66
1:F:246:TYR:CE1	1:N:263:PRO:CG	2.78	0.65
1:I:210:PRO:HG3	1:I:222:ARG:HH22	1.60	0.65
1:L:189:LEU:O	1:L:194:ARG:NE	2.29	0.65
1:A:212:LEU:CB	1:C:139:GLU:OE2	2.40	0.65
1:E:239:LEU:HD11	1:F:113:PHE:HB3	1.79	0.65
1:I:158:SER:HA	1:K:153:ASP:O	1.97	0.65
1:I:211:VAL:CG2	1:K:207:ARG:HG3	2.18	0.65
1:E:160:SER:OG	1:E:276:ARG:NH1	2.29	0.65
1:B:209:ARG:HD2	1:B:222:ARG:CZ	2.27	0.65
1:F:246:TYR:CG	1:N:263:PRO:HG2	2.32	0.65
1:L:243:THR:HG22	3:L:402:HOH:O	1.95	0.65
1:N:211:VAL:HG13	1:N:215:GLN:HG3	1.78	0.65
1:B:216:LEU:HD23	1:B:222:ARG:CD	2.23	0.64
1:C:153:ASP:OD1	1:C:155:HIS:ND1	2.29	0.64
1:I:156:PHE:CD1	1:K:208:GLU:OE1	2.50	0.64
1:P:185:GLU:HG2	1:P:193:THR:CG2	2.27	0.64
1:H:139:GLU:OE1	1:H:206:ALA:HB1	1.97	0.64
1:O:262:SER:HG	1:O:264:GLU:HG3	1.61	0.64
1:D:161:GLU:HB2	1:D:276:ARG:HH21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:PHE:CE2	1:K:211:VAL:HG12	2.33	0.64
1:J:139:GLU:HG3	1:J:207:ARG:HG3	1.79	0.64
1:L:172:ASN:ND2	3:L:402:HOH:O	2.29	0.64
1:M:206:ALA:O	1:N:140:ARG:NH1	2.25	0.64
1:N:215:GLN:H	1:N:215:GLN:CD	2.01	0.64
1:F:251:LYS:HE2	1:F:257:ARG:NH2	2.11	0.63
1:A:153:ASP:O	1:C:158:SER:HB3	1.99	0.63
1:G:207:ARG:HH11	1:H:100:THR:HG1	1.46	0.63
1:J:133:VAL:H	1:J:205:THR:HG21	1.64	0.63
1:E:157:ARG:HG2	1:E:159:SER:HB2	1.80	0.63
1:P:96:GLU:HA	1:P:124:ASN:HB3	1.81	0.63
1:K:198:ARG:CZ	1:L:116:ILE:HG22	2.27	0.63
1:M:195:VAL:HB	1:M:217:LEU:CD2	2.28	0.63
1:I:212:LEU:HD11	1:I:216:LEU:O	1.99	0.63
1:M:138:TRP:HE1	1:M:154:MET:HG3	1.64	0.63
1:D:216:LEU:HD12	1:D:222:ARG:CZ	2.29	0.63
1:K:266:THR:HG21	1:M:122:LYS:HA	1.81	0.62
1:E:162:ILE:HD13	1:E:276:ARG:HG2	1.79	0.62
1:C:185:GLU:OE1	1:C:188:PRO:N	2.32	0.62
1:E:204:ASP:HB3	1:E:207:ARG:HH12	1.63	0.62
1:N:215:GLN:OE1	1:N:215:GLN:N	2.23	0.62
1:P:159:SER:CB	1:P:162:ILE:HG12	2.27	0.62
1:E:126:GLN:OE1	1:F:222:ARG:NE	2.32	0.62
1:I:126:GLN:HE22	1:J:221:PRO:HA	1.64	0.62
1:N:185:GLU:CG	1:N:193:THR:HG21	2.30	0.62
1:K:153:ASP:OD1	1:K:155:HIS:HB2	2.00	0.61
1:O:239:LEU:HD13	1:P:116:ILE:CD1	2.29	0.61
1:L:218:ASP:N	1:L:218:ASP:OD2	2.32	0.61
1:L:232:ARG:NH1	1:L:252:ASP:OD2	2.33	0.61
1:I:276:ARG:HB2	3:I:402:HOH:O	2.01	0.61
1:M:134:LEU:CA	1:M:154:MET:HE1	2.29	0.61
1:L:213:THR:CG2	1:L:243:THR:OG1	2.49	0.61
1:A:160:SER:O	1:A:161:GLU:HG2	2.01	0.61
1:C:185:GLU:OE1	1:C:187:GLU:CA	2.48	0.61
1:C:140:ARG:HH12	1:D:207:ARG:NH2	1.98	0.61
1:C:185:GLU:CG	1:C:193:THR:HG21	2.31	0.61
1:I:206:ALA:CB	1:J:145:ARG:HH12	2.12	0.61
1:N:191:GLU:O	1:N:195:VAL:HG23	2.00	0.61
1:P:194:ARG:NH2	1:P:217:LEU:HD21	2.15	0.61
1:B:215:GLN:C	1:B:216:LEU:HD12	2.21	0.60
1:L:189:LEU:O	1:L:194:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:277:ARG:O	1:P:277:ARG:HG2	1.98	0.60
1:J:211:VAL:H	1:J:215:GLN:HE22	1.50	0.60
1:L:290:GLU:OE2	1:L:293:LYS:HD2	2.01	0.60
1:O:217:LEU:H	1:O:220:GLN:NE2	1.99	0.60
1:E:159:SER:OG	1:E:160:SER:N	2.30	0.60
1:E:205:THR:H	1:E:207:ARG:NH1	2.00	0.60
1:N:154:MET:HG3	1:N:155:HIS:H	1.65	0.60
1:B:218:ASP:O	1:B:219:LYS:HG2	2.02	0.60
1:J:211:VAL:HG12	1:J:213:THR:H	1.67	0.59
1:E:157:ARG:HD2	1:E:157:ARG:O	2.02	0.59
1:H:133:VAL:O	1:H:205:THR:HA	2.02	0.59
1:O:217:LEU:H	1:O:220:GLN:HE21	1.50	0.59
1:B:108:PRO:HD3	3:B:305:HOH:O	2.03	0.59
1:B:134:LEU:HD21	1:B:211:VAL:HG21	1.85	0.59
1:J:276:ARG:HE	1:L:95:MET:HE2	1.67	0.59
1:K:184:GLN:N	1:K:184:GLN:OE1	2.36	0.59
1:M:162:ILE:O	1:M:162:ILE:HG23	2.01	0.59
1:B:160:SER:OG	1:B:161:GLU:OE1	2.19	0.59
1:C:139:GLU:CG	1:C:207:ARG:HH21	2.16	0.59
1:M:205:THR:HG21	3:M:401:HOH:O	2.02	0.58
1:P:174:TYR:CE1	1:P:214:VAL:HG11	2.38	0.58
1:A:156:PHE:HA	1:C:154:MET:SD	2.43	0.58
1:F:209:ARG:O	1:F:209:ARG:HG2	2.02	0.58
1:P:212:LEU:HB2	1:P:215:GLN:HA	1.84	0.58
1:G:134:LEU:HD13	1:G:212:LEU:HB3	1.86	0.58
1:I:209:ARG:HB3	1:K:207:ARG:H	1.68	0.58
1:L:290:GLU:OE2	1:L:290:GLU:HA	2.03	0.58
1:P:216:LEU:C	1:P:217:LEU:HG	2.23	0.58
1:L:172:ASN:HD22	1:L:243:THR:CG2	2.16	0.57
1:J:139:GLU:HG3	1:J:207:ARG:CG	2.34	0.57
1:O:213:THR:HG22	1:O:214:VAL:H	1.68	0.57
1:I:156:PHE:HA	1:K:154:MET:CG	2.20	0.57
1:K:198:ARG:CZ	1:L:116:ILE:CG2	2.83	0.57
1:F:191:GLU:O	1:F:195:VAL:HG23	2.03	0.57
1:B:134:LEU:CD2	1:B:211:VAL:HG21	2.35	0.57
1:F:169:THR:HG22	1:F:171:MET:HE2	1.87	0.57
1:P:185:GLU:HG2	1:P:193:THR:HG21	1.86	0.57
1:A:217:LEU:H	1:A:220:GLN:NE2	2.03	0.57
1:L:96:GLU:HA	1:L:124:ASN:HB3	1.87	0.57
1:B:193:THR:HA	1:B:196:LYS:HZ2	1.68	0.56
1:P:132:GLU:OE2	1:P:140:ARG:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LEU:HB2	1:C:215:GLN:HA	1.86	0.56
1:I:155:HIS:O	1:I:156:PHE:HB2	2.04	0.56
1:P:140:ARG:HD2	1:P:145:ARG:NH1	2.20	0.56
1:A:156:PHE:CG	1:A:157:ARG:N	2.73	0.56
1:G:172:ASN:HD22	1:G:243:THR:CG2	2.19	0.56
1:I:133:VAL:HG12	1:I:134:LEU:HG	1.86	0.56
1:I:210:PRO:CG	1:I:222:ARG:HH22	2.19	0.56
1:L:213:THR:HG22	1:L:214:VAL:H	1.69	0.56
1:E:169:THR:O	1:E:298:LYS:HE2	2.06	0.56
1:N:100:THR:HG23	1:N:130:ILE:HD13	1.88	0.56
1:A:207:ARG:O	1:A:210:PRO:HD2	2.06	0.56
1:D:263:PRO:HB2	1:P:171:MET:HG3	1.87	0.56
1:G:173:VAL:CG2	1:G:260:VAL:HG22	2.36	0.56
1:L:213:THR:HG21	1:L:243:THR:OG1	2.06	0.56
1:O:157:ARG:HA	1:O:157:ARG:HH11	1.70	0.56
1:B:96:GLU:HA	1:B:124:ASN:HB3	1.88	0.56
1:F:194:ARG:NH2	1:F:215:GLN:O	2.38	0.56
1:A:135:ALA:HA	1:C:209:ARG:HE	1.70	0.55
1:I:156:PHE:HD2	1:I:157:ARG:H	1.53	0.55
1:B:273:MET:HE3	1:B:291:ILE:CD1	2.34	0.55
1:G:204:ASP:HB2	1:G:209:ARG:HB3	1.88	0.55
1:G:157:ARG:HD3	1:G:157:ARG:N	2.20	0.55
1:J:139:GLU:CD	1:J:207:ARG:HG2	2.27	0.55
1:J:276:ARG:NE	1:L:95:MET:HE2	2.21	0.55
1:P:169:THR:HG23	1:P:268:GLU:HG2	1.89	0.55
1:C:135:ALA:CB	1:C:206:ALA:HB3	2.36	0.55
1:A:217:LEU:H	1:A:220:GLN:HE21	1.54	0.55
1:F:96:GLU:HA	1:F:124:ASN:HB3	1.89	0.55
1:N:185:GLU:HG2	1:N:193:THR:HG21	1.87	0.55
1:N:209:ARG:HE	1:N:222:ARG:HH12	1.54	0.55
1:I:104:GLU:OE2	1:I:134:LEU:HD23	2.07	0.55
1:J:143:GLN:HA	1:L:96:GLU:CG	2.37	0.55
1:M:266:THR:HG21	1:O:122:LYS:HA	1.89	0.55
1:O:205:THR:HB	1:O:207:ARG:HH12	1.72	0.55
1:A:207:ARG:HG2	1:B:145:ARG:HH12	1.72	0.55
1:G:206:ALA:HB1	1:H:140:ARG:HH12	1.72	0.55
1:G:211:VAL:HG22	1:G:216:LEU:CD2	2.36	0.55
1:G:138:TRP:CE2	1:G:154:MET:HG3	2.42	0.55
1:G:207:ARG:NH1	1:H:100:THR:HG1	1.99	0.55
1:N:104:GLU:OE2	1:N:134:LEU:HD22	2.07	0.55
1:A:136:GLY:CA	1:A:205:THR:HG23	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:GLY:HA2	1:E:296:ASN:HD22	1.72	0.54
1:E:277:ARG:NH1	1:E:280:MET:SD	2.80	0.54
1:E:134:LEU:HD21	3:E:305:HOH:O	2.07	0.54
1:H:104:GLU:OE2	1:H:134:LEU:HD22	2.06	0.54
1:M:104:GLU:OE2	1:M:134:LEU:HD23	2.08	0.54
1:M:142:GLU:HG2	1:M:156:PHE:CE1	2.42	0.54
1:P:162:ILE:HG13	1:P:162:ILE:O	2.06	0.54
1:C:139:GLU:OE1	1:C:206:ALA:HB2	2.08	0.54
1:O:221:PRO:HA	1:P:126:GLN:HE21	1.70	0.54
1:L:104:GLU:OE2	1:L:134:LEU:HD22	2.08	0.54
1:E:243:THR:HG22	3:E:304:HOH:O	2.08	0.54
1:M:172:ASN:ND2	1:M:269:ILE:HD12	2.23	0.54
1:B:273:MET:HE1	1:B:288:LEU:HA	1.90	0.53
1:E:156:PHE:HD1	1:E:157:ARG:NE	2.03	0.53
1:E:104:GLU:OE2	1:E:134:LEU:HD23	2.07	0.53
1:P:104:GLU:OE2	1:P:134:LEU:HD22	2.08	0.53
1:P:185:GLU:HG3	1:P:186:PRO:HD2	1.90	0.53
1:J:143:GLN:HA	1:L:96:GLU:HG3	1.91	0.53
1:H:171:MET:CE	1:H:268:GLU:HG2	2.39	0.53
1:C:157:ARG:NH2	1:C:160:SER:HB3	2.24	0.53
1:C:266:THR:HG21	1:E:122:LYS:HA	1.91	0.53
1:L:294:LEU:HB2	1:L:295:PHE:CE1	2.44	0.53
1:G:155:HIS:O	1:G:157:ARG:CZ	2.57	0.53
1:A:205:THR:O	1:A:207:ARG:NE	2.42	0.52
1:A:213:THR:O	1:A:214:VAL:HB	2.09	0.52
1:B:143:GLN:HA	1:D:96:GLU:HG3	1.92	0.52
1:F:172:ASN:ND2	1:F:269:ILE:HD12	2.24	0.52
1:M:116:ILE:HD12	1:N:239:LEU:HD13	1.90	0.52
1:C:208:GLU:O	1:C:211:VAL:HG22	2.09	0.52
1:E:133:VAL:HG12	1:E:134:LEU:HG	1.92	0.52
1:E:298:LYS:HE3	1:G:293:LYS:HZ2	1.75	0.52
1:B:189:LEU:HD21	1:B:262:SER:HB3	1.90	0.52
1:P:106:LEU:HD22	1:P:245:PRO:HG3	1.91	0.52
1:G:213:THR:HG21	1:G:216:LEU:HB2	1.91	0.52
1:D:172:ASN:ND2	1:D:269:ILE:HD12	2.25	0.52
1:F:171:MET:HE3	1:N:264:GLU:HG3	1.91	0.52
1:G:239:LEU:HD13	1:H:116:ILE:HD12	1.92	0.52
1:I:156:PHE:O	1:K:156:PHE:CD2	2.62	0.52
1:N:154:MET:CG	1:N:155:HIS:N	2.73	0.52
1:B:204:ASP:OD2	1:B:204:ASP:N	2.41	0.52
1:H:96:GLU:HA	1:H:124:ASN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:286:TRP:CZ2	1:J:290:GLU:HG3	2.45	0.52
1:M:185:GLU:HG3	1:M:187:GLU:N	2.24	0.52
1:K:295:PHE:O	1:K:298:LYS:HG2	2.10	0.52
1:L:171:MET:CE	1:L:268:GLU:HG2	2.40	0.52
1:B:209:ARG:HG3	1:B:216:LEU:CG	2.38	0.51
1:D:133:VAL:HB	1:D:204:ASP:HA	1.93	0.51
1:C:277:ARG:HG2	1:C:277:ARG:HH11	1.75	0.51
1:L:189:LEU:C	1:L:194:ARG:HE	2.14	0.51
1:N:96:GLU:HA	1:N:124:ASN:HB3	1.93	0.51
1:P:185:GLU:HG2	1:P:193:THR:HG23	1.93	0.51
1:A:159:SER:HA	1:C:156:PHE:HE2	1.75	0.51
1:N:286:TRP:CZ2	1:N:290:GLU:HG3	2.46	0.51
1:E:133:VAL:HB	1:E:204:ASP:O	2.09	0.51
1:J:208:GLU:OE2	1:J:210:PRO:HD2	2.10	0.51
1:K:122:LYS:HA	1:O:266:THR:HG21	1.92	0.51
1:N:172:ASN:ND2	1:N:269:ILE:HD12	2.25	0.51
1:J:159:SER:C	1:J:161:GLU:H	2.13	0.51
1:N:133:VAL:HG23	1:N:205:THR:H	1.75	0.51
1:N:212:LEU:C	1:N:215:GLN:NE2	2.64	0.51
1:N:209:ARG:NE	1:N:222:ARG:HH12	2.09	0.51
1:P:136:GLY:HA2	1:P:206:ALA:HB3	1.93	0.51
1:P:277:ARG:O	1:P:277:ARG:CG	2.58	0.51
1:G:134:LEU:CD1	1:G:212:LEU:HB3	2.41	0.50
1:M:211:VAL:HG12	1:M:212:LEU:N	2.25	0.50
1:G:214:VAL:O	1:G:215:GLN:NE2	2.44	0.50
1:D:286:TRP:CZ2	1:D:290:GLU:HG3	2.46	0.50
1:G:139:GLU:O	1:G:143:GLN:HG3	2.11	0.50
1:K:134:LEU:HD13	1:K:211:VAL:HG13	1.92	0.50
1:C:122:LYS:HA	1:G:266:THR:HG21	1.93	0.50
1:M:138:TRP:HE1	1:M:154:MET:HE2	1.77	0.50
1:D:171:MET:CE	1:D:268:GLU:HG2	2.41	0.50
1:P:286:TRP:CZ2	1:P:290:GLU:HG3	2.47	0.50
1:G:286:TRP:CZ2	1:G:290:GLU:HG3	2.47	0.50
1:L:106:LEU:HD22	1:L:245:PRO:HG3	1.94	0.50
1:A:156:PHE:CD1	1:C:154:MET:SD	2.94	0.49
1:D:209:ARG:O	1:D:211:VAL:HG12	2.11	0.49
1:A:212:LEU:CD1	1:C:139:GLU:OE2	2.58	0.49
1:C:116:ILE:HD12	1:D:239:LEU:HD13	1.94	0.49
1:C:154:MET:O	1:C:156:PHE:CD2	2.65	0.49
1:O:239:LEU:HD11	1:P:113:PHE:HB3	1.93	0.49
1:B:209:ARG:HD3	1:B:216:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:138:TRP:NE1	1:G:154:MET:HG3	2.27	0.49
1:K:296:ASN:OD1	1:O:297:GLY:HA2	2.12	0.49
1:P:157:ARG:HE	1:P:164:SER:HB2	1.78	0.49
1:A:135:ALA:HA	1:C:209:ARG:NE	2.28	0.49
1:H:133:VAL:HB	1:H:204:ASP:O	2.12	0.49
1:A:212:LEU:HD12	1:C:206:ALA:HA	1.93	0.49
1:B:216:LEU:HD12	1:B:216:LEU:N	2.27	0.49
1:H:286:TRP:CZ2	1:H:290:GLU:HG3	2.48	0.49
1:N:211:VAL:CG1	1:N:215:GLN:HG3	2.42	0.49
1:C:289:ARG:NH2	1:G:268:GLU:OE1	2.45	0.49
1:D:209:ARG:HG2	1:D:210:PRO:N	2.27	0.49
1:B:189:LEU:N	1:B:189:LEU:HD22	2.27	0.49
1:E:275:TRP:HE1	1:E:277:ARG:NH1	2.11	0.49
1:I:155:HIS:HA	1:K:156:PHE:HB2	1.94	0.49
1:M:203:ALA:HB1	1:M:207:ARG:H	1.78	0.49
1:O:136:GLY:CA	1:O:205:THR:HG23	2.42	0.49
1:F:106:LEU:HD22	1:F:245:PRO:HG3	1.95	0.49
1:K:286:TRP:CZ2	1:K:290:GLU:HG3	2.48	0.49
1:M:138:TRP:HB3	1:M:156:PHE:HD1	1.75	0.49
1:E:286:TRP:CZ2	1:E:290:GLU:HG3	2.47	0.48
1:M:156:PHE:CG	1:M:157:ARG:N	2.81	0.48
1:A:194:ARG:HH11	1:A:215:GLN:HA	1.78	0.48
1:E:266:THR:HG21	1:G:122:LYS:HA	1.95	0.48
1:E:298:LYS:HE3	1:G:293:LYS:HZ3	1.76	0.48
1:G:217:LEU:HG	1:G:218:ASP:N	2.29	0.48
1:G:223:LEU:HD22	1:H:116:ILE:HD13	1.95	0.48
1:E:198:ARG:CZ	1:F:116:ILE:HG22	2.44	0.48
1:L:286:TRP:CZ2	1:L:290:GLU:HG3	2.48	0.48
1:A:286:TRP:CZ2	1:A:290:GLU:HG3	2.48	0.48
1:E:207:ARG:HA	1:F:140:ARG:NH2	2.25	0.48
1:I:286:TRP:CZ2	1:I:290:GLU:HG3	2.48	0.48
1:P:136:GLY:HA3	1:P:205:THR:OG1	2.12	0.48
1:P:212:LEU:HB2	1:P:215:GLN:CA	2.43	0.48
1:A:198:ARG:NE	3:A:402:HOH:O	2.32	0.48
1:B:148:ILE:HG21	1:B:273:MET:HE3	1.95	0.48
1:D:294:LEU:HB2	1:D:295:PHE:CE1	2.48	0.48
1:I:211:VAL:HG22	1:K:207:ARG:HG2	1.93	0.48
1:M:156:PHE:CE2	1:M:162:ILE:HD12	2.49	0.48
1:H:135:ALA:HB3	1:H:208:GLU:HG2	1.95	0.48
1:F:162:ILE:HG12	1:F:276:ARG:HG2	1.95	0.48
1:L:165:ARG:HG3	1:L:275:TRP:CH2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:211:VAL:HG12	1:J:212:LEU:N	2.29	0.47
1:O:286:TRP:CZ2	1:O:290:GLU:HG3	2.48	0.47
1:C:130:ILE:HG13	1:D:207:ARG:HH22	1.78	0.47
1:J:280:MET:O	1:L:279:SER:HA	2.14	0.47
1:N:154:MET:CG	1:N:155:HIS:H	2.26	0.47
1:B:119:LEU:HG	1:B:286:TRP:CZ3	2.49	0.47
1:C:286:TRP:CZ2	1:C:290:GLU:HG3	2.48	0.47
1:M:169:THR:O	1:M:298:LYS:NZ	2.39	0.47
1:M:239:LEU:HD13	1:N:116:ILE:HD12	1.96	0.47
1:N:119:LEU:HG	1:N:286:TRP:CZ3	2.49	0.47
1:P:213:THR:HB	1:P:243:THR:HG21	1.96	0.47
1:F:171:MET:CE	1:N:264:GLU:HG3	2.45	0.47
1:J:134:LEU:HD11	1:J:211:VAL:HG13	1.95	0.47
1:M:106:LEU:HD22	1:M:245:PRO:HG3	1.97	0.47
1:B:148:ILE:HG21	1:B:273:MET:CE	2.45	0.47
1:E:276:ARG:NH2	1:E:278:ASP:OD2	2.43	0.47
1:J:207:ARG:HD3	1:J:208:GLU:HB2	1.97	0.47
1:O:212:LEU:HD23	1:O:213:THR:O	2.13	0.47
1:C:160:SER:O	1:C:162:ILE:HG13	2.14	0.47
1:C:295:PHE:HA	1:C:298:LYS:HD3	1.95	0.47
1:D:119:LEU:HG	1:D:286:TRP:CZ3	2.50	0.47
1:J:96:GLU:HA	1:J:124:ASN:HB3	1.97	0.47
1:N:133:VAL:HG23	1:N:204:ASP:HA	1.96	0.47
1:E:280:MET:HE3	1:E:280:MET:HA	1.96	0.47
1:O:136:GLY:HA2	1:O:205:THR:HG23	1.97	0.47
1:G:136:GLY:HA3	1:G:205:THR:HB	1.97	0.47
1:K:106:LEU:HD22	1:K:245:PRO:HG3	1.97	0.47
1:E:160:SER:HG	1:E:276:ARG:NH1	2.12	0.47
1:A:160:SER:O	1:A:162:ILE:HG12	2.15	0.47
1:N:171:MET:CE	1:N:268:GLU:HG2	2.45	0.47
1:O:213:THR:HG22	1:O:214:VAL:N	2.30	0.47
1:C:268:GLU:OE2	1:E:289:ARG:NH2	2.48	0.46
1:E:226:SER:HB2	1:F:131:THR:H	1.81	0.46
1:M:286:TRP:CZ2	1:M:290:GLU:HG3	2.50	0.46
1:H:119:LEU:HG	1:H:286:TRP:CZ3	2.50	0.46
1:M:189:LEU:CD2	1:M:262:SER:HB3	2.45	0.46
1:E:162:ILE:HD13	1:E:276:ARG:CG	2.45	0.46
1:E:239:LEU:HD13	1:F:116:ILE:HD12	1.98	0.46
1:G:207:ARG:HH22	1:H:98:HIS:HB3	1.79	0.46
1:J:119:LEU:HG	1:J:286:TRP:CZ3	2.51	0.46
1:J:160:SER:C	1:J:161:GLU:HG3	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:282:GLU:HA	1:K:282:GLU:OE1	2.15	0.46
1:L:119:LEU:HG	1:L:286:TRP:CZ3	2.51	0.46
1:P:140:ARG:HD2	1:P:145:ARG:HH12	1.80	0.46
1:D:273:MET:HE1	1:D:291:ILE:HB	1.97	0.46
1:K:239:LEU:HD11	1:L:113:PHE:CB	2.41	0.46
1:E:209:ARG:NE	1:E:210:PRO:HD2	2.30	0.46
1:F:119:LEU:HG	1:F:286:TRP:CZ3	2.50	0.46
1:P:119:LEU:HG	1:P:286:TRP:CZ3	2.51	0.46
1:B:286:TRP:CZ2	1:B:290:GLU:HG3	2.51	0.46
1:M:189:LEU:HD21	1:M:262:SER:HB3	1.97	0.46
1:M:277:ARG:HA	1:M:277:ARG:HD3	1.69	0.46
1:A:106:LEU:HD22	1:A:245:PRO:HG3	1.97	0.46
1:C:138:TRP:CE2	1:C:154:MET:HG2	2.51	0.46
1:C:209:ARG:HB3	1:C:210:PRO:HD3	1.97	0.46
1:F:246:TYR:CD1	1:N:263:PRO:HG3	2.46	0.46
1:F:263:PRO:HG3	1:N:246:TYR:CE1	2.51	0.46
1:J:167:LEU:HD21	1:J:273:MET:CE	2.46	0.46
1:C:280:MET:HE2	1:C:284:LYS:HE2	1.97	0.46
1:P:213:THR:CG2	1:P:243:THR:HG21	2.46	0.46
1:E:106:LEU:HD22	1:E:245:PRO:HG3	1.97	0.45
1:P:157:ARG:O	1:P:157:ARG:HG2	2.17	0.45
1:B:113:PHE:N	1:B:114:PRO:CD	2.80	0.45
1:F:289:ARG:CZ	1:F:289:ARG:HB3	2.47	0.45
1:J:211:VAL:HG12	1:J:212:LEU:H	1.80	0.45
1:D:273:MET:SD	1:D:288:LEU:CD2	3.05	0.45
1:G:106:LEU:HD22	1:G:245:PRO:HG3	1.98	0.45
1:H:216:LEU:HD21	1:H:222:ARG:HE	1.81	0.45
1:H:113:PHE:N	1:H:114:PRO:CD	2.80	0.45
1:P:214:VAL:HG23	1:P:216:LEU:H	1.81	0.45
1:A:155:HIS:CD2	1:A:155:HIS:H	2.33	0.45
1:B:161:GLU:HA	1:B:277:ARG:NE	2.30	0.45
1:E:116:ILE:HD12	1:F:239:LEU:HD13	1.99	0.45
1:G:195:VAL:CG2	1:G:219:LYS:HG3	2.47	0.45
1:K:113:PHE:N	1:K:114:PRO:CD	2.80	0.45
1:B:216:LEU:N	1:B:216:LEU:CD1	2.79	0.45
1:E:98:HIS:CG	1:F:207:ARG:CZ	2.99	0.45
1:H:263:PRO:HG3	1:L:246:TYR:CE1	2.51	0.45
1:D:113:PHE:N	1:D:114:PRO:CD	2.80	0.45
1:H:208:GLU:O	1:H:210:PRO:HD3	2.17	0.45
1:K:160:SER:C	1:K:161:GLU:HG2	2.37	0.45
1:H:159:SER:HB3	1:H:162:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:106:LEU:HD22	1:J:245:PRO:HG3	1.97	0.45
1:J:255:GLU:OE1	1:J:255:GLU:HA	2.17	0.45
1:H:157:ARG:NE	1:H:164:SER:OG	2.46	0.45
1:I:106:LEU:HD22	1:I:245:PRO:HG3	1.98	0.45
1:J:113:PHE:N	1:J:114:PRO:CD	2.80	0.45
1:M:205:THR:HG23	1:M:207:ARG:NH2	2.32	0.45
1:A:209:ARG:HA	1:A:209:ARG:HD3	1.83	0.44
1:D:106:LEU:HD22	1:D:245:PRO:HG3	1.98	0.44
1:E:160:SER:OG	1:E:276:ARG:CZ	2.65	0.44
1:G:195:VAL:HG21	1:G:219:LYS:HG3	1.99	0.44
1:G:213:THR:CG2	1:G:216:LEU:HB2	2.47	0.44
1:L:157:ARG:O	1:L:157:ARG:HG2	2.17	0.44
1:M:277:ARG:NH1	1:M:280:MET:SD	2.90	0.44
1:B:194:ARG:HH22	1:B:217:LEU:HD21	1.79	0.44
1:D:246:TYR:CG	1:P:263:PRO:HG2	2.53	0.44
1:I:154:MET:O	1:I:157:ARG:NH1	2.50	0.44
1:K:160:SER:O	1:K:162:ILE:HG13	2.16	0.44
1:L:191:GLU:HG3	1:L:194:ARG:NH1	2.31	0.44
1:C:113:PHE:N	1:C:114:PRO:CD	2.80	0.44
1:D:273:MET:SD	1:D:288:LEU:HD23	2.58	0.44
1:J:211:VAL:O	1:J:212:LEU:HD13	2.17	0.44
1:C:214:VAL:O	1:C:215:GLN:HG3	2.17	0.44
1:E:209:ARG:NE	1:E:209:ARG:HA	2.32	0.44
1:H:106:LEU:HD22	1:H:245:PRO:HG3	1.99	0.44
1:I:156:PHE:HD1	1:K:208:GLU:OE1	1.98	0.44
1:N:136:GLY:HA3	1:N:205:THR:HB	1.99	0.44
1:O:113:PHE:N	1:O:114:PRO:CD	2.81	0.44
1:E:113:PHE:N	1:E:114:PRO:CD	2.80	0.44
1:F:113:PHE:N	1:F:114:PRO:CD	2.80	0.44
1:D:216:LEU:HD12	1:D:222:ARG:NH2	2.32	0.44
1:O:214:VAL:HG12	1:O:215:GLN:OE1	2.18	0.44
1:A:276:ARG:HB3	1:A:278:ASP:OD1	2.18	0.44
1:B:104:GLU:OE2	1:B:134:LEU:HD12	2.17	0.44
1:B:171:MET:CE	1:B:268:GLU:HG2	2.47	0.44
1:B:286:TRP:CE2	1:B:290:GLU:HG3	2.52	0.44
1:C:106:LEU:HD22	1:C:245:PRO:HG3	2.00	0.44
1:F:215:GLN:H	1:F:215:GLN:HG3	1.12	0.44
1:I:277:ARG:HA	1:I:277:ARG:HD3	1.84	0.44
1:P:191:GLU:O	1:P:195:VAL:HG23	2.18	0.44
1:L:113:PHE:N	1:L:114:PRO:CD	2.81	0.44
1:L:189:LEU:O	1:L:194:ARG:CZ	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:TYR:CE1	1:P:263:PRO:HG3	2.53	0.43
1:G:113:PHE:N	1:G:114:PRO:CD	2.81	0.43
1:L:213:THR:HG22	1:L:214:VAL:N	2.31	0.43
1:B:106:LEU:HD22	1:B:245:PRO:HG3	2.00	0.43
1:M:113:PHE:N	1:M:114:PRO:CD	2.80	0.43
1:P:212:LEU:HG	1:P:216:LEU:HG	2.01	0.43
1:A:113:PHE:N	1:A:114:PRO:CD	2.81	0.43
1:F:159:SER:OG	1:F:162:ILE:HB	2.18	0.43
1:F:246:TYR:CZ	1:N:263:PRO:HD3	2.53	0.43
1:G:206:ALA:O	1:G:208:GLU:N	2.52	0.43
1:P:113:PHE:N	1:P:114:PRO:CD	2.80	0.43
1:B:95:MET:CG	1:D:276:ARG:NH1	2.81	0.43
1:C:216:LEU:HD21	1:C:222:ARG:HE	1.83	0.43
1:E:194:ARG:NH1	1:E:217:LEU:HD13	2.33	0.43
1:I:113:PHE:N	1:I:114:PRO:CD	2.81	0.43
1:J:134:LEU:CD1	1:J:211:VAL:HG13	2.48	0.43
1:K:239:LEU:HD13	1:L:116:ILE:CD1	2.48	0.43
1:N:113:PHE:N	1:N:114:PRO:CD	2.81	0.43
1:P:163:ASN:HB2	1:P:275:TRP:CE2	2.54	0.43
1:A:157:ARG:O	1:A:158:SER:OG	2.36	0.43
1:B:210:PRO:HA	1:B:215:GLN:HG2	2.00	0.43
1:B:210:PRO:HA	1:B:215:GLN:HB3	2.01	0.43
1:E:208:GLU:O	1:E:208:GLU:HG2	2.18	0.43
1:I:280:MET:HE3	1:I:280:MET:HA	2.00	0.43
1:L:142:GLU:OE2	1:L:156:PHE:HD2	2.01	0.43
1:L:249:VAL:HG23	1:L:253:ILE:HD11	1.99	0.43
1:N:251:LYS:HD3	1:N:257:ARG:HH22	1.84	0.43
1:O:106:LEU:HD22	1:O:245:PRO:HG3	2.01	0.43
1:M:222:ARG:HG2	1:N:126:GLN:OE1	2.18	0.43
1:C:160:SER:C	1:C:161:GLU:HG3	2.40	0.42
1:D:157:ARG:NE	1:D:164:SER:OG	2.49	0.42
1:P:132:GLU:OE1	1:P:205:THR:HB	2.19	0.42
1:B:209:ARG:N	1:B:210:PRO:CD	2.82	0.42
1:B:211:VAL:H	1:B:215:GLN:HG2	1.83	0.42
1:M:252:ASP:OD1	1:M:252:ASP:N	2.51	0.42
1:I:159:SER:N	1:K:156:PHE:HE2	2.17	0.42
1:L:294:LEU:HB2	1:L:295:PHE:CD1	2.54	0.42
1:N:128:ALA:HB1	1:N:130:ILE:HD11	2.02	0.42
1:N:286:TRP:CE2	1:N:290:GLU:HG3	2.55	0.42
1:G:182:ILE:HD13	1:G:241:VAL:HG21	2.01	0.42
1:I:277:ARG:NH1	1:I:280:MET:SD	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:157:ARG:NE	1:L:164:SER:OG	2.51	0.42
1:H:156:PHE:HE2	1:H:209:ARG:HH12	1.66	0.42
1:G:209:ARG:HE	1:G:210:PRO:HD2	1.85	0.42
1:H:163:ASN:HB2	1:H:275:TRP:CE2	2.55	0.42
1:H:194:ARG:CZ	1:H:214:VAL:HG12	2.50	0.42
1:L:108:PRO:HD3	3:L:407:HOH:O	2.19	0.42
1:N:106:LEU:HD22	1:N:245:PRO:HG3	2.01	0.42
1:I:159:SER:H	1:K:156:PHE:HE2	1.66	0.42
1:J:279:SER:HA	1:L:280:MET:O	2.20	0.42
1:M:163:ASN:HB2	1:M:275:TRP:CE2	2.54	0.42
1:J:211:VAL:N	1:J:215:GLN:HE22	2.16	0.42
1:L:213:THR:CG2	1:L:214:VAL:H	2.33	0.42
1:P:195:VAL:HG23	1:P:217:LEU:HD13	2.02	0.42
1:J:273:MET:HB3	1:J:273:MET:HE2	1.57	0.42
1:N:202:VAL:HA	1:N:225:VAL:O	2.20	0.42
1:B:273:MET:CE	1:B:288:LEU:HA	2.50	0.42
1:E:217:LEU:H	1:E:220:GLN:NE2	2.18	0.42
1:H:277:ARG:HH11	1:H:277:ARG:HG3	1.84	0.42
1:J:181:PRO:HA	1:J:184:GLN:OE1	2.19	0.42
1:L:163:ASN:HB2	1:L:275:TRP:CE2	2.55	0.42
1:O:142:GLU:OE2	1:O:160:SER:OG	2.28	0.42
1:B:163:ASN:HB2	1:B:275:TRP:CE2	2.54	0.41
1:D:163:ASN:HB2	1:D:275:TRP:CE2	2.55	0.41
1:K:268:GLU:OE2	1:M:289:ARG:NH2	2.52	0.41
1:N:163:ASN:HB2	1:N:275:TRP:CE2	2.55	0.41
1:B:202:VAL:HA	1:B:225:VAL:O	2.20	0.41
1:H:217:LEU:H	1:H:220:GLN:NE2	2.18	0.41
1:N:157:ARG:NE	1:N:164:SER:OG	2.47	0.41
1:N:182:ILE:O	1:N:185:GLU:HB2	2.20	0.41
1:B:209:ARG:HB2	1:B:216:LEU:HD13	2.01	0.41
1:C:212:LEU:HB3	1:C:216:LEU:H	1.85	0.41
1:G:202:VAL:HA	1:G:225:VAL:O	2.20	0.41
1:H:217:LEU:H	1:H:220:GLN:HE21	1.67	0.41
1:I:189:LEU:HD13	1:I:189:LEU:HA	1.94	0.41
1:J:163:ASN:HB2	1:J:275:TRP:CE2	2.55	0.41
1:J:251:LYS:HD3	1:J:257:ARG:NH2	2.22	0.41
1:F:286:TRP:CZ2	1:F:290:GLU:HG3	2.55	0.41
1:I:159:SER:HA	1:K:156:PHE:CE2	2.55	0.41
1:P:194:ARG:CZ	1:P:217:LEU:HD21	2.50	0.41
1:H:171:MET:HE1	1:H:268:GLU:HG2	2.02	0.41
1:L:100:THR:HG23	1:L:130:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:163:ASN:HB2	1:M:275:TRP:CZ2	2.56	0.41
1:O:157:ARG:HA	1:O:157:ARG:NH1	2.35	0.41
1:O:163:ASN:HB2	1:O:275:TRP:CE2	2.56	0.41
1:C:163:ASN:HB2	1:C:275:TRP:CE2	2.56	0.41
1:H:181:PRO:HA	1:H:184:GLN:OE1	2.20	0.41
1:H:263:PRO:HG3	1:L:246:TYR:CD1	2.56	0.41
1:I:136:GLY:HA3	1:K:209:ARG:NH2	2.35	0.41
1:K:262:SER:HA	1:K:263:PRO:HD3	1.96	0.41
1:O:207:ARG:HA	1:P:140:ARG:HH12	1.86	0.41
1:A:159:SER:HB2	1:C:155:HIS:HB2	2.03	0.41
1:A:159:SER:CB	1:C:155:HIS:HB2	2.51	0.41
1:G:203:ALA:HB1	1:G:207:ARG:HA	2.02	0.41
1:H:133:VAL:HG21	1:H:203:ALA:O	2.21	0.41
1:I:202:VAL:HA	1:I:225:VAL:O	2.20	0.41
1:L:215:GLN:HG3	1:L:216:LEU:O	2.20	0.41
1:M:202:VAL:HA	1:M:225:VAL:O	2.20	0.41
1:A:194:ARG:NH1	1:A:215:GLN:HA	2.36	0.41
1:F:163:ASN:HB2	1:F:275:TRP:CE2	2.56	0.41
1:J:143:GLN:O	1:L:98:HIS:CD2	2.74	0.41
1:A:134:LEU:HA	1:A:154:MET:HE1	2.02	0.41
1:A:155:HIS:O	1:A:156:PHE:CB	2.68	0.41
1:B:206:ALA:HA	1:B:224:THR:HG21	2.03	0.41
1:C:134:LEU:HB3	1:C:210:PRO:HG2	2.02	0.41
1:G:122:LYS:NZ	1:G:282:GLU:HG2	2.36	0.41
1:J:202:VAL:HA	1:J:225:VAL:O	2.21	0.41
1:K:234:ALA:HA	1:L:113:PHE:CE2	2.56	0.41
1:O:202:VAL:HA	1:O:225:VAL:O	2.20	0.41
1:A:154:MET:O	1:C:156:PHE:HB3	2.21	0.41
1:A:298:LYS:NZ	3:A:401:HOH:O	2.05	0.41
1:C:154:MET:O	1:C:156:PHE:HD2	2.04	0.41
1:C:185:GLU:HG3	1:C:193:THR:CG2	2.42	0.41
1:D:128:ALA:HB1	1:D:130:ILE:HD11	2.02	0.41
1:D:171:MET:HG3	1:P:263:PRO:HB2	2.01	0.41
1:D:202:VAL:HA	1:D:225:VAL:O	2.20	0.41
1:E:138:TRP:CG	1:E:157:ARG:NH2	2.89	0.41
1:F:286:TRP:CE2	1:F:290:GLU:HG3	2.56	0.41
1:K:202:VAL:HA	1:K:225:VAL:O	2.20	0.41
1:L:202:VAL:HA	1:L:225:VAL:O	2.21	0.41
1:P:216:LEU:O	1:P:217:LEU:CD2	2.68	0.41
1:A:180:HIS:HE1	1:A:197:TYR:CD2	2.39	0.40
1:A:204:ASP:OD2	1:C:207:ARG:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLN:OE1	1:A:236:LEU:HD12	2.21	0.40
1:C:202:VAL:HA	1:C:225:VAL:O	2.20	0.40
1:E:170:LEU:HB3	1:E:269:ILE:HG23	2.03	0.40
1:F:202:VAL:HA	1:F:225:VAL:O	2.20	0.40
1:I:153:ASP:CG	1:K:157:ARG:O	2.59	0.40
1:M:96:GLU:OE1	1:M:96:GLU:HA	2.21	0.40
1:D:193:THR:HA	1:D:196:LYS:HE2	2.02	0.40
1:E:217:LEU:H	1:E:220:GLN:HE21	1.69	0.40
1:F:263:PRO:HG3	1:N:246:TYR:CD1	2.56	0.40
1:I:216:LEU:HD13	1:I:217:LEU:N	2.36	0.40
1:L:193:THR:HA	1:L:196:LYS:HE2	2.03	0.40
1:N:157:ARG:O	1:N:157:ARG:HG2	2.21	0.40
1:J:157:ARG:HH22	1:J:160:SER:HB3	1.86	0.40
1:B:189:LEU:HD21	1:B:262:SER:CB	2.51	0.40
1:E:98:HIS:CE1	1:E:126:GLN:HG3	2.57	0.40
1:J:169:THR:HG22	1:J:270:ASP:OD1	2.21	0.40
1:M:262:SER:HA	1:M:263:PRO:HD3	1.95	0.40
1:N:277:ARG:HH11	1:N:277:ARG:HG3	1.86	0.40
1:C:296:ASN:OD1	3:C:401:HOH:O	2.22	0.40
1:E:98:HIS:CB	1:F:207:ARG:NH2	2.52	0.40
1:E:202:VAL:HA	1:E:225:VAL:O	2.21	0.40
1:E:211:VAL:CG1	1:E:212:LEU:N	2.84	0.40
1:K:170:LEU:HB3	1:K:269:ILE:HG23	2.04	0.40

All (7) 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:L:165:ARG:CZ	1:P:160:SER:O[9_544]	1.23	0.97
1:L:165:ARG:NH2	1:P:160:SER:O[9_544]	1.48	0.72
1:L:165:ARG:NE	1:P:160:SER:O[9_544]	1.58	0.62
1:E:209:ARG:NH2	1:G:208:GLU:OE2[3_655]	1.87	0.33
1:M:209:ARG:NH2	1:O:208:GLU:O[2_555]	2.09	0.11
1:D:165:ARG:NH2	1:H:160:SER:O[5_445]	2.12	0.08
1:M:156:PHE:O	1:O:154:MET:CE[2_555]	2.15	0.05

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	200/207 (97%)	188 (94%)	9 (4%)	3 (2%)	10 14
1	B	202/207 (98%)	191 (95%)	11 (5%)	0	100 100
1	C	200/207 (97%)	192 (96%)	8 (4%)	0	100 100
1	D	202/207 (98%)	196 (97%)	6 (3%)	0	100 100
1	E	200/207 (97%)	188 (94%)	12 (6%)	0	100 100
1	F	203/207 (98%)	196 (97%)	7 (3%)	0	100 100
1	G	200/207 (97%)	189 (94%)	10 (5%)	1 (0%)	29 43
1	H	201/207 (97%)	190 (94%)	11 (6%)	0	100 100
1	I	199/207 (96%)	185 (93%)	11 (6%)	3 (2%)	10 14
1	J	202/207 (98%)	192 (95%)	9 (4%)	1 (0%)	29 43
1	K	200/207 (97%)	190 (95%)	9 (4%)	1 (0%)	29 43
1	L	201/207 (97%)	196 (98%)	5 (2%)	0	100 100
1	M	201/207 (97%)	191 (95%)	9 (4%)	1 (0%)	29 43
1	N	203/207 (98%)	198 (98%)	5 (2%)	0	100 100
1	O	200/207 (97%)	189 (94%)	11 (6%)	0	100 100
1	P	197/207 (95%)	191 (97%)	6 (3%)	0	100 100
All	All	3211/3312 (97%)	3062 (95%)	139 (4%)	10 (0%)	41 56

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	PHE
1	A	214	VAL
1	I	156	PHE
1	I	161	GLU
1	K	155	HIS
1	I	205	THR

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Mol	Chain	Res	Type
1	G	207	ARG
1	A	213	THR
1	J	160	SER
1	M	214	VAL

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	173/177 (98%)	162 (94%)	11 (6%)	17	27
1	B	173/177 (98%)	162 (94%)	11 (6%)	17	27
1	C	173/177 (98%)	163 (94%)	10 (6%)	20	31
1	D	173/177 (98%)	158 (91%)	15 (9%)	10	14
1	E	173/177 (98%)	160 (92%)	13 (8%)	13	20
1	F	175/177 (99%)	161 (92%)	14 (8%)	12	18
1	G	173/177 (98%)	160 (92%)	13 (8%)	13	20
1	H	174/177 (98%)	161 (92%)	13 (8%)	13	20
1	I	172/177 (97%)	158 (92%)	14 (8%)	11	17
1	J	173/177 (98%)	161 (93%)	12 (7%)	15	23
1	K	173/177 (98%)	168 (97%)	5 (3%)	42	60
1	L	174/177 (98%)	160 (92%)	14 (8%)	12	18
1	M	174/177 (98%)	161 (92%)	13 (8%)	13	20
1	N	175/177 (99%)	162 (93%)	13 (7%)	13	21
1	O	173/177 (98%)	163 (94%)	10 (6%)	20	31
1	P	172/177 (97%)	158 (92%)	14 (8%)	11	17
All	All	2773/2832 (98%)	2578 (93%)	195 (7%)	15	23

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	ARG
1	A	161	GLU
1	A	179	ASP
1	A	204	ASP
1	A	205	THR
1	A	207	ARG
1	A	216	LEU
1	A	217	LEU
1	A	218	ASP
1	A	276	ARG
1	A	277	ARG
1	B	159	SER
1	B	179	ASP
1	B	204	ASP
1	B	207	ARG
1	B	209	ARG
1	B	212	LEU
1	B	216	LEU
1	B	222	ARG
1	B	248	MET
1	B	277	ARG
1	B	278	ASP
1	C	158	SER
1	C	161	GLU
1	C	163	ASN
1	C	179	ASP
1	C	205	THR
1	C	207	ARG
1	C	212	LEU
1	C	214	VAL
1	C	222	ARG
1	C	277	ARG
1	D	124	ASN
1	D	159	SER
1	D	161	GLU
1	D	179	ASP
1	D	189	LEU
1	D	207	ARG
1	D	209	ARG
1	D	212	LEU
1	D	213	THR
1	D	214	VAL
1	D	216	LEU

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Mol	Chain	Res	Type
1	D	218	ASP
1	D	276	ARG
1	D	277	ARG
1	D	289	ARG
1	E	142	GLU
1	E	154	MET
1	E	156	PHE
1	E	157	ARG
1	E	161	GLU
1	E	179	ASP
1	E	194	ARG
1	E	207	ARG
1	E	209	ARG
1	E	212	LEU
1	E	215	GLN
1	E	217	LEU
1	E	218	ASP
1	F	95	MET
1	F	154	MET
1	F	155	HIS
1	F	157	ARG
1	F	159	SER
1	F	189	LEU
1	F	194	ARG
1	F	196	LYS
1	F	209	ARG
1	F	212	LEU
1	F	267	SER
1	F	278	ASP
1	F	289	ARG
1	F	298	LYS
1	G	139	GLU
1	G	155	HIS
1	G	158	SER
1	G	161	GLU
1	G	179	ASP
1	G	182	ILE
1	G	191	GLU
1	G	196	LYS
1	G	204	ASP
1	G	211	VAL
1	G	212	LEU

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Mol	Chain	Res	Type
1	G	218	ASP
1	G	222	ARG
1	H	145	ARG
1	H	165	ARG
1	H	202	VAL
1	H	207	ARG
1	H	208	GLU
1	H	209	ARG
1	H	222	ARG
1	H	233	GLN
1	H	251	LYS
1	H	267	SER
1	H	277	ARG
1	H	278	ASP
1	H	285	SER
1	I	97	THR
1	I	157	ARG
1	I	165	ARG
1	I	179	ASP
1	I	189	LEU
1	I	204	ASP
1	I	207	ARG
1	I	209	ARG
1	I	212	LEU
1	I	214	VAL
1	I	218	ASP
1	I	222	ARG
1	I	276	ARG
1	I	277	ARG
1	J	95	MET
1	J	155	HIS
1	J	159	SER
1	J	188	PRO
1	J	189	LEU
1	J	207	ARG
1	J	209	ARG
1	J	214	VAL
1	J	216	LEU
1	J	267	SER
1	J	277	ARG
1	J	278	ASP
1	K	154	MET

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Mol	Chain	Res	Type
1	K	158	SER
1	K	211	VAL
1	K	212	LEU
1	K	296	ASN
1	L	124	ASN
1	L	158	SER
1	L	159	SER
1	L	161	GLU
1	L	179	ASP
1	L	207	ARG
1	L	211	VAL
1	L	212	LEU
1	L	215	GLN
1	L	216	LEU
1	L	219	LYS
1	L	267	SER
1	L	277	ARG
1	L	278	ASP
1	M	98	HIS
1	M	154	MET
1	M	162	ILE
1	M	163	ASN
1	M	165	ARG
1	M	179	ASP
1	M	187	GLU
1	M	213	THR
1	M	229	GLU
1	M	252	ASP
1	M	276	ARG
1	M	277	ARG
1	M	298	LYS
1	N	154	MET
1	N	159	SER
1	N	163	ASN
1	N	205	THR
1	N	207	ARG
1	N	208	GLU
1	N	214	VAL
1	N	215	GLN
1	N	216	LEU
1	N	267	SER
1	N	277	ARG

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Mol	Chain	Res	Type
1	N	278	ASP
1	N	298	LYS
1	O	155	HIS
1	O	158	SER
1	O	163	ASN
1	O	179	ASP
1	O	205	THR
1	O	207	ARG
1	O	211	VAL
1	O	215	GLN
1	O	218	ASP
1	O	277	ARG
1	P	140	ARG
1	P	157	ARG
1	P	158	SER
1	P	164	SER
1	P	166	LYS
1	P	169	THR
1	P	179	ASP
1	P	190	SER
1	P	211	VAL
1	P	218	ASP
1	P	222	ARG
1	P	267	SER
1	P	277	ARG
1	P	280	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	155	HIS
1	A	220	GLN
1	E	220	GLN
1	G	172	ASN
1	G	215	GLN
1	H	143	GLN
1	H	220	GLN
1	I	126	GLN
1	L	172	ASN
1	L	296	ASN
1	M	143	GLN
1	O	220	GLN

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Mol	Chain	Res	Type
1	O	233	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 15 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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	202/207 (97%)	-0.22	0 100 100	34, 51, 73, 97	0
1	B	204/207 (98%)	-0.12	4 (1%) 65 61	28, 56, 72, 92	0
1	C	202/207 (97%)	-0.21	1 (0%) 91 90	34, 53, 76, 88	0
1	D	204/207 (98%)	-0.05	6 (2%) 51 48	39, 56, 76, 95	0
1	E	202/207 (97%)	-0.21	2 (0%) 82 81	31, 51, 73, 83	0
1	F	205/207 (99%)	-0.12	5 (2%) 59 55	29, 52, 73, 115	0
1	G	202/207 (97%)	-0.20	5 (2%) 57 53	30, 51, 78, 87	0
1	H	203/207 (98%)	-0.03	7 (3%) 45 41	33, 53, 78, 95	0
1	I	201/207 (97%)	-0.20	2 (0%) 82 81	32, 52, 72, 93	0
1	J	204/207 (98%)	-0.06	2 (0%) 82 81	26, 57, 73, 85	0
1	K	202/207 (97%)	-0.20	1 (0%) 91 90	37, 53, 70, 84	0
1	L	203/207 (98%)	-0.11	2 (0%) 82 81	37, 55, 71, 93	0
1	M	203/207 (98%)	-0.20	2 (0%) 82 81	32, 52, 76, 96	0
1	N	205/207 (99%)	-0.12	3 (1%) 73 71	29, 53, 69, 111	0
1	O	202/207 (97%)	-0.28	1 (0%) 91 90	34, 51, 76, 91	0
1	P	201/207 (97%)	-0.10	2 (0%) 82 81	33, 54, 72, 81	0
All	All	3245/3312 (97%)	-0.15	45 (1%) 75 73	26, 53, 74, 115	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	217	LEU	5.2
1	H	158	SER	4.0
1	N	121	ALA	4.0
1	D	212	LEU	3.5
1	H	211	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	212	LEU	3.4
1	H	94	HIS	3.1
1	F	210	PRO	3.0
1	I	297	GLY	3.0
1	D	254	ALA	2.9
1	D	217	LEU	2.8
1	D	121	ALA	2.8
1	B	211	VAL	2.7
1	G	217	LEU	2.6
1	D	213	THR	2.6
1	C	195	VAL	2.6
1	I	217	LEU	2.5
1	L	158	SER	2.5
1	P	210	PRO	2.5
1	G	192	VAL	2.5
1	F	286	TRP	2.5
1	B	121	ALA	2.4
1	P	209	ARG	2.4
1	G	187	GLU	2.4
1	J	210	PRO	2.4
1	F	157	ARG	2.4
1	B	254	ALA	2.4
1	B	158	SER	2.4
1	E	192	VAL	2.4
1	K	197	TYR	2.4
1	N	210	PRO	2.4
1	H	156	PHE	2.4
1	G	188	PRO	2.3
1	H	157	ARG	2.2
1	N	211	VAL	2.2
1	O	197	TYR	2.2
1	M	197	TYR	2.2
1	L	209	ARG	2.1
1	F	211	VAL	2.1
1	E	195	VAL	2.1
1	M	217	LEU	2.1
1	D	120	ALA	2.1
1	J	158	SER	2.1
1	G	216	LEU	2.0
1	H	122	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	A	302	1/1	0.85	0.17	37,37,37,37	0
2	NA	F	301	1/1	0.89	0.36	40,40,40,40	0
2	NA	G	301	1/1	0.91	0.23	40,40,40,40	0
2	NA	C	301	1/1	0.94	0.26	32,32,32,32	0
2	NA	H	301	1/1	0.94	0.19	44,44,44,44	0
2	NA	L	302	1/1	0.94	0.22	38,38,38,38	0
2	NA	D	301	1/1	0.95	0.19	49,49,49,49	0
2	NA	L	301	1/1	0.96	0.19	46,46,46,46	0
2	NA	N	301	1/1	0.96	0.41	58,58,58,58	0
2	NA	P	301	1/1	0.96	0.19	43,43,43,43	0
2	NA	I	301	1/1	0.97	0.31	26,26,26,26	0
2	NA	O	301	1/1	0.97	0.34	32,32,32,32	0
2	NA	M	301	1/1	0.97	0.25	39,39,39,39	0
2	NA	A	301	1/1	0.99	0.20	33,33,33,33	0
2	NA	J	301	1/1	0.99	0.15	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.