



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2016 – 11:40 AM EDT

PDB ID : 5K98
Title : Structure of HipA-HipB-O2-O3 complex
Authors : Schumacher, M.
Deposited on : 2016-05-31
Resolution : 3.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
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-20027790

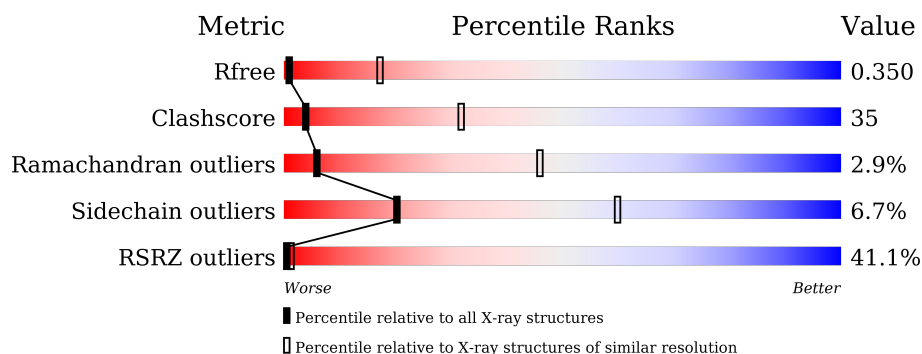
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.99 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	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

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

Mol	Chain	Length	Quality of chain
1	A	448	<div> <div>38%</div> <div>48%</div> <div>40%</div> <div>8%</div> </div>
1	D	448	<div> <div>39%</div> <div>49%</div> <div>38%</div> <div>8%</div> </div>
2	B	91	<div> <div>25%</div> <div>34%</div> <div>37%</div> <div>7%</div> <div>22%</div> </div>
2	P	91	<div> <div>25%</div> <div>36%</div> <div>33%</div> <div>9%</div> <div>22%</div> </div>
3	T	23	<div> <div>57%</div> <div>13%</div> <div>65%</div> <div>22%</div> </div>
4	E	23	<div> <div>52%</div> <div>22%</div> <div>35%</div> <div>43%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8605 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 Serine/threonine-protein kinase HipA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3270	2098	570	590	12			
1	D	414	Total	C	N	O	S	0	0	0
			3270	2098	570	590	12			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP P23874
A	-6	HIS	-	expression tag	UNP P23874
A	-5	HIS	-	expression tag	UNP P23874
A	-4	HIS	-	expression tag	UNP P23874
A	-3	HIS	-	expression tag	UNP P23874
A	-2	HIS	-	expression tag	UNP P23874
A	-1	HIS	-	expression tag	UNP P23874
A	0	SER	-	expression tag	UNP P23874
A	1	ARG	-	expression tag	UNP P23874
A	309	GLN	ASP	engineered mutation	UNP P23874
D	-7	MET	-	initiating methionine	UNP P23874
D	-6	HIS	-	expression tag	UNP P23874
D	-5	HIS	-	expression tag	UNP P23874
D	-4	HIS	-	expression tag	UNP P23874
D	-3	HIS	-	expression tag	UNP P23874
D	-2	HIS	-	expression tag	UNP P23874
D	-1	HIS	-	expression tag	UNP P23874
D	0	SER	-	expression tag	UNP P23874
D	1	ARG	-	expression tag	UNP P23874
D	309	GLN	ASP	engineered mutation	UNP P23874

- Molecule 2 is a protein called Antitoxin HipB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total	C	N	O	S	0	0	0
			564	358	95	108	3			
2	P	71	Total	C	N	O	S	0	0	0
			564	358	95	108	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP M9IJX7
B	-1	SER	-	expression tag	UNP M9IJX7
B	0	HIS	-	expression tag	UNP M9IJX7
P	-2	GLY	-	expression tag	UNP M9IJX7
P	-1	SER	-	expression tag	UNP M9IJX7
P	0	HIS	-	expression tag	UNP M9IJX7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	23	Total	C	N	O	P	0	0	0
			465	223	83	137	22			

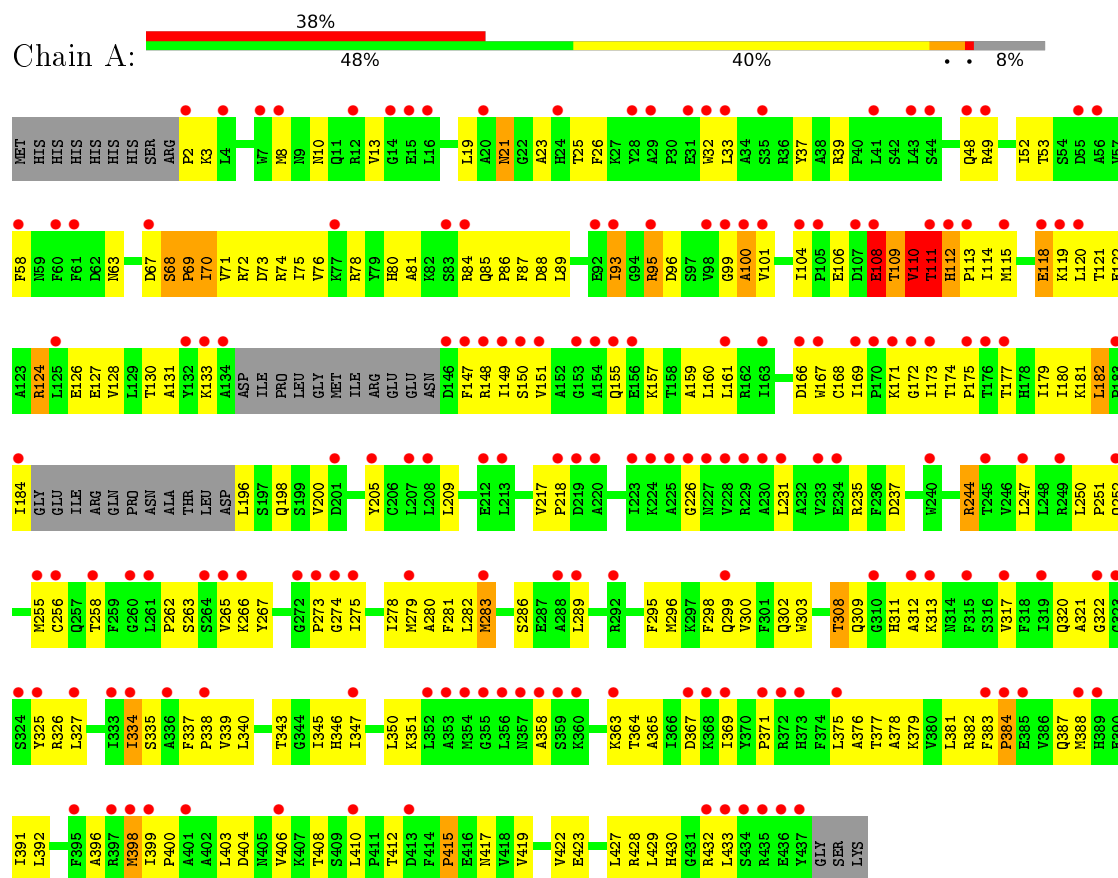
- Molecule 4 is a DNA chain called DNA (5'-D(*CP*TP*AP*TP*CP*CP*CP*CP*TP*TP*AP*AP*GP*GP*GP*GP*AP*TP*AP*GP*GP*GP*A)-3').

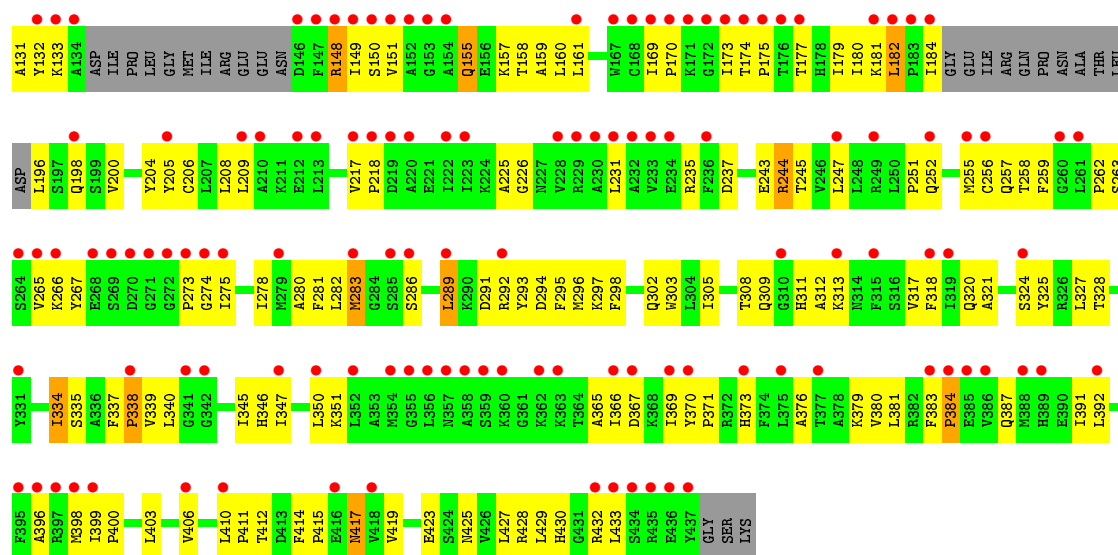
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	23	Total	C	N	O	P	0	0	0
			472	225	90	135	22			

3 Residue-property plots

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: Serine/threonine-protein kinase HipA





● Molecule 2: Antitoxin HipB



● Molecule 2: Antitoxin HipB



C700	T701	A702	T703	G704	G705	C706	C707	T708	T709	A710	A711	G712	G713	G714	G715	A716	T717	A718	G719	G720	G721	A722

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	214.04Å 146.83Å 53.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.08 – 3.99 121.08 – 3.99	Depositor EDS
% Data completeness (in resolution range)	92.2 (121.08-3.99) 92.4 (121.08-3.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 4.01Å)	Xtriage
Refinement program	PHENIX 1.6.4 _486	Depositor
R, R_{free}	0.350 , 0.375 0.323 , 0.350	Depositor DCC
R_{free} test set	1398 reflections (10.02%)	DCC
Wilson B-factor (Å ²)	120.1	Xtriage
Anisotropy	0.930	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 108.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	8605	wwPDB-VP
Average B, all atoms (Å ²)	179.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.73 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.6243e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	0.91	8/3343 (0.2%)	0.73	7/4530 (0.2%)
1	D	0.67	9/3343 (0.3%)	0.75	11/4530 (0.2%)
2	B	0.54	0/572	0.65	0/771
2	P	0.48	0/572	0.65	1/771 (0.1%)
3	T	1.02	1/520 (0.2%)	1.56	8/800 (1.0%)
4	E	1.00	3/530 (0.6%)	1.98	21/817 (2.6%)
All	All	0.79	21/8880 (0.2%)	0.94	48/12219 (0.4%)

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

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	VAL	CA-CB	30.12	2.18	1.54
1	A	110	VAL	CB-CG1	28.62	2.12	1.52
1	D	109	THR	CA-CB	15.28	1.93	1.53
1	D	107	ASP	CB-CG	11.98	1.76	1.51
1	D	109	THR	CA-C	10.09	1.79	1.52
1	A	111	THR	N-CA	9.89	1.66	1.46
1	A	110	VAL	CA-C	7.55	1.72	1.52
1	D	283	MET	CG-SD	6.92	1.99	1.81
1	D	398	MET	CG-SD	6.64	1.98	1.81
1	A	283	MET	CG-SD	6.37	1.97	1.81
3	T	708	DT	C1'-N1	6.30	1.57	1.49
1	D	107	ASP	CA-CB	6.16	1.67	1.53
1	D	110	VAL	CA-C	6.07	1.68	1.52
1	A	398	MET	CG-SD	5.91	1.96	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	715	DG	N7-C5	5.65	1.42	1.39
4	E	713	DG	N3-C4	5.38	1.39	1.35
1	D	108	GLU	CB-CG	5.25	1.62	1.52
1	A	111	THR	CA-CB	5.20	1.66	1.53
4	E	702	DA	C3'-O3'	-5.16	1.37	1.44
1	D	107	ASP	CA-C	5.07	1.66	1.52
1	A	112	HIS	N-CA	5.07	1.56	1.46

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	713	DG	O4'-C1'-N9	23.20	124.24	108.00
4	E	715	DG	O4'-C1'-N9	16.66	119.66	108.00
1	A	111	THR	N-CA-CB	15.95	140.61	110.30
3	T	708	DT	O4'-C1'-N1	11.79	116.25	108.00
1	D	109	THR	CA-CB-CG2	10.08	126.51	112.40
4	E	716	DA	O4'-C1'-N9	9.63	114.74	108.00
4	E	713	DG	N3-C4-C5	-9.54	123.83	128.60
1	D	84	ARG	NE-CZ-NH1	-9.43	115.59	120.30
1	D	109	THR	O-C-N	-9.37	107.70	122.70
1	A	110	VAL	CA-CB-CG1	9.27	124.80	110.90
1	A	110	VAL	CB-CA-C	9.03	128.56	111.40
4	E	710	DA	O4'-C1'-N9	8.29	113.80	108.00
1	D	107	ASP	CB-CG-OD1	8.18	125.66	118.30
1	D	107	ASP	CB-CA-C	8.04	126.48	110.40
4	E	712	DG	O4'-C1'-N9	7.90	113.53	108.00
2	P	38	LYS	CD-CE-NZ	7.69	129.38	111.70
3	T	716	DA	O4'-C1'-N9	7.56	113.30	108.00
3	T	715	DG	O4'-C1'-N9	7.10	112.97	108.00
4	E	709	DT	O4'-C1'-N1	7.07	112.95	108.00
3	T	701	DT	O4'-C1'-C2'	-7.04	100.27	105.90
4	E	715	DG	C4-C5-N7	-7.01	108.00	110.80
1	D	110	VAL	N-CA-C	6.95	129.77	111.00
4	E	713	DG	C8-N9-C4	-6.84	103.66	106.40
4	E	715	DG	N9-C4-C5	6.74	108.09	105.40
4	E	718	DA	O4'-C1'-N9	6.52	112.56	108.00
1	A	111	THR	N-CA-C	-6.15	94.39	111.00
1	A	70	ILE	CB-CA-C	-6.04	99.52	111.60
4	E	713	DG	O4'-C4'-C3'	5.93	109.56	106.00
4	E	713	DG	N3-C4-N9	5.85	129.51	126.00
4	E	715	DG	N7-C8-N9	5.75	115.97	113.10
3	T	708	DT	C6-N1-C2	-5.74	118.43	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	706	DC	O4'-C1'-N1	5.74	112.02	108.00
4	E	715	DG	C8-N9-C4	-5.73	104.11	106.40
1	A	111	THR	CA-CB-OG1	5.59	120.74	109.00
3	T	697	DT	O4'-C1'-N1	5.59	111.91	108.00
4	E	713	DG	C4'-C3'-C2'	-5.56	98.10	103.10
3	T	708	DT	N3-C4-O4	5.54	123.22	119.90
1	D	109	THR	CB-CA-C	5.53	126.52	111.60
1	D	108	GLU	C-N-CA	-5.41	108.19	121.70
4	E	713	DG	O4'-C1'-C2'	-5.30	101.66	105.90
1	D	107	ASP	OD1-CG-OD2	-5.29	113.24	123.30
4	E	715	DG	C5-C6-O6	5.26	131.75	128.60
1	D	110	VAL	CB-CA-C	-5.15	101.61	111.40
1	A	68	SER	N-CA-CB	-5.14	102.78	110.50
4	E	701	DT	O4'-C1'-C2'	-5.13	101.79	105.90
4	E	701	DT	C1'-O4'-C4'	-5.08	105.02	110.10
3	T	710	DA	O4'-C1'-N9	5.04	111.53	108.00
1	D	111	THR	N-CA-CB	5.04	119.88	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3270	0	3313	236	10
1	D	3270	0	3313	214	10
2	B	564	0	574	52	0
2	P	564	0	574	48	0
3	T	465	0	261	37	0
4	E	472	0	260	55	0
All	All	8605	0	8295	582	10

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 35.

All (582) 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:D:109:THR:C	1:D:109:THR:CA	1.79	1.51
1:D:107:ASP:CB	1:D:107:ASP:CG	1.76	1.50
1:D:109:THR:CA	1:D:109:THR:CB	1.93	1.42
1:A:110:VAL:CB	1:A:110:VAL:CG1	2.12	1.27
1:A:68:SER:OG	1:A:70:ILE:HD12	1.31	1.25
1:A:112:HIS:CG	1:A:173:ILE:HG23	1.71	1.22
1:A:110:VAL:CB	1:A:110:VAL:CA	2.18	1.22
2:B:38:LYS:HD2	4:E:715:DG:C6	1.76	1.19
1:A:118:GLU:HB2	1:A:171:LYS:HE3	1.24	1.17
1:D:110:VAL:HG12	1:D:110:VAL:O	1.35	1.13
1:D:104:ILE:HG22	1:D:108:GLU:HB3	1.31	1.11
1:D:110:VAL:HG11	1:D:112:HIS:CE1	1.87	1.08
1:D:124:ARG:HH11	1:D:124:ARG:HB3	0.95	1.07
1:D:148:ARG:HG3	1:D:148:ARG:HH11	1.18	1.04
1:D:206:CYS:SG	1:D:305:ILE:HD12	1.97	1.03
1:A:95:ARG:NE	1:A:112:HIS:HE1	1.58	1.01
1:A:95:ARG:CD	1:A:112:HIS:CE1	2.45	1.00
1:A:110:VAL:CB	1:A:110:VAL:HA	1.92	0.99
1:D:106:GLU:O	1:D:107:ASP:C	2.02	0.96
1:D:124:ARG:NH1	1:D:124:ARG:HB3	1.80	0.95
2:P:39:GLN:HE22	4:E:702:DA:H62	1.06	0.95
1:A:112:HIS:HB2	1:A:173:ILE:HG12	1.48	0.94
1:A:345:ILE:H	1:A:345:ILE:HD12	1.33	0.94
1:A:95:ARG:NE	1:A:112:HIS:CE1	2.36	0.93
1:A:95:ARG:HD3	1:A:112:HIS:ND1	1.84	0.93
1:D:345:ILE:H	1:D:345:ILE:HD12	1.33	0.92
1:A:68:SER:HG	1:A:70:ILE:HD12	1.34	0.91
1:D:20:ALA:O	1:D:22:GLY:N	2.03	0.91
1:A:112:HIS:CD2	1:A:173:ILE:HG23	2.05	0.90
1:A:429:LEU:HD23	1:A:432:ARG:HH12	1.34	0.90
1:A:112:HIS:CB	1:A:173:ILE:HG23	2.02	0.90
1:A:118:GLU:HB2	1:A:171:LYS:CE	2.01	0.89
1:D:110:VAL:HG11	1:D:112:HIS:NE2	1.86	0.89
1:D:105:PRO:HB2	1:D:108:GLU:HB2	1.54	0.89
1:D:110:VAL:O	1:D:112:HIS:N	2.06	0.89
3:T:713:DG:H2"	2:P:38:LYS:HD3	1.54	0.88
1:D:399:ILE:HB	1:D:430:HIS:HD2	1.38	0.87
1:D:106:GLU:O	1:D:107:ASP:O	1.93	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:707:DC:H2''	4:E:708:DT:H5'	1.54	0.87
3:T:700:DC:H42	4:E:719:DG:H1	1.22	0.87
1:D:399:ILE:HB	1:D:430:HIS:CD2	2.09	0.87
1:A:399:ILE:HB	1:A:430:HIS:HD2	1.40	0.85
1:D:429:LEU:HD23	1:D:432:ARG:HH12	1.41	0.85
1:A:99:GLY:HA2	1:A:252:GLN:HG2	1.55	0.85
2:B:38:LYS:HD2	4:E:715:DG:C5	2.11	0.85
1:D:124:ARG:HH11	1:D:124:ARG:CB	1.86	0.85
1:A:63:ASN:OD1	1:A:263:SER:HB3	1.76	0.85
2:B:27:THR:OG1	2:B:30:GLU:HG2	1.78	0.83
1:D:104:ILE:HG22	1:D:108:GLU:CB	2.07	0.83
4:E:709:DT:H1'	4:E:710:DA:H5'	1.59	0.83
2:B:38:LYS:HE2	4:E:713:DG:H2''	1.60	0.83
1:A:399:ILE:HB	1:A:430:HIS:CD2	2.13	0.83
1:D:96:ASP:HB3	1:D:149:ILE:HG23	1.59	0.83
1:D:428:ARG:HH11	1:D:428:ARG:HG2	1.42	0.83
1:A:112:HIS:CB	1:A:173:ILE:N	2.42	0.82
1:A:95:ARG:HD3	1:A:112:HIS:HD1	1.43	0.82
1:A:112:HIS:HB3	1:A:173:ILE:N	1.95	0.82
1:D:110:VAL:O	1:D:111:THR:C	2.19	0.81
2:B:38:LYS:HE2	4:E:713:DG:C2'	2.10	0.81
1:A:429:LEU:HD23	1:A:432:ARG:NH1	1.94	0.81
1:A:403:LEU:HD13	1:A:423:GLU:HG3	1.63	0.81
4:E:706:DC:H1'	4:E:707:DC:H5'	1.60	0.81
1:A:112:HIS:HB2	1:A:173:ILE:HG23	1.62	0.80
1:D:99:GLY:HA2	1:D:252:GLN:HG2	1.64	0.80
2:B:38:LYS:CE	4:E:713:DG:H2''	2.11	0.80
3:T:704:DC:O2	4:E:716:DA:H2	1.65	0.79
1:A:119:LYS:HA	1:A:168:CYS:SG	2.22	0.79
1:A:200:VAL:HG13	1:A:231:LEU:HB2	1.65	0.79
1:A:124:ARG:HH11	1:A:124:ARG:HB3	1.48	0.78
3:T:702:DA:N1	4:E:718:DA:H2	1.82	0.78
3:T:705:DC:C4	4:E:714:DG:O6	2.36	0.78
1:A:76:VAL:HG13	1:A:81:ALA:HB3	1.64	0.77
1:A:95:ARG:HD3	1:A:112:HIS:CE1	2.16	0.77
1:A:112:HIS:HB3	1:A:172:GLY:CA	2.15	0.77
1:D:110:VAL:O	1:D:110:VAL:CG1	2.21	0.77
3:T:702:DA:H2''	3:T:703:DT:H5''	1.66	0.77
1:D:109:THR:HB	1:D:109:THR:CA	2.14	0.77
3:T:698:DC:H2''	3:T:699:DC:C5	2.20	0.77
3:T:712:DG:H4'	3:T:713:DG:H5'	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:LYS:HA	1:D:283:MET:HE1	1.66	0.76
1:D:169:ILE:HG23	1:D:170:PRO:HD2	1.69	0.75
1:D:109:THR:O	1:D:110:VAL:HB	1.86	0.75
1:A:112:HIS:HB2	1:A:173:ILE:CG1	2.17	0.74
1:D:105:PRO:CB	1:D:108:GLU:HB2	2.17	0.74
1:D:383:PHE:CD1	1:D:384:PRO:HD2	2.23	0.74
1:A:151:VAL:HG12	1:A:157:LYS:HE3	1.69	0.74
1:A:49:ARG:HD2	2:B:23:GLN:HG2	1.70	0.74
2:B:7:ILE:HG23	2:B:12:GLN:HG2	1.70	0.74
2:P:39:GLN:NE2	4:E:702:DA:H62	1.85	0.74
1:D:20:ALA:C	1:D:22:GLY:H	1.91	0.73
1:D:69:PRO:HA	1:D:72:ARG:HG3	1.70	0.73
1:A:95:ARG:HD2	1:A:148:ARG:HB2	1.71	0.73
1:A:112:HIS:CB	1:A:173:ILE:H	2.02	0.72
1:D:72:ARG:O	1:D:76:VAL:HG23	1.90	0.72
2:B:10:PRO:HG2	2:B:50:ASP:OD1	1.89	0.72
1:D:76:VAL:HG22	1:D:89:LEU:HD21	1.71	0.72
1:D:392:LEU:HD22	1:D:433:LEU:HD21	1.72	0.71
1:A:21:ASN:HD21	1:A:23:ALA:CB	2.03	0.71
1:D:204:TYR:CZ	1:D:208:LEU:HD11	2.24	0.71
1:D:109:THR:O	1:D:110:VAL:CB	2.36	0.71
1:A:69:PRO:O	1:A:72:ARG:HB2	1.90	0.71
1:A:339:VAL:O	1:A:339:VAL:HG12	1.91	0.70
1:D:76:VAL:HG13	1:D:81:ALA:HB3	1.72	0.70
1:A:111:THR:HG21	1:A:114:ILE:HD11	1.74	0.70
1:D:109:THR:C	1:D:109:THR:HA	2.08	0.69
2:B:38:LYS:CD	4:E:713:DG:H2"	2.22	0.69
1:A:399:ILE:CB	1:A:430:HIS:HD2	2.06	0.69
1:A:95:ARG:HG2	1:A:112:HIS:CE1	2.28	0.69
1:A:85:GLN:HE21	1:A:86:PRO:HD2	1.59	0.69
1:A:21:ASN:HD21	1:A:23:ALA:HB3	1.58	0.68
1:D:120:LEU:HD22	1:D:124:ARG:NH1	2.09	0.68
1:D:384:PRO:HG2	1:D:387:GLN:NE2	2.08	0.68
1:A:298:PHE:O	1:A:302:GLN:HG3	1.93	0.68
1:A:71:VAL:O	1:A:75:ILE:HD13	1.94	0.68
1:D:148:ARG:HH11	1:D:148:ARG:CG	2.03	0.68
1:A:111:THR:HG23	1:A:112:HIS:N	2.08	0.68
1:D:76:VAL:HG21	1:D:84:ARG:HG3	1.76	0.68
3:T:701:DT:O2	3:T:702:DA:C5	2.46	0.68
1:A:280:ALA:O	1:A:283:MET:HB2	1.94	0.68
1:A:71:VAL:O	1:A:74:ARG:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:ARG:HG3	1:D:148:ARG:NH1	1.98	0.67
1:D:71:VAL:O	1:D:75:ILE:HD13	1.95	0.67
1:D:286:SER:HA	2:P:8:TYR:CE2	2.29	0.67
1:D:5:VAL:HG23	1:D:106:GLU:HA	1.76	0.67
1:A:428:ARG:HG2	1:A:428:ARG:HH11	1.60	0.67
1:D:76:VAL:HG21	1:D:84:ARG:CG	2.26	0.66
1:D:58:PHE:CE1	1:D:86:PRO:HG2	2.30	0.66
1:A:112:HIS:HB2	1:A:173:ILE:CG2	2.24	0.66
1:A:96:ASP:HB3	1:A:149:ILE:HG23	1.78	0.66
2:P:6:LYS:NZ	2:P:74:LYS:HE3	2.10	0.66
1:A:95:ARG:CG	1:A:112:HIS:CE1	2.78	0.66
1:A:161:LEU:HD12	1:A:177:THR:HG23	1.77	0.66
2:B:56:THR:OG1	4:E:712:DG:H5"	1.96	0.66
2:B:55:THR:O	2:B:59:LYS:HG3	1.96	0.66
1:D:179:ILE:HD11	1:D:235:ARG:CZ	2.26	0.65
1:A:112:HIS:CD2	1:A:173:ILE:CG2	2.79	0.65
1:D:26:PHE:O	1:D:52:ILE:HG12	1.97	0.65
3:T:704:DC:O2	4:E:716:DA:C2	2.49	0.65
2:B:17:MET:SD	2:B:45:PHE:CZ	2.89	0.64
1:A:112:HIS:HB2	1:A:173:ILE:N	2.12	0.64
1:A:13:VAL:HG13	1:A:32:TRP:CE2	2.33	0.64
1:A:383:PHE:CD1	1:A:384:PRO:HD2	2.32	0.64
2:B:37:ILE:HB	4:E:713:DG:OP2	1.97	0.64
1:A:244:ARG:HG2	1:A:244:ARG:HH11	1.61	0.64
1:D:399:ILE:CB	1:D:430:HIS:HD2	2.08	0.63
2:P:19:LEU:CD2	2:P:23:GLN:HG3	2.29	0.63
1:A:111:THR:CG2	1:A:112:HIS:N	2.59	0.63
3:T:716:DA:H61	4:E:703:DT:H3	1.46	0.63
2:P:35:ILE:HG13	2:P:36:GLY:H	1.63	0.63
2:P:6:LYS:HZ1	2:P:74:LYS:HE3	1.63	0.63
2:B:17:MET:SD	2:B:45:PHE:HZ	2.21	0.63
1:D:429:LEU:HD23	1:D:432:ARG:NH1	2.12	0.63
1:A:175:PRO:HB2	1:A:247:LEU:HD23	1.81	0.63
1:A:112:HIS:HB2	1:A:173:ILE:CB	2.30	0.62
1:D:3:LYS:O	1:D:106:GLU:N	2.32	0.62
1:A:112:HIS:HB3	1:A:173:ILE:H	1.60	0.62
1:D:182:LEU:H	1:D:182:LEU:HD22	1.64	0.62
1:D:345:ILE:N	1:D:345:ILE:HD12	2.12	0.62
2:B:38:LYS:HG3	4:E:713:DG:C2'	2.30	0.62
1:A:112:HIS:CG	1:A:173:ILE:CG2	2.67	0.62
1:D:345:ILE:H	1:D:345:ILE:CD1	2.09	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:55:THR:O	2:P:59:LYS:HG3	2.00	0.62
1:A:119:LYS:HG3	1:A:166:ASP:CB	2.30	0.62
1:D:95:ARG:HB2	1:D:148:ARG:O	1.99	0.62
1:A:115:MET:CE	1:A:174:THR:HG23	2.30	0.61
1:D:179:ILE:HG12	1:D:235:ARG:HG2	1.83	0.61
1:A:68:SER:HB3	1:A:71:VAL:HG23	1.82	0.61
1:A:110:VAL:CA	1:A:110:VAL:HB	2.27	0.61
1:D:151:VAL:HG12	1:D:157:LYS:HE3	1.82	0.61
2:B:59:LYS:HA	1:D:283:MET:CE	2.29	0.61
1:D:244:ARG:HG2	1:D:244:ARG:HH11	1.63	0.61
2:B:64:LEU:O	2:B:66:LEU:HD13	2.00	0.61
1:A:75:ILE:HG22	1:A:89:LEU:HD22	1.83	0.61
1:A:205:TYR:HD1	1:A:410:LEU:HD21	1.65	0.61
1:D:175:PRO:HB2	1:D:247:LEU:HD23	1.81	0.61
4:E:712:DG:C6	4:E:713:DG:C2	2.89	0.61
1:A:159:ALA:O	1:A:160:LEU:HD23	2.00	0.60
1:A:274:GLY:O	1:A:278:ILE:HG12	2.01	0.60
1:A:256:CYS:SG	1:A:313:LYS:HG3	2.42	0.60
2:P:64:LEU:O	2:P:66:LEU:HD13	2.00	0.60
1:A:13:VAL:HG13	1:A:32:TRP:NE1	2.16	0.60
2:B:52:THR:HB	2:P:54:LEU:HD12	1.83	0.60
1:A:382:ARG:HD3	3:T:714:DG:OP1	2.01	0.60
1:D:21:ASN:HD22	1:D:22:GLY:N	1.98	0.60
1:A:120:LEU:HD22	1:A:124:ARG:HH11	1.66	0.60
1:A:110:VAL:O	1:A:111:THR:O	2.20	0.60
2:B:38:LYS:CD	4:E:715:DG:C6	2.70	0.60
1:D:281:PHE:HE2	1:D:317:VAL:HG11	1.66	0.59
1:A:320:GLN:OE1	1:A:326:ARG:HG2	2.02	0.59
1:D:21:ASN:HD22	1:D:21:ASN:C	2.05	0.59
1:A:184:ILE:HD12	1:A:196:LEU:HB2	1.84	0.59
2:P:7:ILE:HG23	2:P:12:GLN:HG2	1.83	0.59
1:D:303:TRP:HE1	1:D:369:ILE:HB	1.67	0.59
1:A:58:PHE:CE1	1:A:86:PRO:HG2	2.38	0.59
1:A:21:ASN:ND2	1:A:23:ALA:CB	2.65	0.59
2:B:26:TRP:HA	2:B:30:GLU:OE1	2.03	0.58
1:D:108:GLU:HG3	1:D:110:VAL:CG2	2.33	0.58
3:T:718:DA:H2	4:E:702:DA:C2	2.21	0.58
3:T:715:DG:O6	2:P:38:LYS:NZ	2.31	0.58
1:A:72:ARG:O	1:A:76:VAL:HG23	2.03	0.58
1:D:110:VAL:CG1	1:D:112:HIS:CE1	2.77	0.58
3:T:712:DG:H2"	3:T:713:DG:C8	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ASN:OD1	1:D:263:SER:HB3	2.03	0.58
1:A:89:LEU:O	1:A:93:ILE:HD13	2.03	0.58
2:B:38:LYS:HE2	4:E:713:DG:C8	2.39	0.58
1:A:112:HIS:O	1:A:113:PRO:C	2.38	0.58
1:A:339:VAL:O	1:A:345:ILE:HB	2.04	0.58
1:D:159:ALA:O	1:D:160:LEU:HD23	2.03	0.58
1:D:347:ILE:HG13	1:D:367:ASP:HB2	1.86	0.58
1:D:19:LEU:HD12	1:D:23:ALA:HB3	1.85	0.58
3:T:711:DA:N1	4:E:710:DA:H5"	2.19	0.58
1:A:10:ASN:HD21	1:A:173:ILE:HD12	1.69	0.58
1:A:345:ILE:CD1	1:A:345:ILE:H	2.09	0.58
1:A:217:VAL:HB	1:A:218:PRO:HD2	1.85	0.58
1:D:370:TYR:CD2	1:D:432:ARG:HD3	2.39	0.58
1:D:48:GLN:HB2	2:P:22:GLN:HE22	1.68	0.58
1:A:48:GLN:HB2	2:B:22:GLN:HE22	1.68	0.57
1:D:157:LYS:HD3	1:D:181:LYS:HE2	1.86	0.57
1:A:112:HIS:HB2	1:A:173:ILE:H	1.68	0.57
1:D:21:ASN:HD21	1:D:23:ALA:HB3	1.69	0.57
1:D:303:TRP:NE1	1:D:369:ILE:HB	2.20	0.57
1:A:19:LEU:HB2	1:A:23:ALA:HB3	1.87	0.57
1:A:387:GLN:O	1:A:391:ILE:HG13	2.04	0.57
1:A:112:HIS:HB3	1:A:172:GLY:C	2.25	0.57
2:P:17:MET:SD	2:P:45:PHE:CZ	2.98	0.57
1:A:85:GLN:HB2	1:A:88:ASP:OD2	2.04	0.57
1:A:322:GLY:HA2	2:B:5:GLN:NE2	2.20	0.56
1:A:108:GLU:HG3	1:A:110:VAL:HG23	1.86	0.56
1:A:104:ILE:CD1	1:A:112:HIS:NE2	2.69	0.56
3:T:712:DG:H2"	3:T:713:DG:N7	2.19	0.56
1:D:124:ARG:O	1:D:128:VAL:HG23	2.05	0.56
2:B:69:THR:OG1	2:P:4:PHE:HB3	2.05	0.56
4:E:702:DA:H2"	4:E:703:DT:H71	1.88	0.56
1:A:179:ILE:HD11	1:A:235:ARG:CZ	2.35	0.56
4:E:707:DC:H2"	4:E:708:DT:C5'	2.33	0.56
1:D:298:PHE:O	1:D:302:GLN:HG3	2.06	0.56
1:D:308:THR:HG22	1:D:351:LYS:O	2.06	0.56
1:A:108:GLU:O	1:A:109:THR:C	2.42	0.56
1:A:75:ILE:CG2	1:A:89:LEU:HD22	2.36	0.56
1:D:339:VAL:O	1:D:345:ILE:HB	2.06	0.55
1:A:161:LEU:CD1	1:A:177:THR:HG23	2.36	0.55
2:P:17:MET:SD	2:P:45:PHE:HZ	2.30	0.55
3:T:718:DA:C2	4:E:702:DA:C2	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:714:DG:H2''	4:E:715:DG:O4'	2.06	0.55
2:P:39:GLN:HE22	4:E:702:DA:N6	1.89	0.55
1:A:21:ASN:ND2	1:A:23:ALA:HB2	2.21	0.55
1:D:337:PHE:C	1:D:339:VAL:H	2.08	0.55
1:A:399:ILE:HG22	1:A:400:PRO:N	2.19	0.55
1:D:200:VAL:HG13	1:D:231:LEU:HB2	1.89	0.55
1:A:26:PHE:O	1:A:52:ILE:HG12	2.07	0.55
1:A:281:PHE:CZ	1:A:325:TYR:CE2	2.95	0.55
1:A:130:THR:HA	1:A:133:LYS:NZ	2.22	0.55
1:D:347:ILE:HD12	1:D:350:LEU:HD12	1.89	0.55
1:A:85:GLN:NE2	1:A:86:PRO:HD2	2.21	0.55
1:D:282:LEU:HD21	1:D:327:LEU:HD13	1.88	0.55
1:A:308:THR:HG22	1:A:351:LYS:O	2.07	0.54
1:D:115:MET:HE2	1:D:174:THR:HG23	1.89	0.54
4:E:717:DT:O2	4:E:718:DA:C2	2.60	0.54
1:A:19:LEU:HB2	1:A:21:ASN:HD21	1.72	0.54
1:A:384:PRO:HG2	1:A:387:GLN:NE2	2.22	0.54
1:D:130:THR:HA	1:D:133:LYS:NZ	2.22	0.54
1:A:347:ILE:HD12	1:A:350:LEU:HD12	1.88	0.54
1:D:370:TYR:H	1:D:373:HIS:HD1	1.55	0.54
4:E:712:DG:C5	4:E:713:DG:C4	2.95	0.54
1:D:339:VAL:HG12	1:D:339:VAL:O	2.07	0.54
1:D:428:ARG:NH1	1:D:428:ARG:HG2	2.16	0.54
2:B:35:ILE:HG23	2:B:63:SER:HB3	1.87	0.54
1:D:104:ILE:HG22	1:D:108:GLU:CG	2.38	0.54
1:D:427:LEU:HA	1:D:430:HIS:HB3	1.90	0.54
1:D:85:GLN:HE21	1:D:86:PRO:HD2	1.71	0.54
1:A:112:HIS:HB3	1:A:172:GLY:HA3	1.87	0.54
4:E:702:DA:C2'	4:E:703:DT:H71	2.38	0.54
1:A:303:TRP:NE1	1:A:369:ILE:HB	2.23	0.54
1:A:93:ILE:H	1:A:93:ILE:HD13	1.72	0.54
1:D:198:GLN:HE22	1:D:415:PRO:HB3	1.74	0.53
1:D:52:ILE:HD13	1:D:52:ILE:N	2.22	0.53
3:T:713:DG:C4	3:T:714:DG:N7	2.77	0.53
2:B:54:LEU:O	2:B:58:PHE:HD1	1.90	0.53
1:D:206:CYS:HG	1:D:305:ILE:HD12	1.73	0.53
3:T:702:DA:C2'	3:T:703:DT:H5''	2.35	0.53
1:A:104:ILE:HD12	1:A:112:HIS:NE2	2.22	0.53
1:A:278:ILE:HG21	1:A:295:PHE:CE1	2.42	0.53
2:B:35:ILE:HG21	2:B:59:LYS:O	2.09	0.53
1:D:71:VAL:O	1:D:75:ILE:CD1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:LYS:HG3	1:A:166:ASP:HB3	1.89	0.53
1:D:104:ILE:CG2	1:D:108:GLU:HG2	2.38	0.53
2:B:6:LYS:HZ1	2:B:74:LYS:HG3	1.73	0.53
4:E:700:DC:H2''	4:E:701:DT:O5'	2.08	0.53
1:A:19:LEU:HD12	1:A:23:ALA:HB3	1.91	0.53
1:A:120:LEU:HD22	1:A:124:ARG:HB3	1.92	0.52
1:A:182:LEU:HD22	1:A:182:LEU:H	1.73	0.52
1:A:345:ILE:N	1:A:345:ILE:HD12	2.14	0.52
1:D:85:GLN:NE2	1:D:86:PRO:HD2	2.24	0.52
2:P:58:PHE:HA	2:P:61:LEU:HB2	1.91	0.52
1:D:410:LEU:HD13	1:D:419:VAL:HG22	1.90	0.52
1:D:108:GLU:HG3	1:D:110:VAL:HG23	1.90	0.52
1:D:291:ASP:O	1:D:292:ARG:C	2.48	0.52
2:P:19:LEU:HD22	2:P:23:GLN:HG3	1.91	0.52
1:A:95:ARG:HE	1:A:112:HIS:HE1	1.52	0.52
1:D:243:GLU:CB	1:D:245:THR:HG23	2.40	0.52
1:A:19:LEU:HB2	1:A:21:ASN:ND2	2.25	0.52
1:D:21:ASN:ND2	1:D:23:ALA:H	2.07	0.52
1:D:237:ASP:HB3	1:D:252:GLN:OE1	2.10	0.52
2:P:53:THR:HG22	2:P:55:THR:H	1.75	0.52
1:D:370:TYR:CE2	1:D:432:ARG:HD3	2.45	0.51
2:B:35:ILE:CG2	2:B:63:SER:HB3	2.40	0.51
1:D:96:ASP:CB	1:D:149:ILE:HG23	2.37	0.51
2:B:69:THR:HG22	2:P:69:THR:HG23	1.92	0.51
1:A:209:LEU:HA	1:A:406:VAL:HG21	1.91	0.51
4:E:716:DA:H2''	4:E:717:DT:H5'	1.93	0.51
2:P:53:THR:HG22	2:P:54:LEU:N	2.25	0.51
4:E:717:DT:C2	4:E:718:DA:C6	2.98	0.51
1:A:399:ILE:CB	1:A:430:HIS:CD2	2.87	0.51
1:A:148:ARG:HG3	1:A:148:ARG:HH11	1.76	0.51
1:D:205:TYR:HD1	1:D:410:LEU:HD21	1.75	0.51
2:B:38:LYS:CG	4:E:713:DG:H2''	2.41	0.51
2:P:7:ILE:HG23	2:P:12:GLN:CG	2.40	0.51
1:D:255:MET:HB2	1:D:312:ALA:O	2.10	0.50
1:D:79:TYR:O	1:D:80:HIS:C	2.49	0.50
1:A:275:ILE:HG22	1:A:381:LEU:HD11	1.93	0.50
1:D:19:LEU:HB2	1:D:21:ASN:HD21	1.76	0.50
1:D:110:VAL:CG1	1:D:112:HIS:NE2	2.66	0.50
1:D:295:PHE:O	1:D:296:MET:C	2.49	0.50
1:D:320:GLN:O	1:D:321:ALA:C	2.50	0.50
1:D:428:ARG:HH11	1:D:428:ARG:CG	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:CZ	1:A:148:ARG:HG3	2.41	0.50
2:B:31:LEU:O	2:B:35:ILE:HG12	2.12	0.50
2:B:61:LEU:HD21	2:P:70:LEU:HD22	1.92	0.50
1:A:255:MET:HB2	1:A:312:ALA:O	2.12	0.50
1:A:33:LEU:HD11	1:A:48:GLN:O	2.10	0.50
1:A:347:ILE:HG13	1:A:367:ASP:HB2	1.93	0.50
1:D:376:ALA:O	1:D:379:LYS:HB2	2.12	0.50
1:A:175:PRO:HG2	1:A:247:LEU:HB3	1.94	0.50
1:A:428:ARG:HG2	1:A:428:ARG:NH1	2.26	0.50
1:D:380:VAL:HG23	1:D:381:LEU:N	2.27	0.50
1:D:387:GLN:O	1:D:391:ILE:HG13	2.11	0.50
4:E:718:DA:H2'	4:E:718:DA:OP2	2.12	0.50
2:B:7:ILE:HG23	2:B:12:GLN:CG	2.42	0.49
1:A:337:PHE:C	1:A:339:VAL:H	2.15	0.49
1:D:104:ILE:O	1:D:105:PRO:O	2.29	0.49
1:D:169:ILE:CG2	1:D:170:PRO:HD2	2.42	0.49
1:D:161:LEU:CD1	1:D:177:THR:HG23	2.42	0.49
1:D:371:PRO:HB3	1:D:392:LEU:HD13	1.95	0.49
1:D:33:LEU:HD11	1:D:48:GLN:O	2.12	0.49
1:A:100:ALA:HB3	1:A:251:PRO:HA	1.95	0.49
1:D:262:PRO:O	1:D:265:VAL:HG22	2.12	0.49
1:A:198:GLN:HE22	1:A:415:PRO:HB3	1.78	0.49
1:D:21:ASN:ND2	1:D:23:ALA:CB	2.76	0.49
2:P:6:LYS:NZ	2:P:74:LYS:HG3	2.28	0.49
3:T:703:DT:H1'	3:T:704:DC:H5'	1.94	0.49
1:A:376:ALA:O	1:A:379:LYS:HB2	2.13	0.49
1:A:375:LEU:HD23	1:A:388:MET:HG2	1.94	0.49
1:D:125:LEU:HD23	1:D:225:ALA:HB2	1.93	0.49
1:D:149:ILE:HG22	1:D:150:SER:H	1.78	0.49
1:D:266:LYS:HD2	1:D:311:HIS:CD2	2.47	0.49
1:A:179:ILE:HG12	1:A:235:ARG:HG2	1.94	0.48
1:A:151:VAL:CG1	1:A:157:LYS:HE3	2.41	0.48
1:A:237:ASP:HB3	1:A:252:GLN:OE1	2.13	0.48
1:A:182:LEU:N	1:A:182:LEU:HD13	2.28	0.48
1:A:275:ILE:CG2	1:A:381:LEU:HD11	2.43	0.48
1:A:404:ASP:O	1:A:408:THR:HG23	2.14	0.48
1:A:384:PRO:HB2	1:A:387:GLN:HB2	1.95	0.48
1:A:340:LEU:HD23	1:A:345:ILE:HG22	1.96	0.48
1:D:161:LEU:HD12	1:D:177:THR:HG23	1.94	0.48
1:D:115:MET:CE	1:D:174:THR:HG23	2.43	0.48
2:P:42:ILE:HD13	2:P:60:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LEU:CD2	1:A:432:ARG:HH12	2.17	0.48
1:D:280:ALA:O	1:D:283:MET:HB2	2.14	0.48
1:D:318:PHE:CD1	1:D:328:THR:HG22	2.49	0.48
2:P:53:THR:CG2	2:P:54:LEU:N	2.76	0.48
4:E:712:DG:O6	4:E:713:DG:C2	2.67	0.48
2:B:17:MET:HG3	2:P:70:LEU:HD11	1.94	0.48
1:D:309:GLN:HG3	1:D:334:ILE:CG2	2.44	0.48
1:D:148:ARG:NH1	1:D:148:ARG:CG	2.69	0.47
1:D:93:ILE:HG12	1:D:93:ILE:O	2.13	0.47
2:P:31:LEU:O	2:P:35:ILE:HG12	2.14	0.47
1:A:303:TRP:HE1	1:A:369:ILE:HB	1.78	0.47
1:D:104:ILE:HG22	1:D:108:GLU:HG2	1.96	0.47
1:D:209:LEU:HA	1:D:406:VAL:HG21	1.97	0.47
1:A:358:ALA:HB2	1:A:363:LYS:H	1.78	0.47
1:D:414:PHE:CD2	1:D:415:PRO:HD2	2.50	0.47
1:D:414:PHE:CG	1:D:415:PRO:HD2	2.50	0.47
1:D:399:ILE:CB	1:D:430:HIS:CD2	2.88	0.47
1:D:46:PRO:O	1:D:47:LEU:C	2.53	0.47
3:T:705:DC:N4	4:E:714:DG:O6	2.47	0.47
1:A:3:LYS:HD2	1:A:106:GLU:OE1	2.15	0.47
1:A:115:MET:HE2	1:A:174:THR:HG23	1.95	0.47
2:B:19:LEU:CD2	2:B:23:GLN:HG3	2.45	0.47
3:T:710:DA:H5"	4:E:711:DA:C2	2.49	0.47
2:B:38:LYS:HG3	4:E:713:DG:H2"	1.95	0.47
2:P:56:THR:O	2:P:59:LYS:HB2	2.15	0.47
1:A:429:LEU:CD2	1:A:432:ARG:NH1	2.72	0.47
3:T:708:DT:H3	4:E:712:DG:H22	1.62	0.47
3:T:703:DT:H2"	3:T:704:DC:OP2	2.14	0.47
1:A:351:LYS:HD2	1:A:365:ALA:HA	1.97	0.47
1:A:300:VAL:O	1:A:303:TRP:HB3	2.15	0.47
1:A:392:LEU:HD22	1:A:433:LEU:HD21	1.97	0.47
1:A:68:SER:HB3	1:A:71:VAL:CG2	2.45	0.47
1:D:108:GLU:HG3	1:D:110:VAL:HG21	1.97	0.47
1:D:309:GLN:HG3	1:D:334:ILE:HG23	1.97	0.47
1:D:256:CYS:SG	1:D:313:LYS:HG3	2.55	0.46
1:D:60:PHE:CE1	1:D:257:GLN:NE2	2.83	0.46
2:P:26:TRP:HA	2:P:30:GLU:OE1	2.15	0.46
1:A:371:PRO:HB3	1:A:392:LEU:HD13	1.97	0.46
1:D:337:PHE:O	1:D:339:VAL:N	2.49	0.46
1:D:399:ILE:HG22	1:D:400:PRO:N	2.31	0.46
4:E:702:DA:H2"	4:E:703:DT:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:HD12	2:P:52:THR:HB	1.97	0.46
2:B:53:THR:HG22	2:B:55:THR:H	1.80	0.46
1:D:311:HIS:CE1	1:D:313:LYS:HB2	2.51	0.46
1:D:396:ALA:O	1:D:430:HIS:NE2	2.47	0.46
2:B:6:LYS:NZ	2:B:74:LYS:HG3	2.30	0.46
4:E:717:DT:O2	4:E:718:DA:N1	2.49	0.46
1:A:375:LEU:HD23	1:A:388:MET:CG	2.45	0.46
1:D:182:LEU:N	1:D:182:LEU:HD22	2.30	0.46
1:D:184:ILE:HD12	1:D:196:LEU:HB2	1.98	0.46
1:D:204:TYR:CE2	1:D:208:LEU:HD11	2.51	0.46
1:A:110:VAL:O	1:A:111:THR:C	2.54	0.46
1:A:382:ARG:CD	3:T:714:DG:OP1	2.63	0.46
1:A:399:ILE:HG22	1:A:400:PRO:CD	2.46	0.46
2:B:22:GLN:C	2:B:24:ASN:H	2.19	0.46
1:A:273:PRO:HD2	1:A:312:ALA:HB2	1.98	0.46
1:A:76:VAL:HG22	1:A:89:LEU:HD21	1.97	0.46
1:D:109:THR:HA	1:D:109:THR:CB	2.27	0.45
1:D:114:ILE:HD13	1:D:173:ILE:HD11	1.97	0.45
1:A:25:THR:HG22	1:A:53:THR:HG22	1.99	0.45
1:D:158:THR:OG1	1:D:159:ALA:N	2.49	0.45
1:A:396:ALA:O	1:A:430:HIS:NE2	2.48	0.45
1:D:370:TYR:CZ	1:D:432:ARG:NE	2.83	0.45
1:A:115:MET:CE	1:A:115:MET:HA	2.47	0.45
1:A:296:MET:O	1:A:299:GLN:N	2.50	0.45
1:A:2:PRO:O	1:A:87:PHE:HZ	2.00	0.45
1:A:99:GLY:O	1:A:250:LEU:O	2.34	0.45
1:D:13:VAL:HG13	1:D:32:TRP:CE2	2.52	0.45
1:D:21:ASN:HD21	1:D:23:ALA:CB	2.29	0.45
1:D:410:LEU:HD13	1:D:419:VAL:CG2	2.46	0.45
3:T:714:DG:OP2	3:T:714:DG:H3'	2.17	0.45
1:A:68:SER:HG	1:A:70:ILE:CD1	2.17	0.45
1:D:274:GLY:O	1:D:278:ILE:HG12	2.17	0.45
1:D:293:TYR:O	1:D:294:ASP:C	2.55	0.45
1:D:297:LYS:HG3	1:D:391:ILE:HG23	1.99	0.45
1:A:126:GLU:O	1:A:130:THR:HG23	2.17	0.45
1:A:126:GLU:OE2	1:A:226:GLY:HA3	2.17	0.45
1:A:37:TYR:HB3	1:A:39:ARG:HH21	1.82	0.45
1:D:100:ALA:HB3	1:D:251:PRO:HA	1.98	0.45
1:D:104:ILE:O	1:D:105:PRO:C	2.55	0.45
4:E:707:DC:C2'	4:E:708:DT:H5'	2.37	0.45
2:P:55:THR:O	2:P:56:THR:C	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:O	1:A:147:PHE:CD1	2.70	0.44
1:A:351:LYS:CD	1:A:365:ALA:HA	2.47	0.44
1:D:282:LEU:HD23	1:D:282:LEU:HA	1.89	0.44
4:E:712:DG:N7	4:E:713:DG:C5	2.84	0.44
3:T:709:DT:H2''	3:T:710:DA:O5'	2.17	0.44
1:A:427:LEU:HA	1:A:430:HIS:HB3	1.98	0.44
1:D:157:LYS:CD	1:D:181:LYS:HE2	2.48	0.44
3:T:712:DG:OP1	2:P:53:THR:N	2.34	0.44
1:A:110:VAL:C	1:A:111:THR:O	2.53	0.44
1:A:104:ILE:HD11	1:A:112:HIS:NE2	2.32	0.44
1:D:410:LEU:CD1	1:D:419:VAL:HG22	2.47	0.44
2:P:54:LEU:O	2:P:58:PHE:HD1	1.99	0.44
1:A:130:THR:HA	1:A:133:LYS:CE	2.48	0.44
1:A:429:LEU:O	1:A:432:ARG:HB2	2.17	0.44
1:A:262:PRO:O	1:A:265:VAL:HG22	2.18	0.44
4:E:708:DT:H1'	4:E:709:DT:C4	2.52	0.44
1:A:410:LEU:HD13	1:A:419:VAL:HG22	1.99	0.44
1:A:430:HIS:ND1	1:A:430:HIS:C	2.71	0.44
1:D:320:GLN:HB2	1:D:324:SER:HB2	1.99	0.44
1:A:118:GLU:HB2	1:A:171:LYS:NZ	2.31	0.44
1:A:283:MET:HE1	2:P:59:LYS:HA	1.99	0.44
1:D:273:PRO:HD2	1:D:312:ALA:HB2	1.99	0.44
1:D:340:LEU:HD23	1:D:345:ILE:HG22	1.99	0.44
1:D:425:ASN:HD22	1:D:425:ASN:H	1.66	0.44
1:A:320:GLN:O	1:A:321:ALA:C	2.57	0.44
1:D:110:VAL:CG1	1:D:112:HIS:CD2	3.01	0.44
1:D:8:MET:HE3	1:D:101:VAL:HG12	2.00	0.44
1:A:100:ALA:CB	1:A:251:PRO:HA	2.48	0.43
1:D:243:GLU:O	1:D:245:THR:HG23	2.17	0.43
4:E:700:DC:C5	4:E:701:DT:H73	2.53	0.43
2:P:6:LYS:HZ1	2:P:74:LYS:HG3	1.83	0.43
1:D:98:VAL:HG12	1:D:99:GLY:N	2.33	0.43
1:D:160:LEU:HG	1:D:180:ILE:HD12	2.00	0.43
1:D:258:THR:HG22	1:D:259:PHE:CD2	2.53	0.43
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.29	0.43
1:A:266:LYS:HD2	1:A:311:HIS:CD2	2.53	0.43
1:A:337:PHE:O	1:A:339:VAL:N	2.51	0.43
1:D:120:LEU:HD22	1:D:124:ARG:HH11	1.81	0.43
1:A:95:ARG:NH2	1:A:148:ARG:NH1	2.67	0.43
1:D:266:LYS:HD2	1:D:311:HIS:CE1	2.53	0.43
1:D:98:VAL:HG12	1:D:99:GLY:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:717:DT:C2	4:E:718:DA:N1	2.86	0.43
1:A:124:ARG:O	1:A:128:VAL:HG23	2.19	0.43
2:B:38:LYS:HD2	4:E:715:DG:N1	2.27	0.43
1:A:52:ILE:N	1:A:52:ILE:HD13	2.33	0.43
1:A:21:ASN:N	1:A:21:ASN:ND2	2.67	0.43
1:A:182:LEU:HD22	1:A:182:LEU:N	2.34	0.43
1:A:279:MET:HG3	1:A:381:LEU:HD13	2.00	0.43
1:D:21:ASN:ND2	1:D:23:ALA:N	2.67	0.43
1:D:337:PHE:C	1:D:339:VAL:N	2.72	0.42
1:D:337:PHE:N	1:D:338:PRO:CD	2.82	0.42
1:A:120:LEU:HD11	1:A:169:ILE:HG13	2.01	0.42
1:A:149:ILE:HG22	1:A:150:SER:H	1.83	0.42
1:A:120:LEU:HB2	1:A:167:TRP:O	2.20	0.42
2:B:38:LYS:CG	4:E:713:DG:C2'	2.96	0.42
2:B:65:GLU:O	2:B:66:LEU:HD12	2.18	0.42
1:D:217:VAL:HB	1:D:218:PRO:HD2	2.01	0.42
2:P:38:LYS:HB2	2:P:38:LYS:HE2	1.35	0.42
1:A:112:HIS:O	1:A:114:ILE:N	2.53	0.42
1:A:296:MET:O	1:A:299:GLN:HB2	2.19	0.42
2:B:62:GLN:NE2	2:P:8:TYR:HB3	2.35	0.42
3:T:701:DT:C2	3:T:702:DA:C5	3.07	0.42
1:A:84:ARG:HE	1:A:84:ARG:HB2	1.69	0.42
1:D:120:LEU:HD11	1:D:169:ILE:HG13	2.02	0.42
1:A:127:GLU:O	1:A:131:ALA:HB2	2.20	0.42
1:A:343:THR:OG1	1:A:345:ILE:HD13	2.19	0.42
1:D:155:GLN:HG2	1:D:184:ILE:HG12	2.02	0.42
1:D:428:ARG:NH1	1:D:428:ARG:CG	2.79	0.42
3:T:707:DC:H42	4:E:713:DG:H21	1.68	0.42
1:A:309:GLN:HG3	1:A:334:ILE:HG23	2.01	0.42
1:A:334:ILE:HG12	1:A:335:SER:N	2.34	0.42
1:A:398:MET:O	1:A:399:ILE:C	2.56	0.42
1:A:96:ASP:OD2	1:A:175:PRO:HA	2.19	0.42
3:T:712:DG:P	2:P:53:THR:H	2.42	0.42
1:A:75:ILE:HG22	1:A:89:LEU:CD2	2.50	0.42
1:D:334:ILE:HG12	1:D:335:SER:N	2.34	0.42
1:D:275:ILE:CG2	1:D:381:LEU:HD11	2.50	0.42
1:D:403:LEU:HD13	1:D:423:GLU:HG3	2.01	0.42
1:A:282:LEU:HD21	1:A:327:LEU:HD13	2.01	0.41
1:D:13:VAL:HG13	1:D:32:TRP:NE1	2.34	0.41
3:T:705:DC:N3	4:E:714:DG:O6	2.52	0.41
2:P:39:GLN:HE21	2:P:39:GLN:HB3	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:O	1:A:93:ILE:CD1	2.68	0.41
1:D:21:ASN:HD22	1:D:23:ALA:H	1.66	0.41
1:D:410:LEU:HA	1:D:411:PRO:HD2	1.89	0.41
3:T:712:DG:C4'	3:T:713:DG:H5'	2.43	0.41
1:A:382:ARG:NE	3:T:714:DG:OP1	2.53	0.41
1:A:205:TYR:HE2	1:A:422:VAL:HG11	1.84	0.41
1:D:160:LEU:HB2	1:D:180:ILE:HD11	2.02	0.41
1:D:351:LYS:CD	1:D:365:ALA:HA	2.49	0.41
2:P:28:GLN:OE1	2:P:43:SER:HB2	2.20	0.41
2:P:58:PHE:O	2:P:59:LYS:C	2.56	0.41
1:D:266:LYS:HE2	1:D:267:TYR:HE1	1.85	0.41
1:D:76:VAL:HG21	1:D:84:ARG:HG2	2.00	0.41
1:D:128:VAL:O	1:D:131:ALA:HB3	2.20	0.41
1:D:281:PHE:CZ	1:D:325:TYR:CE2	3.08	0.41
1:A:157:LYS:HD3	1:A:181:LYS:HE2	2.02	0.41
1:D:266:LYS:HD2	1:D:311:HIS:CG	2.56	0.41
2:B:68:MET:HE3	2:B:68:MET:HB2	1.95	0.41
1:D:180:ILE:HA	1:D:231:LEU:O	2.20	0.41
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.73	0.41
1:A:286:SER:HA	2:B:8:TYR:CE2	2.56	0.41
1:D:120:LEU:HD21	1:D:169:ILE:HD12	2.02	0.41
3:T:714:DG:N7	2:P:38:LYS:NZ	2.63	0.41
1:A:120:LEU:HD22	1:A:124:ARG:NH1	2.35	0.41
1:A:205:TYR:CD1	1:A:410:LEU:HD21	2.52	0.41
2:B:34:LYS:HE2	1:D:289:LEU:HD23	2.02	0.41
1:D:149:ILE:HG22	1:D:150:SER:N	2.36	0.41
4:E:712:DG:C5	4:E:713:DG:C5	3.09	0.41
1:A:108:GLU:C	1:A:110:VAL:N	2.74	0.41
1:A:13:VAL:HG13	1:A:32:TRP:CD1	2.55	0.41
1:A:295:PHE:O	1:A:296:MET:C	2.57	0.40
1:A:205:TYR:CE2	1:A:422:VAL:HG11	2.55	0.40
1:A:70:ILE:HG13	1:A:70:ILE:H	1.57	0.40
1:D:182:LEU:N	1:D:182:LEU:HD13	2.36	0.40
2:P:60:ILE:O	2:P:64:LEU:HG	2.20	0.40
2:B:67:SER:N	2:P:71:CYS:O	2.51	0.40
1:A:174:THR:HA	1:A:175:PRO:HD3	1.86	0.40
1:A:196:LEU:N	1:A:196:LEU:HD22	2.36	0.40
1:A:281:PHE:HE2	1:A:317:VAL:HG11	1.86	0.40
1:A:85:GLN:HE21	1:A:86:PRO:CD	2.32	0.40
1:D:366:ILE:HG22	1:D:367:ASP:N	2.34	0.40
3:T:712:DG:OP2	2:P:52:THR:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ILE:HA	1:A:231:LEU:O	2.21	0.40
1:A:266:LYS:HE2	1:A:267:TYR:HE1	1.86	0.40
2:B:34:LYS:HE2	1:D:289:LEU:CD2	2.51	0.40
1:D:4:LEU:HD23	1:D:105:PRO:HA	2.02	0.40
1:A:337:PHE:C	1:A:339:VAL:N	2.74	0.40
1:A:377:THR:O	1:A:378:ALA:C	2.58	0.40
1:A:399:ILE:CB	1:A:400:PRO:HD3	2.51	0.40
1:A:121:THR:H	1:A:124:ARG:HB2	1.87	0.40
1:A:112:HIS:CB	1:A:173:ILE:HG12	2.35	0.40
1:D:21:ASN:HD22	1:D:23:ALA:N	2.19	0.40
1:D:337:PHE:HB2	1:D:338:PRO:HD3	2.03	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:VAL:CB	1:D:109:THR:C[3_456]	1.68	0.52
1:A:110:VAL:CA	1:D:110:VAL:N[3_456]	1.94	0.26
1:A:110:VAL:CG1	1:D:109:THR:O[3_456]	1.95	0.25
1:A:110:VAL:O	1:D:110:VAL:N[3_456]	2.00	0.20
1:A:110:VAL:CB	1:D:110:VAL:N[3_456]	2.09	0.11
1:A:110:VAL:C	1:D:110:VAL:N[3_456]	2.10	0.10
1:A:67:ASP:O	1:D:84:ARG:NH1[3_455]	2.15	0.05
1:A:340:LEU:O	1:D:417:ASN:OD1[4_465]	2.15	0.05
1:A:110:VAL:CB	1:D:109:THR:CA[3_456]	2.15	0.05
1:A:110:VAL:CG1	1:D:109:THR:C[3_456]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	408/448 (91%)	353 (86%)	45 (11%)	10 (2%)	7 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	408/448 (91%)	353 (86%)	41 (10%)	14 (3%)	5	43
2	B	69/91 (76%)	63 (91%)	5 (7%)	1 (1%)	14	59
2	P	69/91 (76%)	63 (91%)	3 (4%)	3 (4%)	3	35
All	All	954/1078 (88%)	832 (87%)	94 (10%)	28 (3%)	6	46

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	ARG
1	A	108	GLU
1	A	110	VAL
1	D	20	ALA
1	D	21	ASN
1	D	95	ARG
1	D	108	GLU
1	A	78	ARG
1	A	80	HIS
1	D	80	HIS
1	D	110	VAL
1	D	111	THR
1	A	100	ALA
2	B	23	GLN
1	D	105	PRO
1	A	384	PRO
1	D	113	PRO
1	A	415	PRO
1	D	109	THR
1	D	132	TYR
1	D	384	PRO
2	P	36	GLY
2	P	50	ASP
1	A	109	THR
1	D	338	PRO
1	A	338	PRO
1	D	226	GLY
2	P	35	ILE

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	351/382 (92%)	328 (93%)	23 (7%)	21	60
1	D	351/382 (92%)	332 (95%)	19 (5%)	27	67
2	B	64/83 (77%)	57 (89%)	7 (11%)	8	38
2	P	64/83 (77%)	57 (89%)	7 (11%)	8	38
All	All	830/930 (89%)	774 (93%)	56 (7%)	20	60

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	21	ASN
1	A	69	PRO
1	A	73	ASP
1	A	93	ILE
1	A	101	VAL
1	A	108	GLU
1	A	110	VAL
1	A	111	THR
1	A	118	GLU
1	A	122	GLU
1	A	124	ARG
1	A	155	GLN
1	A	182	LEU
1	A	244	ARG
1	A	258	THR
1	A	289	LEU
1	A	308	THR
1	A	334	ILE
1	A	346	HIS
1	A	364	THR
1	A	412	THR
1	A	417	ASN
2	B	4	PHE
2	B	5	GLN
2	B	12	GLN
2	B	13	LEU
2	B	19	LEU

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Mol	Chain	Res	Type
2	B	61	LEU
2	B	66	LEU
1	D	8	MET
1	D	21	ASN
1	D	73	ASP
1	D	84	ARG
1	D	93	ILE
1	D	107	ASP
1	D	108	GLU
1	D	118	GLU
1	D	122	GLU
1	D	124	ARG
1	D	148	ARG
1	D	155	GLN
1	D	182	LEU
1	D	244	ARG
1	D	289	LEU
1	D	334	ILE
1	D	346	HIS
1	D	412	THR
1	D	417	ASN
2	P	5	GLN
2	P	12	GLN
2	P	13	LEU
2	P	19	LEU
2	P	39	GLN
2	P	61	LEU
2	P	66	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	21	ASN
1	A	85	GLN
1	A	198	GLN
1	A	227	ASN
1	A	357	ASN
1	A	387	GLN
2	B	5	GLN
2	B	12	GLN
2	B	22	GLN

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Mol	Chain	Res	Type
2	B	39	GLN
1	D	10	ASN
1	D	21	ASN
1	D	85	GLN
1	D	198	GLN
1	D	216	ASN
1	D	387	GLN
1	D	417	ASN
1	D	425	ASN
2	P	5	GLN
2	P	12	GLN
2	P	22	GLN
2	P	39	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	414/448 (92%)	2.13	171 (41%) 0 1	155, 179, 191, 199	0
1	D	414/448 (92%)	2.09	176 (42%) 0 1	157, 179, 191, 206	0
2	B	71/91 (78%)	1.57	23 (32%) 1 1	162, 176, 183, 185	0
2	P	71/91 (78%)	1.69	23 (32%) 1 1	158, 175, 187, 190	0
3	T	23/23 (100%)	2.31	13 (56%) 0 1	168, 186, 195, 198	0
4	E	23/23 (100%)	2.93	12 (52%) 0 1	166, 191, 196, 204	0
All	All	1016/1124 (90%)	2.06	418 (41%) 0 1	155, 179, 191, 206	0

All (418) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	GLY	20.9
1	D	273	PRO	13.1
1	A	229	ARG	11.5
1	D	230	ALA	11.2
1	A	100	ALA	11.1
1	D	229	ARG	10.9
2	P	73	THR	10.7
1	D	146	ASP	10.5
1	A	146	ASP	10.5
1	A	273	PRO	10.3
1	A	149	ILE	10.2
1	A	132	TYR	9.4
1	A	147	PHE	9.0
2	B	8	TYR	8.8
1	A	112	HIS	8.7
1	D	218	PRO	8.7
1	A	434	SER	8.7
1	D	175	PRO	8.6
1	A	148	ARG	8.5

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Mol	Chain	Res	Type	RSRZ
2	P	74	LYS	8.4
1	D	147	PHE	8.4
1	D	151	VAL	8.4
1	D	219	ASP	8.2
1	A	225	ALA	8.1
4	E	710	DA	7.9
1	A	84	ARG	7.8
4	E	720	DG	7.8
1	D	49	ARG	7.6
4	E	707	DC	7.6
1	A	355	GLY	7.5
1	D	183	PRO	7.5
1	D	434	SER	7.4
1	D	149	ILE	7.3
1	A	437	TYR	7.3
1	A	255	MET	7.3
1	A	228	VAL	7.0
1	D	272	GLY	7.0
1	D	150	SER	7.0
1	A	2	PRO	7.0
2	P	5	GLN	6.9
1	D	220	ALA	6.9
1	A	12	ARG	6.9
1	D	231	LEU	6.8
2	P	72	ASP	6.7
1	A	98	VAL	6.6
1	D	359	SER	6.5
2	B	73	THR	6.5
1	A	118	GLU	6.4
1	A	107	ASP	6.3
1	A	120	LEU	6.2
1	D	395	PHE	6.1
1	A	134	ALA	6.0
1	D	111	THR	6.0
1	D	176	THR	6.0
1	A	67	ASP	5.9
1	D	397	ARG	5.9
1	A	113	PRO	5.9
1	D	223	ILE	5.9
1	D	2	PRO	5.8
1	A	16	LEU	5.8
1	A	223	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	112	HIS	5.7
1	D	270	ASP	5.7
1	D	134	ALA	5.7
1	D	435	ARG	5.6
1	D	117	TRP	5.6
1	A	83	SER	5.6
1	A	111	THR	5.6
1	A	435	ARG	5.6
1	D	31	GLU	5.5
1	D	249	ARG	5.4
1	D	118	GLU	5.4
2	B	68	MET	5.4
1	A	15	GLU	5.4
2	P	6	LYS	5.4
1	D	383	PHE	5.3
4	E	706	DC	5.3
1	D	148	ARG	5.3
1	A	183	PRO	5.3
1	A	150	SER	5.3
1	A	433	LEU	5.2
1	D	358	ALA	5.2
2	P	23	GLN	5.2
1	A	220	ALA	5.2
1	A	167	TRP	5.2
1	A	105	PRO	5.1
1	D	129	LEU	5.1
1	D	15	GLU	5.1
1	D	437	TYR	5.1
1	A	265	VAL	5.1
1	A	383	PHE	5.0
1	A	49	ARG	5.0
1	D	213	LEU	5.0
1	D	24	HIS	5.0
1	A	31	GLU	4.9
1	D	99	GLY	4.9
1	D	385	GLU	4.9
1	A	176	THR	4.8
1	D	132	TYR	4.8
1	D	170	PRO	4.8
1	D	50	GLY	4.8
1	D	355	GLY	4.7
1	A	256	CYS	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	101	VAL	4.7
1	A	363	LYS	4.7
1	D	120	LEU	4.7
1	D	433	LEU	4.7
1	A	354	MET	4.7
4	E	708	DT	4.7
2	B	5	GLN	4.6
1	A	406	VAL	4.6
1	D	396	ALA	4.6
2	B	74	LYS	4.6
2	B	6	LYS	4.6
2	P	4	PHE	4.6
1	A	398	MET	4.5
1	D	171	LYS	4.5
1	D	313	LYS	4.5
1	D	52	ILE	4.5
1	A	60	PHE	4.5
1	D	271	GLY	4.5
1	D	367	ASP	4.4
1	D	115	MET	4.4
2	B	62	GLN	4.4
1	D	356	LEU	4.4
1	A	172	GLY	4.4
1	A	28	TYR	4.4
1	D	78	ARG	4.4
1	A	224	LYS	4.4
1	D	116	ALA	4.4
1	A	413	ASP	4.4
1	D	360	LYS	4.4
1	A	175	PRO	4.3
1	A	119	LYS	4.3
1	A	357	ASN	4.3
1	D	153	GLY	4.3
1	D	363	LYS	4.3
1	A	324	SER	4.2
1	D	154	ALA	4.2
1	D	60	PHE	4.2
1	D	212	GLU	4.2
1	A	274	GLY	4.2
1	D	95	ARG	4.2
1	D	324	SER	4.2
1	D	110	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	93	ILE	4.2
3	T	708	DT	4.2
1	D	26	PHE	4.1
1	A	108	GLU	4.1
1	D	286	SER	4.1
1	D	265	VAL	4.1
1	A	399	ILE	4.1
1	D	279	MET	4.0
1	D	173	ILE	4.0
2	B	7	ILE	4.0
2	B	46	GLU	4.0
1	D	32	TRP	4.0
1	D	174	THR	3.9
1	A	207	LEU	3.9
1	A	313	LYS	3.9
1	D	315	PHE	3.9
1	D	261	LEU	3.9
1	A	356	LEU	3.9
1	A	272	GLY	3.8
1	D	283	MET	3.8
3	T	710	DA	3.8
1	D	373	HIS	3.8
1	D	410	LEU	3.8
1	A	245	THR	3.8
1	A	219	ASP	3.8
1	A	385	GLU	3.8
1	A	173	ILE	3.8
1	A	371	PRO	3.8
2	P	62	GLN	3.8
3	T	709	DT	3.7
1	A	133	LYS	3.7
1	D	399	ILE	3.7
1	D	16	LEU	3.7
1	D	377	THR	3.7
1	D	168	CYS	3.7
1	A	436	GLU	3.7
2	B	69	THR	3.7
1	A	151	VAL	3.6
3	T	698	DC	3.6
1	D	217	VAL	3.6
2	B	37	ILE	3.5
1	A	43	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	358	ALA	3.5
1	D	388	MET	3.5
2	P	8	TYR	3.5
1	A	347	ILE	3.5
1	D	342	GLY	3.5
1	D	384	PRO	3.5
1	A	171	LYS	3.5
3	T	707	DC	3.5
4	E	719	DG	3.5
1	A	227	ASN	3.5
1	D	255	MET	3.5
2	P	69	THR	3.5
1	A	44	SER	3.5
1	D	398	MET	3.5
1	A	218	PRO	3.5
1	D	275	ILE	3.5
2	B	70	LEU	3.5
1	A	395	PHE	3.5
1	D	12	ARG	3.4
1	D	228	VAL	3.4
1	D	98	VAL	3.4
1	D	357	ASN	3.4
3	T	699	DC	3.4
1	A	41	LEU	3.4
2	B	28	GLN	3.4
1	A	161	LEU	3.4
1	A	373	HIS	3.3
1	D	184	ILE	3.3
1	A	247	LEU	3.3
1	A	261	LEU	3.3
1	A	389	HIS	3.3
1	D	41	LEU	3.3
4	E	705	DC	3.3
1	A	310	GLY	3.3
1	A	166	ASP	3.2
1	D	11	GLN	3.2
1	D	106	GLU	3.2
4	E	718	DA	3.2
1	D	97	SER	3.1
1	D	167	TRP	3.1
2	P	39	GLN	3.1
2	P	28	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	4	LEU	3.1
1	D	389	HIS	3.1
2	P	7	ILE	3.1
1	A	360	LYS	3.1
3	T	697	DT	3.1
1	D	177	THR	3.0
1	A	154	ALA	3.0
1	D	113	PRO	3.0
1	D	352	LEU	3.0
1	A	177	THR	3.0
2	P	40	ALA	3.0
1	A	156	GLU	3.0
1	A	353	ALA	3.0
1	A	319	ILE	3.0
1	A	184	ILE	2.9
1	D	108	GLU	2.9
1	A	289	LEU	2.9
2	B	39	GLN	2.9
1	A	240	TRP	2.9
1	D	256	CYS	2.9
4	E	722	DA	2.9
3	T	700	DC	2.9
1	D	51	ASN	2.9
1	D	436	GLU	2.9
1	A	33	LEU	2.9
2	P	20	VAL	2.9
1	D	43	LEU	2.9
1	A	260	GLY	2.8
1	A	384	PRO	2.8
1	D	133	LYS	2.8
1	A	29	ALA	2.8
1	A	115	MET	2.8
1	D	94	GLY	2.8
1	D	172	GLY	2.8
1	A	14	GLY	2.8
1	A	322	GLY	2.8
1	D	48	GLN	2.8
1	A	104	ILE	2.8
1	D	236	PHE	2.8
1	D	233	VAL	2.8
1	A	170	PRO	2.8
1	A	323	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	372	ARG	2.8
1	A	312	ALA	2.8
1	A	169	ILE	2.7
1	A	338	PRO	2.7
2	B	35	ILE	2.7
2	P	12	GLN	2.7
1	A	212	GLU	2.7
1	A	401	ALA	2.7
1	D	369	ILE	2.7
2	P	30	GLU	2.7
4	E	709	DT	2.7
1	D	74	ARG	2.7
1	D	25	THR	2.7
1	A	249	ARG	2.7
1	A	275	ILE	2.7
1	A	352	LEU	2.7
1	D	161	LEU	2.7
1	A	397	ARG	2.6
2	B	43	SER	2.6
1	D	152	ALA	2.6
2	P	31	LEU	2.6
1	A	368	LYS	2.6
1	A	55	ASP	2.6
1	D	169	ILE	2.6
3	T	706	DC	2.6
1	A	359	SER	2.6
1	A	432	ARG	2.6
4	E	721	DG	2.6
1	D	289	LEU	2.6
2	B	47	ASN	2.6
1	D	84	ARG	2.6
1	D	198	GLN	2.6
1	D	205	TYR	2.6
2	P	70	LEU	2.6
1	A	292	ARG	2.5
1	D	318	PHE	2.5
1	D	209	LEU	2.5
1	D	362	LYS	2.5
1	D	268	GLU	2.5
1	D	347	ILE	2.5
1	A	279	MET	2.5
1	A	283	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	260	GLY	2.5
1	D	53	THR	2.5
1	A	367	ASP	2.5
3	T	704	DC	2.5
2	B	23	GLN	2.5
1	D	310	GLY	2.5
1	D	93	ILE	2.5
1	A	201	ASP	2.5
1	D	56	ALA	2.5
1	D	418	VAL	2.5
1	D	92	GLU	2.5
1	D	354	MET	2.4
1	D	264	SER	2.4
1	D	266	LYS	2.4
2	P	24	ASN	2.4
1	D	247	LEU	2.4
1	A	233	VAL	2.4
1	D	392	LEU	2.4
1	A	388	MET	2.4
1	D	274	GLY	2.4
1	A	56	ALA	2.4
2	P	43	SER	2.4
1	A	153	GLY	2.4
1	D	100	ALA	2.4
1	A	163	ILE	2.4
1	A	266	LYS	2.4
1	A	205	TYR	2.3
1	D	28	TYR	2.3
1	A	95	ARG	2.3
1	D	432	ARG	2.3
1	A	35	SER	2.3
1	A	264	SER	2.3
1	A	226	GLY	2.3
1	A	336	ALA	2.3
1	D	182	LEU	2.3
1	A	230	ALA	2.3
1	A	325	TYR	2.3
1	D	406	VAL	2.3
1	D	35	SER	2.3
1	A	410	LEU	2.3
1	D	292	ARG	2.3
1	A	231	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	350	LEU	2.3
3	T	701	DT	2.3
1	A	32	TRP	2.3
1	A	155	GLN	2.3
1	A	58	PHE	2.3
1	D	222	ILE	2.2
3	T	714	DG	2.2
1	A	24	HIS	2.2
2	P	42	ILE	2.2
1	D	252	GLN	2.2
2	B	26	TRP	2.2
1	D	29	ALA	2.2
1	D	370	TYR	2.2
1	D	70	ILE	2.2
1	D	269	SER	2.2
2	B	31	LEU	2.2
1	A	375	LEU	2.2
1	D	366	ILE	2.2
1	D	416	GLU	2.2
1	A	317	VAL	2.2
1	D	234	GLU	2.2
1	D	210	ALA	2.2
1	D	232	ALA	2.2
4	E	713	DG	2.2
1	D	72	ARG	2.2
1	A	7	TRP	2.2
1	A	48	GLN	2.2
1	A	208	LEU	2.2
1	A	61	PHE	2.2
1	D	331	TYR	2.2
1	A	334	ILE	2.2
1	A	369	ILE	2.2
1	D	57	VAL	2.1
1	D	3	LYS	2.1
2	B	12	GLN	2.1
1	A	20	ALA	2.1
2	B	22	GLN	2.1
1	A	213	LEU	2.1
1	A	327	LEU	2.1
1	A	92	GLU	2.1
1	D	80	HIS	2.1
1	A	258	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	338	PRO	2.1
1	D	319	ILE	2.1
1	D	77	LYS	2.1
1	D	285	SER	2.1
1	A	252	GLN	2.1
1	D	375	LEU	2.1
1	A	315	PHE	2.1
1	A	288	ALA	2.1
3	T	718	DA	2.1
1	A	8	MET	2.0
1	A	125	LEU	2.0
1	D	386	VAL	2.0
1	D	87	PHE	2.0
1	D	181	LYS	2.0
1	A	77	LYS	2.0
2	B	30	GLU	2.0
2	P	68	MET	2.0
1	A	333	ILE	2.0
1	A	299	GLN	2.0
1	A	234	GLU	2.0
1	D	341	GLY	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.