Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2025 – 02:34 PM JST

PDB ID	:	8YQ0
Title	:	Crystal structure of human phosphoribosyl pyrophosphate synthetase 1(PRPS1) chimera swapped with three residues from PRPS2
Authors	:	Zhang, L.; Zhang, L.
Deposited on	:	2024-03-18
Resolution	:	3.10 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:

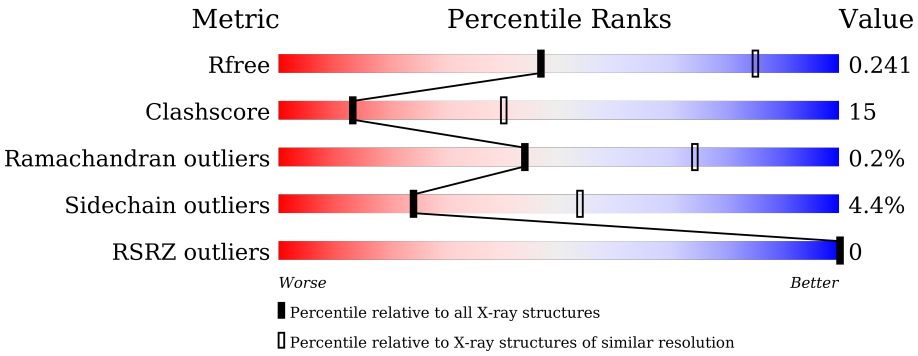
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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	321	71% 23%
1	B	321	68% 25%
1	C	321	65% 28%
1	D	321	71% 23%
1	E	321	65% 27%
1	F	321	71% 23%

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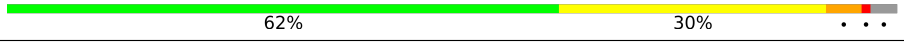
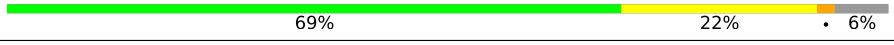
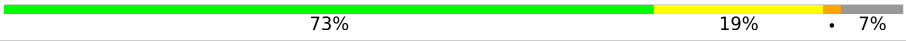
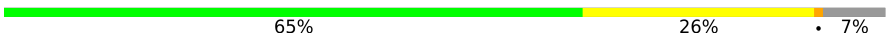
Mol	Chain	Length	Quality of chain
1	G	321	
1	H	321	
1	I	321	
1	J	321	
1	K	321	
1	L	321	
1	M	321	
1	N	321	
1	O	321	
1	P	321	
1	Q	321	
1	R	321	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 42231 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 Ribose-phosphate pyrophosphokinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2382	1496	418	451	17			
1	B	312	Total	C	N	O	S	0	0	0
			2382	1496	418	451	17			
1	C	309	Total	C	N	O	S	0	0	0
			2354	1479	412	446	17			
1	D	310	Total	C	N	O	S	0	0	0
			2362	1485	413	447	17			
1	E	312	Total	C	N	O	S	0	0	0
			2379	1494	418	450	17			
1	F	312	Total	C	N	O	S	0	0	0
			2382	1496	418	451	17			
1	G	311	Total	C	N	O	S	0	0	0
			2373	1491	417	448	17			
1	H	301	Total	C	N	O	S	0	0	0
			2291	1434	405	435	17			
1	I	313	Total	C	N	O	S	0	0	0
			2390	1500	419	454	17			
1	J	300	Total	C	N	O	S	0	1	0
			2295	1437	407	434	17			
1	K	311	Total	C	N	O	S	0	0	0
			2368	1488	414	449	17			
1	L	298	Total	C	N	O	S	0	0	0
			2267	1421	399	430	17			
1	M	298	Total	C	N	O	S	0	0	0
			2267	1421	399	430	17			
1	N	310	Total	C	N	O	S	0	0	0
			2362	1485	413	447	17			
1	O	298	Total	C	N	O	S	0	0	0
			2272	1424	402	429	17			
1	P	313	Total	C	N	O	S	0	0	0
			2390	1500	419	454	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	300	Total	C	N	O	S	0	0	0
			2285	1431	404	433	17			
1	R	313	Total	C	N	O	S	0	0	0
			2388	1499	419	453	17			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP P60891
A	103	VAL	-	insertion	UNP P60891
A	104	GLY	-	insertion	UNP P60891
A	105	GLU	-	insertion	UNP P60891
B	1	SER	-	expression tag	UNP P60891
B	103	VAL	-	insertion	UNP P60891
B	104	GLY	-	insertion	UNP P60891
B	105	GLU	-	insertion	UNP P60891
C	1	SER	-	expression tag	UNP P60891
C	103	VAL	-	insertion	UNP P60891
C	104	GLY	-	insertion	UNP P60891
C	105	GLU	-	insertion	UNP P60891
D	1	SER	-	expression tag	UNP P60891
D	103	VAL	-	insertion	UNP P60891
D	104	GLY	-	insertion	UNP P60891
D	105	GLU	-	insertion	UNP P60891
E	1	SER	-	expression tag	UNP P60891
E	103	VAL	-	insertion	UNP P60891
E	104	GLY	-	insertion	UNP P60891
E	105	GLU	-	insertion	UNP P60891
F	1	SER	-	expression tag	UNP P60891
F	103	VAL	-	insertion	UNP P60891
F	104	GLY	-	insertion	UNP P60891
F	105	GLU	-	insertion	UNP P60891
G	1	SER	-	expression tag	UNP P60891
G	103	VAL	-	insertion	UNP P60891
G	104	GLY	-	insertion	UNP P60891
G	105	GLU	-	insertion	UNP P60891
H	1	SER	-	expression tag	UNP P60891
H	103	VAL	-	insertion	UNP P60891
H	104	GLY	-	insertion	UNP P60891
H	105	GLU	-	insertion	UNP P60891
I	1	SER	-	expression tag	UNP P60891
I	103	VAL	-	insertion	UNP P60891

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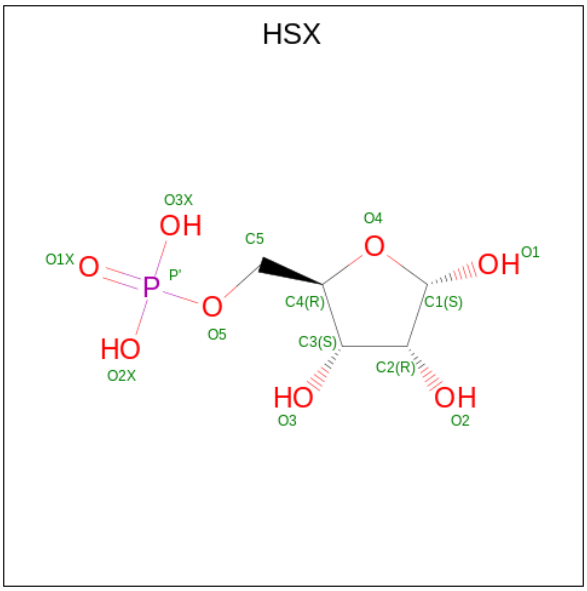
Chain	Residue	Modelled	Actual	Comment	Reference
I	104	GLY	-	insertion	UNP P60891
I	105	GLU	-	insertion	UNP P60891
J	1	SER	-	expression tag	UNP P60891
J	103	VAL	-	insertion	UNP P60891
J	104	GLY	-	insertion	UNP P60891
J	105	GLU	-	insertion	UNP P60891
K	1	SER	-	expression tag	UNP P60891
K	103	VAL	-	insertion	UNP P60891
K	104	GLY	-	insertion	UNP P60891
K	105	GLU	-	insertion	UNP P60891
L	1	SER	-	expression tag	UNP P60891
L	103	VAL	-	insertion	UNP P60891
L	104	GLY	-	insertion	UNP P60891
L	105	GLU	-	insertion	UNP P60891
M	1	SER	-	expression tag	UNP P60891
M	103	VAL	-	insertion	UNP P60891
M	104	GLY	-	insertion	UNP P60891
M	105	GLU	-	insertion	UNP P60891
N	1	SER	-	expression tag	UNP P60891
N	103	VAL	-	insertion	UNP P60891
N	104	GLY	-	insertion	UNP P60891
N	105	GLU	-	insertion	UNP P60891
O	1	SER	-	expression tag	UNP P60891
O	103	VAL	-	insertion	UNP P60891
O	104	GLY	-	insertion	UNP P60891
O	105	GLU	-	insertion	UNP P60891
P	1	SER	-	expression tag	UNP P60891
P	103	VAL	-	insertion	UNP P60891
P	104	GLY	-	insertion	UNP P60891
P	105	GLU	-	insertion	UNP P60891
Q	1	SER	-	expression tag	UNP P60891
Q	103	VAL	-	insertion	UNP P60891
Q	104	GLY	-	insertion	UNP P60891
Q	105	GLU	-	insertion	UNP P60891
R	1	SER	-	expression tag	UNP P60891
R	103	VAL	-	insertion	UNP P60891
R	104	GLY	-	insertion	UNP P60891
R	105	GLU	-	insertion	UNP P60891

- Molecule 2 is 5-O-phosphono-alpha-D-ribofuranose (three-letter code: HSX) (formula: $C_5H_{11}O_8P$) (labeled as "Ligand of Interest" by depositor).



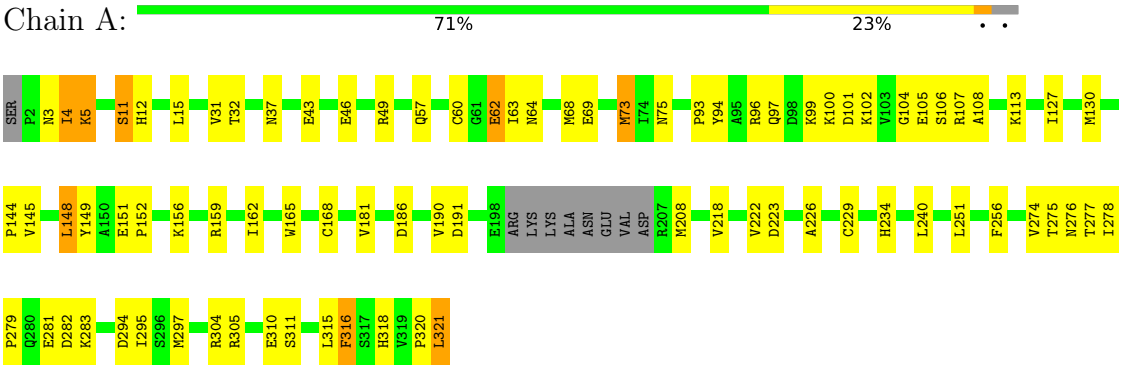
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O P 14 5 8 1	0	0
2	F	1	Total C O P 14 5 8 1	0	0
2	O	1	Total C O P 14 5 8 1	0	0

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.

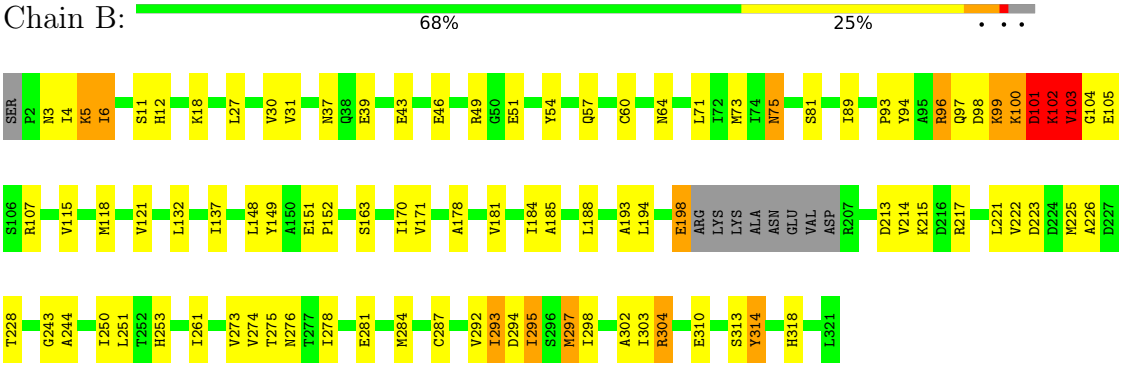
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain A:



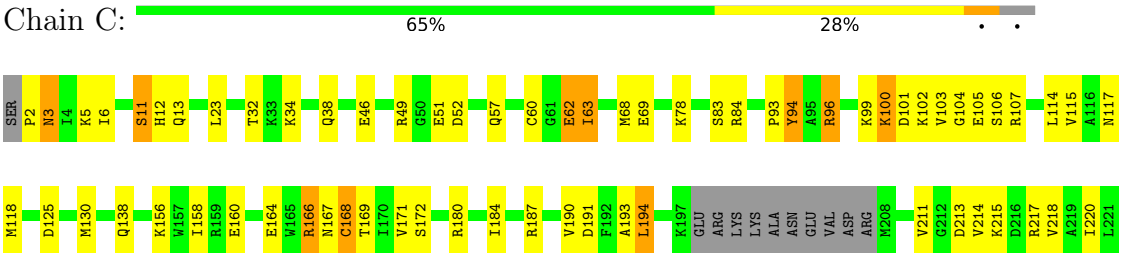
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain B:



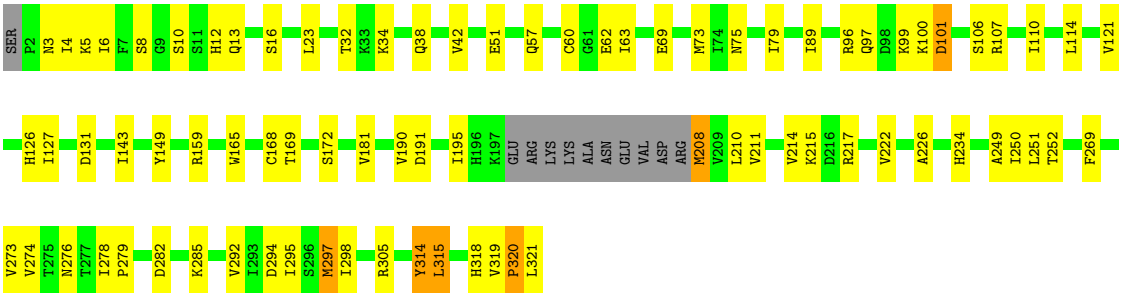
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain C:



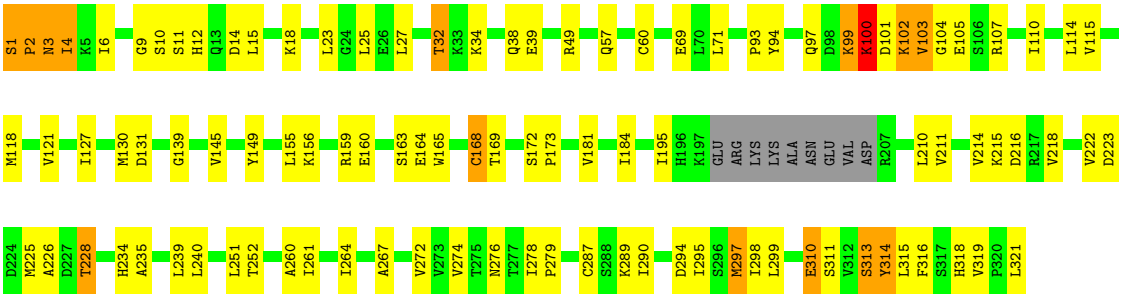
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain D:



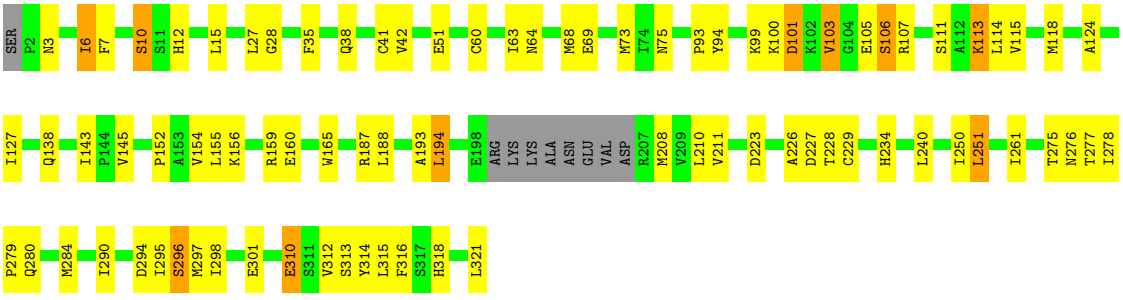
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain E:



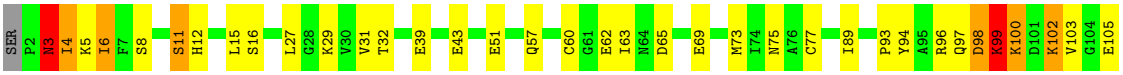
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

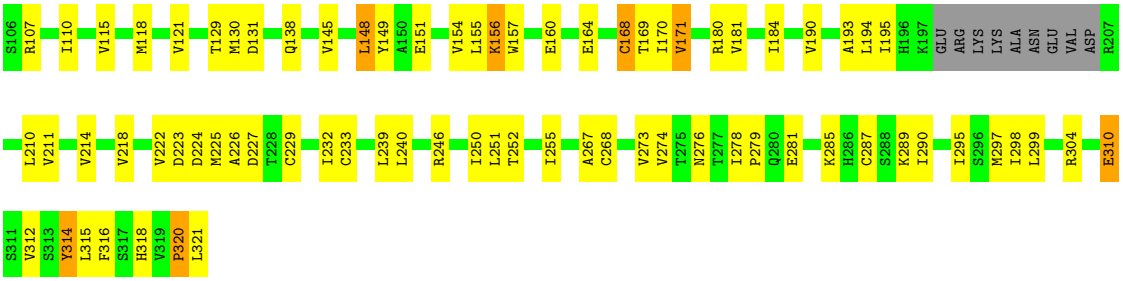
Chain F:



• Molecule 1: Ribose-phosphate pyrophosphokinase 1

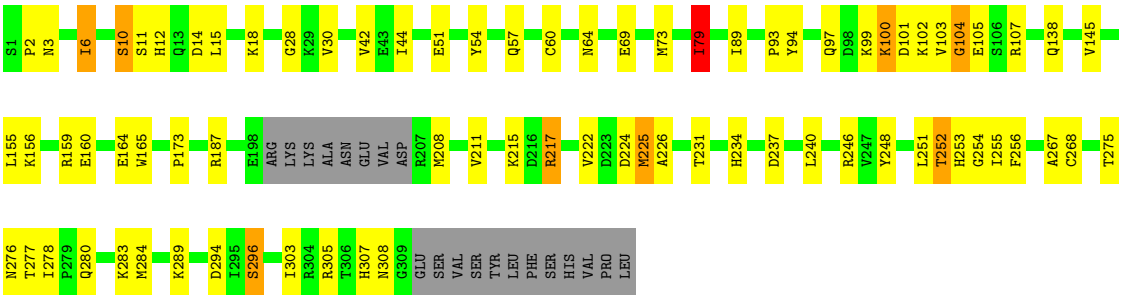
Chain G:





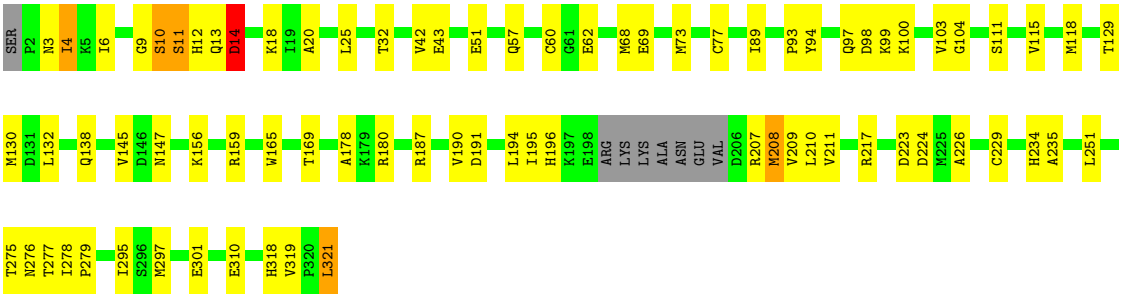
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain H:



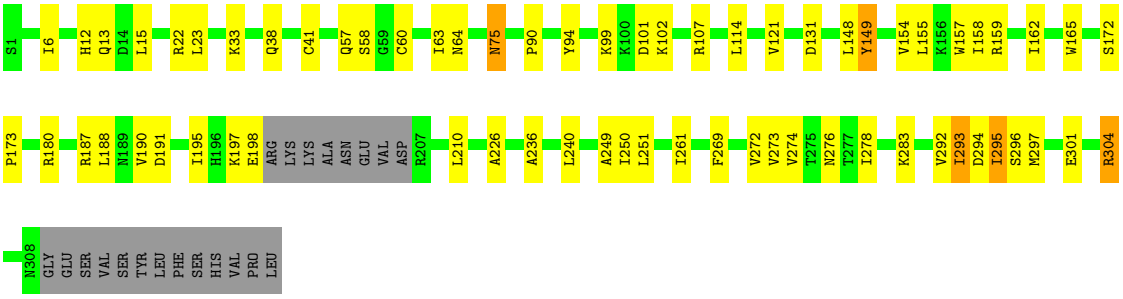
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain I:



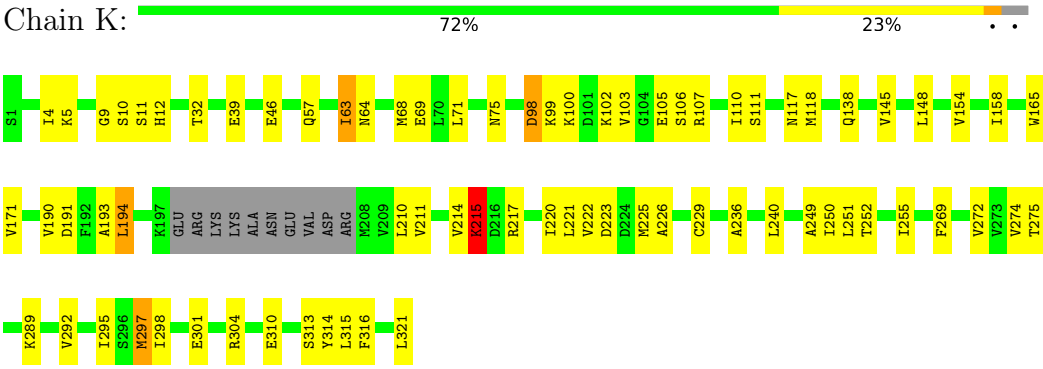
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain J:



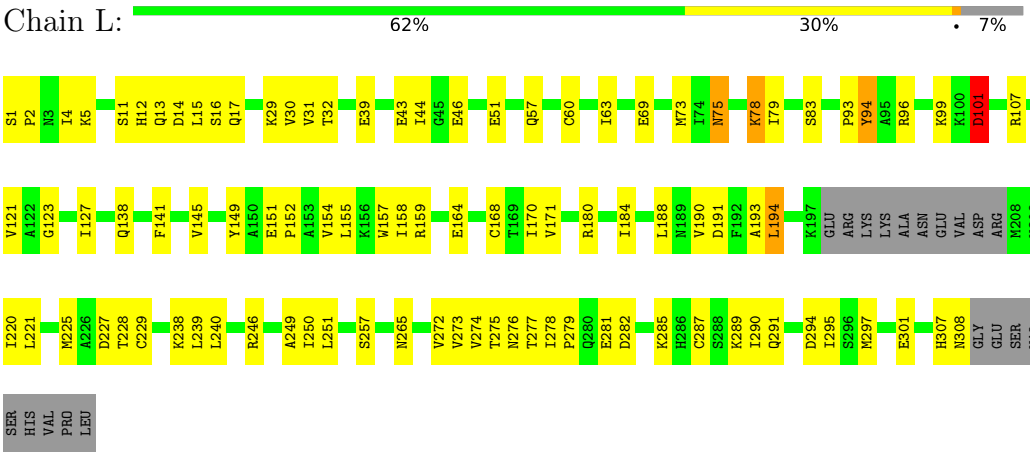
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain K:



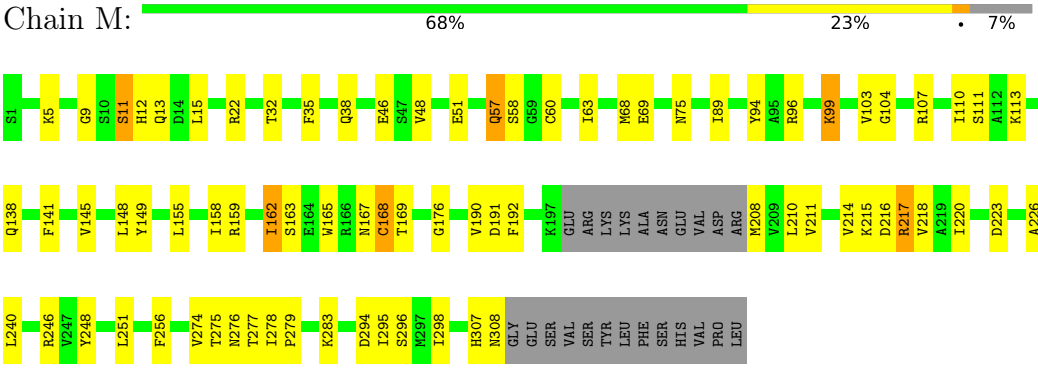
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain L:



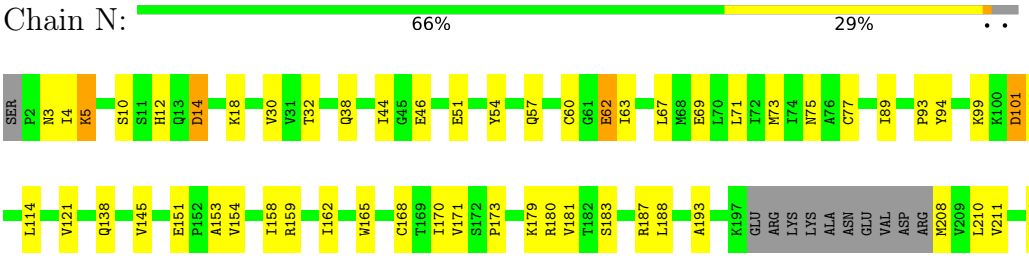
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain M:



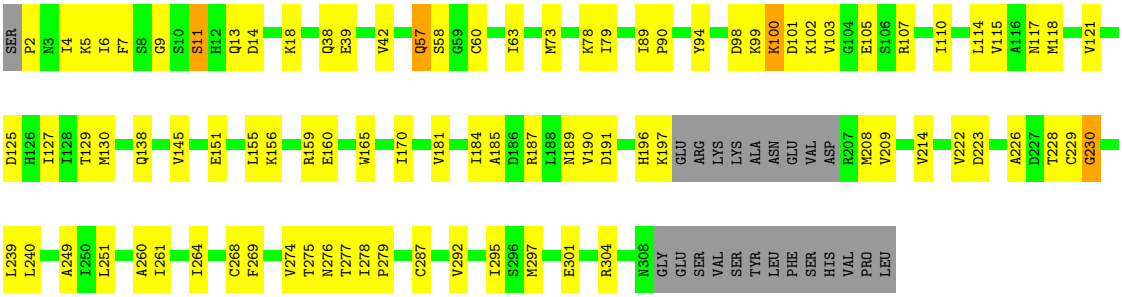
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain N:



• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain O:

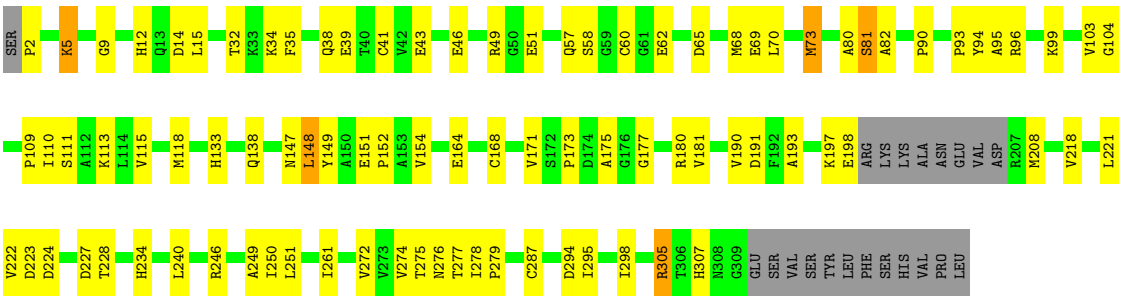


• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain P:

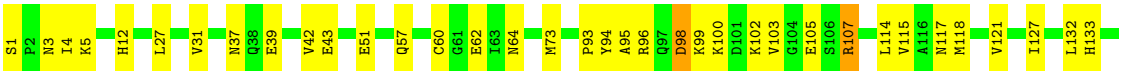
• Molecule 1: Ribose-phosphate pyrophosphokinase 1

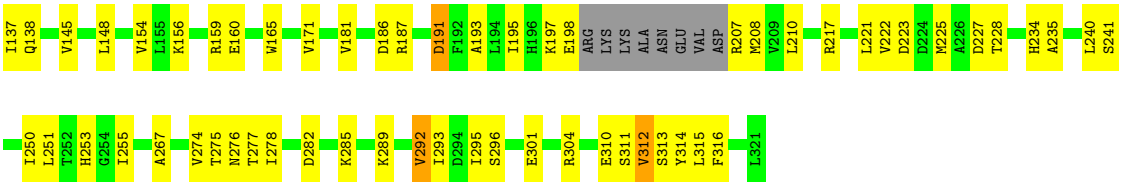
Chain Q:



• Molecule 1: Ribose-phosphate pyrophosphokinase 1

Chain R:




I137
Q138
V145
L148
V154
L155
K156
R159
E160
W165
V171
V181
D186
R187
D191
F192
A193
L194
I195
H196
K197
E198
ARG
LYS
LYS
ALA
ASN
GLU
VAL
ASP
R207
M208
V209
L210
R217
L221
V222
D223
D224
M225
A226
D227
T228
H234
A235
L240
S241
I250
L251
T252
H253
G254
I255
A267
V274
T275
N276
T277
I278
D282
K285
K289
V292
I293
D294
I295
S296
E301
R304
E310
S311
V312
S313
Y314
L315
F316
L321

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	108.08Å 108.08Å 659.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.10 50.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.01-3.10) 98.8 (50.01-3.10)	Depositor EDS
R_{merge}	0.54	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.75 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.196 , 0.250 0.198 , 0.241	Depositor DCC
R_{free} test set	6691 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.429 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	42231	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.99	10/2417 (0.4%)	0.92	0/3269
1	B	0.97	8/2417 (0.3%)	0.90	0/3269
1	C	0.93	6/2389 (0.3%)	0.96	0/3232
1	D	0.81	2/2397 (0.1%)	0.88	0/3243
1	E	1.08	5/2414 (0.2%)	0.99	3/3266 (0.1%)
1	F	1.00	6/2417 (0.2%)	0.92	0/3269
1	G	1.00	9/2408 (0.4%)	0.98	4/3257 (0.1%)
1	H	1.03	9/2322 (0.4%)	0.93	1/3139 (0.0%)
1	I	0.83	2/2425 (0.1%)	0.90	0/3280
1	J	0.74	3/2329 (0.1%)	0.87	1/3148 (0.0%)
1	K	0.83	2/2403 (0.1%)	0.93	3/3252 (0.1%)
1	L	0.76	1/2298 (0.0%)	0.91	2/3108 (0.1%)
1	M	0.81	5/2298 (0.2%)	0.88	0/3108
1	N	0.82	3/2397 (0.1%)	0.91	0/3243
1	O	0.89	6/2303 (0.3%)	0.90	0/3113
1	P	0.72	2/2425 (0.1%)	0.91	1/3280 (0.0%)
1	Q	0.96	6/2316 (0.3%)	0.92	0/3130
1	R	0.84	0/2423	0.91	0/3278
All	All	0.90	85/42798 (0.2%)	0.92	15/57884 (0.0%)

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	168	CYS	CB-SG	-8.45	1.67	1.82
1	H	254	GLY	C-O	-8.27	1.10	1.23
1	N	77	CYS	CB-SG	-7.58	1.69	1.82
1	B	105	GLU	CD-OE2	-6.91	1.18	1.25
1	F	106	SER	CB-OG	-6.73	1.33	1.42
1	M	104	GLY	CA-C	-6.66	1.41	1.51
1	G	77	CYS	CB-SG	-6.58	1.71	1.82
1	G	314	TYR	CE2-CZ	-6.57	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	104	GLY	C-O	-6.34	1.13	1.23
1	G	168	CYS	CB-SG	-6.29	1.71	1.82
1	B	5	LYS	C-O	-6.26	1.11	1.23
1	A	11	SER	CA-CB	-6.25	1.43	1.52
1	C	62	GLU	CD-OE1	-6.14	1.18	1.25
1	G	105	GLU	CD-OE1	-6.10	1.19	1.25
1	B	104	GLY	C-O	-5.97	1.14	1.23
1	E	314	TYR	CE1-CZ	-5.95	1.30	1.38
1	E	10	SER	C-O	-5.92	1.12	1.23
1	A	149	TYR	CE1-CZ	-5.91	1.30	1.38
1	O	229	CYS	CB-SG	-5.91	1.72	1.81
1	I	77	CYS	CB-SG	-5.87	1.72	1.81
1	F	113	LYS	C-O	-5.83	1.12	1.23
1	H	6	ILE	C-O	-5.83	1.12	1.23
1	E	168	CYS	CB-SG	-5.81	1.72	1.81
1	H	28	GLY	C-O	-5.76	1.14	1.23
1	H	224	ASP	C-O	-5.76	1.12	1.23
1	B	314	TYR	CE1-CZ	-5.73	1.31	1.38
1	O	6	ILE	C-O	-5.72	1.12	1.23
1	B	6	ILE	C-O	-5.71	1.12	1.23
1	O	230	GLY	C-O	-5.71	1.14	1.23
1	M	46	GLU	CD-OE1	-5.69	1.19	1.25
1	C	62	GLU	CD-OE2	-5.67	1.19	1.25
1	P	5	LYS	C-O	-5.65	1.12	1.23
1	G	31	VAL	C-O	-5.65	1.12	1.23
1	Q	148	LEU	C-O	-5.65	1.12	1.23
1	I	14	ASP	C-O	-5.64	1.12	1.23
1	G	171	VAL	C-O	-5.58	1.12	1.23
1	M	46	GLU	CD-OE2	-5.57	1.19	1.25
1	B	194	LEU	C-O	-5.53	1.12	1.23
1	N	5	LYS	C-O	-5.53	1.12	1.23
1	O	5	LYS	C-O	-5.50	1.12	1.23
1	G	11	SER	CA-CB	-5.49	1.44	1.52
1	K	229	CYS	C-O	-5.48	1.12	1.23
1	A	149	TYR	CE2-CZ	-5.46	1.31	1.38
1	L	94	TYR	CE2-CZ	-5.46	1.31	1.38
1	F	111	SER	CA-CB	-5.43	1.44	1.52
1	E	228	THR	CB-CG2	-5.43	1.34	1.52
1	H	105	GLU	CD-OE2	-5.43	1.19	1.25
1	F	105	GLU	CD-OE2	-5.41	1.19	1.25
1	J	295	ILE	C-O	-5.39	1.13	1.23
1	Q	5	LYS	C-O	-5.37	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	LEU	C-O	-5.35	1.13	1.23
1	A	144	PRO	C-O	-5.34	1.12	1.23
1	H	222	VAL	C-O	-5.33	1.13	1.23
1	A	5	LYS	C-O	-5.32	1.13	1.23
1	Q	81	SER	CA-CB	-5.31	1.45	1.52
1	F	111	SER	CB-OG	-5.30	1.35	1.42
1	C	11	SER	CB-OG	-5.28	1.35	1.42
1	J	293	ILE	C-O	-5.25	1.13	1.23
1	B	105	GLU	CD-OE1	-5.23	1.19	1.25
1	A	106	SER	C-O	-5.23	1.13	1.23
1	A	149	TYR	CB-CG	-5.23	1.43	1.51
1	C	94	TYR	CE1-CZ	-5.20	1.31	1.38
1	C	60	CYS	CB-SG	-5.19	1.73	1.81
1	C	314	TYR	CE1-CZ	-5.17	1.31	1.38
1	A	105	GLU	CG-CD	-5.17	1.44	1.51
1	J	94	TYR	CE1-CZ	-5.17	1.31	1.38
1	P	94	TYR	CE1-CZ	-5.16	1.31	1.38
1	O	94	TYR	CE1-CZ	-5.14	1.31	1.38
1	B	314	TYR	CE2-CZ	-5.13	1.31	1.38
1	H	79	ILE	C-O	-5.13	1.13	1.23
1	G	310	GLU	CD-OE1	-5.12	1.20	1.25
1	N	14	ASP	C-O	-5.12	1.13	1.23
1	H	6	ILE	N-CA	-5.12	1.36	1.46
1	E	287	CYS	CB-SG	-5.11	1.73	1.81
1	Q	109	PRO	C-O	-5.11	1.13	1.23
1	D	315	LEU	C-O	-5.10	1.13	1.23
1	M	104	GLY	C-O	-5.09	1.15	1.23
1	O	7	PHE	C-O	-5.09	1.13	1.23
1	G	148	LEU	C-O	-5.08	1.13	1.23
1	Q	149	TYR	CE1-CZ	-5.08	1.31	1.38
1	A	149	TYR	CZ-OH	-5.04	1.29	1.37
1	F	105	GLU	CA-CB	-5.04	1.42	1.53
1	H	104	GLY	C-O	-5.04	1.15	1.23
1	D	314	TYR	CE2-CZ	-5.03	1.32	1.38
1	K	64	ASN	C-O	-5.01	1.13	1.23

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	3	ASN	CB-CA-C	9.05	128.51	110.40
1	G	100	LYS	N-CA-C	-7.23	91.49	111.00
1	L	101	ASP	C-N-CA	7.16	139.59	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	2	PRO	C-N-CA	6.42	137.75	121.70
1	G	99	LYS	CB-CA-C	-5.97	98.45	110.40
1	H	225	MET	CB-CG-SD	-5.86	94.83	112.40
1	J	149	TYR	CB-CA-C	-5.83	98.74	110.40
1	E	2	PRO	N-CD-CG	-5.81	94.48	103.20
1	K	168	CYS	CB-CA-C	-5.57	99.27	110.40
1	E	99	LYS	C-N-CA	5.42	135.25	121.70
1	E	100	LYS	N-CA-C	-5.39	96.45	111.00
1	K	168	CYS	N-CA-CB	-5.22	101.21	110.60
1	L	101	ASP	CB-CA-C	5.21	120.81	110.40
1	K	215	LYS	CB-CA-C	-5.16	100.08	110.40
1	G	102	LYS	N-CA-CB	5.08	119.74	110.60

There are no chirality outliers.

There are no planarity outliers.

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	2382	0	2421	70	0
1	B	2382	0	2421	96	0
1	C	2354	0	2388	95	0
1	D	2362	0	2402	72	0
1	E	2379	0	2419	97	0
1	F	2382	0	2421	76	0
1	G	2373	0	2415	105	0
1	H	2291	0	2334	62	0
1	I	2390	0	2425	63	0
1	J	2295	0	2345	49	0
1	K	2368	0	2409	77	0
1	L	2267	0	2313	90	0
1	M	2267	0	2313	76	0
1	N	2362	0	2402	67	0
1	O	2272	0	2319	73	0
1	P	2390	0	2425	62	0
1	Q	2285	0	2328	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	2388	0	2428	82	0
2	B	14	0	0	1	0
2	F	14	0	0	2	0
2	O	14	0	0	4	0
All	All	42231	0	42928	1243	0

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

All (1243) 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:H:225:MET:HE1	1:H:255:ILE:CD1	1.56	1.36
1:C:213:ASP:O	1:C:217:ARG:NH2	1.60	1.30
1:B:11:SER:HB2	1:B:57:GLN:OE1	1.36	1.25
1:I:11:SER:HB2	1:I:57:GLN:OE1	1.07	1.23
1:B:4:ILE:HG22	1:G:310:GLU:O	1.40	1.18
1:M:9:GLY:HA3	1:M:57:GLN:HE22	1.06	1.16
1:B:310:GLU:O	1:G:4:ILE:CG2	1.96	1.13
1:H:225:MET:HE1	1:H:255:ILE:HD11	1.16	1.13
1:E:310:GLU:OE1	1:P:310:GLU:OE1	1.64	1.12
1:D:208:MET:HE1	1:D:234:HIS:HB3	1.17	1.11
1:E:226:ALA:HB2	1:E:251:LEU:HD13	1.27	1.11
1:H:225:MET:CE	1:H:255:ILE:CD1	2.29	1.09
1:I:11:SER:CB	1:I:57:GLN:OE1	1.99	1.09
1:D:121:VAL:HG11	1:E:121:VAL:HG11	1.30	1.09
1:E:99:LYS:HE3	1:E:101:ASP:OD1	1.50	1.09
1:G:43:GLU:CD	1:L:99:LYS:HE3	1.73	1.09
1:F:310:GLU:OE1	1:K:310:GLU:OE1	1.70	1.09
1:M:9:GLY:HA3	1:M:57:GLN:NE2	1.68	1.09
1:K:226:ALA:HB2	1:K:251:LEU:HD13	1.36	1.08
1:L:12:HIS:HE1	1:L:276:ASN:O	1.35	1.08
1:O:226:ALA:O	2:O:1001:HSX:O1	1.68	1.07
1:K:168:CYS:HB3	1:K:190:VAL:HG11	1.36	1.06
1:H:226:ALA:HB2	1:H:251:LEU:HD13	1.36	1.06
1:H:225:MET:HE1	1:H:255:ILE:HD12	1.38	1.05
1:P:100:LYS:NZ	1:Q:43:GLU:OE1	1.89	1.05
1:C:96:ARG:H	1:C:96:ARG:HD2	1.22	1.04
1:G:43:GLU:OE2	1:L:99:LYS:HE3	1.54	1.04
1:H:226:ALA:HB2	1:H:251:LEU:CD1	1.88	1.04
1:R:99:LYS:HB2	1:R:107:ARG:CD	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:ALA:C	1:F:194:LEU:HD23	1.78	1.03
1:E:102:LYS:O	1:E:105:GLU:O	1.76	1.03
1:M:12:HIS:HE1	1:M:15:LEU:HB2	1.20	1.01
1:D:169:THR:HB	1:D:217:ARG:HH11	1.23	1.00
1:O:103:VAL:CG2	1:P:187:ARG:NH1	2.24	1.00
1:B:310:GLU:O	1:G:4:ILE:HG22	1.59	1.00
1:M:162:ILE:HD11	1:M:218:VAL:HG21	1.41	0.99
1:R:99:LYS:CB	1:R:107:ARG:HD3	1.92	0.98
1:O:9:GLY:HA3	1:O:57:GLN:HE22	1.26	0.98
1:C:246:ARG:HD2	1:C:270:GLU:HG3	1.45	0.97
1:B:4:ILE:CG2	1:G:310:GLU:O	2.12	0.96
1:H:225:MET:CE	1:H:255:ILE:HD11	1.95	0.96
1:M:12:HIS:CE1	1:M:15:LEU:HB2	2.00	0.96
1:F:99:LYS:O	1:F:107:ARG:NH1	1.98	0.95
1:M:211:VAL:HG12	1:N:211:VAL:HG12	1.45	0.95
1:O:9:GLY:HA3	1:O:57:GLN:NE2	1.80	0.94
1:B:11:SER:CB	1:B:57:GLN:OE1	2.16	0.94
1:H:225:MET:CE	1:H:255:ILE:HD12	1.95	0.93
1:I:208:MET:HE2	1:I:234:HIS:HB3	1.48	0.93
1:I:10:SER:OG	1:I:69:GLU:OE2	1.86	0.93
1:A:12:HIS:HE1	1:A:276:ASN:O	1.52	0.93
1:F:310:GLU:O	1:K:4:ILE:HG22	1.69	0.91
1:R:99:LYS:HB2	1:R:107:ARG:HD3	1.49	0.90
1:E:100:LYS:HB2	1:E:107:ARG:NH2	1.87	0.90
1:G:100:LYS:NZ	1:L:43:GLU:OE2	2.05	0.90
1:R:99:LYS:HB2	1:R:107:ARG:HD2	1.52	0.89
1:L:99:LYS:O	1:L:107:ARG:HD2	1.70	0.89
1:J:301:GLU:OE2	1:J:304[B]:ARG:NH1	2.05	0.89
1:C:103:VAL:O	1:D:149:TYR:HD2	1.55	0.89
1:H:99:LYS:O	1:H:107:ARG:HD2	1.72	0.89
1:G:12:HIS:HD2	1:G:279:PRO:HG3	1.38	0.88
1:M:12:HIS:CE1	1:M:15:LEU:CB	2.55	0.88
1:G:121:VAL:HG11	1:L:121:VAL:HG11	1.55	0.88
1:K:194:LEU:HD21	1:L:194:LEU:CD2	2.03	0.88
1:I:11:SER:HB2	1:I:57:GLN:CD	1.93	0.87
1:K:194:LEU:CD2	1:L:194:LEU:HD21	2.04	0.87
1:L:12:HIS:CE1	1:L:276:ASN:O	2.26	0.86
1:F:99:LYS:HD2	1:F:101:ASP:OD1	1.75	0.86
1:P:5:LYS:NZ	1:P:51:GLU:OE1	2.09	0.86
1:A:100:LYS:H	1:A:107:ARG:HH21	1.20	0.85
1:N:14:ASP:OD2	1:N:18:LYS:NZ	2.08	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:98:ASP:O	1:O:100:LYS:HD3	1.77	0.85
1:G:43:GLU:OE2	1:L:99:LYS:CE	2.24	0.85
1:A:310:GLU:OE2	1:R:310:GLU:OE1	1.95	0.85
1:M:11:SER:OG	1:M:57:GLN:HG3	1.77	0.85
1:K:297:MET:HG2	1:K:298:ILE:N	1.91	0.84
1:O:301:GLU:OE1	1:O:304:ARG:NH2	2.10	0.84
1:R:181:VAL:HG12	1:R:222:VAL:HG22	1.60	0.83
1:L:14:ASP:O	1:L:15:LEU:C	2.11	0.83
1:B:297:MET:HG2	1:B:298:ILE:N	1.90	0.83
1:M:168:CYS:SG	1:M:169:THR:N	2.49	0.83
1:I:208:MET:CE	1:I:234:HIS:HB3	2.07	0.83
1:C:99:LYS:HB2	1:C:107:ARG:HE	1.44	0.83
1:H:101:ASP:O	1:H:102:LYS:HB2	1.79	0.83
1:Q:227:ASP:OD1	1:Q:228:THR:N	2.13	0.82
1:D:63:ILE:HD11	1:E:39:GLU:HA	1.61	0.81
1:B:102:LYS:NZ	1:B:102:LYS:HB3	1.95	0.81
1:R:100:LYS:O	1:R:107:ARG:NH2	2.14	0.80
1:E:211:VAL:HG12	1:F:211:VAL:HG12	1.62	0.80
1:F:310:GLU:OE2	1:K:304:ARG:NH2	2.14	0.80
1:E:310:GLU:O	1:P:4:ILE:HG22	1.82	0.80
1:R:99:LYS:HB3	1:R:107:ARG:HD3	1.62	0.80
1:D:79:ILE:HD11	1:E:110:ILE:HG12	1.63	0.79
1:B:11:SER:HB2	1:B:57:GLN:CD	2.02	0.79
1:N:63:ILE:HD11	1:O:39:GLU:HA	1.64	0.79
1:C:2:PRO:HB3	1:N:312:VAL:HG23	1.65	0.79
1:I:169:THR:HG23	1:I:217:ARG:HD3	1.64	0.79
1:L:11:SER:OG	1:L:57:GLN:OE1	1.99	0.79
1:M:38:GLN:NE2	1:R:62:GLU:OE1	2.16	0.79
1:D:99:LYS:HG3	1:D:101:ASP:H	1.47	0.78
1:K:168:CYS:HB3	1:K:190:VAL:CG1	2.14	0.78
1:C:214:VAL:HG11	1:C:239:LEU:CD2	2.14	0.78
1:I:60:CYS:HB3	1:I:278:ILE:HG12	1.64	0.77
1:G:12:HIS:CD2	1:G:279:PRO:HG3	2.18	0.77
1:M:96:ARG:HH22	1:R:37:ASN:HD22	1.28	0.77
1:B:93:PRO:O	1:B:94:TYR:HB2	1.83	0.77
1:C:226:ALA:HB2	1:C:251:LEU:HD13	1.65	0.77
1:D:99:LYS:HB2	1:D:107:ARG:HD2	1.67	0.77
1:A:4:ILE:CG2	1:R:310:GLU:O	2.33	0.77
1:B:295:ILE:HA	1:B:297:MET:HE2	1.65	0.77
1:A:12:HIS:CE1	1:A:276:ASN:O	2.37	0.76
1:A:181:VAL:HG12	1:A:222:VAL:HG22	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:VAL:HG13	1:D:320:PRO:HD2	1.66	0.76
1:A:4:ILE:HG22	1:R:310:GLU:O	1.85	0.76
1:B:101:ASP:O	1:B:103:VAL:N	2.18	0.76
1:G:164:GLU:CD	1:G:246:ARG:HH22	1.88	0.76
1:Q:5:LYS:HE2	1:Q:46:GLU:OE1	1.85	0.76
1:R:191:ASP:OD1	1:R:191:ASP:N	2.17	0.76
1:A:99:LYS:HD2	1:A:101:ASP:HA	1.67	0.76
1:A:320:PRO:O	1:A:321:LEU:CB	2.29	0.76
1:M:12:HIS:HD2	1:M:279:PRO:HD3	1.49	0.76
1:J:294:ASP:OD1	1:J:296:SER:OG	2.04	0.75
1:B:297:MET:HG2	1:B:298:ILE:H	1.50	0.75
1:Q:51:GLU:O	1:Q:82:ALA:O	2.03	0.75
1:H:10:SER:OG	1:H:69:GLU:OE1	2.05	0.75
1:M:35:PHE:HE2	1:R:98:ASP:OD2	1.68	0.75
1:L:138:GLN:NE2	1:L:145:VAL:O	2.20	0.74
1:O:103:VAL:HG22	1:P:187:ARG:NH1	2.01	0.74
1:C:166:ARG:CG	1:C:166:ARG:HH21	2.00	0.74
1:K:252:THR:O	1:K:275:THR:HG22	1.86	0.74
1:O:103:VAL:HG23	1:P:187:ARG:NH1	2.02	0.74
1:B:31:VAL:HG23	1:B:43:GLU:HB2	1.67	0.74
1:P:246:ARG:NH1	1:P:248:TYR:OH	2.21	0.74
1:A:320:PRO:O	1:A:321:LEU:HB2	1.89	0.73
1:B:99:LYS:CB	1:B:107:ARG:HD2	2.19	0.73
1:C:100:LYS:N	1:C:107:ARG:NH2	2.36	0.73
1:E:211:VAL:HG12	1:F:211:VAL:CG1	2.18	0.73
1:C:168:CYS:SG	1:C:169:THR:N	2.61	0.73
1:H:12:HIS:CE1	1:H:15:LEU:HB2	2.24	0.73
1:M:99:LYS:O	1:M:99:LYS:HG3	1.87	0.73
1:B:6:ILE:HG22	1:B:27:LEU:CD2	2.18	0.73
1:D:63:ILE:HG12	1:E:38:GLN:HB3	1.71	0.73
1:C:3:ASN:N	1:C:3:ASN:HD22	1.87	0.73
1:K:9:GLY:HA3	1:K:57:GLN:NE2	2.02	0.73
1:O:156:LYS:HE3	1:O:160:GLU:OE1	1.89	0.73
1:G:225:MET:HE2	1:G:255:ILE:HD11	1.70	0.73
1:K:194:LEU:HD21	1:L:194:LEU:HD21	1.65	0.72
1:F:193:ALA:C	1:F:194:LEU:CD2	2.57	0.72
1:C:211:VAL:HG12	1:D:211:VAL:CG1	2.19	0.72
1:J:261:ILE:HD11	1:J:283:LYS:HD2	1.71	0.72
1:B:181:VAL:HG12	1:B:222:VAL:HG22	1.70	0.72
1:D:13:GLN:HG3	1:D:13:GLN:O	1.90	0.71
1:M:12:HIS:HE1	1:M:15:LEU:CB	1.93	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:32:THR:HG21	1:L:69:GLU:OE2	1.90	0.71
1:M:12:HIS:ND1	1:M:15:LEU:HB3	2.06	0.71
1:M:226:ALA:HB2	1:M:251:LEU:HD22	1.71	0.71
1:Q:80:ALA:O	1:Q:81:SER:HB2	1.91	0.71
1:C:5:LYS:HD2	1:C:51:GLU:OE1	1.91	0.70
1:P:226:ALA:HB2	1:P:251:LEU:HD13	1.73	0.70
1:K:194:LEU:HD21	1:L:194:LEU:HD23	1.72	0.70
1:M:35:PHE:CE2	1:R:98:ASP:OD2	2.44	0.70
1:C:211:VAL:CG1	1:D:211:VAL:HG12	2.21	0.70
1:M:223:ASP:HB3	1:M:251:LEU:HD23	1.72	0.70
1:G:96:ARG:NH2	1:G:227:ASP:OD2	2.24	0.70
1:G:75:ASN:OD1	1:L:110:ILE:HG23	1.91	0.70
1:Q:115:VAL:HA	1:Q:118:MET:HE2	1.73	0.70
1:F:193:ALA:O	1:F:194:LEU:CD2	2.40	0.69
1:F:12:HIS:HE1	1:F:276:ASN:O	1.76	0.69
1:K:194:LEU:HD22	1:L:194:LEU:HD21	1.72	0.69
1:M:12:HIS:CE1	1:M:15:LEU:HB3	2.27	0.69
1:M:12:HIS:CD2	1:M:279:PRO:HD3	2.27	0.69
1:A:305:ARG:NH2	1:A:316:PHE:CD1	2.60	0.69
1:B:102:LYS:HB3	1:B:102:LYS:HZ1	1.55	0.69
1:K:171:VAL:HA	1:K:193:ALA:O	1.93	0.69
1:M:5:LYS:HD2	1:M:51:GLU:HG2	1.75	0.69
1:M:12:HIS:HD2	1:M:279:PRO:CD	2.05	0.69
1:B:225:MET:HG3	1:B:253:HIS:HB2	1.75	0.69
1:B:121:VAL:HG11	1:C:117:ASN:HB3	1.75	0.69
1:D:12:HIS:HE1	1:D:276:ASN:O	1.76	0.69
1:O:60:CYS:HB3	1:O:278:ILE:HG12	1.74	0.69
1:C:164:GLU:OE1	1:C:246:ARG:NH2	2.26	0.69
1:L:31:VAL:HG23	1:L:43:GLU:HB2	1.75	0.69
1:C:211:VAL:HG12	1:D:211:VAL:HG12	1.75	0.68
1:B:6:ILE:HG22	1:B:27:LEU:HD23	1.74	0.68
1:F:194:LEU:HD23	1:F:194:LEU:N	2.07	0.68
1:L:5:LYS:HD2	1:L:51:GLU:OE1	1.93	0.68
1:F:226:ALA:HB2	1:F:251:LEU:HD22	1.76	0.68
1:G:98:ASP:OD1	1:G:98:ASP:N	2.14	0.68
1:H:99:LYS:O	1:H:107:ARG:CD	2.41	0.68
1:L:93:PRO:O	1:L:94:TYR:HB2	1.94	0.68
1:G:43:GLU:CD	1:L:99:LYS:CE	2.59	0.68
1:M:99:LYS:HD3	1:M:107:ARG:HB2	1.76	0.67
1:L:168:CYS:HB2	1:L:218:VAL:HG13	1.74	0.67
1:P:102:LYS:HD2	1:P:107:ARG:NH1	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:75:ASN:OD1	1:Q:110:ILE:HG23	1.93	0.67
1:E:226:ALA:HB2	1:E:251:LEU:CD1	2.15	0.67
1:M:246:ARG:NH1	1:M:248:TYR:OH	2.27	0.67
1:L:78:LYS:HD3	1:L:123:GLY:O	1.95	0.67
1:C:103:VAL:O	1:D:149:TYR:CD2	2.44	0.66
1:H:156:LYS:CE	1:H:160:GLU:OE2	2.43	0.66
1:K:249:ALA:HB3	1:K:272:VAL:HG23	1.77	0.66
1:B:31:VAL:CG2	1:B:43:GLU:HB2	2.26	0.66
1:G:121:VAL:CG1	1:L:121:VAL:HG11	2.26	0.66
1:B:275:THR:HG22	1:B:295:ILE:HG12	1.77	0.66
1:C:168:CYS:HB2	1:C:218:VAL:HG23	1.76	0.66
1:E:226:ALA:CB	1:E:251:LEU:HD13	2.15	0.66
1:R:31:VAL:CG2	1:R:43:GLU:HB2	2.25	0.66
1:O:214:VAL:HG11	1:O:239:LEU:HD22	1.77	0.66
1:G:3:ASN:HD22	1:G:3:ASN:H	1.42	0.66
1:G:5:LYS:NZ	1:G:51:GLU:OE2	2.28	0.65
1:K:138:GLN:NE2	1:K:145:VAL:O	2.29	0.65
1:N:170:ILE:HD11	1:N:188:LEU:HD12	1.77	0.65
1:F:301:GLU:OE1	1:F:314:TYR:OH	2.12	0.65
1:G:321:LEU:HD12	1:G:321:LEU:C	2.16	0.65
1:N:3:ASN:N	1:N:3:ASN:OD1	2.25	0.65
1:B:275:THR:CG2	1:B:295:ILE:HG12	2.27	0.65
1:C:96:ARG:H	1:C:96:ARG:CD	1.98	0.65
1:H:12:HIS:CE1	1:H:15:LEU:CB	2.80	0.65
1:I:14:ASP:OD1	1:I:18:LYS:HE3	1.96	0.65
1:B:6:ILE:CG2	1:B:27:LEU:HD23	2.26	0.65
1:C:6:ILE:HD11	1:C:23:LEU:HD12	1.77	0.65
1:I:190:VAL:HG12	1:I:191:ASP:H	1.62	0.65
1:A:315:LEU:HD11	1:A:318:HIS:NE2	2.12	0.65
1:B:96:ARG:HD2	1:B:225:MET:SD	2.36	0.65
1:E:103:VAL:HG13	1:F:187:ARG:NH2	2.12	0.65
1:B:99:LYS:HB2	1:B:107:ARG:HD2	1.77	0.64
1:A:104:GLY:O	1:B:149:TYR:N	2.26	0.64
1:P:169:THR:HB	1:P:217:ARG:HH12	1.61	0.64
1:R:115:VAL:HA	1:R:118:MET:HE2	1.80	0.64
1:P:79:ILE:HG21	1:Q:110:ILE:HD11	1.80	0.64
1:I:208:MET:CE	1:I:234:HIS:CB	2.74	0.64
1:N:5:LYS:HE2	1:N:46:GLU:OE2	1.96	0.64
1:K:9:GLY:HA3	1:K:57:GLN:CD	2.18	0.64
1:Q:148:LEU:HD13	1:Q:298:ILE:HG22	1.80	0.64
1:F:310:GLU:O	1:K:4:ILE:CG2	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:THR:HG21	1:G:69:GLU:OE1	1.98	0.64
1:M:190:VAL:HG12	1:M:191:ASP:H	1.63	0.64
1:Q:197:LYS:O	1:Q:198:GLU:HB2	1.98	0.64
1:D:190:VAL:HG12	1:D:191:ASP:H	1.61	0.64
1:E:101:ASP:O	1:E:103:VAL:N	2.32	0.63
1:J:63:ILE:HD13	1:K:39:GLU:HG3	1.81	0.63
1:D:276:ASN:OD1	1:D:295:ILE:HG13	1.98	0.63
1:A:190:VAL:HG12	1:A:191:ASP:H	1.63	0.63
1:G:100:LYS:O	1:G:107:ARG:NH2	2.32	0.63
1:K:297:MET:HG2	1:K:298:ILE:H	1.64	0.63
1:E:225:MET:O	1:E:251:LEU:HD22	1.97	0.63
1:B:132:LEU:HD13	1:B:137:ILE:HB	1.81	0.63
1:E:214:VAL:HG11	1:E:239:LEU:HD22	1.79	0.63
1:L:250:ILE:HG12	1:L:273:VAL:CG2	2.29	0.63
1:G:3:ASN:HD22	1:G:3:ASN:N	1.94	0.63
1:P:6:ILE:HD11	1:P:23:LEU:HD12	1.81	0.63
1:A:60:CYS:HB3	1:A:278:ILE:HG12	1.80	0.63
1:E:311:SER:O	1:E:313:SER:N	2.27	0.62
1:J:294:ASP:CG	1:J:296:SER:HG	2.01	0.62
1:G:11:SER:HB2	1:G:57:GLN:OE1	1.99	0.62
1:A:3:ASN:OD1	1:A:3:ASN:N	2.28	0.62
1:A:168:CYS:HB2	1:A:218:VAL:HG13	1.82	0.62
1:C:215:LYS:O	1:C:243:GLY:O	2.17	0.62
1:C:166:ARG:HH21	1:C:166:ARG:HG2	1.63	0.62
1:I:3:ASN:N	1:I:3:ASN:OD1	2.32	0.62
1:M:11:SER:OG	1:M:57:GLN:CG	2.47	0.62
1:P:256:PHE:HB2	1:P:283:LYS:HD3	1.82	0.62
1:A:276:ASN:OD1	1:A:295:ILE:HG13	2.00	0.62
1:C:3:ASN:HD22	1:C:3:ASN:H	1.47	0.62
1:F:208:MET:HE1	1:F:234:HIS:HB3	1.82	0.62
1:H:156:LYS:HE3	1:H:160:GLU:OE2	2.00	0.62
1:Q:32:THR:HB	1:Q:69:GLU:OE2	1.98	0.62
1:E:1:SER:HB2	1:E:3:ASN:OD1	1.99	0.62
1:E:100:LYS:O	1:E:107:ARG:NH2	2.28	0.62
1:E:1:SER:O	1:P:309:GLY:O	2.18	0.62
1:F:313:SER:O	1:F:314:TYR:C	2.30	0.62
1:H:252:THR:HG22	1:H:253:HIS:CG	2.35	0.62
1:R:99:LYS:O	1:R:99:LYS:HG3	2.00	0.62
1:M:11:SER:HB3	1:M:58:SER:H	1.65	0.61
1:M:294:ASP:OD1	1:M:296:SER:OG	2.15	0.61
1:R:197:LYS:O	1:R:198:GLU:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:VAL:HG21	1:C:242:ALA:HB3	1.82	0.61
1:F:60:CYS:HB3	1:F:278:ILE:HG12	1.81	0.61
1:I:169:THR:CG2	1:I:217:ARG:HD3	2.30	0.61
1:K:158:ILE:HD12	1:K:220:ILE:HD13	1.82	0.61
1:B:57:GLN:O	1:B:89:ILE:HA	2.00	0.61
1:H:99:LYS:HD3	1:H:101:ASP:OD1	2.01	0.61
1:M:158:ILE:HD12	1:M:220:ILE:HD13	1.82	0.61
1:I:10:SER:OG	1:I:69:GLU:CD	2.38	0.61
1:K:98:ASP:N	1:K:98:ASP:OD1	2.34	0.61
1:R:138:GLN:NE2	1:R:145:VAL:O	2.34	0.61
1:Q:96:ARG:NH2	1:Q:227:ASP:OD2	2.33	0.61
1:B:99:LYS:HB3	1:B:107:ARG:HD2	1.81	0.61
1:J:295:ILE:HD12	1:J:295:ILE:C	2.21	0.61
1:P:60:CYS:HB3	1:P:278:ILE:HG12	1.82	0.61
1:G:39:GLU:HA	1:L:63:ILE:HD11	1.82	0.61
1:N:99:LYS:HB2	1:N:107:ARG:HD2	1.82	0.61
1:K:215:LYS:HD2	1:K:215:LYS:O	2.00	0.60
1:A:31:VAL:HB	1:A:43:GLU:HG3	1.83	0.60
1:N:158:ILE:HG13	1:N:162:ILE:HD12	1.81	0.60
1:A:281:GLU:HG2	1:A:282:ASP:N	2.16	0.60
1:C:96:ARG:HD2	1:C:96:ARG:N	2.07	0.60
1:E:172:SER:HB2	1:E:181:VAL:HG21	1.84	0.60
1:Q:305:ARG:HH21	1:Q:305:ARG:HG3	1.64	0.60
1:C:93:PRO:O	1:C:94:TYR:HB2	2.01	0.60
1:Q:93:PRO:O	1:Q:94:TYR:HB2	2.01	0.60
1:B:97:GLN:O	1:B:97:GLN:HG3	1.99	0.60
1:F:193:ALA:O	1:F:194:LEU:HD23	1.98	0.60
1:Q:12:HIS:HE1	1:Q:276:ASN:O	1.85	0.60
1:R:156:LYS:HE2	1:R:160:GLU:OE2	2.01	0.60
1:D:62:GLU:HA	1:E:38:GLN:HG2	1.84	0.60
1:B:93:PRO:HB2	1:B:94:TYR:HD2	1.66	0.60
1:P:251:LEU:O	1:P:274:VAL:HA	2.01	0.60
1:C:310:GLU:O	1:N:4:ILE:HG22	2.01	0.60
1:D:114:LEU:HD21	1:E:71:LEU:HB3	1.84	0.60
1:G:6:ILE:HG22	1:G:27:LEU:HD23	1.83	0.60
1:G:43:GLU:CG	1:L:99:LYS:HE3	2.32	0.60
1:L:14:ASP:O	1:L:17:GLN:N	2.35	0.60
1:P:100:LYS:NZ	1:Q:43:GLU:CD	2.55	0.60
1:B:3:ASN:HB2	1:B:51:GLU:OE1	2.01	0.60
1:D:169:THR:HB	1:D:217:ARG:NH1	2.05	0.60
1:G:184:ILE:HD11	1:G:222:VAL:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:226:ALA:HB2	1:J:251:LEU:HD13	1.82	0.60
1:R:276:ASN:OD1	1:R:295:ILE:HG13	2.02	0.59
1:A:93:PRO:O	1:A:94:TYR:HB2	2.01	0.59
1:E:294:ASP:O	1:E:297:MET:HE1	2.03	0.59
1:G:100:LYS:NZ	1:L:43:GLU:CD	2.55	0.59
1:G:240:LEU:HG	1:G:268:CYS:SG	2.42	0.59
1:F:99:LYS:HB2	1:F:107:ARG:HH11	1.66	0.59
1:N:158:ILE:HD13	1:N:188:LEU:HD11	1.83	0.59
1:Q:154:VAL:HG13	1:Q:250:ILE:HG21	1.84	0.59
1:D:99:LYS:CB	1:D:107:ARG:HD2	2.32	0.59
1:E:12:HIS:HE1	1:E:276:ASN:O	1.86	0.59
1:N:214:VAL:HG21	1:N:239:LEU:HD22	1.83	0.59
1:A:11:SER:OG	1:A:57:GLN:OE1	2.17	0.59
1:K:10:SER:H	1:K:57:GLN:HE22	1.51	0.59
1:K:71:LEU:HD11	1:K:118:MET:HE3	1.85	0.59
1:I:97:GLN:HG3	1:I:97:GLN:O	2.02	0.59
1:P:297:MET:HG2	1:P:298:ILE:N	2.17	0.59
1:K:102:LYS:O	1:K:105:GLU:O	2.21	0.59
1:O:99:LYS:HB2	1:O:107:ARG:HE	1.68	0.59
1:C:158:ILE:HD12	1:C:220:ILE:HD13	1.84	0.58
1:G:11:SER:CB	1:G:57:GLN:OE1	2.51	0.58
1:B:121:VAL:CG1	1:C:117:ASN:HB3	2.32	0.58
1:C:156:LYS:O	1:C:160:GLU:HG2	2.03	0.58
1:G:276:ASN:OD1	1:G:295:ILE:HG13	2.03	0.58
1:K:11:SER:OG	1:K:57:GLN:OE1	2.12	0.58
1:H:14:ASP:OD2	1:H:18:LYS:NZ	2.36	0.58
1:I:211:VAL:HG23	1:I:211:VAL:O	2.02	0.58
1:L:13:GLN:O	1:L:13:GLN:HG3	2.03	0.58
1:E:103:VAL:HG12	1:E:103:VAL:O	2.04	0.58
1:E:211:VAL:CG1	1:F:211:VAL:HG12	2.33	0.58
1:I:104:GLY:O	1:J:149:TYR:N	2.36	0.58
1:M:11:SER:CB	1:M:58:SER:H	2.17	0.58
1:E:99:LYS:CE	1:E:101:ASP:OD1	2.41	0.58
1:K:110:ILE:HG13	1:K:111:SER:H	1.68	0.58
1:N:181:VAL:HG12	1:N:222:VAL:HG22	1.85	0.58
1:N:278:ILE:HG23	1:N:279:PRO:HD2	1.85	0.58
1:E:34:LYS:NZ	1:E:38:GLN:HG3	2.19	0.58
1:E:93:PRO:O	1:E:94:TYR:HB2	2.03	0.58
1:O:57:GLN:O	1:O:89:ILE:HA	2.03	0.58
1:E:15:LEU:HD13	1:E:276:ASN:ND2	2.19	0.58
1:Q:14:ASP:O	1:Q:15:LEU:C	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:129:THR:HG22	1:I:130:MET:N	2.18	0.58
1:K:158:ILE:HD11	1:K:250:ILE:HD12	1.85	0.58
1:L:251:LEU:O	1:L:274:VAL:HA	2.03	0.58
1:Q:62:GLU:OE1	1:Q:65:ASP:N	2.26	0.58
1:N:12:HIS:HE1	1:N:276:ASN:O	1.87	0.57
1:C:190:VAL:HG12	1:C:191:ASP:H	1.69	0.57
1:C:251:LEU:O	1:C:274:VAL:HA	2.04	0.57
1:E:32:THR:HG23	1:E:32:THR:O	2.04	0.57
1:M:215:LYS:O	1:M:217:ARG:HD3	2.04	0.57
1:C:102:LYS:HD3	1:C:107:ARG:HG3	1.86	0.57
1:G:12:HIS:CE1	1:G:15:LEU:CB	2.88	0.57
1:B:275:THR:HG21	1:B:295:ILE:HG21	1.86	0.57
1:H:225:MET:HE2	1:H:255:ILE:HD12	1.84	0.57
1:N:251:LEU:O	1:N:274:VAL:HA	2.05	0.57
1:O:230:GLY:HA3	2:O:1001:HSX:O2X	2.03	0.57
1:D:34:LYS:NZ	1:D:38:GLN:OE1	2.34	0.57
1:D:172:SER:HB2	1:D:181:VAL:HG21	1.87	0.57
1:Q:222:VAL:HG12	1:Q:250:ILE:HB	1.86	0.57
1:B:181:VAL:HG12	1:B:222:VAL:CG2	2.34	0.57
1:C:167:ASN:O	1:C:168:CYS:HB3	2.03	0.57
1:A:12:HIS:CE1	1:A:15:LEU:HB2	2.40	0.57
1:B:171:VAL:HA	1:B:193:ALA:O	2.05	0.57
1:I:169:THR:HG22	1:I:191:ASP:HB2	1.87	0.57
1:L:14:ASP:O	1:L:16:SER:N	2.38	0.57
1:G:60:CYS:HB3	1:G:278:ILE:HG12	1.84	0.57
1:O:197:LYS:HE2	1:O:208:MET:HE1	1.86	0.57
1:N:159:ARG:HG2	1:N:165:TRP:CZ2	2.40	0.57
1:C:103:VAL:HG13	1:C:104:GLY:N	2.19	0.56
1:P:7:PHE:O	1:P:8:SER:HB3	2.04	0.56
1:Q:276:ASN:ND2	1:Q:294:ASP:OD1	2.36	0.56
1:C:214:VAL:HG11	1:C:239:LEU:HD22	1.85	0.56
1:I:132:LEU:CG	1:I:147:ASN:OD1	2.53	0.56
1:J:158:ILE:HG23	1:J:162:ILE:HD12	1.86	0.56
1:K:110:ILE:HG13	1:K:111:SER:N	2.21	0.56
1:B:214:VAL:HG12	1:B:244:ALA:HB2	1.87	0.56
1:I:129:THR:HG22	1:I:130:MET:H	1.71	0.56
1:I:132:LEU:HG	1:I:147:ASN:OD1	2.04	0.56
1:I:180:ARG:CZ	1:I:224:ASP:HB3	2.36	0.56
1:K:99:LYS:O	1:K:99:LYS:HG3	2.03	0.56
1:L:170:ILE:HD13	1:L:184:ILE:HG22	1.87	0.56
1:R:274:VAL:O	1:R:292:VAL:HA	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:ASP:HB3	1:G:251:LEU:CD2	2.35	0.56
1:H:156:LYS:HE2	1:H:160:GLU:OE2	2.05	0.56
1:C:13:GLN:O	1:C:13:GLN:HG3	2.05	0.56
1:C:190:VAL:HG12	1:C:191:ASP:N	2.20	0.56
1:J:114:LEU:HD13	1:K:75:ASN:HD22	1.69	0.56
1:I:115:VAL:HA	1:I:118:MET:HE2	1.88	0.56
1:B:226:ALA:HB2	1:B:251:LEU:HG	1.88	0.56
1:G:100:LYS:HZ2	1:L:43:GLU:CD	2.09	0.56
1:D:276:ASN:ND2	1:D:294:ASP:OD1	2.39	0.56
1:M:138:GLN:NE2	1:M:145:VAL:O	2.38	0.56
1:K:99:LYS:HD3	1:K:107:ARG:HB2	1.87	0.56
1:M:12:HIS:CE1	1:M:15:LEU:H	2.24	0.56
1:R:171:VAL:HG22	1:R:193:ALA:HB3	1.88	0.56
1:G:32:THR:HG21	1:G:69:GLU:CD	2.26	0.55
1:H:256:PHE:HB2	1:H:283:LYS:HD3	1.89	0.55
1:M:251:LEU:O	1:M:274:VAL:HA	2.06	0.55
1:I:42:VAL:HG11	1:I:73:MET:HG2	1.87	0.55
1:A:99:LYS:HG2	1:A:101:ASP:H	1.71	0.55
1:E:311:SER:HB3	1:P:25:LEU:HD21	1.89	0.55
1:H:164:GLU:OE1	1:H:164:GLU:N	2.39	0.55
1:I:132:LEU:HD12	1:I:147:ASN:OD1	2.06	0.55
1:I:301:GLU:HG2	1:I:319:VAL:HG21	1.88	0.55
1:J:38:GLN:HB2	1:K:63:ILE:HG23	1.88	0.55
1:M:162:ILE:HD11	1:M:218:VAL:CG2	2.27	0.55
1:N:38:GLN:HB2	1:O:63:ILE:HG12	1.88	0.55
1:I:276:ASN:OD1	1:I:295:ILE:HG13	2.06	0.55
1:L:75:ASN:HD22	1:L:75:ASN:C	2.08	0.55
1:H:93:PRO:O	1:H:94:TYR:HB2	2.06	0.55
1:K:313:SER:O	1:K:315:LEU:HD22	2.06	0.55
1:R:301:GLU:OE1	1:R:314:TYR:OH	2.23	0.55
1:F:193:ALA:O	1:F:194:LEU:HD22	2.06	0.55
1:I:3:ASN:HB2	1:I:51:GLU:HA	1.89	0.55
1:L:1:SER:N	1:L:2:PRO:HD3	2.21	0.55
1:F:127:ILE:HB	1:F:145:VAL:HG22	1.87	0.55
1:O:11:SER:HB2	1:O:57:GLN:CD	2.27	0.55
1:B:99:LYS:HE2	1:B:101:ASP:CG	2.27	0.55
1:D:121:VAL:HG11	1:E:121:VAL:CG1	2.20	0.55
1:O:89:ILE:O	1:O:129:THR:HG23	2.07	0.55
1:H:138:GLN:NE2	1:H:145:VAL:O	2.39	0.55
1:L:155:LEU:O	1:L:158:ILE:HG22	2.07	0.55
1:M:48:VAL:O	1:M:51:GLU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:CG2	1:B:27:LEU:CD2	2.83	0.55
1:L:151:GLU:HA	1:L:154:VAL:HG22	1.87	0.55
1:M:276:ASN:OD1	1:M:295:ILE:HG13	2.07	0.55
1:N:305:ARG:HB2	1:N:314:TYR:HE1	1.72	0.55
1:Q:181:VAL:HG12	1:Q:222:VAL:CG2	2.37	0.55
1:D:79:ILE:HD11	1:E:110:ILE:CG1	2.36	0.54
1:H:60:CYS:HB3	1:H:278:ILE:HG12	1.89	0.54
1:Q:181:VAL:HG12	1:Q:222:VAL:HG23	1.88	0.54
1:Q:305:ARG:NH1	1:R:105:GLU:OE2	2.40	0.54
1:G:12:HIS:CE1	1:G:15:LEU:HB2	2.41	0.54
1:I:275:THR:OG1	1:I:277:THR:HG23	2.06	0.54
1:K:269:PHE:O	1:K:289:LYS:HD3	2.08	0.54
1:Q:171:VAL:HG22	1:Q:193:ALA:HB3	1.88	0.54
1:C:226:ALA:CB	1:C:251:LEU:HD13	2.36	0.54
1:D:60:CYS:HB3	1:D:278:ILE:HG12	1.89	0.54
1:I:57:GLN:O	1:I:89:ILE:HA	2.07	0.54
1:D:75:ASN:HD22	1:E:114:LEU:HD13	1.73	0.54
1:E:251:LEU:O	1:E:274:VAL:HA	2.07	0.54
1:F:152:PRO:HB2	1:F:321:LEU:HD21	1.88	0.54
1:K:168:CYS:O	1:K:190:VAL:HG13	2.07	0.54
1:P:115:VAL:HA	1:P:118:MET:HE2	1.89	0.54
1:P:297:MET:HG2	1:P:298:ILE:H	1.71	0.54
1:D:251:LEU:O	1:D:274:VAL:HA	2.07	0.54
1:L:127:ILE:HB	1:L:145:VAL:HG13	1.90	0.54
1:O:138:GLN:NE2	1:O:145:VAL:O	2.40	0.54
1:B:54:TYR:CE2	1:B:303:ILE:HG23	2.41	0.54
1:E:261:ILE:HD13	1:E:264:ILE:HD11	1.90	0.54
1:G:11:SER:HB2	1:G:57:GLN:CD	2.28	0.54
1:I:62:GLU:C	1:I:62:GLU:OE1	2.46	0.54
1:K:214:VAL:O	1:K:214:VAL:HG23	2.07	0.54
1:L:171:VAL:HA	1:L:193:ALA:O	2.07	0.54
1:N:276:ASN:OD1	1:N:295:ILE:HG13	2.07	0.54
1:Q:12:HIS:CE1	1:Q:15:LEU:HB2	2.43	0.54
1:A:315:LEU:HD11	1:A:318:HIS:CD2	2.42	0.54
1:J:6:ILE:HD11	1:J:23:LEU:HD12	1.90	0.54
1:M:162:ILE:O	1:M:162:ILE:HG13	2.06	0.54
1:H:30:VAL:O	1:H:30:VAL:HG13	2.07	0.54
1:J:274:VAL:O	1:J:292:VAL:HA	2.08	0.54
1:M:208:MET:HE1	1:M:234:HIS:HB3	1.90	0.54
1:N:305:ARG:HB2	1:N:314:TYR:CE1	2.43	0.54
1:F:194:LEU:CD2	1:F:194:LEU:N	2.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:O	1:G:4:ILE:HG23	2.01	0.53
1:I:180:ARG:NH1	1:I:224:ASP:HB3	2.22	0.53
1:K:10:SER:N	1:K:57:GLN:HE22	2.06	0.53
1:K:251:LEU:O	1:K:274:VAL:HA	2.09	0.53
1:A:168:CYS:CB	1:A:218:VAL:HG13	2.39	0.53
1:B:101:ASP:N	1:B:101:ASP:OD1	2.39	0.53
1:G:154:VAL:HG13	1:G:250:ILE:HG21	1.90	0.53
1:G:298:ILE:HD11	1:G:321:LEU:HD22	1.89	0.53
1:H:64:ASN:OD1	1:I:68:MET:HG3	2.09	0.53
1:N:311:SER:O	1:N:313:SER:N	2.41	0.53
1:R:225:MET:HB2	1:R:253:HIS:HB2	1.90	0.53
1:B:64:ASN:ND2	1:C:68:MET:HG2	2.24	0.53
1:A:311:SER:HB2	1:R:4:ILE:HG22	1.90	0.53
1:G:12:HIS:CE1	1:G:15:LEU:HB3	2.44	0.53
1:G:214:VAL:HG11	1:G:239:LEU:HD22	1.89	0.53
1:O:11:SER:HB2	1:O:57:GLN:OE1	2.08	0.53
1:D:190:VAL:HG12	1:D:191:ASP:N	2.24	0.53
1:E:102:LYS:C	1:E:104:GLY:H	2.11	0.53
1:H:155:LEU:HD11	1:H:187:ARG:HD3	1.90	0.53
1:K:57:GLN:NE2	1:K:69:GLU:OE2	2.42	0.53
1:Q:227:ASP:CG	1:Q:228:THR:H	2.10	0.53
1:R:100:LYS:CB	1:R:100:LYS:NZ	2.72	0.53
1:A:99:LYS:CD	1:A:101:ASP:HA	2.39	0.53
1:E:115:VAL:HA	1:E:118:MET:HE2	1.88	0.53
1:E:97:GLN:O	1:E:99:LYS:HG2	2.09	0.53
1:E:102:LYS:O	1:E:105:GLU:N	2.35	0.53
1:J:261:ILE:HD11	1:J:283:LYS:CD	2.38	0.53
1:O:115:VAL:HA	1:O:118:MET:HE2	1.91	0.53
1:J:155:LEU:HD11	1:J:187:ARG:HG2	1.91	0.53
1:L:190:VAL:HG12	1:L:191:ASP:H	1.73	0.53
1:A:68:MET:HG3	1:F:64:ASN:OD1	2.09	0.53
1:E:234:HIS:O	1:E:235:ALA:C	2.44	0.53
1:M:159:ARG:HG2	1:M:165:TRP:CZ2	2.44	0.53
1:F:276:ASN:OD1	1:F:295:ILE:HG13	2.08	0.52
1:J:64:ASN:ND2	1:K:68:MET:HG2	2.24	0.52
1:J:251:LEU:O	1:J:274:VAL:HA	2.09	0.52
1:A:11:SER:CB	1:A:57:GLN:OE1	2.57	0.52
1:E:278:ILE:HG23	1:E:279:PRO:HD2	1.92	0.52
1:K:158:ILE:CD1	1:K:220:ILE:HD13	2.39	0.52
1:L:190:VAL:HG12	1:L:191:ASP:N	2.25	0.52
1:M:110:ILE:HG13	1:M:111:SER:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:31:VAL:HG22	1:R:43:GLU:HB2	1.91	0.52
1:B:96:ARG:HD2	1:B:225:MET:CE	2.40	0.52
1:E:57:GLN:NE2	1:E:69:GLU:OE1	2.40	0.52
1:E:195:ILE:HG13	1:E:210:LEU:HD12	1.92	0.52
1:G:89:ILE:O	1:G:129:THR:HG23	2.09	0.52
1:G:170:ILE:HD12	1:G:184:ILE:HG13	1.90	0.52
1:G:251:LEU:O	1:G:274:VAL:HA	2.09	0.52
1:Q:276:ASN:OD1	1:Q:295:ILE:HG13	2.10	0.52
1:C:275:THR:OG1	1:C:295:ILE:HG12	2.10	0.52
1:E:297:MET:HG2	1:E:298:ILE:N	2.23	0.52
1:J:249:ALA:HB3	1:J:272:VAL:HG22	1.92	0.52
1:D:6:ILE:HD11	1:D:23:LEU:HD12	1.92	0.52
1:B:99:LYS:HB3	1:B:107:ARG:CD	2.40	0.52
1:L:1:SER:HB3	1:L:4:ILE:HG21	1.92	0.52
1:N:275:THR:OG1	1:N:277:THR:HG23	2.10	0.52
1:O:103:VAL:CG2	1:P:187:ARG:CZ	2.88	0.52
1:P:226:ALA:CB	1:P:251:LEU:HD13	2.40	0.52
1:G:168:CYS:HB2	1:G:218:VAL:O	2.10	0.52
1:K:226:ALA:HB2	1:K:251:LEU:CD1	2.25	0.52
1:O:2:PRO:O	1:O:2:PRO:HG2	2.10	0.52
1:Q:12:HIS:CE1	1:Q:276:ASN:O	2.62	0.52
1:C:314:TYR:CD1	1:C:314:TYR:C	2.84	0.51
1:D:32:THR:HG23	1:D:69:GLU:OE2	2.09	0.51
1:F:284:MET:HE3	1:F:290:ILE:HG22	1.91	0.51
1:G:314:TYR:CD1	1:G:314:TYR:C	2.84	0.51
1:C:213:ASP:HB3	1:C:217:ARG:HH22	1.75	0.51
1:G:115:VAL:HA	1:G:118:MET:HE2	1.92	0.51
1:J:6:ILE:HD11	1:J:23:LEU:CD1	2.40	0.51
1:E:260:ALA:O	1:E:264:ILE:HG12	2.09	0.51
1:O:170:ILE:HD12	1:O:185:ALA:HA	1.92	0.51
1:O:240:LEU:HG	1:O:268:CYS:SG	2.50	0.51
1:A:281:GLU:HG2	1:A:282:ASP:H	1.75	0.51
1:C:102:LYS:HE2	1:C:105:GLU:HG3	1.92	0.51
1:J:60:CYS:HB3	1:J:278:ILE:HG12	1.90	0.51
1:J:121:VAL:HG11	1:K:117:ASN:HB3	1.93	0.51
1:C:278:ILE:HG23	1:C:279:PRO:HD2	1.92	0.51
1:E:127:ILE:HB	1:E:145:VAL:HG13	1.92	0.51
1:F:6:ILE:HG22	1:F:27:LEU:HD23	1.93	0.51
1:F:107:ARG:HH11	1:F:107:ARG:HG3	1.75	0.51
1:J:121:VAL:CG1	1:K:117:ASN:HB3	2.41	0.51
1:L:228:THR:O	1:L:229:CYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:223:ASP:O	1:Q:251:LEU:HA	2.10	0.51
1:C:12:HIS:HE1	1:C:276:ASN:O	1.94	0.51
1:F:208:MET:CE	1:F:234:HIS:HB3	2.40	0.51
1:L:29:LYS:HG3	1:L:46:GLU:HG2	1.92	0.51
1:A:276:ASN:ND2	1:A:294:ASP:OD1	2.42	0.51
1:B:293:ILE:O	1:B:293:ILE:HG12	2.06	0.51
1:F:12:HIS:CE1	1:F:276:ASN:O	2.60	0.51
1:Q:60:CYS:HB3	1:Q:278:ILE:HG12	1.91	0.51
1:I:223:ASP:O	1:I:251:LEU:HA	2.10	0.51
1:K:171:VAL:O	1:K:221:LEU:HA	2.10	0.51
1:N:223:ASP:HB3	1:N:251:LEU:HD12	1.92	0.51
1:O:103:VAL:HG22	1:P:187:ARG:HH11	1.73	0.51
1:Q:138:GLN:HE21	1:Q:147:ASN:HB3	1.75	0.51
1:R:171:VAL:HA	1:R:193:ALA:O	2.11	0.51
1:B:261:ILE:HG23	1:B:287:CYS:HB2	1.91	0.51
1:N:54:TYR:CE2	1:N:303:ILE:HG23	2.46	0.51
1:B:3:ASN:N	1:B:3:ASN:ND2	2.59	0.51
1:D:226:ALA:HB2	1:D:251:LEU:HG	1.92	0.51
1:P:215:LYS:O	1:P:215:LYS:HG3	2.10	0.51
1:R:117:ASN:O	1:R:121:VAL:HG23	2.11	0.51
1:P:276:ASN:OD1	1:P:295:ILE:HG13	2.11	0.50
1:D:297:MET:HG2	1:D:298:ILE:N	2.26	0.50
1:E:168:CYS:HB2	1:E:218:VAL:O	2.10	0.50
1:I:89:ILE:O	1:I:129:THR:HG23	2.11	0.50
1:J:195:ILE:HG13	1:J:210:LEU:CD1	2.41	0.50
1:L:227:ASP:OD1	1:L:257:SER:OG	2.20	0.50
1:Q:34:LYS:NZ	1:Q:38:GLN:OE1	2.36	0.50
1:E:1:SER:CB	1:E:2:PRO:CD	2.89	0.50
1:F:6:ILE:HG22	1:F:27:LEU:CD2	2.42	0.50
1:G:151:GLU:HG3	1:G:184:ILE:HG22	1.93	0.50
1:L:265:ASN:HA	1:L:289:LYS:NZ	2.26	0.50
1:O:197:LYS:HE2	1:O:208:MET:CE	2.41	0.50
1:G:3:ASN:N	1:G:3:ASN:ND2	2.60	0.50
1:K:165:TRP:O	1:K:168:CYS:HB2	2.10	0.50
1:O:78:LYS:HE2	1:O:125:ASP:OD2	2.11	0.50
1:O:151:GLU:OE2	1:O:187:ARG:NH1	2.43	0.50
1:D:278:ILE:HG23	1:D:279:PRO:HD2	1.94	0.50
1:A:162:ILE:O	1:A:165:TRP:HB3	2.12	0.50
1:E:100:LYS:HB2	1:E:107:ARG:HH21	1.73	0.50
1:I:226:ALA:HB2	1:I:251:LEU:HG	1.93	0.50
1:O:190:VAL:HG12	1:O:191:ASP:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:VAL:HA	1:C:118:MET:HE2	1.93	0.50
1:J:22:ARG:NH2	1:J:296:SER:OG	2.45	0.50
1:K:106:SER:HB3	1:L:149:TYR:OH	2.11	0.50
1:E:156:LYS:O	1:E:160:GLU:HG2	2.12	0.50
1:G:129:THR:HG22	1:G:130:MET:N	2.27	0.50
1:I:208:MET:CE	1:I:234:HIS:C	2.79	0.50
1:K:194:LEU:CD2	1:L:194:LEU:CD2	2.71	0.50
1:N:171:VAL:HG21	1:N:239:LEU:HD21	1.93	0.50
1:L:30:VAL:HG22	1:L:44:ILE:HA	1.93	0.50
1:B:60:CYS:HB3	1:B:278:ILE:HG12	1.94	0.49
1:B:275:THR:HG22	1:B:276:ASN:H	1.77	0.49
1:B:275:THR:HG21	1:B:295:ILE:CG2	2.42	0.49
1:H:294:ASP:OD1	1:H:296:SER:HB3	2.11	0.49
1:I:190:VAL:HG12	1:I:191:ASP:N	2.26	0.49
1:I:226:ALA:HB1	1:I:229:CYS:SG	2.52	0.49
1:J:33:LYS:HG3	1:J:41:CYS:HB3	1.93	0.49
1:N:75:ASN:OD1	1:O:110:ILE:HG23	2.12	0.49
1:N:121:VAL:HG11	1:O:121:VAL:HG11	1.94	0.49
1:A:130:MET:HG3	1:A:148:LEU:O	2.11	0.49
1:C:2:PRO:HA	1:N:310:GLU:O	2.12	0.49
1:G:281:GLU:OE2	1:G:285:LYS:HE3	2.12	0.49
1:N:5:LYS:NZ	1:N:51:GLU:OE1	2.44	0.49
1:A:32:THR:HB	1:A:69:GLU:OE2	2.12	0.49
1:B:275:THR:CG2	1:B:295:ILE:CG2	2.90	0.49
1:C:172:SER:HB3	1:C:194:LEU:HB2	1.94	0.49
1:E:60:CYS:HB3	1:E:278:ILE:HG12	1.93	0.49
1:A:100:LYS:C	1:A:102:LYS:H	2.15	0.49
1:F:10:SER:OG	1:F:69:GLU:OE1	2.29	0.49
1:F:223:ASP:HB3	1:F:251:LEU:HD23	1.94	0.49
1:H:97:GLN:O	1:H:99:LYS:N	2.46	0.49
1:O:260:ALA:O	1:O:264:ILE:HG12	2.13	0.49
1:E:223:ASP:HB3	1:E:251:LEU:HD23	1.95	0.49
1:A:181:VAL:HG12	1:A:222:VAL:CG2	2.38	0.49
1:C:11:SER:OG	1:C:57:GLN:OE1	2.15	0.49
1:C:99:LYS:HG3	1:C:101:ASP:HA	1.95	0.49
1:D:57:GLN:O	1:D:89:ILE:HA	2.13	0.49
1:L:210:LEU:HD11	1:L:239:LEU:HD23	1.95	0.49
1:M:169:THR:HG21	1:M:214:VAL:HG12	1.95	0.49
1:O:223:ASP:O	1:O:251:LEU:HA	2.13	0.49
1:Q:180:ARG:CZ	1:Q:224:ASP:HB3	2.42	0.49
1:R:99:LYS:CB	1:R:107:ARG:CD	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:SER:OG	1:D:32:THR:HG22	2.11	0.49
1:E:9:GLY:HA3	1:E:57:GLN:OE1	2.13	0.49
1:G:5:LYS:NZ	1:G:51:GLU:HG3	2.28	0.49
1:H:42:VAL:HG11	1:H:73:MET:HG3	1.95	0.49
1:M:117:ASN:HB3	1:R:121:VAL:HG11	1.94	0.49
1:A:256:PHE:O	1:A:283:LYS:HE2	2.12	0.49
1:E:14:ASP:OD2	1:E:18:LYS:NZ	2.41	0.49
1:F:12:HIS:CE1	1:F:15:LEU:HB2	2.47	0.49
1:F:294:ASP:OD1	1:F:296:SER:HB3	2.12	0.49
1:H:12:HIS:CE1	1:H:15:LEU:HB3	2.48	0.49
1:Q:5:LYS:CE	1:Q:46:GLU:OE1	2.60	0.49
1:B:170:ILE:HD11	1:B:188:LEU:HD12	1.95	0.49
1:C:211:VAL:CG1	1:D:211:VAL:CG1	2.86	0.49
1:D:168:CYS:SG	1:D:169:THR:N	2.86	0.49
1:F:156:LYS:HE3	1:F:160:GLU:OE2	2.13	0.49
1:M:162:ILE:CD1	1:M:218:VAL:HG21	2.29	0.49
1:N:101:ASP:N	1:N:101:ASP:OD1	2.45	0.49
1:O:129:THR:HG22	1:O:130:MET:H	1.78	0.49
1:E:276:ASN:OD1	1:E:295:ILE:HG13	2.12	0.49
1:H:159:ARG:HG2	1:H:165:TRP:CE2	2.48	0.49
1:A:100:LYS:HB3	1:A:107:ARG:HH22	1.77	0.48
1:B:275:THR:CG2	1:B:295:ILE:HG23	2.43	0.48
1:B:314:TYR:CD1	1:B:314:TYR:C	2.85	0.48
1:H:159:ARG:HG2	1:H:165:TRP:CZ2	2.48	0.48
1:K:11:SER:CB	1:K:57:GLN:OE1	2.60	0.48
1:K:148:LEU:HD22	1:K:316:PHE:CZ	2.48	0.48
1:K:225:MET:SD	1:K:255:ILE:CD1	3.01	0.48
1:M:208:MET:CE	1:M:234:HIS:HB3	2.43	0.48
1:O:159:ARG:HG2	1:O:165:TRP:CE2	2.48	0.48
1:B:297:MET:SD	1:B:297:MET:N	2.86	0.48
1:D:62:GLU:HG2	1:E:38:GLN:HE21	1.78	0.48
1:F:226:ALA:HA	2:F:1001:HSX:O2	2.13	0.48
1:M:68:MET:HG2	1:R:64:ASN:ND2	2.28	0.48
1:N:30:VAL:HG22	1:N:44:ILE:HA	1.95	0.48
1:D:42:VAL:HG11	1:D:73:MET:HG2	1.95	0.48
1:E:267:ALA:O	1:E:289:LYS:NZ	2.46	0.48
1:K:275:THR:CG2	1:K:277:THR:HG23	2.44	0.48
1:N:168:CYS:HB2	1:N:218:VAL:HG13	1.94	0.48
1:C:96:ARG:HG2	1:C:96:ARG:HH11	1.79	0.48
1:D:159:ARG:HG2	1:D:165:TRP:CZ2	2.48	0.48
1:F:298:ILE:HG23	1:F:316:PHE:HZ	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:LEU:C	1:G:194:LEU:HD12	2.34	0.48
1:O:58:SER:HA	1:O:90:PRO:HD2	1.95	0.48
1:P:63:ILE:HD13	1:Q:39:GLU:HG3	1.94	0.48
1:E:215:LYS:HG3	1:E:216:ASP:OD2	2.14	0.48
1:F:276:ASN:ND2	1:F:294:ASP:OD1	2.45	0.48
1:L:31:VAL:CG2	1:L:43:GLU:HB2	2.43	0.48
1:M:275:THR:OG1	1:M:277:THR:HG23	2.14	0.48
1:R:99:LYS:HD3	1:R:107:ARG:HG3	1.94	0.48
1:G:138:GLN:NE2	1:G:145:VAL:O	2.47	0.48
1:R:60:CYS:HB3	1:R:278:ILE:HG12	1.95	0.48
1:R:154:VAL:HG13	1:R:250:ILE:HG21	1.96	0.48
1:G:320:PRO:O	1:G:320:PRO:HG2	2.12	0.48
1:I:94:TYR:CD2	1:I:111:SER:HB3	2.48	0.48
1:M:63:ILE:HD11	1:R:39:GLU:HA	1.95	0.48
1:P:102:LYS:HG2	1:P:102:LYS:O	2.11	0.48
1:Q:251:LEU:O	1:Q:274:VAL:HA	2.13	0.48
1:R:223:ASP:HB3	1:R:251:LEU:HD12	1.96	0.48
1:D:169:THR:HG21	1:D:214:VAL:HG23	1.94	0.48
1:E:159:ARG:HG2	1:E:165:TRP:CZ2	2.48	0.48
1:G:15:LEU:HD11	1:G:299:LEU:HD12	1.96	0.48
1:K:275:THR:HG23	1:K:277:THR:HG23	1.96	0.48
1:A:97:GLN:HE22	1:A:108:ALA:C	2.17	0.48
1:G:93:PRO:O	1:G:94:TYR:HB2	2.12	0.48
1:H:215:LYS:O	1:H:217:ARG:HD3	2.14	0.48
1:J:195:ILE:HG13	1:J:210:LEU:HD13	1.95	0.48
1:R:98:ASP:OD1	1:R:98:ASP:N	2.30	0.48
1:B:310:GLU:O	1:G:4:ILE:HG21	2.04	0.48
1:C:3:ASN:N	1:C:3:ASN:ND2	2.58	0.48
1:E:1:SER:HB3	1:E:2:PRO:CD	2.44	0.48
1:F:103:VAL:O	1:F:103:VAL:HG23	2.14	0.48
1:M:141:PHE:CD1	1:M:145:VAL:HG21	2.49	0.48
1:C:106:SER:HB3	1:D:149:TYR:OH	2.14	0.47
1:D:127:ILE:HD11	1:D:143:ILE:HD11	1.95	0.47
1:F:3:ASN:HB3	1:F:51:GLU:HA	1.95	0.47
1:H:12:HIS:HE1	1:H:15:LEU:HB2	1.75	0.47
1:I:132:LEU:CD1	1:I:147:ASN:OD1	2.62	0.47
1:L:278:ILE:HG23	1:L:279:PRO:HD2	1.97	0.47
1:L:281:GLU:HG2	1:L:282:ASP:N	2.29	0.47
1:N:138:GLN:NE2	1:N:145:VAL:O	2.47	0.47
1:N:225:MET:HG3	1:N:253:HIS:HB2	1.96	0.47
1:O:129:THR:HG22	1:O:130:MET:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:101:ASP:N	1:L:101:ASP:OD1	2.47	0.47
1:A:275:THR:OG1	1:A:277:THR:HG23	2.14	0.47
1:G:180:ARG:CZ	1:G:224:ASP:HB3	2.44	0.47
1:O:156:LYS:O	1:O:160:GLU:HG3	2.15	0.47
1:R:251:LEU:O	1:R:274:VAL:HA	2.13	0.47
1:E:172:SER:HA	1:E:173:PRO:HD3	1.71	0.47
1:G:12:HIS:HE1	1:G:15:LEU:HB2	1.77	0.47
1:H:57:GLN:O	1:H:89:ILE:HA	2.15	0.47
1:M:32:THR:O	1:M:32:THR:HG22	2.13	0.47
1:O:100:LYS:N	1:O:100:LYS:CD	2.73	0.47
1:O:196:HIS:O	1:O:209:VAL:HG12	2.14	0.47
1:Q:278:ILE:HG23	1:Q:279:PRO:HD2	1.96	0.47
1:A:186:ASP:OD2	1:B:198:GLU:HG3	2.15	0.47
1:B:294:ASP:O	1:B:297:MET:CE	2.62	0.47
1:C:99:LYS:HB2	1:C:107:ARG:NE	2.22	0.47
1:E:130:MET:HG3	1:E:299:LEU:HD21	1.97	0.47
1:F:261:ILE:HD12	1:F:261:ILE:H	1.79	0.47
1:H:280:GLN:O	1:H:284:MET:HG3	2.14	0.47
1:J:6:ILE:CD1	1:J:23:LEU:HD12	2.43	0.47
1:N:171:VAL:HG22	1:N:193:ALA:HB3	1.96	0.47
1:P:8:SER:HB2	1:P:16:SER:HB3	1.96	0.47
1:R:3:ASN:OD1	1:R:3:ASN:N	2.46	0.47
1:R:100:LYS:NZ	1:R:100:LYS:HB2	2.30	0.47
1:A:251:LEU:O	1:A:274:VAL:HA	2.14	0.47
1:B:75:ASN:HD22	1:B:75:ASN:C	2.17	0.47
1:C:180:ARG:CZ	1:C:224:ASP:HB3	2.44	0.47
1:D:250:ILE:HD12	1:D:273:VAL:HB	1.96	0.47
1:E:131:ASP:OD2	1:E:252:THR:HG21	2.15	0.47
1:E:184:ILE:HD12	1:E:222:VAL:HG11	1.96	0.47
1:J:154:VAL:HG13	1:J:250:ILE:HG21	1.96	0.47
1:N:62:GLU:HG2	1:O:38:GLN:NE2	2.29	0.47
1:Q:190:VAL:HG12	1:Q:191:ASP:N	2.29	0.47
1:A:190:VAL:HG12	1:A:191:ASP:N	2.29	0.47
1:A:223:ASP:HB3	1:A:251:LEU:HD12	1.96	0.47
1:C:250:ILE:C	1:C:251:LEU:HG	2.34	0.47
1:O:197:LYS:HB3	1:O:208:MET:HE2	1.96	0.47
1:R:295:ILE:HG13	1:R:295:ILE:H	1.60	0.47
1:H:12:HIS:CE1	1:H:276:ASN:O	2.67	0.47
1:Q:240:LEU:HD23	1:Q:240:LEU:HA	1.63	0.47
1:C:103:VAL:O	1:C:103:VAL:HG22	2.14	0.47
1:E:311:SER:CB	1:P:25:LEU:HD21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:209:VAL:HG23	1:I:209:VAL:O	2.13	0.47
1:J:159:ARG:HG2	1:J:165:TRP:CZ2	2.50	0.47
1:K:100:LYS:O	1:K:107:ARG:NH2	2.44	0.47
1:L:275:THR:OG1	1:L:277:THR:HG23	2.15	0.47
1:L:282:ASP:OD1	1:L:285:LYS:HE3	2.15	0.47
1:N:57:GLN:O	1:N:89:ILE:HA	2.14	0.47
1:R:159:ARG:HG2	1:R:165:TRP:CE2	2.50	0.47
1:B:49:ARG:HD3	1:B:81:SER:HB2	1.96	0.46
1:B:93:PRO:HB2	1:B:94:TYR:CD2	2.49	0.46
1:C:294:ASP:OD1	1:C:296:SER:OG	2.30	0.46
1:D:249:ALA:O	1:D:250:ILE:HD13	2.16	0.46
1:K:225:MET:SD	1:K:255:ILE:HD11	2.55	0.46
1:M:60:CYS:HB3	1:M:278:ILE:HG12	1.96	0.46
1:M:307:HIS:O	1:M:308:ASN:HB2	2.14	0.46
1:Q:138:GLN:HE21	1:Q:147:ASN:CB	2.28	0.46
1:H:225:MET:O	1:H:225:MET:HG3	2.14	0.46
1:I:10:SER:OG	1:I:69:GLU:OE1	2.32	0.46
1:J:13:GLN:O	1:J:13:GLN:HG2	2.16	0.46
1:L:30:VAL:HG11	1:L:73:MET:CE	2.45	0.46
1:M:278:ILE:HG23	1:M:279:PRO:HD2	1.97	0.46
1:N:71:LEU:HB3	1:O:114:LEU:HD21	1.96	0.46
1:C:214:VAL:HG11	1:C:239:LEU:HD23	1.97	0.46
1:P:184:ILE:HD12	1:P:222:VAL:HG11	1.97	0.46
1:R:171:VAL:O	1:R:221:LEU:HA	2.15	0.46
1:G:223:ASP:HB3	1:G:251:LEU:HD23	1.97	0.46
1:N:32:THR:HB	1:N:69:GLU:OE2	2.16	0.46
1:A:159:ARG:HG2	1:A:165:TRP:CZ2	2.50	0.46
1:E:310:GLU:O	1:P:4:ILE:CG2	2.57	0.46
1:K:9:GLY:CA	1:K:57:GLN:NE2	2.76	0.46
1:O:261:ILE:HG23	1:O:287:CYS:HB2	1.98	0.46
1:P:64:ASN:OD1	1:Q:68:MET:HG3	2.15	0.46
1:P:321:LEU:H	1:P:321:LEU:HD23	1.80	0.46
1:A:101:ASP:O	1:A:102:LYS:HB2	2.16	0.46
1:B:115:VAL:HA	1:B:118:MET:HE2	1.96	0.46
1:B:251:LEU:O	1:B:274:VAL:HA	2.16	0.46
1:F:275:THR:OG1	1:F:277:THR:HG23	2.15	0.46
1:K:278:ILE:HG23	1:K:279:PRO:HD2	1.97	0.46
1:N:30:VAL:HG11	1:N:73:MET:HE3	1.96	0.46
1:Q:198:GLU:HA	1:R:186:ASP:OD2	2.16	0.46
1:R:42:VAL:HG11	1:R:73:MET:HG2	1.98	0.46
1:A:5:LYS:HE2	1:A:46:GLU:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:VAL:HG11	1:F:73:MET:HG2	1.98	0.46
1:H:246:ARG:NH1	1:H:248:TYR:OH	2.44	0.46
1:L:60:CYS:HB3	1:L:278:ILE:HG12	1.98	0.46
1:R:132:LEU:HD13	1:R:137:ILE:HB	1.98	0.46
1:C:171:VAL:HA	1:C:193:ALA:O	2.16	0.46
1:E:321:LEU:HD23	1:E:321:LEU:HA	1.71	0.46
1:F:278:ILE:HG23	1:F:279:PRO:HD2	1.98	0.46
1:L:249:ALA:HB3	1:L:272:VAL:HG22	1.98	0.46
1:N:222:VAL:HA	1:N:250:ILE:O	2.15	0.46
1:A:62:GLU:HG2	1:F:38:GLN:NE2	2.30	0.46
1:A:305:ARG:NH2	1:A:316:PHE:HD1	2.10	0.46
1:B:71:LEU:HB3	1:C:114:LEU:HD21	1.98	0.46
1:I:93:PRO:HB2	1:I:94:TYR:HD1	1.81	0.46
1:I:208:MET:HE3	1:I:234:HIS:C	2.35	0.46
1:M:210:LEU:HD11	1:M:239:LEU:HD23	1.98	0.46
1:G:149:TYR:N	1:H:104:GLY:O	2.47	0.46
1:I:115:VAL:HA	1:I:118:MET:CE	2.46	0.46
1:L:151:GLU:O	1:L:154:VAL:HG22	2.16	0.46
1:M:32:THR:HG21	1:M:69:GLU:CD	2.36	0.46
1:N:228:THR:HG22	1:N:263:ARG:NH1	2.31	0.46
1:O:103:VAL:HG23	1:P:187:ARG:HH12	1.79	0.46
1:R:37:ASN:OD1	1:R:37:ASN:C	2.55	0.46
1:C:11:SER:CB	1:C:57:GLN:OE1	2.64	0.45
1:K:223:ASP:O	1:K:251:LEU:HA	2.16	0.45
1:F:99:LYS:CB	1:F:107:ARG:HH11	2.29	0.45
1:J:75:ASN:C	1:J:75:ASN:HD22	2.20	0.45
1:A:97:GLN:NE2	1:A:108:ALA:O	2.49	0.45
1:B:223:ASP:O	1:B:251:LEU:HA	2.17	0.45
1:C:96:ARG:CD	1:C:96:ARG:N	2.72	0.45
1:E:1:SER:HB3	1:E:2:PRO:HD3	1.99	0.45
1:G:6:ILE:HG22	1:G:27:LEU:CD2	2.46	0.45
1:N:274:VAL:O	1:N:292:VAL:HA	2.15	0.45
1:O:102:LYS:HD2	1:O:107:ARG:CZ	2.47	0.45
1:Q:35:PHE:CE2	1:Q:41:CYS:HB2	2.51	0.45
1:Q:208:MET:HE1	1:Q:234:HIS:O	2.17	0.45
1:D:274:VAL:O	1:D:292:VAL:HA	2.16	0.45
1:H:240:LEU:HG	1:H:268:CYS:SG	2.57	0.45
1:L:14:ASP:HB3	1:L:15:LEU:H	1.40	0.45
1:L:157:TRP:CZ2	1:L:273:VAL:HG11	2.51	0.45
1:F:138:GLN:NE2	1:F:145:VAL:O	2.49	0.45
1:H:30:VAL:HG23	1:H:44:ILE:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:64:ASN:HD21	1:K:68:MET:HG2	1.81	0.45
1:M:11:SER:OG	1:M:57:GLN:CD	2.55	0.45
1:O:184:ILE:HD11	1:O:222:VAL:HG11	1.97	0.45
1:Q:307:HIS:O	1:Q:307:HIS:CG	2.70	0.45
1:P:240:LEU:HD23	1:P:240:LEU:HA	1.67	0.45
1:C:5:LYS:HZ3	1:C:46:GLU:HG2	1.81	0.45
1:C:252:THR:O	1:C:275:THR:CG2	2.65	0.45
1:G:223:ASP:O	1:G:251:LEU:HA	2.17	0.45
1:H:159:ARG:HA	1:H:165:TRP:CD1	2.52	0.45
1:A:278:ILE:HG23	1:A:279:PRO:HD2	1.99	0.45
1:B:96:ARG:HD2	1:B:225:MET:HE1	1.98	0.45
1:E:311:SER:O	1:E:311:SER:OG	2.30	0.45
1:F:240:LEU:HD23	1:F:240:LEU:HA	1.59	0.45
1:M:208:MET:HE2	1:M:208:MET:HB2	1.93	0.45
1:N:173:PRO:HG3	1:N:221:LEU:HD22	1.98	0.45
1:O:14:ASP:OD1	1:O:18:LYS:NZ	2.50	0.45
1:P:151:GLU:HB3	1:P:152:PRO:HD3	1.99	0.45
1:Q:95:ALA:HB1	1:Q:133:HIS:HB3	1.98	0.45
1:A:64:ASN:OD1	1:F:68:MET:HG2	2.16	0.45
1:B:275:THR:HG22	1:B:276:ASN:N	2.31	0.45
1:C:252:THR:O	1:C:275:THR:HG22	2.16	0.45
1:I:32:THR:HG22	1:I:42:VAL:HG22	1.99	0.45
1:L:99:LYS:O	1:L:107:ARG:NH2	2.50	0.45
1:L:273:VAL:HG12	1:L:291:GLN:HB2	1.99	0.45
1:M:149:TYR:OH	1:N:106:SER:HB3	2.17	0.45
1:N:180:ARG:CZ	1:N:224:ASP:HB3	2.47	0.45
1:O:251:LEU:O	1:O:274:VAL:HA	2.17	0.45
1:P:5:LYS:HZ3	1:P:51:GLU:HG3	1.82	0.45
1:R:181:VAL:HG12	1:R:222:VAL:CG2	2.39	0.45
1:G:287:CYS:HB3	1:G:290:ILE:HD12	1.99	0.45
1:H:275:THR:OG1	1:H:277:THR:HG23	2.17	0.45
1:J:12:HIS:CE1	1:J:15:LEU:H	2.35	0.45
1:O:170:ILE:HG22	1:O:181:VAL:HG13	1.98	0.45
1:Q:164:GLU:OE2	1:Q:246:ARG:NH1	2.50	0.45
1:Q:275:THR:OG1	1:Q:277:THR:HG23	2.17	0.45
1:R:93:PRO:O	1:R:94:TYR:HB2	2.16	0.45
1:R:127:ILE:HB	1:R:145:VAL:HG13	1.98	0.45
1:R:314:TYR:CD1	1:R:314:TYR:C	2.90	0.45
1:A:208:MET:HE1	1:A:234:HIS:C	2.38	0.44
1:D:195:ILE:HG13	1:D:210:LEU:HG	1.99	0.44
1:D:217:ARG:HH21	1:D:217:ARG:HD3	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:ARG:NH1	1:F:107:ARG:HG3	2.31	0.44
1:G:121:VAL:HG11	1:L:121:VAL:CG1	2.39	0.44
1:K:210:LEU:HD23	1:K:211:VAL:N	2.32	0.44
1:M:158:ILE:CD1	1:M:220:ILE:HD13	2.46	0.44
1:P:157:TRP:CH2	1:P:273:VAL:HG21	2.52	0.44
1:P:240:LEU:HG	1:P:268:CYS:SG	2.56	0.44
1:R:208:MET:HE2	1:R:234:HIS:HB3	1.99	0.44
1:R:227:ASP:HB3	1:R:228:THR:H	1.63	0.44
1:B:250:ILE:HG12	1:B:273:VAL:HB	1.99	0.44
1:F:124:ALA:O	1:F:143:ILE:HD13	2.18	0.44
1:F:284:MET:HE2	1:F:290:ILE:O	2.17	0.44
1:L:240:LEU:HD23	1:L:240:LEU:HA	1.62	0.44
1:F:7:PHE:CE1	1:F:28:GLY:HA3	2.52	0.44
1:F:113:LYS:O	1:F:114:LEU:C	2.53	0.44
1:M:96:ARG:HH22	1:R:37:ASN:ND2	2.04	0.44
1:N:210:LEU:HD23	1:N:211:VAL:N	2.32	0.44
1:P:4:ILE:HG21	1:P:4:ILE:HD13	1.62	0.44
1:Q:222:VAL:HA	1:Q:250:ILE:O	2.16	0.44
1:C:166:ARG:HH21	1:C:166:ARG:HG3	1.80	0.44
1:F:312:VAL:O	1:F:312:VAL:HG12	2.18	0.44
1:H:102:LYS:HG3	1:H:107:ARG:NH1	2.33	0.44
1:I:208:MET:HE1	1:I:234:HIS:CB	2.45	0.44
1:N:246:ARG:NH1	1:N:248:TYR:OH	2.48	0.44
1:R:27:LEU:HD12	1:R:27:LEU:H	1.82	0.44
1:B:151:GLU:HB3	1:B:152:PRO:HD3	1.99	0.44
1:C:164:GLU:CD	1:C:246:ARG:HH22	2.19	0.44
1:G:225:MET:CE	1:G:255:ILE:HD11	2.45	0.44
1:K:154:VAL:HG13	1:K:250:ILE:HG21	2.00	0.44
1:L:158:ILE:HG21	1:L:188:LEU:HD11	2.00	0.44
1:N:114:LEU:HD12	1:N:114:LEU:HA	1.81	0.44
1:A:63:ILE:HG12	1:F:38:GLN:HB2	1.99	0.44
1:B:99:LYS:HB2	1:B:100:LYS:H	1.29	0.44
1:D:32:THR:HG22	1:D:32:THR:O	2.17	0.44
1:F:115:VAL:HA	1:F:118:MET:HE2	1.99	0.44
1:F:159:ARG:HG2	1:F:165:TRP:CZ2	2.52	0.44
1:O:103:VAL:O	1:P:149:TYR:HD2	2.00	0.44
1:O:261:ILE:HD13	1:O:264:ILE:HD11	1.99	0.44
1:A:101:ASP:O	1:A:102:LYS:CB	2.65	0.44
1:F:154:VAL:HG13	1:F:250:ILE:HG21	2.00	0.44
1:G:157:TRP:CH2	1:G:273:VAL:HG21	2.52	0.44
1:G:171:VAL:HA	1:G:193:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:LYS:NZ	1:I:321:LEU:HD23	2.33	0.44
1:L:158:ILE:HD11	1:L:220:ILE:HD13	2.00	0.44
1:B:102:LYS:NZ	1:B:102:LYS:CB	2.72	0.44
1:G:12:HIS:ND1	1:G:15:LEU:HB3	2.33	0.44
1:G:110:ILE:HD11	1:L:79:ILE:HD11	1.98	0.44
1:J:58:SER:HA	1:J:90:PRO:HD2	2.00	0.44
1:M:190:VAL:HG12	1:M:191:ASP:N	2.30	0.44
1:P:49:ARG:O	1:R:312:VAL:HG12	2.18	0.44
1:B:213:ASP:HB3	1:B:217:ARG:NH2	2.32	0.44
1:C:102:LYS:HG3	1:C:102:LYS:O	2.17	0.44
1:C:158:ILE:CD1	1:C:220:ILE:HD13	2.48	0.44
1:C:184:ILE:HD12	1:C:222:VAL:HG11	2.00	0.44
1:J:295:ILE:C	1:J:295:ILE:CD1	2.85	0.44
1:L:171:VAL:HG11	1:L:239:LEU:HD21	2.00	0.44
1:M:127:ILE:HB	1:M:145:VAL:HG13	2.00	0.44
1:E:223:ASP:O	1:E:251:LEU:HA	2.18	0.43
1:J:293:ILE:HD13	1:J:293:ILE:HG21	1.72	0.43
1:L:151:GLU:HB3	1:L:152:PRO:HD3	2.01	0.43
1:L:171:VAL:O	1:L:221:LEU:HA	2.18	0.43
1:L:307:HIS:O	1:L:308:ASN:HB2	2.16	0.43
1:Q:168:CYS:HB2	1:Q:218:VAL:O	2.18	0.43
1:R:100:LYS:HB2	1:R:100:LYS:HZ2	1.82	0.43
1:B:3:ASN:N	1:B:3:ASN:HD22	2.16	0.43
1:B:228:THR:OG1	2:B:1001:HSX:C5	2.67	0.43
1:D:215:LYS:HE3	1:D:215:LYS:HB2	1.90	0.43
1:G:6:ILE:HG22	1:G:6:ILE:O	2.17	0.43
1:P:58:SER:HB3	1:P:60:CYS:SG	2.59	0.43
1:P:226:ALA:HB1	1:P:229:CYS:SG	2.59	0.43
1:Q:261:ILE:HG23	1:Q:287:CYS:HB2	1.99	0.43
1:R:223:ASP:O	1:R:251:LEU:HA	2.17	0.43
1:R:282:ASP:HA	1:R:285:LYS:HE2	1.98	0.43
1:A:37:ASN:O	1:F:63:ILE:HD12	2.19	0.43
1:E:34:LYS:HZ3	1:E:38:GLN:HG3	1.82	0.43
1:G:62:GLU:HG2	1:G:65:ASP:OD2	2.19	0.43
1:G:96:ARG:NH1	1:G:225:MET:SD	2.88	0.43
1:G:103:VAL:HG12	1:G:103:VAL:O	2.18	0.43
1:H:3:ASN:HB2	1:H:51:GLU:OE2	2.18	0.43
1:N:168:CYS:HB2	1:N:218:VAL:O	2.19	0.43
1:A:63:ILE:HG12	1:A:63:ILE:H	1.64	0.43
1:E:223:ASP:HB3	1:E:251:LEU:CD2	2.48	0.43
1:E:239:LEU:HD23	1:E:239:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:11:SER:HB3	1:G:57:GLN:OE1	2.19	0.43
1:I:4:ILE:HG21	1:I:25:LEU:HD11	2.00	0.43
1:L:276:ASN:ND2	1:L:294:ASP:OD1	2.48	0.43
1:P:310:GLU:H	1:P:310:GLU:HG2	1.42	0.43
1:R:293:ILE:HD13	1:R:293:ILE:HG21	1.77	0.43
1:G:180:ARG:NH1	1:G:224:ASP:HB3	2.33	0.43
1:O:13:GLN:O	1:O:13:GLN:HG3	2.18	0.43
1:P:93:PRO:O	1:P:94:TYR:HB2	2.17	0.43
1:R:222:VAL:HA	1:R:250:ILE:O	2.18	0.43
1:B:148:LEU:HD11	1:B:302:ALA:HB2	2.00	0.43
1:C:130:MET:SD	1:C:295:ILE:HD13	2.58	0.43
1:C:252:THR:HA	1:C:275:THR:HG22	2.00	0.43
1:I:196:HIS:O	1:I:208:MET:HA	2.19	0.43
1:L:250:ILE:HA	1:L:273:VAL:HG23	2.00	0.43
1:Q:69:GLU:O	1:Q:73:MET:HG3	2.18	0.43
1:Q:80:ALA:O	1:Q:81:SER:CB	2.56	0.43
1:Q:305:ARG:HG3	1:Q:305:ARG:NH2	2.33	0.43
1:R:1:SER:HB2	1:R:3:ASN:ND2	2.33	0.43
1:R:5:LYS:HE3	1:R:51:GLU:OE2	2.19	0.43
1:C:167:ASN:HB3	1:C:168:CYS:H	1.52	0.43
1:E:316:PHE:O	1:E:319:VAL:HG22	2.18	0.43
1:G:211:VAL:HB	1:H:211:VAL:HG12	2.01	0.43
1:I:9:GLY:HA3	1:I:57:GLN:OE1	2.18	0.43
1:N:151:GLU:HA	1:N:154:VAL:HG22	2.01	0.43
1:A:127:ILE:HB	1:A:145:VAL:HG22	1.99	0.43
1:A:226:ALA:HB2	1:A:251:LEU:HG	2.00	0.43
1:B:5:LYS:HE2	1:B:46:GLU:OE2	2.18	0.43
1:I:138:GLN:NE2	1:I:145:VAL:O	2.51	0.43
1:I:178:ALA:HB2	1:I:194:LEU:HD21	2.01	0.43
1:I:278:ILE:HG23	1:I:279:PRO:HD2	2.00	0.43
1:O:274:VAL:O	1:O:292:VAL:HA	2.19	0.43
1:Q:93:PRO:HB2	1:Q:94:TYR:HD1	1.84	0.43
1:A:99:LYS:HG2	1:A:101:ASP:N	2.32	0.43
1:D:282:ASP:OD1	1:D:285:LYS:HE2	2.18	0.43
1:G:96:ARG:NH1	1:G:225:MET:HE2	2.34	0.43
1:H:208:MET:HE1	1:H:234:HIS:HB3	1.99	0.43
1:I:195:ILE:HD13	1:I:235:ALA:HB1	2.01	0.43
1:J:236:ALA:HB2	1:J:269:PHE:CE1	2.54	0.43
1:P:281:GLU:CD	1:P:281:GLU:H	2.22	0.43
1:Q:151:GLU:HB3	1:Q:152:PRO:HD3	2.01	0.43
1:B:281:GLU:HA	1:B:284:MET:CE	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:ASP:O	1:B:297:MET:HE2	2.19	0.43
1:H:252:THR:HG22	1:H:253:HIS:CE1	2.54	0.43
1:C:249:ALA:HB2	1:C:269:PHE:CE1	2.54	0.42
1:D:99:LYS:HD3	1:D:107:ARG:HB2	2.01	0.42
1:D:249:ALA:HB2	1:D:269:PHE:CE1	2.54	0.42
1:E:155:LEU:HD21	1:E:184:ILE:HG23	2.00	0.42
1:G:69:GLU:O	1:G:73:MET:HB2	2.19	0.42
1:K:301:GLU:OE1	1:K:314:TYR:OH	2.27	0.42
1:M:63:ILE:HD13	1:M:94:TYR:CE2	2.54	0.42
1:O:276:ASN:OD1	1:O:295:ILE:HG13	2.19	0.42
1:P:223:ASP:O	1:P:251:LEU:HA	2.19	0.42
1:B:148:LEU:HD11	1:B:302:ALA:CB	2.49	0.42
1:B:170:ILE:HD12	1:B:185:ALA:HA	2.01	0.42
1:B:184:ILE:HD12	1:B:222:VAL:HG21	2.00	0.42
1:C:272:VAL:O	1:C:290:ILE:HA	2.20	0.42
1:F:103:VAL:O	1:F:103:VAL:CG2	2.67	0.42
1:F:229:CYS:H	2:F:1001:HSX:C2	2.32	0.42
1:G:155:LEU:HD23	1:G:155:LEU:HA	1.88	0.42
1:H:234:HIS:O	1:H:237:ASP:OD1	2.37	0.42
1:O:278:ILE:HG23	1:O:279:PRO:HD2	2.01	0.42
1:P:313:SER:O	1:P:315:LEU:HD22	2.19	0.42
1:R:115:VAL:HA	1:R:118:MET:CE	2.49	0.42
1:C:138:GLN:OE1	1:D:106:SER:OG	2.37	0.42
1:H:252:THR:CG2	1:H:253:HIS:CE1	3.02	0.42
1:K:222:VAL:HA	1:K:250:ILE:O	2.20	0.42
1:L:287:CYS:HB3	1:L:290:ILE:HD12	2.01	0.42
1:Q:103:VAL:HG21	1:R:187:ARG:NH2	2.35	0.42
1:R:95:ALA:HB1	1:R:133:HIS:HB3	2.01	0.42
1:R:275:THR:OG1	1:R:277:THR:HG23	2.19	0.42
1:C:240:LEU:HD23	1:C:240:LEU:HA	1.85	0.42
1:D:319:VAL:O	1:D:319:VAL:HG12	2.18	0.42
1:K:295:ILE:HG22	1:K:298:ILE:HD12	2.02	0.42
1:N:54:TYR:CD2	1:N:303:ILE:HG23	2.53	0.42
1:R:114:LEU:HD12	1:R:114:LEU:HA	1.81	0.42
1:C:167:ASN:O	1:C:168:CYS:CB	2.64	0.42
1:E:102:LYS:C	1:E:104:GLY:N	2.71	0.42
1:K:5:LYS:HE2	1:K:46:GLU:OE2	2.19	0.42
1:L:164:GLU:OE2	1:L:246:ARG:NH1	2.53	0.42
1:O:249:ALA:HB2	1:O:269:PHE:CE1	2.55	0.42
1:Q:171:VAL:HA	1:Q:193:ALA:O	2.18	0.42
1:Q:173:PRO:HG3	1:Q:221:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:NH1	1:R:310:GLU:OE2	2.53	0.42
1:D:79:ILE:HD13	1:D:79:ILE:HG21	1.86	0.42
1:E:139:GLY:O	1:F:113:LYS:HD2	2.19	0.42
1:F:115:VAL:HA	1:F:118:MET:CE	2.50	0.42
1:F:155:LEU:HD22	1:F:188:LEU:HD21	2.02	0.42
1:G:225:MET:HE2	1:G:255:ILE:CD1	2.45	0.42
1:J:190:VAL:CG1	1:J:191:ASP:N	2.83	0.42
1:M:210:LEU:HD23	1:M:211:VAL:N	2.34	0.42
1:R:27:LEU:HD12	1:R:27:LEU:N	2.35	0.42
1:B:30:VAL:HG21	1:B:73:MET:HE2	2.02	0.42
1:E:100:LYS:O	1:E:101:ASP:C	2.57	0.42
1:E:272:VAL:O	1:E:290:ILE:HA	2.18	0.42
1:M:256:PHE:HB2	1:M:283:LYS:HD3	2.02	0.42
1:N:183:SER:O	1:N:187:ARG:HG3	2.19	0.42
1:N:240:LEU:HD23	1:N:240:LEU:HA	1.71	0.42
1:N:256:PHE:HB2	1:N:283:LYS:HE2	2.01	0.42
1:C:315:LEU:HD12	1:C:315:LEU:HA	1.85	0.42
1:D:131:ASP:OD2	1:D:252:THR:HG21	2.20	0.42
1:E:164:GLU:OE1	1:E:164:GLU:N	2.42	0.42
1:G:63:ILE:HD13	1:L:39:GLU:HG3	2.01	0.42
1:H:54:TYR:CE2	1:H:303:ILE:HG23	2.54	0.42
1:H:107:ARG:NH2	1:I:43:GLU:OE2	2.53	0.42
1:K:240:LEU:HD23	1:K:240:LEU:HA	1.84	0.42
1:L:157:TRP:CE2	1:L:273:VAL:HG11	2.55	0.42
1:M:240:LEU:HA	1:M:240:LEU:HD23	1.67	0.42
1:N:181:VAL:HG12	1:N:222:VAL:CG2	2.50	0.42
1:O:4:ILE:HD13	1:O:4:ILE:HG21	1.65	0.42
1:C:34:LYS:HE3	1:C:38:GLN:HA	2.01	0.42
1:D:314:TYR:CD1	1:D:314:TYR:C	2.93	0.42
1:I:104:GLY:O	1:J:148:LEU:HA	2.20	0.42
1:O:105:GLU:O	1:P:149:TYR:CE2	2.72	0.42
1:O:127:ILE:HB	1:O:145:VAL:HG13	2.01	0.42
1:O:155:LEU:HD23	1:O:155:LEU:HA	1.87	0.42
1:R:240:LEU:HD23	1:R:240:LEU:HA	1.65	0.42
1:C:274:VAL:O	1:C:292:VAL:HA	2.20	0.42
1:G:96:ARG:NH1	1:G:225:MET:CE	2.83	0.42
1:G:240:LEU:HD23	1:G:240:LEU:HA	1.67	0.42
1:H:100:LYS:O	1:H:107:ARG:NH1	2.53	0.42
1:J:131:ASP:HB3	1:J:180:ARG:HH22	1.85	0.42
1:L:158:ILE:HG21	1:L:158:ILE:HD13	1.80	0.42
1:L:276:ASN:OD1	1:L:295:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:13:GLN:O	1:M:13:GLN:CG	2.68	0.42
1:O:190:VAL:HG12	1:O:191:ASP:H	1.85	0.42
1:Q:249:ALA:HB3	1:Q:272:VAL:HG22	2.02	0.42
1:B:37:ASN:O	1:C:63:ILE:HD11	2.19	0.41
1:C:301:GLU:OE1	1:C:301:GLU:HA	2.20	0.41
1:D:305:ARG:HB2	1:D:314:TYR:CE1	2.55	0.41
1:E:155:LEU:HD23	1:E:155:LEU:HA	1.84	0.41
1:O:275:THR:OG1	1:O:277:THR:HG23	2.19	0.41
1:R:227:ASP:HA	1:R:255:ILE:HB	2.02	0.41
1:E:34:LYS:HZ1	1:E:38:GLN:HG3	1.85	0.41
1:E:115:VAL:HA	1:E:118:MET:CE	2.50	0.41
1:J:188:LEU:HD23	1:J:188:LEU:HA	1.86	0.41
1:K:225:MET:SD	1:K:255:ILE:HD12	2.60	0.41
1:O:117:ASN:O	1:O:121:VAL:HG22	2.20	0.41
1:Q:9:GLY:HA3	1:Q:57:GLN:OE1	2.20	0.41
1:A:305:ARG:NH2	1:A:316:PHE:CE1	2.88	0.41
1:C:32:THR:HG21	1:C:69:GLU:CD	2.41	0.41
1:C:103:VAL:O	1:C:104:GLY:C	2.55	0.41
1:D:3:ASN:OD1	1:D:3:ASN:N	2.53	0.41
1:D:181:VAL:HG12	1:D:222:VAL:HB	2.02	0.41
1:E:6:ILE:HG22	1:E:27:LEU:HD23	2.01	0.41
1:F:35:PHE:CE2	1:F:41:CYS:HB2	2.55	0.41
1:F:315:LEU:O	1:F:316:PHE:C	2.57	0.41
1:G:232:ILE:HG13	1:G:233:CYS:N	2.35	0.41
1:J:276:ASN:OD1	1:J:295:ILE:HG13	2.20	0.41
1:K:5:LYS:HZ3	1:K:46:GLU:HG2	1.85	0.41
1:N:159:ARG:HG2	1:N:165:TRP:CE2	2.56	0.41
1:O:57:GLN:HE21	1:O:57:GLN:HB2	1.48	0.41
1:O:184:ILE:HD13	1:O:184:ILE:HG21	1.83	0.41
1:E:149:TYR:OH	1:F:106:SER:HB3	2.20	0.41
1:E:215:LYS:HE3	1:E:216:ASP:OD2	2.20	0.41
1:O:230:GLY:CA	2:O:1001:HSX:O2X	2.68	0.41
1:R:195:ILE:HD13	1:R:235:ALA:HB1	2.03	0.41
1:A:240:LEU:HD23	1:A:240:LEU:HA	1.66	0.41
1:E:12:HIS:CE1	1:E:276:ASN:O	2.70	0.41
1:G:97:GLN:OE1	1:G:99:LYS:HG3	2.21	0.41
1:G:195:ILE:HG13	1:G:210:LEU:HD12	2.02	0.41
1:H:267:ALA:O	1:H:289:LYS:NZ	2.54	0.41
1:J:99:LYS:HE2	1:J:107:ARG:N	2.35	0.41
1:L:5:LYS:NZ	1:L:46:GLU:OE2	2.41	0.41
1:L:141:PHE:CD1	1:L:145:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:208:MET:O	1:N:238:LYS:HE3	2.20	0.41
1:O:264:ILE:HD13	1:O:264:ILE:HG21	1.82	0.41
1:P:159:ARG:HG2	1:P:165:TRP:CZ2	2.55	0.41
1:B:171:VAL:O	1:B:221:LEU:HA	2.20	0.41
1:C:96:ARG:HG2	1:C:96:ARG:NH1	2.34	0.41
1:I:6:ILE:HD11	1:I:20:ALA:HB2	2.03	0.41
1:M:57:GLN:O	1:M:89:ILE:HA	2.19	0.41
1:O:42:VAL:HG11	1:O:73:MET:HG2	2.02	0.41
1:O:99:LYS:O	1:O:99:LYS:HG2	2.20	0.41
1:O:228:THR:OG1	2:O:1001:HSX:O4	2.39	0.41
1:B:214:VAL:CG1	1:B:244:ALA:HB2	2.50	0.41
1:E:225:MET:C	1:E:251:LEU:HD22	2.40	0.41
1:F:227:ASP:HB3	1:F:228:THR:H	1.64	0.41
1:G:131:ASP:OD2	1:G:252:THR:HG21	2.19	0.41
1:H:2:PRO:O	1:H:307:HIS:NE2	2.36	0.41
1:J:172:SER:HA	1:J:173:PRO:HD3	1.95	0.41
1:K:215:LYS:O	1:K:215:LYS:CG	2.69	0.41
1:L:117:ASN:O	1:L:121:VAL:HG22	2.21	0.41
1:M:176:GLY:HA2	1:N:179:LYS:HG2	2.02	0.41
1:P:6:ILE:HD11	1:P:23:LEU:CD1	2.48	0.41
1:P:275:THR:OG1	1:P:277:THR:HG23	2.21	0.41
1:Q:138:GLN:NE2	1:Q:147:ASN:HB3	2.34	0.41
1:R:195:ILE:HG13	1:R:210:LEU:HD12	2.03	0.41
1:B:4:ILE:HG21	1:G:310:GLU:O	2.15	0.41
1:C:190:VAL:CG1	1:C:191:ASP:H	2.33	0.41
1:E:23:LEU:HB2	1:E:25:LEU:HD12	2.03	0.41
1:K:32:THR:HG21	1:K:69:GLU:CD	2.41	0.41
1:K:274:VAL:O	1:K:292:VAL:HA	2.20	0.41
1:L:96:ARG:NH1	1:L:225:MET:SD	2.94	0.41
1:L:297:MET:HE2	1:L:301:GLU:OE1	2.21	0.41
1:M:113:LYS:HE2	1:M:117:ASN:OD1	2.21	0.41
1:P:184:ILE:CD1	1:P:222:VAL:HG11	2.51	0.41
1:P:261:ILE:HG23	1:P:287:CYS:HB2	2.02	0.41
1:R:267:ALA:O	1:R:289:LYS:NZ	2.54	0.41
1:A:99:LYS:HG3	1:A:107:ARG:HB2	2.03	0.41
1:B:275:THR:HG23	1:B:295:ILE:HG23	2.03	0.41
1:B:276:ASN:OD1	1:B:295:ILE:HG13	2.21	0.41
1:B:304:ARG:HE	1:G:304:ARG:HD2	1.86	0.41
1:D:5:LYS:HE3	1:D:51:GLU:OE2	2.21	0.41
1:D:126:HIS:N	1:D:143:ILE:HD12	2.36	0.41
1:G:96:ARG:HH12	1:G:225:MET:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:156:LYS:O	1:G:160:GLU:HG2	2.21	0.41
1:G:168:CYS:O	1:G:190:VAL:HG12	2.20	0.41
1:G:226:ALA:HB1	1:G:229:CYS:SG	2.60	0.41
1:J:157:TRP:CH2	1:J:273:VAL:HG21	2.56	0.41
1:J:197:LYS:O	1:J:198:GLU:HB2	2.21	0.41
1:K:190:VAL:CG1	1:K:191:ASP:N	2.84	0.41
1:L:155:LEU:HD23	1:L:155:LEU:HA	1.90	0.41
1:M:148:LEU:HD13	1:M:298:ILE:HG22	2.02	0.41
1:N:18:LYS:HB2	1:N:18:LYS:HE2	1.83	0.41
1:N:60:CYS:HB3	1:N:278:ILE:HG12	2.02	0.41
1:N:93:PRO:HB2	1:N:94:TYR:HD1	1.86	0.41
1:N:311:SER:O	1:N:312:VAL:HB	2.20	0.41
1:P:208:MET:HB2	1:P:208:MET:HE3	1.57	0.41
1:A:4:ILE:HG23	1:R:311:SER:HB2	2.02	0.41
1:C:78:LYS:NZ	1:C:125:ASP:OD1	2.46	0.41
1:D:210:LEU:HD23	1:D:211:VAL:N	2.36	0.41
1:F:280:GLN:O	1:F:284:MET:HG3	2.21	0.41
1:H:252:THR:HG22	1:H:253:HIS:CD2	2.56	0.41
1:M:167:ASN:O	1:M:217:ARG:HG2	2.21	0.41
1:A:100:LYS:HB3	1:A:107:ARG:NH2	2.36	0.40
1:A:151:GLU:HB3	1:A:152:PRO:HD3	2.03	0.40
1:B:37:ASN:HD21	1:B:39:GLU:CD	2.23	0.40
1:B:178:ALA:O	1:B:181:VAL:HG22	2.21	0.40
1:G:170:ILE:HG22	1:G:181:VAL:HG13	2.03	0.40
1:J:99:LYS:HE2	1:J:107:ARG:H	1.85	0.40
1:K:4:ILE:HG21	1:K:4:ILE:HD13	1.88	0.40
1:L:158:ILE:CG2	1:L:159:ARG:N	2.84	0.40
1:M:12:HIS:HD2	1:M:279:PRO:N	2.19	0.40
1:N:153:ALA:HB1	1:N:293:ILE:HG21	2.03	0.40
1:N:228:THR:HG23	1:N:259:PRO:HD2	2.03	0.40
1:B:215:LYS:HD2	1:B:243:GLY:HA3	2.03	0.40
1:D:4:ILE:HG22	1:I:310:GLU:O	2.20	0.40
1:D:10:SER:OG	1:D:32:THR:CG2	2.69	0.40
1:F:93:PRO:O	1:F:94:TYR:HB2	2.21	0.40
1:G:267:ALA:O	1:G:289:LYS:NZ	2.54	0.40
1:I:159:ARG:HG2	1:I:165:TRP:CZ2	2.56	0.40
1:M:22:ARG:HE	1:M:296:SER:HB2	1.86	0.40
1:N:226:ALA:HB2	1:N:251:LEU:HG	2.03	0.40
1:Q:58:SER:HA	1:Q:90:PRO:HD2	2.03	0.40
1:C:52:ASP:OD1	1:C:84:ARG:HB3	2.21	0.40
1:E:4:ILE:O	1:E:4:ILE:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:LYS:O	1:F:100:LYS:C	2.60	0.40
1:G:8:SER:HB2	1:G:16:SER:HB3	2.03	0.40
1:H:173:PRO:HB2	1:H:231:THR:HG22	2.03	0.40
1:J:240:LEU:HD23	1:J:240:LEU:HA	1.62	0.40
1:R:148:LEU:HD22	1:R:316:PHE:CZ	2.56	0.40
1:A:32:THR:HG21	1:A:73:MET:HE1	2.03	0.40
1:A:226:ALA:HB1	1:A:229:CYS:SG	2.62	0.40
1:D:8:SER:HB2	1:D:16:SER:HB3	2.03	0.40
1:D:110:ILE:H	1:D:110:ILE:HG13	1.70	0.40
1:G:4:ILE:HG21	1:G:4:ILE:HD13	1.79	0.40
1:G:57:GLN:O	1:G:89:ILE:HA	2.21	0.40
1:G:194:LEU:HD12	1:G:194:LEU:O	2.22	0.40
1:P:249:ALA:HB3	1:P:272:VAL:HG22	2.02	0.40
1:C:214:VAL:HG21	1:C:242:ALA:CB	2.49	0.40
1:D:4:ILE:HD13	1:D:4:ILE:HG21	1.93	0.40
1:E:240:LEU:HD23	1:E:240:LEU:HA	1.75	0.40
1:E:314:TYR:C	1:E:314:TYR:CD1	2.95	0.40
1:H:79:ILE:O	1:H:79:ILE:CG2	2.69	0.40
1:I:129:THR:CG2	1:I:130:MET:N	2.84	0.40
1:J:236:ALA:HB2	1:J:269:PHE:CZ	2.56	0.40
1:K:236:ALA:HB2	1:K:269:PHE:CE1	2.56	0.40
1:M:117:ASN:HB3	1:R:121:VAL:CG1	2.52	0.40
1:P:248:TYR:CZ	1:P:270:GLU:HG2	2.57	0.40
1:Q:57:GLN:HG2	1:Q:70:LEU:HB2	2.02	0.40
1:Q:175:ALA:O	1:Q:177:GLY:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/321 (96%)	296 (96%)	12 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	308/321 (96%)	289 (94%)	15 (5%)	4 (1%)	10	36
1	C	305/321 (95%)	290 (95%)	15 (5%)	0	100	100
1	D	306/321 (95%)	289 (94%)	17 (6%)	0	100	100
1	E	308/321 (96%)	290 (94%)	16 (5%)	2 (1%)	22	53
1	F	308/321 (96%)	299 (97%)	8 (3%)	1 (0%)	37	68
1	G	307/321 (96%)	292 (95%)	14 (5%)	1 (0%)	37	68
1	H	297/321 (92%)	285 (96%)	12 (4%)	0	100	100
1	I	309/321 (96%)	297 (96%)	12 (4%)	0	100	100
1	J	297/321 (92%)	285 (96%)	12 (4%)	0	100	100
1	K	307/321 (96%)	292 (95%)	15 (5%)	0	100	100
1	L	294/321 (92%)	282 (96%)	12 (4%)	0	100	100
1	M	294/321 (92%)	278 (95%)	15 (5%)	1 (0%)	37	68
1	N	306/321 (95%)	291 (95%)	15 (5%)	0	100	100
1	O	294/321 (92%)	278 (95%)	16 (5%)	0	100	100
1	P	309/321 (96%)	298 (96%)	10 (3%)	1 (0%)	37	68
1	Q	296/321 (92%)	285 (96%)	11 (4%)	0	100	100
1	R	309/321 (96%)	300 (97%)	9 (3%)	0	100	100
All	All	5462/5778 (94%)	5216 (96%)	236 (4%)	10 (0%)	44	74

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	LYS
1	B	101	ASP
1	B	102	LYS
1	B	103	VAL
1	E	100	LYS
1	E	103	VAL
1	P	3	ASN
1	G	99	LYS
1	M	216	ASP
1	F	101	ASP

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	264/272 (97%)	253 (96%)	11 (4%)	25	56
1	B	264/272 (97%)	246 (93%)	18 (7%)	13	40
1	C	261/272 (96%)	244 (94%)	17 (6%)	14	41
1	D	262/272 (96%)	252 (96%)	10 (4%)	28	59
1	E	264/272 (97%)	249 (94%)	15 (6%)	17	46
1	F	264/272 (97%)	253 (96%)	11 (4%)	25	56
1	G	263/272 (97%)	248 (94%)	15 (6%)	17	46
1	H	253/272 (93%)	242 (96%)	11 (4%)	25	55
1	I	265/272 (97%)	248 (94%)	17 (6%)	14	42
1	J	254/272 (93%)	247 (97%)	7 (3%)	38	66
1	K	263/272 (97%)	253 (96%)	10 (4%)	28	59
1	L	251/272 (92%)	244 (97%)	7 (3%)	38	66
1	M	251/272 (92%)	241 (96%)	10 (4%)	27	58
1	N	262/272 (96%)	254 (97%)	8 (3%)	35	63
1	O	251/272 (92%)	244 (97%)	7 (3%)	38	66
1	P	265/272 (97%)	256 (97%)	9 (3%)	32	62
1	Q	252/272 (93%)	245 (97%)	7 (3%)	38	66
1	R	265/272 (97%)	248 (94%)	17 (6%)	14	42
All	All	4674/4896 (96%)	4467 (96%)	207 (4%)	24	54

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	49	ARG
1	A	62	GLU
1	A	73	MET
1	A	75	ASN
1	A	96	ARG

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Mol	Chain	Res	Type
1	A	113	LYS
1	A	156	LYS
1	A	297	MET
1	A	316	PHE
1	A	321	LEU
1	B	12	HIS
1	B	18	LYS
1	B	75	ASN
1	B	96	ARG
1	B	98	ASP
1	B	99	LYS
1	B	101	ASP
1	B	102	LYS
1	B	103	VAL
1	B	163	SER
1	B	198	GLU
1	B	292	VAL
1	B	293	ILE
1	B	295	ILE
1	B	297	MET
1	B	304	ARG
1	B	313	SER
1	B	318	HIS
1	C	3	ASN
1	C	49	ARG
1	C	62	GLU
1	C	63	ILE
1	C	83	SER
1	C	96	ARG
1	C	100	LYS
1	C	166	ARG
1	C	168	CYS
1	C	187	ARG
1	C	194	LEU
1	C	262	SER
1	C	286	HIS
1	C	297	MET
1	C	311	SER
1	C	315	LEU
1	C	316	PHE
1	D	96	ARG
1	D	97	GLN

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Mol	Chain	Res	Type
1	D	100	LYS
1	D	101	ASP
1	D	208	MET
1	D	297	MET
1	D	315	LEU
1	D	318	HIS
1	D	320	PRO
1	D	321	LEU
1	E	1	SER
1	E	3	ASN
1	E	4	ILE
1	E	11	SER
1	E	32	THR
1	E	49	ARG
1	E	102	LYS
1	E	163	SER
1	E	169	THR
1	E	228	THR
1	E	297	MET
1	E	310	GLU
1	E	313	SER
1	E	315	LEU
1	E	318	HIS
1	F	6	ILE
1	F	10	SER
1	F	75	ASN
1	F	103	VAL
1	F	194	LEU
1	F	210	LEU
1	F	251	LEU
1	F	296	SER
1	F	297	MET
1	F	310	GLU
1	F	318	HIS
1	G	3	ASN
1	G	4	ILE
1	G	6	ILE
1	G	29	LYS
1	G	98	ASP
1	G	102	LYS
1	G	148	LEU
1	G	156	LYS

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Mol	Chain	Res	Type
1	G	169	THR
1	G	297	MET
1	G	312	VAL
1	G	315	LEU
1	G	316	PHE
1	G	318	HIS
1	G	320	PRO
1	H	6	ILE
1	H	10	SER
1	H	11	SER
1	H	79	ILE
1	H	100	LYS
1	H	103	VAL
1	H	217	ARG
1	H	252	THR
1	H	296	SER
1	H	305	ARG
1	H	308	ASN
1	I	4	ILE
1	I	10	SER
1	I	11	SER
1	I	12	HIS
1	I	13	GLN
1	I	14	ASP
1	I	98	ASP
1	I	99	LYS
1	I	100	LYS
1	I	103	VAL
1	I	187	ARG
1	I	207	ARG
1	I	208	MET
1	I	210	LEU
1	I	297	MET
1	I	318	HIS
1	I	321	LEU
1	J	57	GLN
1	J	75	ASN
1	J	101	ASP
1	J	102	LYS
1	J	297	MET
1	J	304[A]	ARG
1	J	304[B]	ARG

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Mol	Chain	Res	Type
1	K	12	HIS
1	K	63	ILE
1	K	98	ASP
1	K	103	VAL
1	K	167	ASN
1	K	194	LEU
1	K	215	LYS
1	K	217	ARG
1	K	297	MET
1	K	321	LEU
1	L	75	ASN
1	L	78	LYS
1	L	83	SER
1	L	101	ASP
1	L	180	ARG
1	L	194	LEU
1	L	238	LYS
1	M	11	SER
1	M	57	GLN
1	M	75	ASN
1	M	99	LYS
1	M	103	VAL
1	M	155	LEU
1	M	162	ILE
1	M	163	SER
1	M	192	PHE
1	M	217	ARG
1	N	10	SER
1	N	62	GLU
1	N	67	LEU
1	N	101	ASP
1	N	102	LYS
1	N	103	VAL
1	N	319	VAL
1	N	321	LEU
1	O	11	SER
1	O	57	GLN
1	O	79	ILE
1	O	100	LYS
1	O	101	ASP
1	O	189	ASN
1	O	297	MET

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Mol	Chain	Res	Type
1	P	2	PRO
1	P	4	ILE
1	P	96	ARG
1	P	100	LYS
1	P	102	LYS
1	P	103	VAL
1	P	297	MET
1	P	305	ARG
1	P	310	GLU
1	Q	2	PRO
1	Q	49	ARG
1	Q	73	MET
1	Q	99	LYS
1	Q	111	SER
1	Q	113	LYS
1	Q	305	ARG
1	R	12	HIS
1	R	57	GLN
1	R	96	ARG
1	R	98	ASP
1	R	102	LYS
1	R	103	VAL
1	R	107	ARG
1	R	191	ASP
1	R	207	ARG
1	R	217	ARG
1	R	241	SER
1	R	292	VAL
1	R	296	SER
1	R	304	ARG
1	R	312	VAL
1	R	313	SER
1	R	315	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	75	ASN
1	A	97	GLN
1	B	3	ASN
1	C	3	ASN

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Mol	Chain	Res	Type
1	C	12	HIS
1	D	12	HIS
1	D	75	ASN
1	E	12	HIS
1	F	12	HIS
1	G	3	ASN
1	G	12	HIS
1	H	12	HIS
1	H	57	GLN
1	L	12	HIS
1	M	12	HIS
1	M	57	GLN
1	N	12	HIS
1	O	57	GLN
1	O	97	GLN
1	Q	12	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HSX	O	1001	-	14,14,14	0.77	0	20,21,21	0.94	0
2	HSX	F	1001	-	14,14,14	2.25	5 (35%)	20,21,21	1.79	7 (35%)
2	HSX	B	1001	-	14,14,14	1.03	0	20,21,21	1.49	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HSX	O	1001	-	-	6/6/22/22	0/1/1/1
2	HSX	F	1001	-	-	0/6/22/22	0/1/1/1
2	HSX	B	1001	-	-	3/6/22/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1001	HSX	O3-C3	4.23	1.52	1.43
2	F	1001	HSX	O4-C1	4.12	1.48	1.43
2	F	1001	HSX	O1-C1	2.58	1.47	1.39
2	F	1001	HSX	C3-C4	2.57	1.59	1.53
2	F	1001	HSX	C1-C2	2.12	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1001	HSX	O4-C1-C2	-3.98	99.57	104.46
2	B	1001	HSX	O5-P'-O1X	-3.69	96.13	106.47
2	F	1001	HSX	O1-C1-O4	3.16	115.18	111.13
2	F	1001	HSX	O3-C3-C4	2.62	118.62	111.05
2	B	1001	HSX	P'-O5-C5	-2.54	111.30	118.30
2	F	1001	HSX	C1-C2-C3	2.41	105.31	102.30
2	F	1001	HSX	O3X-P'-O1X	2.35	119.87	110.68
2	F	1001	HSX	O4-C4-C5	2.18	116.55	109.37
2	F	1001	HSX	P'-O5-C5	2.06	123.98	118.30

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1001	HSX	C3-C4-C5-O5
2	O	1001	HSX	C5-O5-P'-O3X
2	O	1001	HSX	C3-C4-C5-O5
2	B	1001	HSX	O4-C4-C5-O5
2	O	1001	HSX	O4-C4-C5-O5
2	O	1001	HSX	C5-O5-P'-O1X
2	B	1001	HSX	C4-C5-O5-P'
2	O	1001	HSX	C4-C5-O5-P'
2	O	1001	HSX	C5-O5-P'-O2X

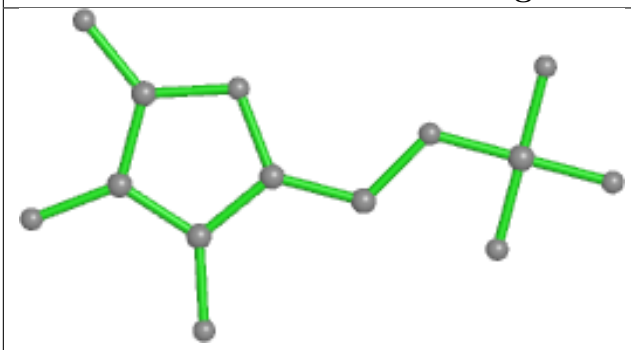
There are no ring outliers.

3 monomers are involved in 7 short contacts:

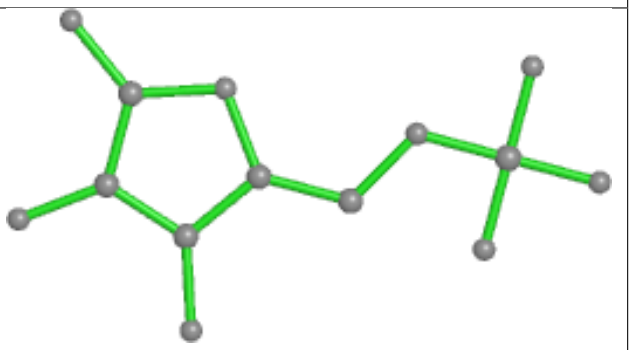
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1001	HSX	4	0
2	F	1001	HSX	2	0
2	B	1001	HSX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

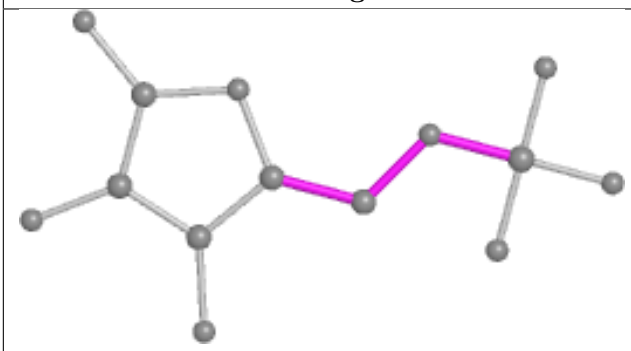
Ligand HSX O 1001



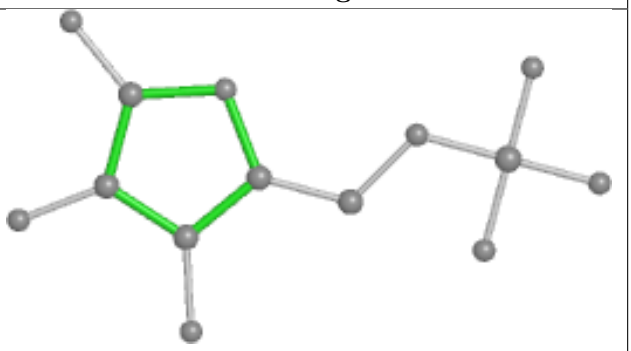
Bond lengths



Bond angles

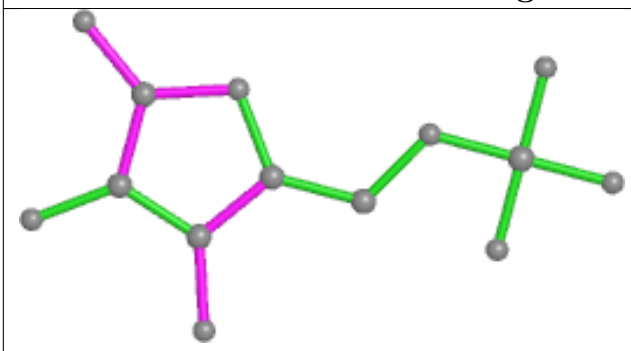


Torsions

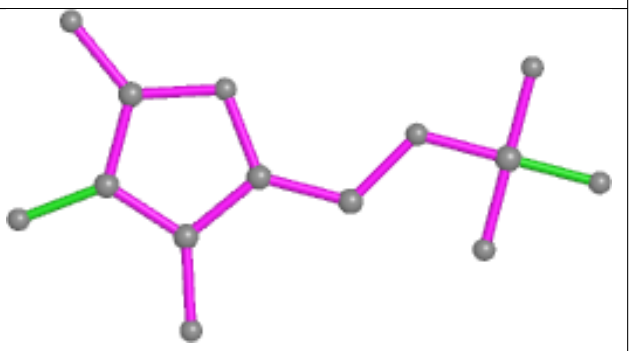


Rings

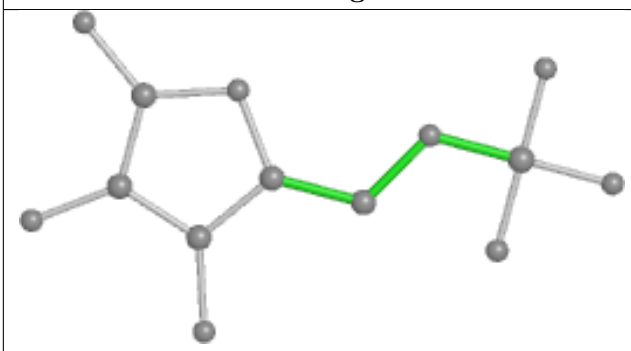
Ligand HSX F 1001



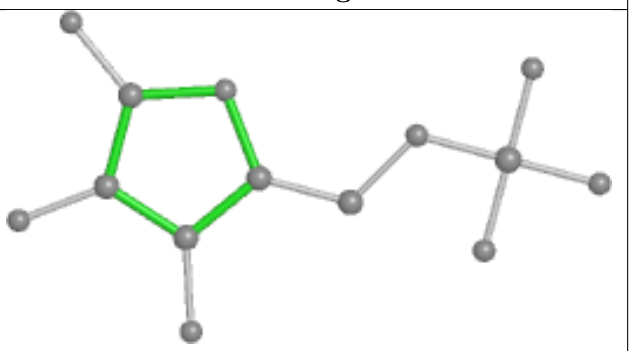
Bond lengths



Bond angles

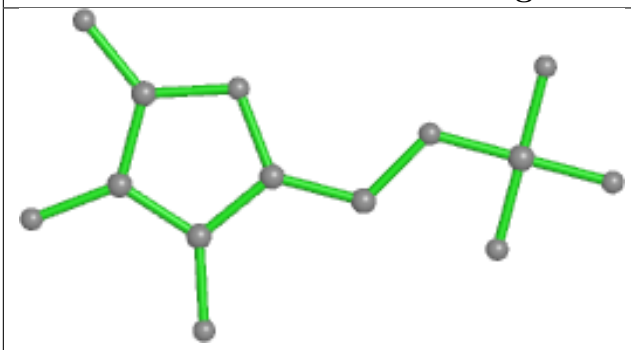


Torsions

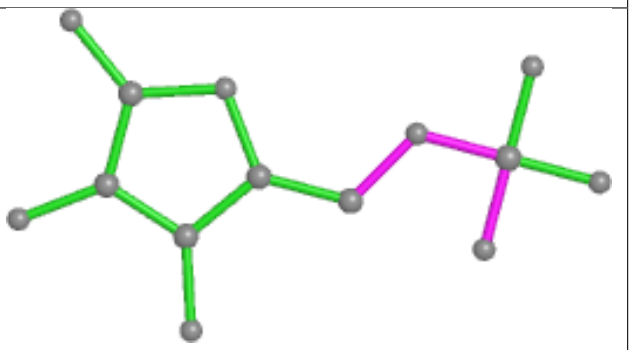


Rings

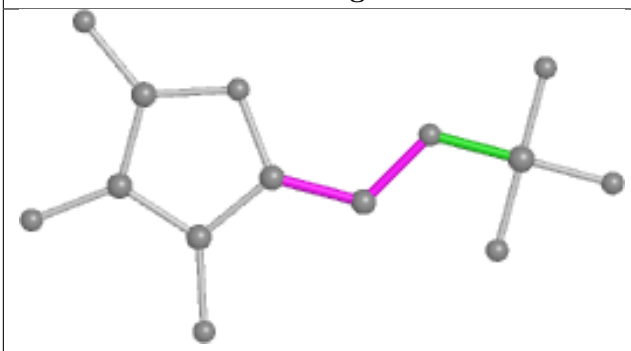
Ligand HSX B 1001



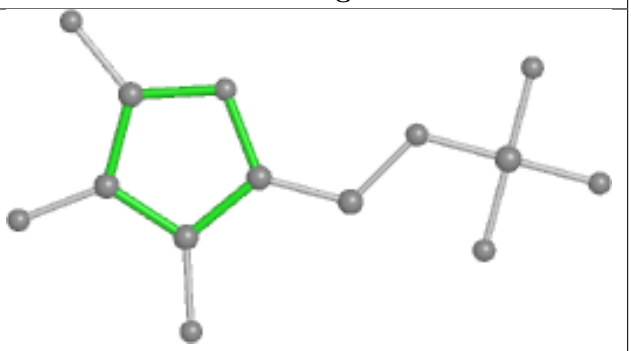
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	312/321 (97%)	-1.65	0	100	100	30, 49, 75, 115	0
1	B	312/321 (97%)	-1.61	0	100	100	34, 54, 78, 111	0
1	C	309/321 (96%)	-1.64	0	100	100	33, 55, 78, 110	0
1	D	310/321 (96%)	-1.64	0	100	100	30, 56, 78, 113	0
1	E	312/321 (97%)	-1.61	0	100	100	35, 55, 81, 102	0
1	F	312/321 (97%)	-1.64	0	100	100	31, 49, 74, 113	0
1	G	311/321 (96%)	-1.63	0	100	100	30, 52, 75, 103	0
1	H	301/321 (93%)	-1.66	0	100	100	33, 50, 69, 111	0
1	I	313/321 (97%)	-1.57	0	100	100	30, 58, 88, 109	0
1	J	300/321 (93%)	-1.59	0	100	100	33, 56, 85, 110	1 (0%)
1	K	311/321 (96%)	-1.64	0	100	100	34, 52, 74, 107	0
1	L	298/321 (92%)	-1.59	0	100	100	30, 61, 84, 107	0
1	M	298/321 (92%)	-1.59	0	100	100	31, 55, 88, 108	0
1	N	310/321 (96%)	-1.59	0	100	100	30, 59, 85, 124	0
1	O	298/321 (92%)	-1.66	0	100	100	32, 51, 71, 100	0
1	P	313/321 (97%)	-1.60	0	100	100	34, 52, 76, 115	0
1	Q	300/321 (93%)	-1.56	0	100	100	38, 63, 86, 109	0
1	R	313/321 (97%)	-1.60	0	100	100	34, 52, 77, 116	0
All	All	5533/5778 (95%)	-1.61	0	100	100	30, 54, 81, 124	1 (0%)

There are no RSRZ outliers to report.

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

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)

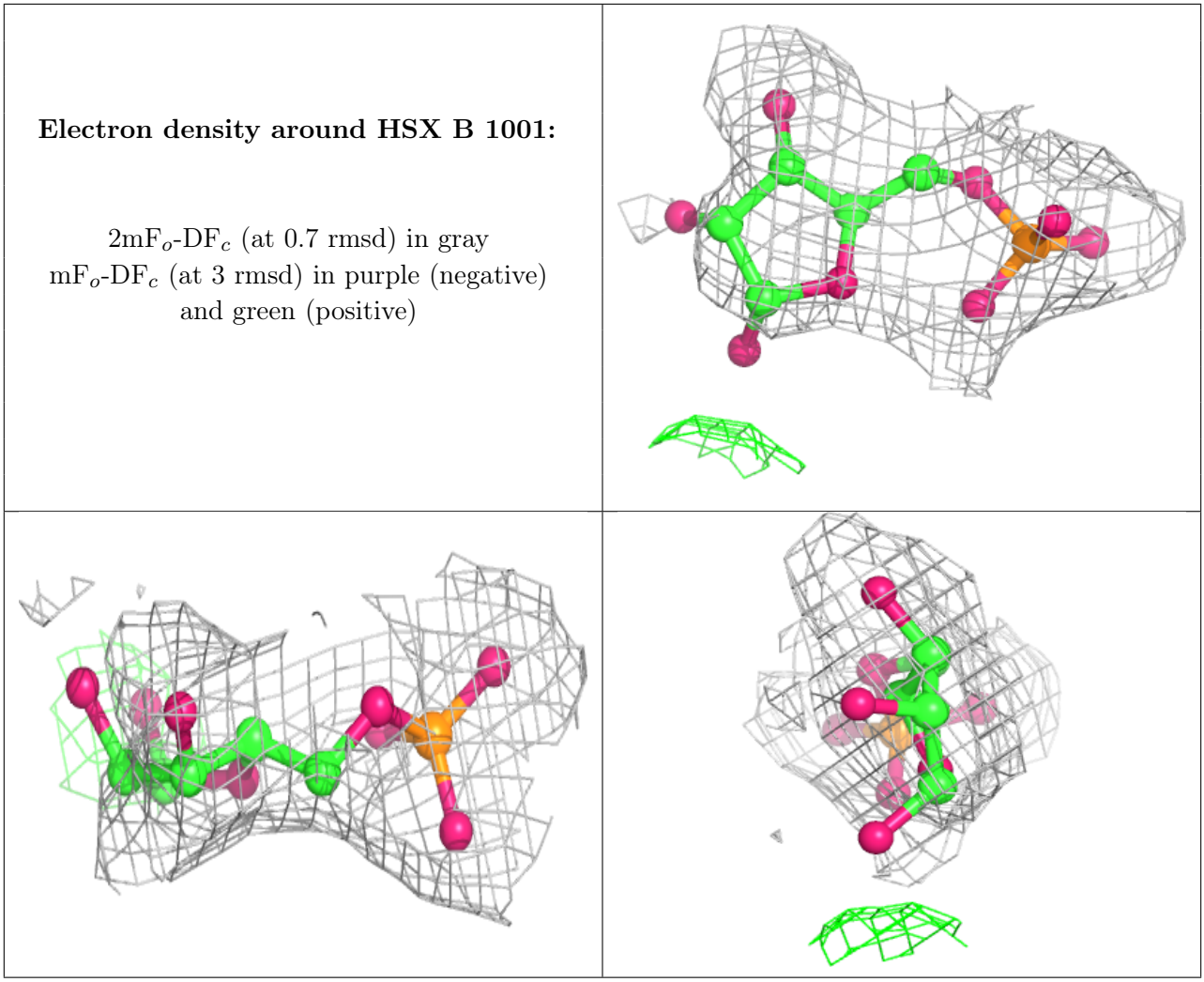
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	HSX	B	1001	14/14	0.95	0.05	83,105,119,136	0
2	HSX	F	1001	14/14	0.98	0.05	76,93,120,129	0
2	HSX	O	1001	14/14	0.98	0.04	78,97,121,144	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

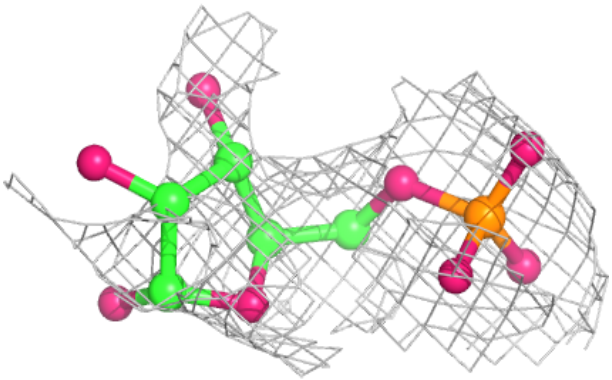
Electron density around HSX B 1001:

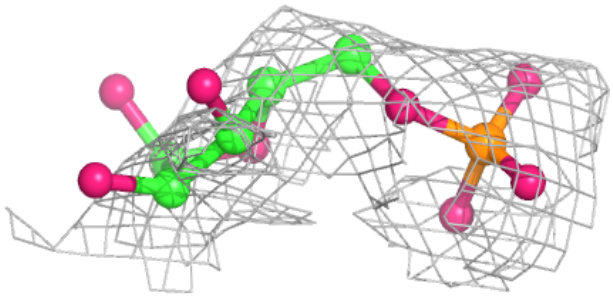
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

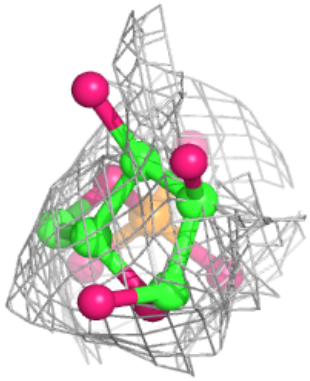


Electron density around HSX F 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

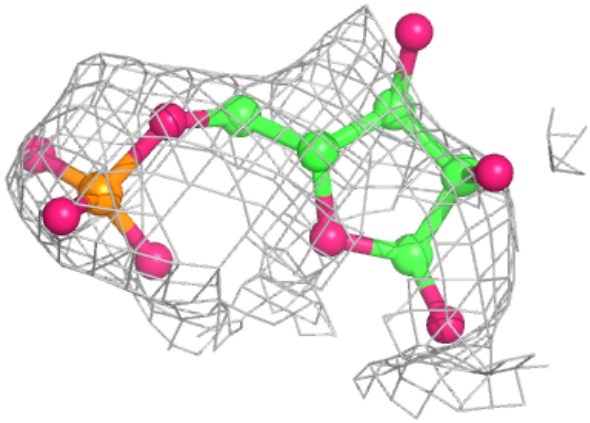


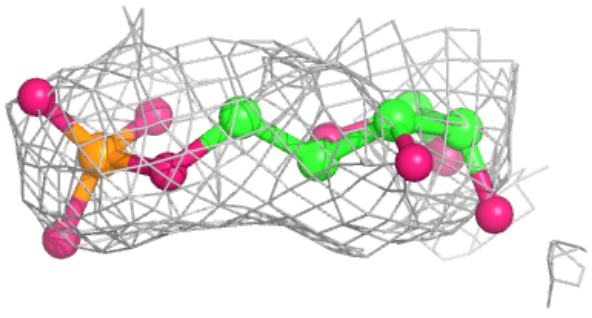


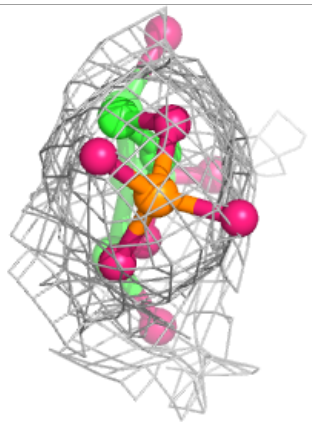


Electron density around HSX O 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.