



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:16 AM UTC

PDB ID : 1ZVV / pdb_00001zvv
Title : Crystal structure of a ccpa-crh-dna complex
Authors : Schumacher, M.A.; Brennan, R.G.; Hillen, W.; Seidel, G.
Deposited on : 2005-06-02
Resolution : 2.98 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

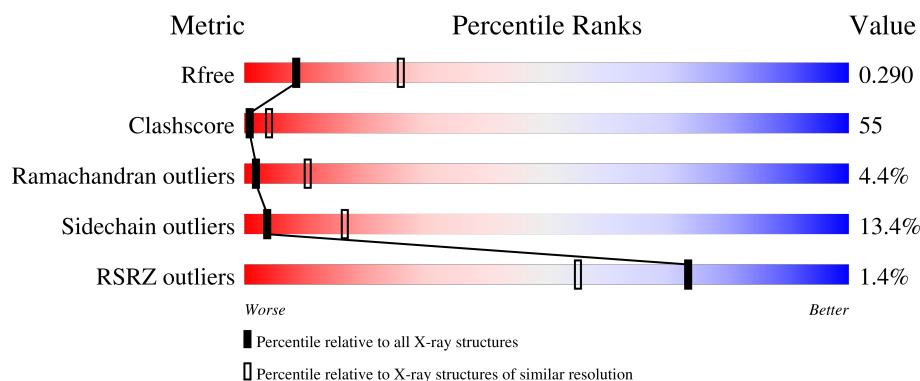
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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.



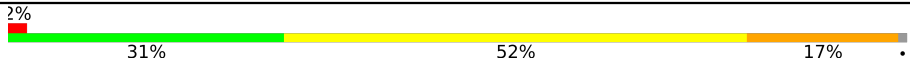
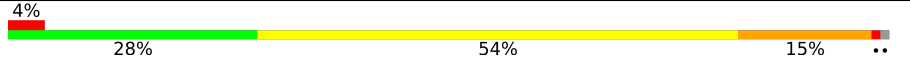
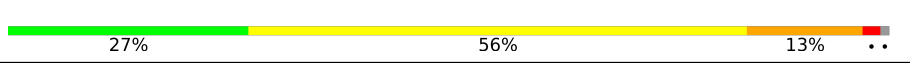
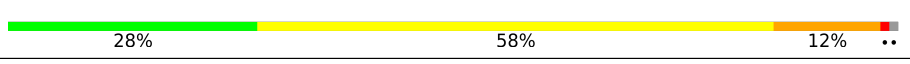
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	16	94% 6%
1	R	16	6% 100%
1	T	16	100%
2	A	332	% 30% 54% 15% .
2	B	332	2% 28% 60% 11% .

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Mol	Chain	Length	Quality of chain
2	G	332	
3	J	85	
3	P	85	
3	W	85	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IOD	G	418	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10661 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 DNA chain called DNA recognition strand CRE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	16	Total	C	N	O	P	0	0	0
			326	156	63	92	15			
1	T	16	Total	C	N	O	P	0	0	0
			326	156	63	92	15			
1	R	16	Total	C	N	O	P	0	0	0
			326	156	63	92	15			

- Molecule 2 is a protein called Glucose-resistance amylase regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	332	Total	C	N	O	S	0	0	0
			2560	1606	437	507	10			
2	B	332	Total	C	N	O	S	0	0	0
			2572	1614	439	509	10			
2	G	329	Total	C	N	O	S	0	0	0
			2538	1593	431	504	10			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	SER	THR	conflict	UNP P46828
A	105	GLN	GLU	conflict	UNP P46828
A	320	GLU	GLN	conflict	UNP P46828
B	87	SER	THR	conflict	UNP P46828
B	105	GLN	GLU	conflict	UNP P46828
B	320	GLU	GLN	conflict	UNP P46828
G	87	SER	THR	conflict	UNP P46828
G	105	GLN	GLU	conflict	UNP P46828
G	320	GLU	GLN	conflict	UNP P46828

- Molecule 3 is a protein called HPr-like protein crh.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	W	84	Total 652	C 407	N 109	O 132	P 1	S 3	0	0	0
3	P	84	Total 652	C 407	N 109	O 132	P 1	S 3	0	0	0
3	J	84	Total 652	C 407	N 109	O 132	P 1	S 3	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	33	ILE	VAL	conflict	UNP O06976
W	55	ILE	VAL	conflict	UNP O06976
W	61	ILE	VAL	conflict	UNP O06976
P	33	ILE	VAL	conflict	UNP O06976
P	55	ILE	VAL	conflict	UNP O06976
P	61	ILE	VAL	conflict	UNP O06976
J	33	ILE	VAL	conflict	UNP O06976
J	55	ILE	VAL	conflict	UNP O06976
J	61	ILE	VAL	conflict	UNP O06976

- Molecule 4 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	1	Total 1	I 1	0	0
4	A	4	Total 4	I 4	0	0
4	B	3	Total 3	I 3	0	0
4	P	1	Total 1	I 1	0	0
4	G	2	Total 2	I 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	6	Total 6	O 6	0	0
5	T	1	Total 1	O 1	0	0
5	A	10	Total 10	O 10	0	0

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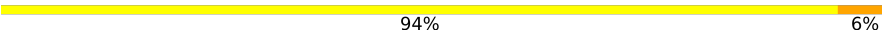
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	W	6	Total 6	O 6	0	0
5	B	9	Total 9	O 9	0	0
5	P	2	Total 2	O 2	0	0
5	G	12	Total 12	O 12	0	0

3 Residue-property plots

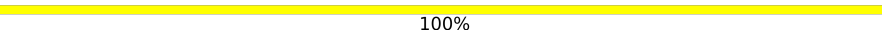
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA recognition strand CRE

Chain O: 

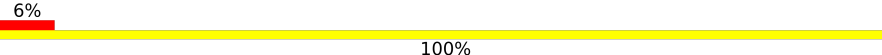
C700
T701
G702
A703
A704
A705
G706
C707
G708
C709
T710
T711
A712
C713
A714
G715

- Molecule 1: DNA recognition strand CRE

Chain T: 

C700
T701
G702
A703
A704
A705
G706
C707
G708
C709
T710
T711
A712
C713
A714
G715

- Molecule 1: DNA recognition strand CRE

Chain R: 

C700
T701
G702
A703
A704
A705
G706
C707
G708
C709
T710
T711
A712
C713
A714
G715

- Molecule 2: Glucose-resistance amylase regulator

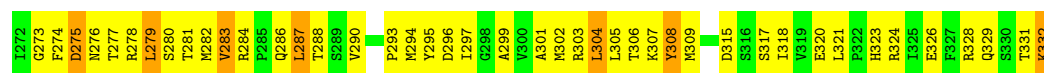
Chain A: 

M1
R2
V3
T4
I5
Y6
D7
V8
A9
R10
E11
A12
S13
V14
S15
M16
A17
T18
I19
V19
S20
R21
V22
V23
N28
V29
K30
P31
S32
T33
R34
K35
K36
V37
L38
E39
T40
R43
L44
G45
Y46
L55
K58
K59
T60
T61
V65
I66
I67
P68
D69
I70
S71
N72
I73
F74

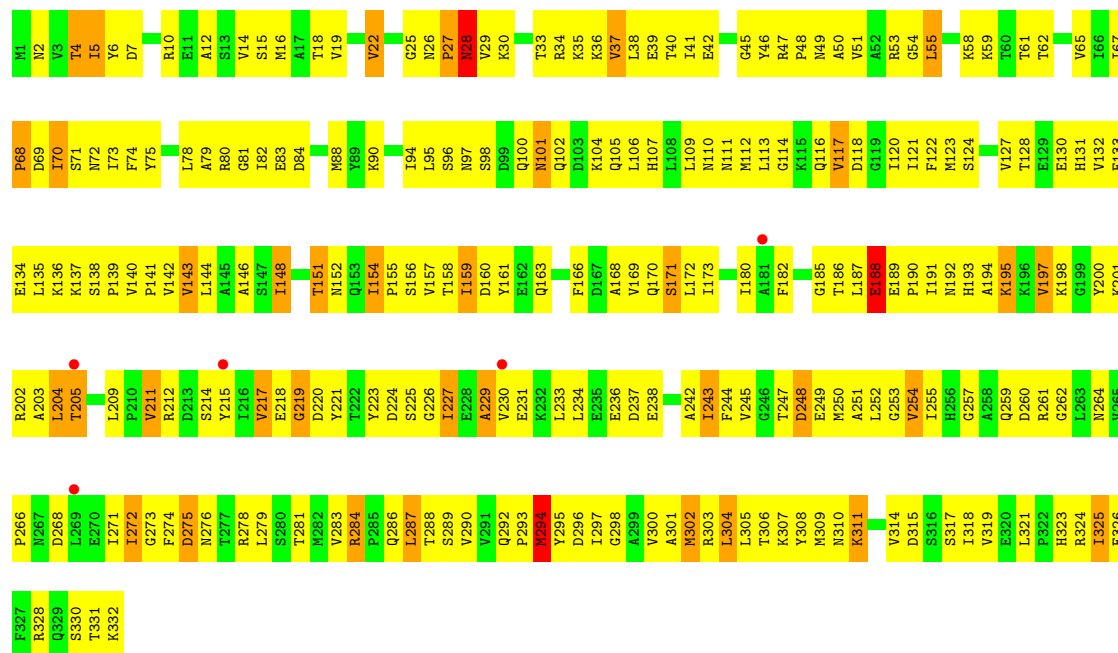
Y75
A76
E77
L78
A79
R80
G81
I82
E83
D84
R85
A86
S87
M88
Y89
N92
I93
I94
L95
S96
N97
A98
D99
Q100
N101
Q102
D103
K104
Q105
L106
L109
M110
N111
M112
E113
G114
K115
Q116
V117
D118
I121
F122
M123
S124
T128
E129
E130
H131
V132
E133
P134
Y135
P139
V140

V143
L144
A146
A147
I148
E149
S150
T151
N152
Q153
I154
P155
S156
V157
T158
I159
D160
I161
E162
Q163
A164
S165
F166
D167
A168
V169
Q170
S171
D174
S175
G176
H177
K178
N179
T180
A181
F182
V183
S184
E188
P189
F190
I191
N192
H193
A194
K195
K196
V197
N198
G199
P200
K201
R202
E206
S207

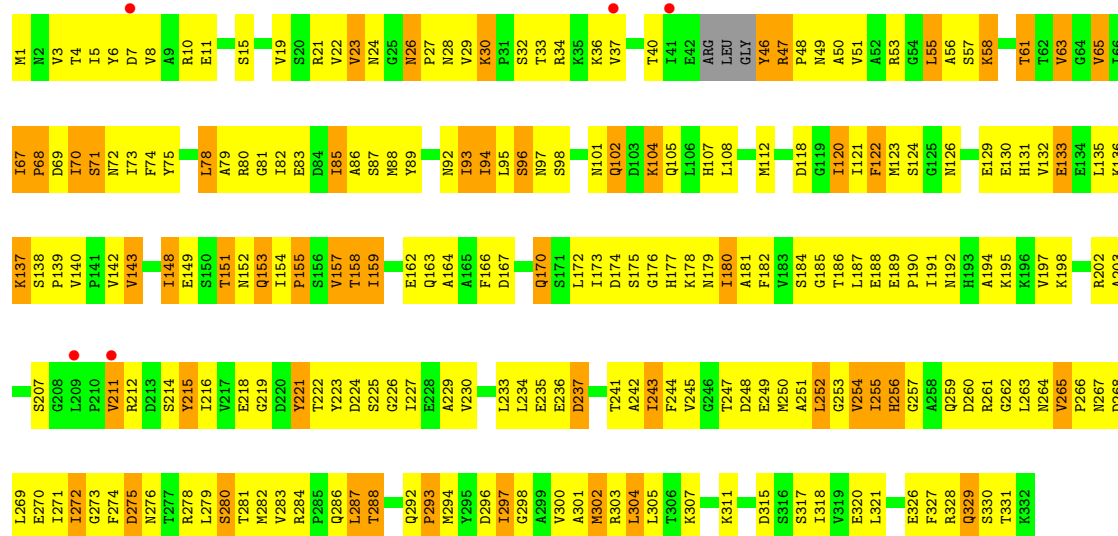
V211
R212
D213
S214
Y215
T216
V217
E218
G219
D220
Y221
T222
Y223
D224
S225
G226
I227
E228
A229
V230
E231
K232
L233
L234
E235
E236
D237
E238
K239
T240
T241
A242
I243
F244
V245
G246
T247
D248
E249
N250
A251
L252
G253
V254
I255
H256
G257
K263
G262
L263
N264
V265
P266
N267
D268
L269
E270
I271



• Molecule 2: Glucose-resistance amylase regulator

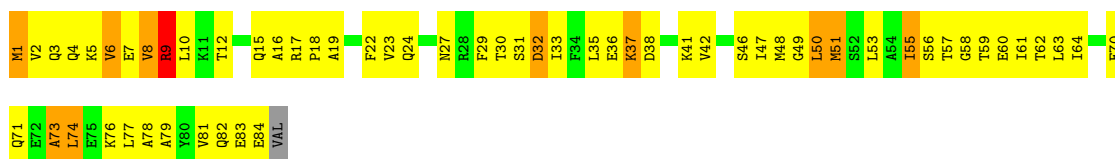


• Molecule 2: Glucose-resistance amylase regulator



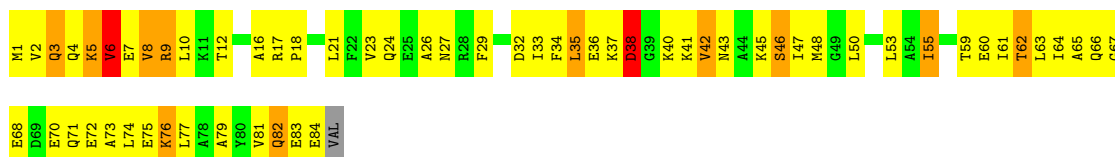
• Molecule 3: HPr-like protein crh





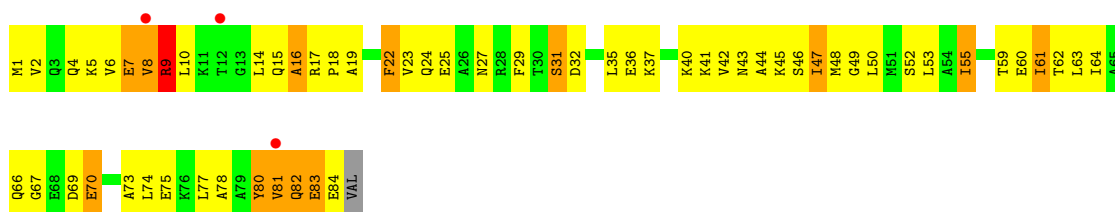
• Molecule 3: HPr-like protein crh

Chain P: 27% 56% 13% ..



• Molecule 3: HPr-like protein crh

Chain J: 4% 28% 54% 15% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	83.69Å 158.10Å 125.47Å 90.00° 100.73° 90.00°	Depositor
Resolution (Å)	79.05 – 2.98 79.05 – 2.98	Depositor EDS
% Data completeness (in resolution range)	93.2 (79.05-2.98) 93.2 (79.05-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.298 0.220 , 0.290	Depositor DCC
R_{free} test set	2450 reflections (7.53%)	wwPDB-VP
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10661	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	O	0.37	0/366	0.80	1/563 (0.2%)
1	R	0.35	0/366	0.79	0/563
1	T	0.36	0/366	0.72	0/563
2	A	0.56	0/2596	1.10	19/3513 (0.5%)
2	B	0.61	0/2610	1.17	17/3536 (0.5%)
2	G	0.61	0/2574	1.14	23/3484 (0.7%)
3	J	0.67	0/645	1.09	5/863 (0.6%)
3	P	0.53	0/645	1.00	2/863 (0.2%)
3	W	0.71	0/645	1.10	2/863 (0.2%)
All	All	0.58	0/10813	1.09	69/14811 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	102	GLN	N-CA-C	9.49	121.31	110.97
2	G	255	ILE	N-CA-C	-9.00	103.08	111.45
2	B	102	GLN	N-CA-C	8.83	120.59	110.97
2	B	254	VAL	N-CA-C	-8.48	104.27	111.56
2	B	2	ASN	N-CA-C	-8.38	101.92	112.90
2	G	280	SER	N-CA-C	-7.57	104.65	114.04
2	G	104	LYS	N-CA-C	-7.26	103.08	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	221	TYR	N-CA-C	-7.16	104.91	112.93
2	G	254	VAL	N-CA-C	-7.11	106.56	113.53
2	B	154	ILE	CA-C-N	7.05	127.45	119.83
2	B	154	ILE	C-N-CA	7.05	127.45	119.83
2	G	252	LEU	N-CA-C	-7.01	102.85	111.33
3	J	22	PHE	N-CA-C	-7.00	103.58	111.07
2	G	5	ILE	N-CA-C	-6.93	103.95	112.76
2	A	150	SER	N-CA-C	6.91	122.76	111.37
3	J	7	GLU	N-CA-C	-6.90	99.51	109.31
2	G	151	THR	N-CA-C	6.90	121.53	113.18
2	A	255	ILE	N-CA-C	-6.87	103.82	110.42
2	G	288	THR	N-CA-C	-6.76	100.97	110.50
2	A	93	ILE	N-CA-C	6.70	119.17	108.85
2	G	215	TYR	N-CA-C	-6.57	104.98	114.12
2	G	139	PRO	N-CA-C	-6.41	106.48	114.68
2	A	5	ILE	N-CA-C	-6.37	103.65	112.50
2	B	156	SER	N-CA-C	6.30	117.76	107.23
2	G	74	PHE	N-CA-C	-6.16	104.19	111.03
2	A	115	LYS	N-CA-C	-6.16	105.62	113.01
3	P	35	LEU	N-CA-C	-6.11	99.76	109.59
2	G	93	ILE	N-CA-C	6.07	116.60	108.11
2	B	188	GLU	N-CA-C	6.04	118.83	111.82
2	A	9	ALA	N-CA-C	-6.02	104.83	111.82
2	A	287	LEU	N-CA-C	6.01	118.45	109.25
2	A	254	VAL	N-CA-C	-5.98	106.98	112.96
2	G	267	ASN	N-CA-C	5.97	120.30	111.04
2	G	315	ASP	N-CA-C	-5.92	104.81	112.68
2	G	243	ILE	N-CA-C	5.85	117.85	108.85
2	A	18	THR	N-CA-C	-5.84	103.71	111.24
2	B	47	ARG	CA-C-N	5.79	125.75	119.78
2	B	47	ARG	C-N-CA	5.79	125.75	119.78
2	A	261	ARG	N-CA-C	-5.79	106.45	112.93
2	G	23	VAL	N-CA-C	-5.76	104.57	113.16
2	B	27	PRO	N-CA-C	-5.76	101.18	110.74
2	G	120	ILE	N-CA-C	5.74	116.34	107.78
2	B	159	ILE	N-CA-C	-5.74	100.02	108.23
2	G	153	GLN	N-CA-C	-5.69	104.92	112.94
2	B	28	ASN	N-CA-C	-5.69	98.68	110.80
3	J	44	ALA	N-CA-C	-5.57	107.06	112.97
1	O	715	DG	C2'-C3'-O3'	-5.52	103.21	111.50
3	W	12	THR	N-CA-C	-5.51	106.55	113.28
2	A	151	THR	N-CA-C	5.51	117.28	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	222	THR	N-CA-C	5.46	118.51	110.59
2	A	8	VAL	N-CA-C	-5.41	104.72	112.35
3	J	48	MET	N-CA-C	5.37	117.95	111.40
2	B	47	ARG	N-CA-C	-5.36	98.11	108.45
2	A	278	ARG	N-CA-C	-5.36	105.84	112.38
2	B	219	GLY	N-CA-C	-5.35	104.95	112.60
2	G	256	HIS	N-CA-C	-5.34	106.46	112.87
2	B	229	ALA	N-CA-C	5.33	117.09	111.28
3	J	24	GLN	N-CA-C	-5.33	106.04	112.54
2	G	287	LEU	N-CA-C	5.31	116.90	108.67
3	W	32	ASP	N-CA-C	-5.24	102.53	110.24
2	A	180	ILE	N-CA-C	5.22	115.37	107.80
3	P	6	VAL	N-CA-C	5.19	120.14	109.34
2	A	245	VAL	N-CA-C	5.12	115.49	108.12
2	A	184	SER	N-CA-C	5.10	118.05	110.14
2	G	157	VAL	N-CA-C	-5.07	102.56	109.55
2	G	297	ILE	N-CA-C	-5.05	106.35	112.76
2	A	221	TYR	N-CA-C	5.04	119.42	113.28
2	B	243	ILE	N-CA-C	5.02	117.05	108.86
2	B	51	VAL	N-CA-C	5.01	115.73	110.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	46	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	326	0	181	38	0
1	R	326	0	181	25	0
1	T	326	0	181	25	0
2	A	2560	0	2580	301	0
2	B	2572	0	2602	280	0
2	G	2538	0	2557	272	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	652	0	668	79	0
3	P	652	0	668	92	0
3	W	652	0	668	86	0
4	A	4	0	0	2	0
4	B	3	0	0	0	0
4	G	2	0	0	3	0
4	O	1	0	0	0	0
4	P	1	0	0	1	0
5	A	10	0	0	0	0
5	B	9	0	0	0	0
5	G	12	0	0	1	0
5	O	6	0	0	0	0
5	P	2	0	0	0	0
5	T	1	0	0	0	0
5	W	6	0	0	0	0
All	All	10661	0	10286	1157	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 55.

All (1157) 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)
2:G:288:THR:HG22	2:G:328:ARG:H	1.08	1.09
3:J:9:ARG:HD2	3:J:82:GLN:NE2	1.69	1.06
2:A:183:VAL:HB	2:A:245:VAL:HG12	1.37	1.06
2:B:230:VAL:HG22	2:B:254:VAL:HG13	1.37	1.05
2:A:288:THR:HG22	2:A:328:ARG:H	0.91	1.04
2:A:288:THR:HG22	2:A:328:ARG:N	1.70	1.03
2:B:252:LEU:HD11	2:B:279:LEU:HB3	1.41	1.03
3:P:33:ILE:HD13	3:P:77:LEU:HD11	1.44	0.99
2:A:245:VAL:HG21	2:A:251:ALA:HB2	1.45	0.96
2:B:227:ILE:HG23	2:B:257:GLY:HA2	1.49	0.95
2:B:65:VAL:O	2:B:112:MET:HE1	1.67	0.94
2:B:284:ARG:HH21	2:B:286:GLN:HG3	1.32	0.94
3:P:36:GLU:HG3	3:P:41:LYS:HB2	1.49	0.93
2:A:143:VAL:HG11	2:A:305:LEU:HB2	1.47	0.93
2:A:230:VAL:HG22	2:A:254:VAL:HG13	1.49	0.93
2:G:29:VAL:HB	2:G:34:ARG:HH21	1.32	0.93
2:G:303:ARG:HH12	2:G:307:LYS:HG3	1.32	0.93
2:A:288:THR:CG2	2:A:328:ARG:H	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:233:LEU:HB3	2:A:240:PRO:HG2	1.48	0.92
2:B:188:GLU:OE1	2:B:189:GLU:HG3	1.69	0.92
1:O:707:DC:H5'	1:O:707:DC:C6	2.03	0.92
2:G:88:MET:HE1	3:J:47:ILE:HD13	1.51	0.92
3:W:31:SER:O	3:W:33:ILE:HG13	1.69	0.91
3:W:7:GLU:HG3	3:W:8:VAL:H	1.35	0.90
2:B:67:ILE:HD11	2:B:75:TYR:HB3	1.51	0.89
2:G:265:VAL:HB	2:G:266:PRO:HD3	1.54	0.89
2:G:223:TYR:CE1	2:G:227:ILE:HD11	2.08	0.89
2:A:307:LYS:HZ1	3:W:48:MET:HG3	1.35	0.89
3:J:7:GLU:HG3	3:J:8:VAL:H	1.34	0.89
2:A:245:VAL:HG23	2:A:273:GLY:HA2	1.56	0.88
2:G:288:THR:HG22	2:G:328:ARG:N	1.88	0.88
3:J:8:VAL:HG23	3:J:81:VAL:HG12	1.55	0.88
1:O:709:DC:H2''	1:O:710:DT:H5''	1.53	0.88
2:A:180:ILE:HG22	2:A:242:ALA:HB3	1.55	0.88
1:R:706:DG:H2''	1:R:707:DC:H5'	1.56	0.88
1:T:700:DC:H2''	1:T:701:DT:O5'	1.75	0.87
2:B:293:PRO:O	2:B:297:ILE:HG12	1.74	0.87
2:G:95:LEU:HD23	2:G:96:SER:N	1.90	0.87
2:A:293:PRO:O	2:A:297:ILE:HG12	1.74	0.87
2:B:70:ILE:HG22	2:B:97:ASN:HD21	1.39	0.87
2:A:305:LEU:HG	2:A:309:MET:HE2	1.57	0.86
2:B:297:ILE:HD13	2:B:321:LEU:HD22	1.57	0.86
2:B:161:TYR:HB2	2:B:195:LYS:HB3	1.55	0.86
2:A:70:ILE:HG22	2:A:97:ASN:HD21	1.41	0.85
1:O:707:DC:H5'	1:O:707:DC:H6	1.40	0.85
2:B:68:PRO:HD3	2:B:123:MET:O	1.76	0.85
2:A:67:ILE:HD11	2:A:75:TYR:HB3	1.57	0.84
2:A:176:GLY:O	2:A:178:LYS:HG3	1.77	0.84
2:G:230:VAL:CG2	2:G:254:VAL:HA	2.07	0.84
1:O:709:DC:H2''	1:O:710:DT:C5'	2.07	0.84
2:B:274:PHE:O	2:B:275:ASP:HB2	1.75	0.84
2:B:190:PRO:HA	2:B:193:HIS:CE1	2.12	0.84
3:W:55:ILE:HD12	3:W:55:ILE:H	1.41	0.84
2:G:95:LEU:HD23	2:G:96:SER:H	1.43	0.84
2:B:252:LEU:HD22	2:B:283:VAL:HG11	1.60	0.83
2:G:148:ILE:HG12	2:G:190:PRO:HB2	1.60	0.83
1:T:705:DA:H2''	1:T:706:DG:OP2	1.78	0.83
3:J:9:ARG:HD2	3:J:82:GLN:HE22	1.39	0.83
3:J:42:VAL:HG11	3:J:53:LEU:HD21	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LEU:HG	2:B:218:GLU:CD	2.04	0.82
3:J:14:LEU:CD1	3:J:55:ILE:HD12	2.08	0.82
2:A:1:MET:CG	2:A:1:MET:CA	2.58	0.82
3:W:36:GLU:HG2	3:W:41:LYS:HB3	1.61	0.82
1:O:700:DC:H5''	2:A:28:ASN:C	2.05	0.81
2:A:22:VAL:HG21	2:A:37:VAL:HG11	1.62	0.81
2:A:154:ILE:HD12	2:A:154:ILE:H	1.45	0.81
1:T:708:DG:H2''	1:T:709:DC:H5''	1.62	0.81
2:B:152:ASN:HD22	2:B:318:ILE:HG12	1.45	0.81
3:J:67:GLY:O	3:J:70:GLU:HG2	1.81	0.81
2:G:101:ASN:HB3	2:G:104:LYS:HB3	1.64	0.80
2:A:149:GLU:HG2	2:A:154:ILE:HD11	1.62	0.80
2:G:19:VAL:O	2:G:22:VAL:HG22	1.80	0.80
2:G:230:VAL:HG22	2:G:254:VAL:HA	1.62	0.80
3:J:9:ARG:HH11	3:J:9:ARG:CG	1.94	0.80
1:O:712:DA:H2''	1:O:713:DC:H5'	1.63	0.80
2:G:286:GLN:HB3	2:G:328:ARG:HB3	1.64	0.80
2:A:113:LEU:HD11	2:A:139:PRO:HD2	1.64	0.80
2:G:78:LEU:HG	2:G:123:MET:HE1	1.63	0.80
2:G:294:MET:HE2	2:G:297:ILE:HD12	1.64	0.80
2:B:67:ILE:CD1	2:B:75:TYR:HB3	2.12	0.79
3:J:63:LEU:HD11	3:J:74:LEU:HG	1.64	0.79
3:P:63:LEU:C	3:P:64:ILE:HD12	2.07	0.79
3:W:8:VAL:HG23	3:W:81:VAL:HG13	1.63	0.79
2:B:58:LYS:O	2:B:59:LYS:HG2	1.83	0.79
2:G:157:VAL:HG11	2:G:301:ALA:HB2	1.64	0.79
1:O:714:DA:H2''	1:O:715:DG:O5'	1.83	0.79
2:B:284:ARG:HH21	2:B:286:GLN:CG	1.96	0.78
2:A:4:THR:HG23	2:A:7:ASP:H	1.47	0.78
2:B:137:LYS:HE2	2:B:137:LYS:HA	1.66	0.78
2:A:70:ILE:O	2:A:70:ILE:HG13	1.82	0.78
2:B:30:LYS:HB3	2:B:33:THR:HG23	1.65	0.78
2:G:181:ALA:HA	2:G:215:TYR:HB3	1.65	0.78
2:G:272:ILE:HD13	2:G:273:GLY:N	1.99	0.77
1:R:714:DA:H1'	1:R:715:DG:H5''	1.67	0.77
2:A:181:ALA:HA	2:A:215:TYR:HB3	1.67	0.77
3:W:2:VAL:HG12	3:W:74:LEU:HD22	1.65	0.77
2:B:223:TYR:CE1	2:B:227:ILE:HD11	2.19	0.77
3:P:8:VAL:HA	3:P:81:VAL:HG12	1.67	0.77
2:B:255:ILE:HG12	2:B:271:ILE:HD12	1.67	0.76
2:G:286:GLN:HB2	2:G:329:GLN:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:148:ILE:HD12	2:G:148:ILE:O	1.84	0.76
2:G:166:PHE:CE1	2:G:170:GLN:HG3	2.20	0.76
2:G:303:ARG:NH1	2:G:307:LYS:HG3	2.00	0.76
2:A:265:VAL:HG22	2:A:269:LEU:HD21	1.66	0.76
3:W:55:ILE:HD12	3:W:55:ILE:N	2.01	0.76
3:W:1:MET:O	3:W:1:MET:HG3	1.85	0.76
3:J:9:ARG:HH11	3:J:9:ARG:HG3	1.49	0.76
3:W:82:GLN:C	3:W:84:GLU:H	1.93	0.75
2:A:239:LYS:H	2:A:239:LYS:HD2	1.51	0.75
2:G:260:ASP:C	2:G:262:GLY:H	1.95	0.75
2:G:236:GLU:HG3	2:G:237:ASP:H	1.51	0.75
1:T:712:DA:H2''	1:T:713:DC:O5'	1.85	0.75
1:O:700:DC:H5''	2:A:29:VAL:N	2.01	0.75
3:J:14:LEU:HD13	3:J:55:ILE:HD12	1.68	0.75
2:B:310:ASN:O	2:B:311:LYS:HG3	1.87	0.74
2:G:159:ILE:HD13	2:G:297:ILE:HD11	1.68	0.74
2:G:303:ARG:NH1	2:G:307:LYS:HE3	2.03	0.74
2:A:22:VAL:HG21	2:A:37:VAL:CG1	2.17	0.74
2:B:173:ILE:HD13	2:B:209:LEU:HD12	1.69	0.74
2:A:212:ARG:H	2:A:212:ARG:HD2	1.52	0.74
3:P:34:PHE:HB2	3:P:64:ILE:HB	1.70	0.74
2:A:183:VAL:HB	2:A:245:VAL:CG1	2.17	0.73
2:A:270:GLU:HG3	2:A:332:LYS:HE3	1.69	0.73
2:G:216:ILE:HD11	4:G:418:IOD:I	2.58	0.73
2:B:295:TYR:OH	3:P:17:ARG:HG3	1.87	0.73
2:G:85:ILE:HG21	2:G:302:MET:HB3	1.71	0.73
2:A:307:LYS:NZ	3:W:48:MET:HG3	2.02	0.73
1:T:702:DG:H2''	1:T:703:DA:C8	2.24	0.73
2:G:70:ILE:H	2:G:97:ASN:ND2	1.86	0.73
2:A:158:THR:O	2:A:320:GLU:HA	1.89	0.72
2:A:105:GLN:HE22	2:A:124:SER:HB2	1.55	0.72
2:A:245:VAL:HG21	2:A:251:ALA:CB	2.19	0.72
2:G:22:VAL:HG11	2:G:37:VAL:HG11	1.70	0.72
2:G:185:GLY:HA3	2:G:221:TYR:CE1	2.24	0.72
2:A:82:ILE:HD13	2:A:121:ILE:HG21	1.71	0.72
3:W:1:MET:HE1	3:W:3:GLN:HB2	1.70	0.72
2:A:60:THR:O	2:A:61:THR:HB	1.89	0.72
1:O:700:DC:H3'	2:A:29:VAL:HA	1.71	0.72
2:B:250:MET:O	2:B:254:VAL:HG23	1.89	0.72
2:G:184:SER:C	2:G:250:MET:HE1	2.15	0.72
2:A:149:GLU:CG	2:A:154:ILE:HD11	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7:GLU:HG3	3:P:9:ARG:H	1.55	0.71
3:P:24:GLN:HG3	4:P:421:IOD:I	2.61	0.71
2:G:283:VAL:HG12	2:G:284:ARG:H	1.55	0.71
2:A:226:GLY:O	2:A:230:VAL:HG23	1.91	0.71
2:G:19:VAL:HA	2:G:22:VAL:HG13	1.72	0.71
3:W:23:VAL:HG23	3:W:50:LEU:HD12	1.72	0.71
2:A:295:TYR:OH	3:W:17:ARG:HG3	1.91	0.71
3:W:23:VAL:CG2	3:W:50:LEU:HD12	2.20	0.71
2:A:215:TYR:OH	2:A:238:GLU:HB3	1.91	0.70
2:B:302:MET:CE	2:B:305:LEU:HD23	2.20	0.70
3:J:82:GLN:C	3:J:84:GLU:H	1.99	0.70
2:B:276:ASN:OD1	2:B:328:ARG:NH2	2.24	0.70
2:A:88:MET:HE2	3:W:24:GLN:HG2	1.73	0.70
2:G:63:VAL:HG21	2:G:302:MET:HE3	1.73	0.70
1:T:702:DG:H8	1:T:702:DG:H5'	1.56	0.70
2:G:85:ILE:CG2	2:G:302:MET:HB3	2.21	0.70
2:A:307:LYS:NZ	3:W:48:MET:HE2	2.06	0.70
3:P:63:LEU:O	3:P:64:ILE:HD12	1.91	0.70
2:G:286:GLN:HB2	2:G:329:GLN:CB	2.22	0.70
2:G:293:PRO:HB2	2:G:296:ASP:HB2	1.73	0.70
1:R:708:DG:H1'	1:R:709:DC:H5''	1.72	0.70
2:G:65:VAL:HG11	2:G:93:ILE:HD11	1.73	0.70
2:A:307:LYS:HZ1	3:W:48:MET:HE2	1.57	0.69
2:G:67:ILE:HD12	2:G:123:MET:SD	2.31	0.69
2:A:101:ASN:O	2:A:105:GLN:HG3	1.91	0.69
2:G:151:THR:OG1	2:G:153:GLN:HG3	1.92	0.69
3:P:42:VAL:HG12	3:P:43:ASN:H	1.58	0.69
2:G:176:GLY:O	2:G:178:LYS:HG3	1.91	0.69
2:A:30:LYS:HE2	2:A:32:SER:HB3	1.75	0.69
2:A:39:GLU:OE1	2:A:43:ARG:HD2	1.92	0.69
3:W:6:VAL:HG12	3:W:82:GLN:HE21	1.58	0.69
2:B:305:LEU:HG	2:B:309:MET:HE2	1.74	0.69
2:A:70:ILE:HG22	2:A:97:ASN:ND2	2.08	0.69
2:B:105:GLN:HE22	2:B:124:SER:CB	2.05	0.69
3:P:66:GLN:HG3	3:P:66:GLN:O	1.92	0.68
3:W:9:ARG:CG	3:W:9:ARG:HH11	2.06	0.68
2:G:4:THR:HG23	2:G:7:ASP:H	1.59	0.68
2:A:287:LEU:C	2:A:328:ARG:HD2	2.18	0.68
3:W:9:ARG:HH11	3:W:9:ARG:HG3	1.58	0.68
2:B:245:VAL:HG21	2:B:254:VAL:HG21	1.76	0.68
2:G:46:TYR:OH	2:G:48:PRO:HA	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:287:LEU:O	2:A:328:ARG:HD2	1.93	0.68
2:B:152:ASN:ND2	2:B:318:ILE:HG12	2.09	0.68
2:G:274:PHE:O	2:G:275:ASP:HB2	1.92	0.68
2:G:57:SER:O	2:G:58:LYS:HB2	1.92	0.68
2:B:29:VAL:HB	2:B:34:ARG:HH21	1.59	0.68
2:G:69:ASP:HA	2:G:97:ASN:HD22	1.59	0.68
3:J:14:LEU:HD12	3:J:55:ILE:HD12	1.75	0.68
2:B:144:LEU:HD21	2:B:154:ILE:HG21	1.75	0.68
2:B:310:ASN:C	2:B:311:LYS:HG3	2.18	0.68
3:W:61:ILE:HD12	3:W:61:ILE:O	1.93	0.67
3:W:4:GLN:HG2	3:W:6:VAL:HG22	1.76	0.67
2:G:63:VAL:HG21	2:G:302:MET:CE	2.24	0.67
2:A:166:PHE:CE1	2:A:170:GLN:HG3	2.30	0.67
2:A:220:ASP:CG	2:A:225:SER:HB3	2.20	0.67
2:G:212:ARG:H	2:G:212:ARG:HD2	1.58	0.67
2:B:248:ASP:HA	2:B:251:ALA:HB3	1.77	0.67
2:G:4:THR:OG1	2:G:6:TYR:HB3	1.95	0.67
2:G:143:VAL:HG12	2:G:305:LEU:HD13	1.74	0.67
2:G:194:ALA:O	2:G:195:LYS:HD2	1.95	0.67
2:B:41:ILE:HG23	2:B:46:TYR:HB3	1.74	0.67
2:B:161:TYR:HB2	2:B:195:LYS:CB	2.23	0.67
2:A:61:THR:HG22	2:A:61:THR:O	1.95	0.67
2:A:157:VAL:CG1	2:A:301:ALA:HB2	2.24	0.67
3:J:36:GLU:O	3:J:61:ILE:HB	1.95	0.67
3:J:37:LYS:HE2	3:J:59:THR:HG21	1.77	0.67
3:P:5:LYS:HG2	3:P:62:THR:HG23	1.76	0.67
3:P:12:THR:HG21	3:P:18:PRO:HG2	1.76	0.67
2:B:159:ILE:HD11	2:B:323:HIS:HB3	1.77	0.66
2:A:270:GLU:CG	2:A:332:LYS:HE3	2.25	0.66
3:W:47:ILE:HD12	3:W:47:ILE:H	1.59	0.66
2:G:98:SER:HB2	2:G:105:GLN:HG2	1.76	0.66
3:P:33:ILE:HD13	3:P:77:LEU:CD1	2.22	0.66
2:A:234:LEU:CD1	2:A:261:ARG:HG3	2.26	0.66
2:G:283:VAL:HG12	2:G:284:ARG:N	2.11	0.66
1:O:706:DG:H2"	1:O:707:DC:OP2	1.96	0.66
3:J:7:GLU:HG3	3:J:8:VAL:N	2.08	0.66
2:G:4:THR:C	2:G:6:TYR:H	2.02	0.65
2:G:21:ARG:HA	2:G:24:ASN:HB2	1.77	0.65
3:P:10:LEU:HD23	3:P:83:GLU:HG2	1.76	0.65
2:G:96:SER:OG	2:G:108:LEU:HD22	1.97	0.65
3:J:4:GLN:OE1	3:J:74:LEU:HD21	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:701:DT:H2''	1:T:702:DG:H5'	1.78	0.65
2:A:4:THR:OG1	2:A:5:ILE:N	2.28	0.65
2:G:330:SER:O	2:G:331:THR:HG23	1.96	0.65
1:O:703:DA:H1'	1:O:704:DA:H5'	1.77	0.65
2:B:318:ILE:N	2:B:318:ILE:HD12	2.11	0.65
2:A:245:VAL:CG2	2:A:251:ALA:HB2	2.23	0.65
2:G:88:MET:HE1	3:J:47:ILE:CD1	2.26	0.65
2:A:230:VAL:HG21	2:A:254:VAL:HA	1.78	0.65
3:J:50:LEU:C	3:J:50:LEU:HD23	2.22	0.65
2:A:306:THR:HA	2:A:309:MET:HE3	1.79	0.65
2:G:4:THR:HG23	2:G:7:ASP:N	2.11	0.65
2:G:287:LEU:O	2:G:328:ARG:HD2	1.97	0.64
2:B:159:ILE:HD12	2:B:293:PRO:HD2	1.79	0.64
1:T:702:DG:H5'	1:T:702:DG:C8	2.32	0.64
2:A:40:THR:O	2:A:44:LEU:HD13	1.96	0.64
2:A:307:LYS:HZ1	3:W:48:MET:CE	2.11	0.64
2:G:157:VAL:CG1	2:G:301:ALA:HB2	2.28	0.64
2:G:230:VAL:HG21	2:G:254:VAL:HA	1.80	0.64
3:J:4:GLN:HG2	3:J:5:LYS:H	1.62	0.64
3:W:7:GLU:HG3	3:W:8:VAL:N	2.10	0.64
3:P:55:ILE:N	3:P:55:ILE:HD12	2.13	0.64
2:G:182:PHE:HE1	2:G:197:VAL:HG22	1.61	0.64
2:B:230:VAL:CG2	2:B:254:VAL:HA	2.27	0.64
3:P:71:GLN:HE21	3:P:75:GLU:CG	2.11	0.64
2:G:105:GLN:HE22	2:G:124:SER:HB2	1.63	0.64
2:A:98:SER:HB2	2:A:105:GLN:HG2	1.80	0.63
2:B:104:LYS:O	2:B:107:HIS:HB3	1.98	0.63
2:G:4:THR:C	2:G:6:TYR:N	2.53	0.63
2:A:30:LYS:HG2	2:A:32:SER:HB3	1.79	0.63
2:B:80:ARG:O	2:B:83:GLU:HB2	1.98	0.63
2:B:98:SER:HB2	2:B:105:GLN:HG2	1.80	0.63
2:G:172:LEU:O	2:G:175:SER:N	2.28	0.63
1:T:703:DA:H1'	1:T:704:DA:H5'	1.81	0.63
2:G:108:LEU:O	2:G:112:MET:HG2	1.98	0.63
2:A:70:ILE:CG2	2:A:97:ASN:HD21	2.11	0.63
2:A:180:ILE:HD13	2:A:180:ILE:H	1.62	0.63
1:O:710:DT:H5'	1:O:710:DT:H6	1.64	0.63
2:G:26:ASN:C	2:G:28:ASN:H	2.07	0.63
3:P:53:LEU:HB3	3:P:55:ILE:CD1	2.27	0.63
2:A:33:THR:O	2:A:36:LYS:HB3	1.99	0.63
2:B:187:LEU:HD21	2:B:218:GLU:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:4:GLN:HG2	3:J:5:LYS:N	2.14	0.62
3:W:8:VAL:HG12	3:W:59:THR:O	1.99	0.62
2:B:158:THR:OG1	2:B:159:ILE:N	2.33	0.62
2:B:227:ILE:HG23	2:B:257:GLY:CA	2.27	0.62
2:G:101:ASN:O	2:G:105:GLN:HG3	2.00	0.62
2:G:184:SER:O	2:G:250:MET:HE1	1.99	0.62
2:A:234:LEU:HD12	2:A:261:ARG:HG3	1.82	0.62
2:B:146:ALA:HB2	2:B:297:ILE:HG21	1.80	0.62
2:G:187:LEU:HD21	4:G:418:IOD:I	2.69	0.62
2:B:198:LYS:O	2:B:202:ARG:HB2	2.00	0.62
2:G:288:THR:HG21	2:G:331:THR:OG1	1.98	0.62
2:A:131:HIS:O	2:A:135:LEU:HD13	1.99	0.62
2:B:105:GLN:HE22	2:B:124:SER:HB2	1.65	0.62
2:B:308:TYR:CZ	2:B:314:VAL:HG21	2.35	0.62
2:G:288:THR:CG2	2:G:328:ARG:H	1.98	0.62
2:A:80:ARG:NH1	2:A:84:ASP:OD1	2.33	0.62
2:G:233:LEU:C	2:G:235:GLU:H	2.08	0.62
2:A:106:LEU:CD2	2:A:110:ASN:HD22	2.13	0.62
3:J:8:VAL:HG23	3:J:81:VAL:CG1	2.28	0.62
2:A:19:VAL:O	2:A:22:VAL:HG22	1.99	0.61
2:B:170:GLN:O	2:B:171:SER:C	2.43	0.61
2:G:252:LEU:HG	2:G:283:VAL:HG21	1.81	0.61
2:A:182:PHE:HB2	2:A:200:TYR:CE2	2.35	0.61
2:A:5:ILE:HG13	2:A:19:VAL:CG1	2.31	0.61
2:G:222:THR:HG21	5:G:425:HOH:O	1.99	0.61
1:R:709:DC:H6	1:R:709:DC:H5'	1.64	0.61
3:P:7:GLU:O	3:P:61:ILE:HD11	1.99	0.61
2:G:263:LEU:HD22	2:G:268:ASP:CG	2.25	0.61
2:A:85:ILE:HG12	2:A:299:ALA:HB1	1.83	0.61
2:A:130:GLU:O	2:A:133:GLU:HG2	2.00	0.61
2:B:161:TYR:CB	2:B:195:LYS:HB3	2.27	0.61
2:A:95:LEU:HD23	2:A:96:SER:N	2.15	0.61
2:B:67:ILE:HD11	2:B:75:TYR:CB	2.27	0.61
2:B:192:ASN:O	2:B:197:VAL:HG22	2.01	0.61
2:A:212:ARG:HD2	2:A:212:ARG:N	2.15	0.61
3:P:7:GLU:HG3	3:P:8:VAL:N	2.15	0.61
2:A:223:TYR:CD1	2:A:223:TYR:C	2.79	0.61
3:P:46:SEP:O2P	3:P:48:MET:HB2	2.00	0.61
2:B:70:ILE:HG12	2:B:70:ILE:O	2.01	0.61
2:G:157:VAL:HG22	2:G:297:ILE:HG23	1.83	0.61
2:B:27:PRO:O	2:B:28:ASN:CG	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:VAL:HG11	2:B:34:ARG:HB2	1.83	0.60
2:G:70:ILE:H	2:G:97:ASN:HD21	1.48	0.60
2:G:241:THR:O	2:G:269:LEU:HA	2.01	0.60
2:A:151:THR:HB	2:A:153:GLN:HE21	1.66	0.60
2:G:121:ILE:HD11	2:G:302:MET:HA	1.83	0.60
1:R:703:DA:H2''	1:R:704:DA:OP2	2.00	0.60
1:R:707:DC:O2	2:G:55:LEU:HD13	2.00	0.60
2:G:276:ASN:OD1	2:G:328:ARG:NH2	2.35	0.60
1:O:713:DC:H2''	1:O:714:DA:OP2	2.01	0.60
2:B:227:ILE:CG2	2:B:257:GLY:HA2	2.29	0.60
2:B:230:VAL:CG2	2:B:254:VAL:HG13	2.24	0.60
3:P:2:VAL:O	3:P:74:LEU:HD22	2.02	0.60
1:T:701:DT:H2''	1:T:702:DG:C8	2.37	0.60
2:A:237:ASP:O	2:A:239:LYS:HD2	2.02	0.60
2:A:270:GLU:CD	2:A:332:LYS:HG2	2.26	0.60
2:A:93:ILE:HG12	2:A:94:ILE:N	2.15	0.60
2:G:170:GLN:HG2	2:G:203:ALA:HB1	1.84	0.60
2:A:154:ILE:HD12	2:A:154:ILE:N	2.12	0.60
2:A:78:LEU:O	2:A:82:ILE:HG13	2.02	0.59
3:J:42:VAL:CG1	3:J:53:LEU:HD21	2.31	0.59
3:J:78:ALA:O	3:J:82:GLN:HB2	2.01	0.59
3:J:8:VAL:HG12	3:J:59:THR:O	2.01	0.59
2:A:66:ILE:HB	2:A:122:PHE:HD2	1.67	0.59
2:A:85:ILE:O	2:A:89:TYR:HD2	1.84	0.59
2:A:115:LYS:O	2:A:116:GLN:HB2	2.02	0.59
2:A:157:VAL:HG11	2:A:301:ALA:HB2	1.83	0.59
2:A:223:TYR:C	2:A:223:TYR:HD1	2.11	0.59
3:P:29:PHE:CZ	3:P:73:ALA:HA	2.38	0.59
2:G:157:VAL:HG13	2:G:297:ILE:HG22	1.85	0.59
2:G:180:ILE:HD13	2:G:180:ILE:H	1.68	0.59
2:B:230:VAL:HG21	2:B:254:VAL:HA	1.84	0.59
3:P:6:VAL:HG12	3:P:7:GLU:H	1.68	0.59
2:G:46:TYR:CD1	2:G:46:TYR:C	2.80	0.59
2:A:149:GLU:OE1	2:A:154:ILE:HD11	2.03	0.59
2:B:237:ASP:O	2:B:238:GLU:HB2	2.02	0.59
2:G:265:VAL:HB	2:G:266:PRO:CD	2.27	0.59
2:B:223:TYR:HE1	2:B:227:ILE:HD11	1.65	0.59
2:B:288:THR:HG22	2:B:330:SER:HB3	1.84	0.59
1:T:708:DG:C2'	1:T:709:DC:H5''	2.31	0.59
2:A:12:ALA:HB3	2:A:14:VAL:HG22	1.85	0.59
2:B:217:VAL:CG1	2:B:233:LEU:HD21	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:36:GLU:HG3	3:J:62:THR:HB	1.84	0.59
3:J:41:LYS:HG2	3:J:42:VAL:N	2.17	0.59
1:R:704:DA:H2''	1:R:705:DA:O5'	2.03	0.59
2:A:274:PHE:O	2:A:275:ASP:HB2	2.02	0.59
3:W:2:VAL:CG1	3:W:74:LEU:HD22	2.32	0.59
1:T:714:DA:H2''	1:T:715:DG:O5'	2.03	0.58
1:R:700:DC:H2'	2:G:28:ASN:O	2.02	0.58
2:B:303:ARG:NH2	2:B:307:LYS:HE2	2.18	0.58
2:G:75:TYR:HD1	2:G:123:MET:HE2	1.68	0.58
1:T:700:DC:O3'	2:B:30:LYS:HB2	2.03	0.58
1:O:709:DC:H2'	1:O:710:DT:H72	1.85	0.58
2:A:102:GLN:CD	2:A:128:THR:HG21	2.29	0.58
2:A:247:THR:HG22	2:A:250:MET:H	1.67	0.58
3:W:37:LYS:HD2	3:W:37:LYS:C	2.28	0.58
1:O:707:DC:H1'	2:A:55:LEU:HD22	1.85	0.58
2:B:110:ASN:O	2:B:111:ASN:C	2.43	0.58
3:P:4:GLN:O	3:P:62:THR:HG22	2.04	0.58
2:G:94:ILE:HG22	2:G:112:MET:HE1	1.85	0.58
2:G:329:GLN:C	2:G:331:THR:H	2.11	0.58
3:J:17:ARG:HG2	3:J:17:ARG:HH11	1.68	0.58
1:O:709:DC:C2'	1:O:710:DT:H5''	2.31	0.58
2:G:294:MET:CE	2:G:297:ILE:HD12	2.32	0.58
2:B:120:ILE:HG22	2:B:142:VAL:HG13	1.86	0.58
2:B:287:LEU:HA	2:B:330:SER:HB2	1.84	0.58
3:P:33:ILE:CD1	3:P:77:LEU:HD11	2.27	0.58
2:B:252:LEU:HD22	2:B:283:VAL:CG1	2.31	0.58
2:A:12:ALA:O	2:A:14:VAL:HG13	2.04	0.57
2:A:143:VAL:CG1	2:A:305:LEU:HB2	2.27	0.57
3:P:50:LEU:C	3:P:50:LEU:HD13	2.28	0.57
3:J:14:LEU:HB2	3:J:55:ILE:HB	1.84	0.57
2:B:109:LEU:HG	2:B:113:LEU:HD12	1.85	0.57
2:B:29:VAL:CG1	2:B:34:ARG:HB2	2.35	0.57
1:R:702:DG:H2''	1:R:703:DA:OP2	2.04	0.57
2:B:194:ALA:O	2:B:198:LYS:HE2	2.04	0.57
2:G:272:ILE:HD13	2:G:272:ILE:C	2.29	0.57
3:J:19:ALA:O	3:J:22:PHE:HB3	2.04	0.57
1:O:709:DC:H2''	1:O:710:DT:H5'	1.85	0.57
2:A:222:THR:O	2:A:225:SER:OG	2.19	0.57
2:A:274:PHE:O	2:A:275:ASP:CB	2.53	0.57
2:B:106:LEU:HD13	2:B:134:GLU:HG2	1.85	0.57
2:B:325:ILE:O	2:B:325:ILE:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:212:ARG:HD2	2:G:212:ARG:N	2.20	0.57
2:A:88:MET:HE2	3:W:24:GLN:CG	2.34	0.57
2:G:30:LYS:HB2	2:G:30:LYS:NZ	2.19	0.57
2:G:259:GLN:HG2	2:G:260:ASP:N	2.18	0.57
3:J:8:VAL:HG13	3:J:8:VAL:O	2.05	0.57
3:J:9:ARG:CD	3:J:82:GLN:HE22	2.12	0.57
1:O:707:DC:C2'	1:O:708:DG:H5''	2.34	0.57
3:W:64:ILE:HD12	3:W:64:ILE:N	2.20	0.57
2:B:55:LEU:HD22	2:B:55:LEU:O	2.04	0.57
2:B:95:LEU:HD23	2:B:96:SER:N	2.20	0.57
2:B:148:ILE:HD11	2:B:191:ILE:HG12	1.87	0.57
3:W:16:ALA:HB3	3:W:18:PRO:HD2	1.87	0.57
3:W:41:LYS:HG3	3:W:41:LYS:O	2.04	0.57
2:B:201:LYS:O	2:B:205:THR:HG23	2.04	0.57
2:B:308:TYR:CE1	2:B:314:VAL:HG21	2.39	0.57
2:G:256:HIS:O	2:G:259:GLN:HB3	2.04	0.57
2:B:173:ILE:HD11	2:B:204:LEU:HD13	1.85	0.56
3:P:7:GLU:HG3	3:P:9:ARG:N	2.21	0.56
2:G:256:HIS:C	2:G:259:GLN:HB3	2.30	0.56
2:A:230:VAL:CG2	2:A:254:VAL:HA	2.34	0.56
3:W:8:VAL:C	3:W:10:LEU:H	2.12	0.56
2:B:245:VAL:CG2	2:B:254:VAL:HG21	2.35	0.56
3:P:27:ASN:HA	3:P:45:LYS:CE	2.35	0.56
3:J:41:LYS:HE2	3:J:64:ILE:HD12	1.87	0.56
1:R:707:DC:C2	2:G:55:LEU:HD13	2.41	0.56
2:A:321:LEU:N	2:A:321:LEU:HD12	2.21	0.56
3:P:67:GLY:O	3:P:68:GLU:C	2.47	0.56
2:G:29:VAL:CG1	2:G:34:ARG:HB2	2.35	0.56
2:G:180:ILE:HD13	2:G:180:ILE:N	2.21	0.56
2:B:30:LYS:HB3	2:B:33:THR:CG2	2.35	0.56
2:B:193:HIS:O	2:B:197:VAL:CG2	2.54	0.56
1:O:715:DG:C2'	2:B:28:ASN:ND2	2.69	0.56
2:B:201:LYS:O	2:B:204:LEU:HB2	2.05	0.56
2:B:29:VAL:HB	2:B:34:ARG:NH2	2.19	0.56
2:G:230:VAL:HG21	2:G:257:GLY:HA3	1.87	0.56
1:O:702:DG:H2''	1:O:703:DA:C8	2.40	0.56
2:A:12:ALA:HA	2:A:36:LYS:NZ	2.19	0.56
3:P:6:VAL:O	3:P:61:ILE:HD12	2.06	0.56
2:A:106:LEU:CD2	2:A:110:ASN:ND2	2.69	0.56
2:G:227:ILE:HA	2:G:253:GLY:O	2.06	0.56
2:B:159:ILE:CD1	2:B:323:HIS:HB3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:35:LYS:HD3	2:A:38:LEU:HD12	1.87	0.55
2:A:288:THR:HA	2:A:326:GLU:O	2.07	0.55
2:B:227:ILE:N	2:B:253:GLY:O	2.39	0.55
3:P:42:VAL:HG12	3:P:43:ASN:N	2.21	0.55
2:B:157:VAL:HG11	2:B:301:ALA:HB2	1.87	0.55
2:B:255:ILE:HD11	2:B:287:LEU:HD13	1.87	0.55
2:G:292:GLN:OE1	2:G:294:MET:HE3	2.06	0.55
2:A:12:ALA:HA	2:A:36:LYS:HZ2	1.71	0.55
3:W:82:GLN:O	3:W:84:GLU:N	2.36	0.55
3:J:43:ASN:OD1	3:J:45:LYS:HB2	2.06	0.55
3:J:81:VAL:C	3:J:83:GLU:H	2.13	0.55
2:A:30:LYS:HB3	2:A:33:THR:OG1	2.07	0.55
2:B:29:VAL:CG2	2:B:34:ARG:HH21	2.19	0.55
3:P:16:ALA:HB3	3:P:18:PRO:HD2	1.89	0.55
2:G:89:TYR:OH	2:G:303:ARG:NE	2.40	0.55
2:A:252:LEU:O	2:A:252:LEU:HD23	2.07	0.55
2:A:65:VAL:HG22	2:A:95:LEU:HA	1.89	0.55
2:A:78:LEU:CD2	2:A:294:MET:SD	2.95	0.55
2:B:266:PRO:HG2	2:B:332:LYS:HE3	1.88	0.55
2:G:82:ILE:CD1	2:G:121:ILE:HG21	2.37	0.55
2:G:85:ILE:O	2:G:88:MET:N	2.40	0.55
2:G:158:THR:HG23	2:G:159:ILE:N	2.22	0.55
3:W:53:LEU:HB2	3:W:55:ILE:HD11	1.89	0.55
2:B:226:GLY:C	2:B:253:GLY:O	2.50	0.55
2:B:304:LEU:HD22	2:B:308:TYR:CE2	2.41	0.55
3:W:8:VAL:HA	3:W:81:VAL:HG12	1.89	0.54
2:A:22:VAL:HG23	2:A:23:VAL:N	2.22	0.54
2:A:202:ARG:O	2:A:206:GLU:HB2	2.07	0.54
3:J:25:GLU:OE2	3:J:25:GLU:HA	2.07	0.54
2:B:81:GLY:O	2:B:82:ILE:C	2.50	0.54
3:P:67:GLY:H	3:P:70:GLU:HB3	1.72	0.54
2:A:181:ALA:HB1	2:A:215:TYR:O	2.07	0.54
2:B:12:ALA:HA	2:B:36:LYS:HE3	1.88	0.54
2:B:144:LEU:HG	2:B:154:ILE:HG22	1.88	0.54
2:G:192:ASN:O	2:G:197:VAL:HG23	2.06	0.54
2:G:328:ARG:HG2	2:G:328:ARG:HH11	1.72	0.54
1:T:710:DT:H4'	1:T:710:DT:OP1	2.07	0.54
2:A:117:VAL:O	2:A:140:VAL:HG11	2.07	0.54
2:A:307:LYS:O	2:A:307:LYS:HG2	2.08	0.54
2:B:157:VAL:CG1	2:B:301:ALA:HB2	2.37	0.54
2:B:302:MET:O	2:B:305:LEU:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:163:GLN:OE1	2:A:163:GLN:HA	2.05	0.54
2:G:81:GLY:O	2:G:82:ILE:C	2.51	0.54
2:G:233:LEU:C	2:G:235:GLU:N	2.63	0.54
1:R:715:DG:H5'	1:R:715:DG:H8	1.73	0.54
2:A:123:MET:HE2	2:A:145:ALA:HB3	1.88	0.54
2:A:180:ILE:HD13	2:A:180:ILE:N	2.23	0.54
3:W:6:VAL:CG1	3:W:82:GLN:HE21	2.19	0.54
2:A:34:ARG:O	2:A:37:VAL:HB	2.08	0.54
2:A:329:GLN:O	2:A:329:GLN:HG2	2.08	0.54
2:B:122:PHE:O	2:B:144:LEU:HA	2.07	0.54
2:B:180:ILE:HG22	2:B:242:ALA:HB3	1.90	0.54
2:G:143:VAL:HG11	2:G:305:LEU:HB2	1.89	0.54
2:G:257:GLY:C	2:G:259:GLN:H	2.13	0.54
1:O:715:DG:H2'	2:B:28:ASN:ND2	2.23	0.53
3:W:9:ARG:CG	3:W:9:ARG:NH1	2.67	0.53
2:B:248:ASP:O	2:B:252:LEU:HG	2.07	0.53
2:G:300:VAL:HG21	2:G:321:LEU:HD11	1.89	0.53
3:J:9:ARG:CG	3:J:9:ARG:NH1	2.59	0.53
2:B:26:ASN:HD22	2:B:27:PRO:HD2	1.73	0.53
2:G:260:ASP:C	2:G:262:GLY:N	2.61	0.53
2:G:269:LEU:HD23	2:G:269:LEU:H	1.72	0.53
1:T:706:DG:H2''	1:T:707:DC:OP2	2.08	0.53
3:P:8:VAL:HG23	3:P:81:VAL:HG13	1.90	0.53
2:G:95:LEU:CD2	2:G:96:SER:N	2.68	0.53
2:B:22:VAL:HG21	2:B:37:VAL:CG1	2.38	0.53
2:B:284:ARG:NH2	2:B:286:GLN:CG	2.68	0.53
3:P:1:MET:O	3:P:1:MET:HG3	2.07	0.53
2:G:75:TYR:CD1	2:G:123:MET:HE2	2.43	0.53
1:O:710:DT:H2''	1:O:711:DT:C6	2.43	0.53
2:A:307:LYS:HZ1	3:W:48:MET:CG	2.15	0.53
3:W:9:ARG:HB2	3:W:82:GLN:O	2.09	0.53
2:B:29:VAL:CB	2:B:34:ARG:HH21	2.20	0.53
2:G:19:VAL:C	2:G:21:ARG:H	2.15	0.53
3:J:35:LEU:HD21	3:J:55:ILE:HD11	1.90	0.53
2:A:151:THR:CB	2:A:153:GLN:HE21	2.21	0.53
2:A:163:GLN:O	2:A:164:ALA:C	2.52	0.53
2:A:198:LYS:O	2:A:202:ARG:HB2	2.09	0.53
2:B:220:ASP:O	2:B:221:TYR:HB2	2.08	0.53
1:R:712:DA:H2''	1:R:713:DC:O5'	2.08	0.53
2:A:324:ARG:NH1	3:W:15:GLN:OE1	2.41	0.53
3:W:47:ILE:HD12	3:W:47:ILE:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:10:LEU:HA	3:P:83:GLU:HG3	1.91	0.53
3:P:27:ASN:HA	3:P:45:LYS:HE2	1.89	0.53
2:G:260:ASP:O	2:G:262:GLY:N	2.42	0.53
3:J:77:LEU:O	3:J:81:VAL:HG23	2.08	0.53
2:A:151:THR:O	2:A:152:ASN:HB2	2.09	0.53
2:G:163:GLN:O	2:G:164:ALA:C	2.51	0.53
2:B:193:HIS:O	2:B:197:VAL:HG23	2.09	0.53
3:W:37:LYS:HD3	3:W:38:ASP:OD1	2.09	0.53
3:W:42:VAL:HG21	3:W:49:GLY:C	2.34	0.53
2:G:3:VAL:O	2:G:3:VAL:HG23	2.08	0.53
2:A:5:ILE:HG13	2:A:19:VAL:HG11	1.90	0.52
2:A:98:SER:O	2:A:100:GLN:N	2.42	0.52
2:A:280:SER:O	2:A:283:VAL:HG23	2.09	0.52
3:P:66:GLN:HA	3:P:70:GLU:OE1	2.10	0.52
2:A:3:VAL:HG23	2:A:3:VAL:O	2.09	0.52
2:A:160:ASP:OD2	2:A:163:GLN:HB2	2.09	0.52
2:B:5:ILE:HD11	2:B:16:MET:O	2.10	0.52
2:B:185:GLY:H	2:B:192:ASN:ND2	2.07	0.52
2:B:306:THR:O	2:B:310:ASN:ND2	2.42	0.52
2:A:78:LEU:O	2:A:78:LEU:HD12	2.10	0.52
2:A:197:VAL:O	2:A:200:TYR:HB3	2.09	0.52
2:G:15:SER:O	2:G:19:VAL:HG23	2.09	0.52
2:A:183:VAL:HG23	2:A:243:ILE:HG21	1.92	0.52
2:B:220:ASP:OD2	2:B:225:SER:HB3	2.09	0.52
2:B:236:GLU:HG2	2:B:237:ASP:H	1.75	0.52
3:J:53:LEU:N	3:J:53:LEU:HD22	2.25	0.52
1:O:707:DC:H2''	1:O:708:DG:H5''	1.92	0.52
1:O:709:DC:H2'	1:O:710:DT:C7	2.39	0.52
2:B:157:VAL:HG13	2:B:157:VAL:O	2.09	0.52
3:P:26:ALA:O	3:P:45:LYS:HE3	2.10	0.52
3:J:82:GLN:O	3:J:84:GLU:N	2.42	0.52
1:O:707:DC:H2''	2:A:55:LEU:CD2	2.40	0.52
2:A:70:ILE:H	2:A:97:ASN:ND2	2.08	0.52
2:B:131:HIS:O	2:B:135:LEU:HD13	2.09	0.52
3:P:55:ILE:CD1	3:P:55:ILE:H	2.22	0.52
2:G:65:VAL:CG1	2:G:93:ILE:HD11	2.39	0.52
1:R:701:DT:H1'	1:R:702:DG:H5'	1.92	0.52
2:A:281:THR:HG22	2:A:328:ARG:NH1	2.24	0.52
3:P:17:ARG:N	3:P:18:PRO:CD	2.73	0.52
3:J:35:LEU:C	3:J:35:LEU:HD23	2.35	0.52
3:P:77:LEU:O	3:P:81:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:712:DA:H4'	1:O:712:DA:OP1	2.09	0.51
2:A:4:THR:CG2	2:A:6:TYR:HB3	2.40	0.51
2:G:72:ASN:OD1	2:G:72:ASN:C	2.53	0.51
1:O:715:DG:C2'	2:B:28:ASN:HD22	2.24	0.51
2:A:30:LYS:HE2	2:A:32:SER:CB	2.39	0.51
2:A:44:LEU:HD12	2:A:44:LEU:N	2.24	0.51
2:A:227:ILE:HD13	2:A:253:GLY:O	2.10	0.51
2:B:46:TYR:HE1	2:B:48:PRO:HG3	1.75	0.51
2:B:166:PHE:CD2	2:B:203:ALA:HB2	2.46	0.51
2:B:170:GLN:HA	2:B:170:GLN:NE2	2.26	0.51
3:P:9:ARG:HB3	3:P:83:GLU:HB2	1.91	0.51
2:G:155:PRO:HA	2:G:317:SER:O	2.09	0.51
3:J:49:GLY:O	3:J:52:SER:HB3	2.10	0.51
2:A:245:VAL:O	2:A:274:PHE:HB2	2.10	0.51
2:A:286:GLN:H	2:A:329:GLN:HB3	1.74	0.51
2:A:293:PRO:HB2	2:A:296:ASP:HB2	1.93	0.51
3:W:82:GLN:C	3:W:84:GLU:N	2.58	0.51
2:B:161:TYR:HB2	2:B:195:LYS:CG	2.40	0.51
2:B:227:ILE:HD13	2:B:253:GLY:O	2.09	0.51
2:G:55:LEU:HD22	2:G:55:LEU:O	2.09	0.51
2:A:67:ILE:O	2:A:97:ASN:HA	2.10	0.51
2:A:85:ILE:HD13	2:A:85:ILE:H	1.74	0.51
2:A:98:SER:C	2:A:100:GLN:H	2.19	0.51
2:G:29:VAL:HB	2:G:34:ARG:NH2	2.14	0.51
2:B:5:ILE:HD13	2:B:16:MET:CG	2.41	0.51
3:P:1:MET:HE3	3:P:64:ILE:HG23	1.91	0.51
2:G:257:GLY:C	2:G:259:GLN:N	2.68	0.51
2:A:270:GLU:OE2	2:A:332:LYS:HG2	2.10	0.51
2:B:62:THR:CG2	2:B:94:ILE:HG13	2.40	0.51
3:P:55:ILE:N	3:P:55:ILE:CD1	2.74	0.51
3:J:8:VAL:C	3:J:10:LEU:H	2.18	0.51
3:J:82:GLN:C	3:J:84:GLU:N	2.64	0.51
2:A:132:VAL:C	2:A:134:GLU:H	2.19	0.51
3:W:35:LEU:C	3:W:35:LEU:HD23	2.35	0.51
2:B:243:ILE:HG22	2:B:244:PHE:N	2.26	0.51
2:B:131:HIS:O	2:B:135:LEU:HB2	2.11	0.51
2:B:188:GLU:OE1	2:B:189:GLU:N	2.44	0.51
2:G:278:ARG:C	2:G:280:SER:H	2.19	0.51
3:J:29:PHE:CE2	3:J:73:ALA:HA	2.46	0.51
2:A:100:GLN:HB2	4:A:411:IOD:I	2.81	0.50
2:B:82:ILE:HD13	2:B:298:GLY:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:VAL:HG11	2:B:301:ALA:CA	2.42	0.50
2:G:162:GLU:OE1	2:G:202:ARG:HD3	2.11	0.50
2:B:293:PRO:HB2	2:B:296:ASP:HB2	1.94	0.50
3:J:9:ARG:HD2	3:J:82:GLN:HE21	1.67	0.50
2:G:82:ILE:HD13	2:G:121:ILE:HG21	1.94	0.50
2:G:166:PHE:CE2	2:G:202:ARG:HG2	2.47	0.50
2:G:275:ASP:OD2	2:G:292:GLN:NE2	2.44	0.50
1:T:701:DT:H2''	1:T:702:DG:C5'	2.41	0.50
2:A:85:ILE:HG21	2:A:303:ARG:HB2	1.93	0.50
2:A:238:GLU:O	2:A:239:LYS:C	2.54	0.50
2:B:5:ILE:HD13	2:B:16:MET:HG3	1.92	0.50
2:B:12:ALA:O	2:B:14:VAL:HG13	2.11	0.50
1:O:707:DC:H2''	2:A:55:LEU:HD21	1.93	0.50
1:R:714:DA:H2''	1:R:715:DG:OP2	2.11	0.50
2:A:296:ASP:OD1	3:W:51:MET:HG2	2.11	0.50
3:W:2:VAL:HG23	3:W:70:GLU:OE2	2.12	0.50
1:T:703:DA:H2''	1:T:704:DA:O5'	2.12	0.50
2:A:95:LEU:HD23	2:A:95:LEU:C	2.36	0.50
2:A:323:HIS:O	2:A:324:ARG:HG3	2.12	0.50
2:A:78:LEU:HD22	2:A:294:MET:SD	2.51	0.50
2:A:98:SER:C	2:A:100:GLN:N	2.66	0.49
2:B:82:ILE:HG23	2:B:302:MET:HG2	1.94	0.49
2:B:245:VAL:HG11	2:B:251:ALA:N	2.27	0.49
2:B:276:ASN:O	2:B:276:ASN:ND2	2.44	0.49
3:J:17:ARG:N	3:J:18:PRO:CD	2.74	0.49
3:J:63:LEU:HD12	3:J:63:LEU:O	2.12	0.49
2:A:39:GLU:HG3	2:A:40:THR:N	2.26	0.49
3:W:36:GLU:HB2	3:W:62:THR:HB	1.94	0.49
2:G:4:THR:CG2	2:G:6:TYR:HB3	2.41	0.49
2:G:157:VAL:HG13	2:G:297:ILE:CG2	2.42	0.49
1:T:702:DG:H2''	1:T:703:DA:H8	1.74	0.49
2:A:270:GLU:HB3	2:A:331:THR:HG22	1.92	0.49
2:B:182:PHE:HB2	2:B:200:TYR:CE2	2.47	0.49
3:P:7:GLU:CG	3:P:8:VAL:N	2.75	0.49
2:G:226:GLY:O	2:G:230:VAL:HG23	2.13	0.49
3:J:74:LEU:HD23	3:J:74:LEU:C	2.36	0.49
2:A:60:THR:H	2:A:118:ASP:CG	2.21	0.49
2:A:85:ILE:CD1	2:A:85:ILE:N	2.76	0.49
2:G:65:VAL:HA	2:G:121:ILE:O	2.12	0.49
3:P:79:ALA:O	3:P:84:GLU:O	2.31	0.49
2:G:61:THR:N	2:G:118:ASP:OD2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:94:ILE:CG2	2:A:112:MET:HE2	2.43	0.49
2:A:277:THR:C	2:A:279:LEU:N	2.69	0.49
2:B:26:ASN:HD22	2:B:26:ASN:C	2.20	0.49
2:B:120:ILE:O	2:B:142:VAL:HA	2.12	0.49
2:B:245:VAL:O	2:B:273:GLY:HA2	2.13	0.49
1:O:710:DT:H5'	1:O:710:DT:C6	2.45	0.49
2:A:145:ALA:C	2:A:147:SER:H	2.19	0.49
2:A:180:ILE:CG2	2:A:242:ALA:HB3	2.34	0.49
3:W:37:LYS:HD2	3:W:37:LYS:O	2.12	0.49
2:B:185:GLY:H	2:B:192:ASN:HD21	1.61	0.49
2:G:151:THR:O	2:G:152:ASN:C	2.54	0.49
2:G:236:GLU:HG3	2:G:237:ASP:N	2.24	0.49
3:J:31:SER:OG	3:J:69:ASP:OD1	2.29	0.49
2:B:173:ILE:HD11	2:B:204:LEU:CD1	2.43	0.49
2:B:306:THR:HA	2:B:309:MET:HE3	1.95	0.49
2:G:270:GLU:HB3	2:G:331:THR:HG22	1.93	0.49
2:A:121:ILE:HD13	2:A:143:VAL:HG13	1.94	0.49
3:W:55:ILE:H	3:W:55:ILE:CD1	2.18	0.49
2:B:182:PHE:HE1	2:B:197:VAL:HG13	1.78	0.49
2:G:143:VAL:CG1	2:G:305:LEU:HD13	2.42	0.49
1:T:710:DT:H2''	1:T:711:DT:O5'	2.12	0.49
2:B:82:ILE:HD12	2:B:121:ILE:CD1	2.43	0.49
2:B:82:ILE:HD12	2:B:121:ILE:HD13	1.95	0.49
2:A:304:LEU:HD23	2:A:304:LEU:O	2.12	0.48
2:B:212:ARG:C	2:B:214:SER:H	2.21	0.48
3:P:3:GLN:O	3:P:4:GLN:HB2	2.13	0.48
2:G:270:GLU:OE1	2:G:331:THR:HG22	2.12	0.48
3:J:4:GLN:HB2	3:J:74:LEU:HD11	1.95	0.48
2:B:39:GLU:HG3	2:B:40:THR:N	2.27	0.48
2:A:149:GLU:C	2:A:149:GLU:OE2	2.56	0.48
3:W:4:GLN:HG2	3:W:6:VAL:CG2	2.42	0.48
3:W:8:VAL:O	3:W:8:VAL:HG13	2.13	0.48
2:B:159:ILE:HG23	2:B:160:ASP:N	2.28	0.48
2:B:187:LEU:CD2	2:B:218:GLU:HB3	2.43	0.48
3:P:71:GLN:HE21	3:P:75:GLU:HG3	1.77	0.48
2:G:249:GLU:HA	2:G:252:LEU:HD13	1.94	0.48
3:W:63:LEU:HD12	3:W:74:LEU:HD12	1.95	0.48
2:B:25:GLY:O	2:B:26:ASN:C	2.56	0.48
2:B:113:LEU:HD22	2:B:139:PRO:HD2	1.95	0.48
3:P:1:MET:O	3:P:1:MET:CG	2.60	0.48
3:P:9:ARG:HB3	3:P:83:GLU:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:63:VAL:HG11	2:G:302:MET:HE1	1.95	0.48
2:G:177:HIS:CE1	2:G:242:ALA:HB2	2.48	0.48
2:A:109:LEU:HG	2:A:110:ASN:N	2.28	0.48
2:A:182:PHE:HD2	2:A:244:PHE:O	1.97	0.48
2:B:194:ALA:O	2:B:198:LYS:HG3	2.12	0.48
2:B:101:ASN:OD1	2:B:101:ASN:C	2.56	0.48
2:A:17:ALA:O	2:A:21:ARG:HG3	2.14	0.48
2:A:326:GLU:HA	2:A:326:GLU:OE2	2.13	0.48
3:W:57:THR:HG22	3:W:58:GLY:N	2.28	0.48
2:B:274:PHE:O	2:B:275:ASP:CB	2.54	0.48
3:P:33:ILE:HA	3:P:64:ILE:O	2.13	0.48
3:J:9:ARG:HB2	3:J:83:GLU:HB2	1.95	0.48
3:J:50:LEU:HD23	3:J:50:LEU:O	2.14	0.48
2:A:66:ILE:HB	2:A:122:PHE:CD2	2.47	0.48
2:A:318:ILE:O	2:A:318:ILE:HG22	2.14	0.48
2:G:97:ASN:O	2:G:108:LEU:HD11	2.13	0.48
2:G:223:TYR:O	2:G:227:ILE:HG13	2.14	0.48
2:G:224:ASP:O	2:G:227:ILE:N	2.46	0.48
2:G:264:ASN:OD1	2:G:266:PRO:HD2	2.14	0.48
2:G:296:ASP:C	2:G:298:GLY:N	2.71	0.48
2:A:68:PRO:HD3	2:A:123:MET:O	2.13	0.48
2:G:85:ILE:O	2:G:86:ALA:C	2.57	0.48
2:G:280:SER:HA	2:G:287:LEU:HB3	1.95	0.48
2:A:256:HIS:O	2:A:257:GLY:C	2.57	0.48
2:B:26:ASN:HD22	2:B:27:PRO:CD	2.26	0.48
2:G:79:ALA:O	2:G:80:ARG:C	2.56	0.48
2:A:194:ALA:O	2:A:195:LYS:HD2	2.14	0.47
3:P:3:GLN:HG2	3:P:4:GLN:H	1.79	0.47
3:P:10:LEU:HA	3:P:83:GLU:CG	2.44	0.47
2:G:98:SER:CB	2:G:105:GLN:HG2	2.43	0.47
3:J:22:PHE:CD2	3:J:50:LEU:HD11	2.49	0.47
2:A:218:GLU:HG2	2:A:219:GLY:H	1.78	0.47
2:G:218:GLU:HG2	2:G:219:GLY:H	1.79	0.47
1:O:708:DG:H2''	1:O:709:DC:O5'	2.14	0.47
1:T:700:DC:H6	1:T:700:DC:O5'	1.97	0.47
3:W:9:ARG:HB2	3:W:83:GLU:HB3	1.96	0.47
2:B:18:THR:O	2:B:19:VAL:C	2.57	0.47
3:W:1:MET:CE	3:W:3:GLN:HB2	2.42	0.47
3:W:31:SER:O	3:W:32:ASP:C	2.58	0.47
3:W:79:ALA:O	3:W:82:GLN:HB2	2.14	0.47
2:B:67:ILE:HA	2:B:123:MET:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:PRO:HA	2:B:193:HIS:ND1	2.27	0.47
2:A:78:LEU:HD23	2:A:294:MET:SD	2.55	0.47
2:A:165:ALA:O	2:A:169:VAL:HG23	2.15	0.47
2:B:169:VAL:HG21	2:B:200:TYR:HA	1.95	0.47
2:B:266:PRO:HB3	2:B:331:THR:HA	1.97	0.47
3:W:17:ARG:O	3:W:18:PRO:C	2.57	0.47
2:B:260:ASP:C	2:B:262:GLY:H	2.22	0.47
3:P:35:LEU:HD13	3:P:50:LEU:HD21	1.96	0.47
1:O:700:DC:H5''	2:A:29:VAL:CA	2.45	0.47
1:R:700:DC:H2'	1:R:700:DC:H6	1.55	0.47
2:A:226:GLY:O	2:A:254:VAL:HG22	2.14	0.47
3:W:17:ARG:N	3:W:18:PRO:CD	2.78	0.47
2:B:79:ALA:O	2:B:80:ARG:C	2.56	0.47
2:B:101:ASN:O	2:B:105:GLN:HG3	2.15	0.47
2:B:230:VAL:HG12	2:B:234:LEU:HG	1.97	0.47
2:B:247:THR:O	2:B:250:MET:N	2.47	0.47
2:B:326:GLU:HB3	2:B:328:ARG:NH1	2.29	0.47
2:G:19:VAL:HA	2:G:22:VAL:CG1	2.43	0.47
2:G:82:ILE:O	2:G:302:MET:HG3	2.15	0.47
2:G:292:GLN:CD	2:G:294:MET:HE3	2.39	0.47
2:G:329:GLN:C	2:G:331:THR:N	2.73	0.47
2:A:265:VAL:HG22	2:A:269:LEU:CD2	2.40	0.47
2:A:73:ILE:O	2:A:76:ALA:HB3	2.15	0.47
2:A:85:ILE:HG12	2:A:299:ALA:CA	2.45	0.47
3:W:5:LYS:NZ	3:W:60:GLU:OE1	2.48	0.47
2:B:168:ALA:O	2:B:171:SER:HB3	2.14	0.47
2:B:186:THR:HG21	2:B:188:GLU:OE2	2.15	0.47
2:B:278:ARG:HA	2:B:281:THR:HG22	1.97	0.47
3:P:37:LYS:NZ	3:P:59:THR:HG21	2.30	0.47
2:G:265:VAL:O	2:G:266:PRO:C	2.57	0.47
2:G:300:VAL:HG21	2:G:321:LEU:HD21	1.97	0.47
2:A:162:GLU:HG3	2:A:199:GLY:CA	2.45	0.47
2:A:264:ASN:H	2:A:268:ASP:CG	2.23	0.47
2:B:35:LYS:O	2:B:36:LYS:C	2.58	0.47
2:B:70:ILE:HG22	2:B:97:ASN:ND2	2.19	0.47
3:P:82:GLN:C	3:P:84:GLU:H	2.22	0.47
2:G:148:ILE:O	2:G:148:ILE:CD1	2.59	0.47
2:B:190:PRO:O	2:B:194:ALA:HB3	2.14	0.46
2:B:252:LEU:HD13	2:B:283:VAL:CG1	2.45	0.46
2:G:4:THR:HG22	2:G:7:ASP:CG	2.40	0.46
2:G:78:LEU:HD23	2:G:294:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:129:GLU:O	2:G:130:GLU:C	2.58	0.46
2:G:236:GLU:O	2:G:237:ASP:C	2.57	0.46
2:G:255:ILE:C	2:G:257:GLY:N	2.72	0.46
2:A:304:LEU:C	2:A:304:LEU:CD2	2.88	0.46
2:B:138:SER:HA	2:B:139:PRO:HD3	1.77	0.46
3:P:53:LEU:HD12	3:P:53:LEU:HA	1.71	0.46
3:P:55:ILE:HD12	3:P:55:ILE:H	1.76	0.46
2:G:105:GLN:HE22	2:G:124:SER:CB	2.28	0.46
2:G:180:ILE:HA	2:G:242:ALA:O	2.15	0.46
1:T:701:DT:H2''	1:T:702:DG:H8	1.78	0.46
2:A:30:LYS:CE	2:A:32:SER:HB3	2.44	0.46
3:W:76:LYS:O	3:W:79:ALA:HB3	2.16	0.46
2:B:62:THR:HG21	2:B:94:ILE:HG13	1.97	0.46
3:P:2:VAL:HG12	3:P:74:LEU:CD2	2.46	0.46
2:G:19:VAL:C	2:G:21:ARG:N	2.70	0.46
2:G:247:THR:HG22	2:G:248:ASP:N	2.29	0.46
1:R:711:DT:H2''	1:R:712:DA:C8	2.51	0.46
2:A:106:LEU:HD11	2:A:134:GLU:OE1	2.14	0.46
2:A:145:ALA:C	2:A:147:SER:N	2.73	0.46
2:B:132:VAL:O	2:B:136:LYS:N	2.46	0.46
2:B:187:LEU:HG	2:B:218:GLU:OE1	2.16	0.46
2:G:120:ILE:HB	2:G:142:VAL:HG22	1.98	0.46
2:G:223:TYR:CZ	2:G:227:ILE:HD11	2.50	0.46
2:G:236:GLU:CG	2:G:237:ASP:H	2.25	0.46
3:J:31:SER:HA	3:J:67:GLY:HA3	1.97	0.46
2:A:68:PRO:HD3	2:A:123:MET:HG3	1.96	0.46
2:B:163:GLN:HA	2:B:163:GLN:NE2	2.30	0.46
2:G:131:HIS:O	2:G:135:LEU:HD22	2.14	0.46
2:G:166:PHE:HE2	2:G:202:ARG:HG2	1.80	0.46
3:J:80:TYR:HD2	3:J:81:VAL:N	2.13	0.46
2:B:49:ASN:O	2:B:50:ALA:C	2.59	0.46
2:B:288:THR:HB	2:B:328:ARG:H	1.80	0.46
2:B:324:ARG:HG2	2:B:325:ILE:H	1.80	0.46
3:P:23:VAL:HG11	3:P:47:ILE:HD12	1.97	0.46
2:G:218:GLU:HG2	2:G:219:GLY:N	2.29	0.46
2:A:217:VAL:HG22	2:A:218:GLU:N	2.31	0.46
2:A:266:PRO:O	2:A:267:ASN:C	2.58	0.46
2:B:112:MET:O	2:B:117:VAL:HG22	2.15	0.46
2:A:222:THR:O	2:A:223:TYR:C	2.59	0.46
2:A:296:ASP:CG	3:W:51:MET:HG2	2.40	0.46
2:B:273:GLY:O	2:B:290:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:3:GLN:HG3	3:P:64:ILE:HG13	1.97	0.46
2:G:32:SER:OG	2:G:33:THR:N	2.47	0.46
2:G:163:GLN:OE1	2:G:202:ARG:NH2	2.47	0.46
2:G:216:ILE:CD1	4:G:418:IOD:I	3.32	0.46
2:A:78:LEU:HD12	2:A:78:LEU:C	2.41	0.46
2:A:160:ASP:OD2	2:A:163:GLN:CB	2.64	0.46
3:W:8:VAL:O	3:W:10:LEU:N	2.49	0.46
3:W:50:LEU:C	3:W:50:LEU:CD2	2.89	0.46
3:P:76:LYS:O	3:P:77:LEU:C	2.59	0.46
2:G:252:LEU:HD12	2:G:252:LEU:N	2.31	0.46
3:J:15:GLN:O	3:J:16:ALA:C	2.59	0.46
2:A:132:VAL:C	2:A:134:GLU:N	2.73	0.46
2:B:27:PRO:O	2:B:27:PRO:HG2	2.16	0.46
2:B:61:THR:N	2:B:118:ASP:OD2	2.43	0.46
2:B:295:TYR:CD1	2:B:295:TYR:C	2.94	0.46
2:G:189:GLU:C	2:G:191:ILE:N	2.73	0.46
1:O:702:DG:O6	2:A:21:ARG:NH2	2.48	0.45
2:A:177:HIS:NE2	2:A:270:GLU:OE2	2.48	0.45
1:O:715:DG:H3'	2:B:28:ASN:ND2	2.31	0.45
2:A:200:TYR:CD1	2:A:200:TYR:C	2.93	0.45
2:A:212:ARG:H	2:A:212:ARG:CD	2.20	0.45
2:A:295:TYR:CE2	3:W:17:ARG:HB2	2.52	0.45
3:W:8:VAL:C	3:W:10:LEU:N	2.73	0.45
2:B:69:ASP:C	2:B:71:SER:H	2.23	0.45
2:B:223:TYR:CD1	2:B:223:TYR:C	2.95	0.45
2:G:46:TYR:HH	2:G:48:PRO:HA	1.81	0.45
2:G:330:SER:O	2:G:331:THR:CG2	2.63	0.45
2:A:30:LYS:CG	2:A:32:SER:HB3	2.46	0.45
2:A:277:THR:C	2:A:279:LEU:H	2.24	0.45
3:W:35:LEU:HD23	3:W:35:LEU:O	2.16	0.45
2:B:26:ASN:HD22	2:B:27:PRO:N	2.15	0.45
3:P:36:GLU:CG	3:P:41:LYS:HB2	2.33	0.45
2:A:166:PHE:CD1	2:A:166:PHE:C	2.94	0.45
2:A:229:ALA:O	2:A:230:VAL:C	2.58	0.45
2:A:264:ASN:O	2:A:268:ASP:HB2	2.16	0.45
2:G:8:VAL:HG13	2:G:40:THR:OG1	2.15	0.45
2:G:293:PRO:O	2:G:294:MET:C	2.57	0.45
2:A:162:GLU:OE2	2:A:202:ARG:NH1	2.41	0.45
2:A:197:VAL:HG22	2:A:216:ILE:HD11	1.99	0.45
2:A:273:GLY:O	2:A:290:VAL:HG23	2.15	0.45
3:W:19:ALA:O	3:W:22:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:66:GLN:O	3:P:66:GLN:CG	2.62	0.45
2:G:252:LEU:HG	2:G:283:VAL:CG2	2.44	0.45
2:A:8:VAL:HG12	2:A:19:VAL:HG22	1.98	0.45
2:A:130:GLU:O	2:A:133:GLU:CG	2.65	0.45
2:A:302:MET:O	2:A:306:THR:HG23	2.16	0.45
2:G:29:VAL:HG12	2:G:34:ARG:HB2	1.98	0.45
1:T:702:DG:C2'	1:T:703:DA:C8	2.98	0.45
1:R:705:DA:H2''	1:R:706:DG:O5'	2.16	0.45
2:A:162:GLU:O	2:A:163:GLN:C	2.58	0.45
2:A:211:VAL:HG23	2:A:211:VAL:O	2.16	0.45
1:R:709:DC:H5'	1:R:709:DC:C6	2.47	0.45
2:G:136:LYS:O	2:G:138:SER:N	2.50	0.45
2:G:304:LEU:O	2:G:304:LEU:CD2	2.65	0.45
2:G:320:GLU:O	2:G:321:LEU:C	2.59	0.45
2:A:22:VAL:CG2	2:A:23:VAL:N	2.80	0.45
3:W:82:GLN:O	3:W:83:GLU:HB3	2.16	0.45
3:P:53:LEU:HB3	3:P:55:ILE:HD11	1.98	0.45
2:G:10:ARG:HA	2:G:10:ARG:NE	2.31	0.45
3:W:50:LEU:C	3:W:50:LEU:HD22	2.42	0.45
2:B:137:LYS:HE2	2:B:137:LYS:CA	2.42	0.45
2:B:201:LYS:HD2	2:B:211:VAL:HG11	1.98	0.45
2:G:197:VAL:O	2:G:198:LYS:C	2.60	0.45
2:G:243:ILE:HG22	2:G:244:PHE:N	2.31	0.45
2:A:4:THR:HG21	2:A:6:TYR:HB3	1.97	0.44
2:A:4:THR:HG22	2:A:7:ASP:OD2	2.16	0.44
2:A:85:ILE:HG12	2:A:299:ALA:CB	2.46	0.44
2:A:170:GLN:O	2:A:171:SER:C	2.59	0.44
2:A:235:GLU:HG2	2:A:261:ARG:NH2	2.33	0.44
2:B:39:GLU:O	2:B:42:GLU:N	2.49	0.44
2:B:219:GLY:HA3	2:B:250:MET:SD	2.57	0.44
2:B:293:PRO:HG2	2:B:297:ILE:HD11	2.00	0.44
3:P:37:LYS:O	3:P:38:ASP:C	2.59	0.44
2:G:69:ASP:OD1	2:G:71:SER:HB2	2.17	0.44
2:G:179:ASN:HB2	2:G:241:THR:HG23	1.99	0.44
2:A:60:THR:N	2:A:118:ASP:OD2	2.46	0.44
2:B:69:ASP:O	2:B:71:SER:N	2.50	0.44
2:B:128:THR:C	2:B:130:GLU:N	2.74	0.44
2:B:137:LYS:O	2:B:138:SER:C	2.60	0.44
2:A:8:VAL:O	2:A:12:ALA:HB3	2.16	0.44
2:A:220:ASP:OD1	2:A:225:SER:HB3	2.17	0.44
2:B:4:THR:HG22	2:B:7:ASP:OD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:LEU:HG	2:B:309:MET:CE	2.42	0.44
3:P:8:VAL:HG12	3:P:59:THR:O	2.17	0.44
1:O:700:DC:H3'	2:A:29:VAL:CA	2.43	0.44
2:A:85:ILE:H	2:A:85:ILE:CD1	2.30	0.44
2:B:15:SER:O	2:B:18:THR:HB	2.17	0.44
2:B:105:GLN:HE22	2:B:124:SER:HB3	1.80	0.44
2:B:201:LYS:HD2	2:B:211:VAL:CG1	2.48	0.44
2:A:76:ALA:O	2:A:79:ALA:HB3	2.18	0.44
2:A:149:GLU:CD	2:A:154:ILE:HD11	2.41	0.44
2:A:190:PRO:C	2:A:192:ASN:H	2.24	0.44
2:B:122:PHE:CE1	2:B:127:VAL:HG22	2.53	0.44
2:B:227:ILE:O	2:B:231:GLU:HG3	2.18	0.44
2:B:264:ASN:O	2:B:268:ASP:HB2	2.18	0.44
2:B:307:LYS:NZ	3:P:48:MET:HE2	2.32	0.44
3:P:55:ILE:HG23	3:P:59:THR:HB	1.98	0.44
2:A:182:PHE:HB2	2:A:200:TYR:CD2	2.52	0.44
2:A:215:TYR:CZ	2:A:238:GLU:HB3	2.53	0.44
2:A:216:ILE:HG23	2:A:216:ILE:O	2.18	0.44
2:A:306:THR:C	2:A:308:TYR:H	2.26	0.44
2:B:295:TYR:C	2:B:295:TYR:HD1	2.25	0.44
3:P:41:LYS:C	3:P:41:LYS:HD2	2.42	0.44
2:G:132:VAL:HG22	2:G:154:ILE:HD12	2.00	0.44
2:G:278:ARG:O	2:G:281:THR:HG22	2.18	0.44
1:T:707:DC:H6	1:T:707:DC:H2'	1.67	0.44
1:R:709:DC:H2''	1:R:710:DT:O5'	2.18	0.44
3:W:23:VAL:O	3:W:27:ASN:ND2	2.51	0.44
2:B:4:THR:OG1	2:B:5:ILE:N	2.50	0.44
2:B:132:VAL:HG13	2:B:154:ILE:CG1	2.48	0.44
2:B:325:ILE:O	2:B:326:GLU:C	2.60	0.44
3:P:1:MET:HA	3:P:65:ALA:O	2.17	0.44
2:B:40:THR:O	2:B:40:THR:HG22	2.17	0.44
2:G:29:VAL:HG11	2:G:34:ARG:HB2	2.00	0.44
2:G:30:LYS:HG2	2:G:32:SER:H	1.83	0.44
2:B:81:GLY:HA2	2:B:295:TYR:CE1	2.53	0.44
2:B:95:LEU:HD23	2:B:95:LEU:C	2.42	0.44
2:G:96:SER:OG	2:G:108:LEU:HD13	2.18	0.44
1:R:714:DA:C1'	1:R:715:DG:H5''	2.45	0.43
2:A:31:PRO:HA	2:A:34:ARG:HB3	2.00	0.43
2:A:104:LYS:HA	4:A:410:IOD:I	2.87	0.43
2:G:269:LEU:HD23	2:G:269:LEU:O	2.18	0.43
3:J:4:GLN:O	3:J:62:THR:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:32:ASP:N	3:J:66:GLN:O	2.50	0.43
1:O:704:DA:H2''	1:O:705:DA:OP2	2.18	0.43
2:A:6:TYR:O	2:A:9:ALA:HB3	2.17	0.43
2:A:168:ALA:O	2:A:171:SER:HB3	2.18	0.43
2:A:225:SER:HA	2:A:228:GLU:OE1	2.18	0.43
3:W:50:LEU:HD22	3:W:50:LEU:O	2.19	0.43
2:B:42:GLU:OE2	2:B:42:GLU:HA	2.18	0.43
2:B:160:ASP:OD1	2:B:163:GLN:N	2.41	0.43
2:B:168:ALA:HB1	2:B:272:ILE:HD11	1.99	0.43
2:G:189:GLU:C	2:G:191:ILE:H	2.25	0.43
2:G:255:ILE:C	2:G:257:GLY:H	2.25	0.43
3:J:7:GLU:OE2	3:J:60:GLU:CG	2.67	0.43
2:A:132:VAL:O	2:A:134:GLU:N	2.51	0.43
2:A:182:PHE:CD2	2:A:182:PHE:C	2.96	0.43
2:A:189:GLU:O	2:A:191:ILE:N	2.51	0.43
2:A:191:ILE:HG22	2:A:191:ILE:O	2.18	0.43
2:B:53:ARG:O	2:B:54:GLY:C	2.62	0.43
2:G:4:THR:HG22	2:G:7:ASP:OD2	2.18	0.43
2:G:158:THR:HG22	2:G:320:GLU:HG2	2.00	0.43
2:A:218:GLU:CG	2:A:219:GLY:H	2.32	0.43
2:B:121:ILE:HD11	2:B:302:MET:HG2	2.00	0.43
2:B:305:LEU:O	2:B:309:MET:HG3	2.19	0.43
2:G:63:VAL:HG21	2:G:302:MET:HE1	2.00	0.43
2:G:283:VAL:CG1	2:G:284:ARG:N	2.80	0.43
2:A:85:ILE:CG1	2:A:299:ALA:HB1	2.47	0.43
2:B:140:VAL:HB	2:B:141:PRO:CD	2.48	0.43
2:B:292:GLN:O	2:B:294:MET:HE2	2.18	0.43
2:G:234:LEU:HD21	2:G:269:LEU:HD13	2.00	0.43
2:G:296:ASP:C	2:G:298:GLY:H	2.27	0.43
2:B:5:ILE:HG12	2:B:19:VAL:HG11	2.00	0.43
2:B:300:VAL:O	2:B:301:ALA:C	2.61	0.43
2:G:67:ILE:CD1	2:G:123:MET:SD	3.03	0.43
2:G:288:THR:HG22	2:G:327:PHE:HA	2.01	0.43
1:O:715:DG:C3'	2:B:28:ASN:ND2	2.82	0.43
2:A:86:ALA:CB	2:A:302:MET:HE2	2.49	0.43
2:A:214:SER:HB3	2:A:236:GLU:OE2	2.18	0.43
2:A:275:ASP:O	2:A:276:ASN:HB3	2.18	0.43
2:B:182:PHE:HE1	2:B:197:VAL:CG1	2.32	0.43
3:P:32:ASP:OD1	3:P:32:ASP:N	2.51	0.43
2:G:211:VAL:O	2:G:211:VAL:HG23	2.18	0.43
2:A:149:GLU:HG2	2:A:154:ILE:CD1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:149:GLU:CG	2:A:149:GLU:O	2.66	0.43
2:B:243:ILE:CG2	2:B:244:PHE:N	2.82	0.43
3:P:41:LYS:HD2	3:P:41:LYS:O	2.18	0.43
2:G:252:LEU:C	2:G:254:VAL:H	2.25	0.43
3:J:4:GLN:CG	3:J:5:LYS:N	2.82	0.43
2:A:105:GLN:HE22	2:A:124:SER:CB	2.29	0.43
2:A:218:GLU:HG2	2:A:219:GLY:N	2.34	0.43
2:A:224:ASP:C	2:A:226:GLY:N	2.77	0.43
2:A:255:ILE:HD13	2:A:271:ILE:HD12	2.01	0.43
2:G:49:ASN:O	2:G:51:VAL:N	2.52	0.43
3:J:9:ARG:C	3:J:83:GLU:HB2	2.43	0.43
3:J:27:ASN:C	3:J:29:PHE:H	2.26	0.43
2:A:287:LEU:HD12	2:A:288:THR:N	2.34	0.43
2:B:74:PHE:O	2:B:75:TYR:C	2.61	0.43
2:B:143:VAL:O	2:B:143:VAL:HG22	2.19	0.43
2:G:33:THR:HA	2:G:36:LYS:HE3	2.01	0.43
2:G:224:ASP:C	2:G:226:GLY:N	2.73	0.43
1:R:705:DA:H5"	1:R:705:DA:H8	1.84	0.42
2:B:72:ASN:O	2:B:74:PHE:N	2.52	0.42
2:B:245:VAL:HG11	2:B:251:ALA:CA	2.48	0.42
3:P:37:LYS:O	3:P:38:ASP:O	2.37	0.42
2:G:47:ARG:HD2	2:G:47:ARG:O	2.19	0.42
3:J:82:GLN:OE1	3:J:82:GLN:HA	2.18	0.42
2:A:22:VAL:HG21	2:A:37:VAL:HG12	1.98	0.42
2:A:84:ASP:O	2:A:85:ILE:C	2.61	0.42
3:P:23:VAL:HG13	3:P:46:SEP:N	2.34	0.42
3:P:37:LYS:HZ3	3:P:59:THR:HG21	1.83	0.42
2:G:101:ASN:O	2:G:102:GLN:C	2.62	0.42
3:J:9:ARG:HB2	3:J:83:GLU:CB	2.50	0.42
2:A:268:ASP:O	2:A:269:LEU:HB3	2.19	0.42
2:A:295:TYR:CD1	2:A:295:TYR:C	2.98	0.42
2:B:6:TYR:HA	2:B:16:MET:HE3	2.00	0.42
2:B:49:ASN:OD1	2:B:49:ASN:C	2.63	0.42
2:B:157:VAL:HG23	2:B:319:VAL:HG12	2.01	0.42
2:G:34:ARG:O	2:G:37:VAL:HB	2.19	0.42
2:G:227:ILE:N	2:G:253:GLY:O	2.52	0.42
3:J:50:LEU:C	3:J:52:SER:H	2.27	0.42
2:A:94:ILE:HG22	2:A:112:MET:HE2	2.01	0.42
2:B:26:ASN:C	2:B:26:ASN:ND2	2.78	0.42
2:B:170:GLN:HA	2:B:170:GLN:HE21	1.84	0.42
2:B:273:GLY:C	2:B:289:SER:HB2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:8:VAL:O	3:P:8:VAL:HG13	2.18	0.42
3:P:38:ASP:OD1	3:P:38:ASP:N	2.51	0.42
2:G:227:ILE:HA	2:G:230:VAL:HG23	2.00	0.42
2:G:252:LEU:HD12	2:G:252:LEU:H	1.84	0.42
3:W:1:MET:C	3:W:1:MET:HE3	2.44	0.42
2:B:36:LYS:O	2:B:39:GLU:HG2	2.20	0.42
2:B:72:ASN:C	2:B:74:PHE:N	2.77	0.42
2:G:33:THR:O	2:G:36:LYS:HB3	2.20	0.42
3:J:50:LEU:C	3:J:50:LEU:CD2	2.91	0.42
2:A:155:PRO:HA	2:A:317:SER:HB3	2.01	0.42
2:A:188:GLU:O	2:A:190:PRO:HD3	2.19	0.42
2:A:190:PRO:O	2:A:194:ALA:HB3	2.20	0.42
2:A:232:LYS:HB2	2:A:232:LYS:HE3	1.84	0.42
2:B:114:GLY:C	2:B:116:GLN:H	2.26	0.42
2:B:157:VAL:HA	2:B:319:VAL:HB	2.01	0.42
2:B:244:PHE:HA	2:B:272:ILE:O	2.20	0.42
3:P:7:GLU:CG	3:P:8:VAL:H	2.33	0.42
2:G:19:VAL:HG13	2:G:22:VAL:HG21	2.02	0.42
2:G:288:THR:HG21	2:G:331:THR:HG1	1.83	0.42
2:A:78:LEU:HG	2:A:123:MET:SD	2.60	0.42
2:B:84:ASP:OD1	2:B:84:ASP:N	2.52	0.42
2:B:113:LEU:CD2	2:B:139:PRO:HD2	2.49	0.42
2:G:82:ILE:HG23	2:G:302:MET:HG2	2.01	0.42
2:G:223:TYR:CD1	2:G:223:TYR:C	2.98	0.42
3:J:74:LEU:O	3:J:75:GLU:C	2.63	0.42
1:T:712:DA:C2'	1:T:713:DC:O5'	2.63	0.42
2:B:45:GLY:O	2:B:46:TYR:C	2.62	0.42
2:B:170:GLN:O	2:B:172:LEU:N	2.52	0.42
2:B:195:LYS:HE3	2:B:198:LYS:NZ	2.34	0.42
2:G:212:ARG:H	2:G:212:ARG:CD	2.25	0.42
2:G:330:SER:C	2:G:331:THR:HG23	2.44	0.42
1:T:702:DG:OP2	2:B:15:SER:HB3	2.20	0.42
2:A:230:VAL:HG22	2:A:254:VAL:CG1	2.36	0.42
3:W:7:GLU:CG	3:W:8:VAL:H	2.19	0.42
3:W:27:ASN:N	3:W:27:ASN:HD22	2.17	0.42
2:B:133:GLU:O	2:B:137:LYS:HG2	2.20	0.42
2:B:170:GLN:HE21	2:B:170:GLN:CA	2.33	0.42
2:B:170:GLN:C	2:B:172:LEU:N	2.77	0.42
3:P:41:LYS:HB3	3:P:41:LYS:HE3	1.77	0.42
2:G:224:ASP:O	2:G:225:SER:C	2.63	0.42
3:J:80:TYR:CD2	3:J:81:VAL:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:160:ASP:OD2	2:A:163:GLN:HG2	2.20	0.42
2:B:155:PRO:HA	2:B:317:SER:O	2.20	0.42
2:G:104:LYS:NZ	2:G:107:HIS:CD2	2.88	0.42
2:G:157:VAL:CG1	2:G:297:ILE:HG22	2.49	0.42
3:J:16:ALA:HB3	3:J:18:PRO:HD2	2.01	0.42
1:O:702:DG:H5''	2:A:15:SER:HB2	2.00	0.41
1:R:715:DG:H5'	1:R:715:DG:C8	2.53	0.41
2:A:60:THR:O	2:A:61:THR:CB	2.62	0.41
3:W:29:PHE:CE2	3:W:73:ALA:HA	2.55	0.41
2:B:5:ILE:CG2	2:B:6:TYR:N	2.83	0.41
2:B:6:TYR:O	2:B:10:ARG:HG2	2.20	0.41
2:B:190:PRO:O	2:B:191:ILE:C	2.63	0.41
3:P:36:GLU:N	3:P:62:THR:O	2.46	0.41
2:G:251:ALA:O	2:G:254:VAL:N	2.49	0.41
2:G:278:ARG:O	2:G:282:MET:HG3	2.20	0.41
3:J:9:ARG:CB	3:J:83:GLU:HB2	2.50	0.41
3:W:29:PHE:CZ	3:W:73:ALA:HA	2.55	0.41
2:B:157:VAL:HG23	2:B:319:VAL:CG1	2.51	0.41
2:G:166:PHE:CE2	2:G:203:ALA:HA	2.55	0.41
2:G:248:ASP:O	2:G:251:ALA:HB3	2.19	0.41
2:G:274:PHE:O	2:G:275:ASP:CB	2.66	0.41
2:G:304:LEU:CD2	2:G:304:LEU:C	2.93	0.41
3:J:36:GLU:HB3	3:J:41:LYS:HA	2.02	0.41
2:A:72:ASN:O	2:A:73:ILE:C	2.63	0.41
2:A:216:ILE:O	2:A:216:ILE:HG12	2.20	0.41
3:W:50:LEU:CD2	3:W:50:LEU:O	2.68	0.41
2:B:212:ARG:C	2:B:214:SER:N	2.78	0.41
1:R:700:DC:H6	2:G:28:ASN:O	2.03	0.41
2:A:131:HIS:O	2:A:132:VAL:C	2.63	0.41
2:A:189:GLU:O	2:A:192:ASN:N	2.53	0.41
2:A:212:ARG:NH1	2:A:212:ARG:HG3	2.35	0.41
2:A:263:LEU:H	2:A:263:LEU:HD12	1.84	0.41
3:P:5:LYS:C	3:P:6:VAL:HG22	2.46	0.41
2:G:189:GLU:HB3	2:G:191:ILE:HG12	2.03	0.41
2:G:247:THR:CG2	2:G:248:ASP:N	2.84	0.41
2:A:86:ALA:HB2	2:A:302:MET:HG2	2.03	0.41
2:B:140:VAL:HB	2:B:141:PRO:HD2	2.03	0.41
2:A:252:LEU:HD23	2:A:252:LEU:C	2.45	0.41
2:B:122:PHE:CD1	2:B:122:PHE:C	2.99	0.41
2:B:217:VAL:HG13	2:B:233:LEU:HD21	2.01	0.41
2:G:22:VAL:HG23	2:G:23:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:124:SER:C	2:G:126:ASN:N	2.75	0.41
2:G:172:LEU:HD13	2:G:180:ILE:HG21	2.02	0.41
2:G:233:LEU:O	2:G:235:GLU:N	2.54	0.41
2:G:245:VAL:HG11	2:G:251:ALA:CA	2.51	0.41
2:G:272:ILE:C	2:G:272:ILE:CD1	2.94	0.41
2:G:286:GLN:HB3	2:G:328:ARG:CB	2.43	0.41
1:R:702:DG:N2	1:R:703:DA:C2	2.89	0.41
2:A:307:LYS:NZ	3:W:48:MET:CE	2.76	0.41
3:W:18:PRO:O	3:W:19:ALA:C	2.63	0.41
3:W:36:GLU:HG2	3:W:41:LYS:CB	2.39	0.41
3:W:78:ALA:O	3:W:82:GLN:HG2	2.20	0.41
2:B:106:LEU:HD21	2:B:131:HIS:CG	2.56	0.41
2:B:226:GLY:O	2:B:230:VAL:HG23	2.20	0.41
2:G:247:THR:HB	2:G:250:MET:CB	2.51	0.41
1:O:701:DT:H1'	1:O:702:DG:N7	2.35	0.41
2:A:65:VAL:O	2:A:65:VAL:HG23	2.19	0.41
2:A:106:LEU:HD21	2:A:134:GLU:CD	2.46	0.41
2:G:49:ASN:C	2:G:51:VAL:N	2.79	0.41
2:G:81:GLY:C	2:G:83:GLU:N	2.78	0.41
2:G:124:SER:C	2:G:126:ASN:H	2.29	0.41
2:G:245:VAL:HG21	2:G:251:ALA:CB	2.51	0.41
2:A:265:VAL:HG13	2:A:269:LEU:O	2.20	0.41
2:B:144:LEU:HG	2:B:154:ILE:CG2	2.51	0.41
2:B:159:ILE:HD13	2:B:159:ILE:HG21	1.81	0.41
2:B:190:PRO:CA	2:B:193:HIS:CE1	2.97	0.41
2:B:209:LEU:HD23	2:B:209:LEU:HA	1.91	0.41
3:P:7:GLU:HG3	3:P:8:VAL:H	1.84	0.41
3:P:8:VAL:HG23	3:P:81:VAL:CG1	2.51	0.41
2:G:137:LYS:HA	2:G:137:LYS:HD3	1.76	0.41
2:G:226:GLY:O	2:G:229:ALA:HB3	2.21	0.41
2:G:251:ALA:O	2:G:252:LEU:C	2.64	0.41
3:J:1:MET:HE2	3:J:64:ILE:HG21	2.03	0.41
3:J:23:VAL:HG11	3:J:47:ILE:HD12	2.02	0.41
2:A:12:ALA:C	2:A:36:LYS:HZ2	2.28	0.41
2:B:141:PRO:HB2	2:B:305:LEU:CD1	2.50	0.41
3:P:71:GLN:O	3:P:72:GLU:C	2.63	0.41
2:G:88:MET:HE3	2:G:89:TYR:CE2	2.57	0.41
2:A:163:GLN:O	2:A:166:PHE:N	2.54	0.40
2:A:295:TYR:CZ	3:W:17:ARG:HA	2.56	0.40
2:A:296:ASP:HB3	2:A:321:LEU:CD2	2.51	0.40
2:B:251:ALA:C	2:B:253:GLY:N	2.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:82:GLN:C	3:P:84:GLU:N	2.78	0.40
2:G:1:MET:HG3	2:G:47:ARG:HH22	1.86	0.40
2:G:133:GLU:O	2:G:133:GLU:OE1	2.38	0.40
2:A:30:LYS:O	2:A:34:ARG:N	2.42	0.40
2:A:46:TYR:CD1	2:A:46:TYR:C	2.99	0.40
2:A:228:GLU:O	2:A:229:ALA:C	2.63	0.40
3:P:2:VAL:C	3:P:3:GLN:O	2.64	0.40
2:G:68:PRO:HD3	2:G:123:MET:HG3	2.02	0.40
2:G:271:ILE:O	2:G:330:SER:OG	2.35	0.40
3:J:1:MET:N	3:J:70:GLU:OE1	2.50	0.40
3:J:8:VAL:C	3:J:10:LEU:N	2.78	0.40
2:A:72:ASN:ND2	2:A:74:PHE:HB3	2.37	0.40
2:A:248:ASP:O	2:A:249:GLU:C	2.64	0.40
2:A:283:VAL:HG12	2:A:284:ARG:H	1.86	0.40
2:B:46:TYR:C	2:B:46:TYR:CD1	2.99	0.40
2:B:180:ILE:O	2:B:180:ILE:HG13	2.21	0.40
2:B:193:HIS:HA	2:B:197:VAL:CG2	2.51	0.40
3:P:59:THR:CG2	3:P:60:GLU:N	2.83	0.40
2:A:287:LEU:O	2:A:328:ARG:CD	2.66	0.40
2:B:157:VAL:HG11	2:B:301:ALA:CB	2.49	0.40
2:G:122:PHE:CD1	2:G:122:PHE:C	3.00	0.40
2:G:172:LEU:O	2:G:173:ILE:C	2.64	0.40
1:R:705:DA:H2''	1:R:706:DG:O4'	2.21	0.40
2:A:35:LYS:C	2:A:37:VAL:N	2.78	0.40
2:A:164:ALA:HA	2:A:323:HIS:CD2	2.56	0.40
2:A:202:ARG:O	2:A:206:GLU:CB	2.70	0.40
2:B:88:MET:HE2	3:P:24:GLN:HG3	2.03	0.40
2:B:217:VAL:CG2	2:B:229:ALA:HB1	2.51	0.40
2:B:223:TYR:HA	2:B:249:GLU:O	2.22	0.40
3:P:36:GLU:HG3	3:P:40:LYS:O	2.22	0.40
2:G:53:ARG:O	2:G:56:ALA:N	2.53	0.40
3:J:23:VAL:CG2	3:J:50:LEU:HD13	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	330/332 (99%)	261 (79%)	54 (16%)	15 (4%)	2	10
2	B	330/332 (99%)	257 (78%)	61 (18%)	12 (4%)	2	14
2	G	325/332 (98%)	242 (74%)	69 (21%)	14 (4%)	2	11
3	J	81/85 (95%)	56 (69%)	19 (24%)	6 (7%)	1	3
3	P	81/85 (95%)	54 (67%)	23 (28%)	4 (5%)	1	9
3	W	81/85 (95%)	65 (80%)	13 (16%)	3 (4%)	2	13
All	All	1228/1251 (98%)	935 (76%)	239 (20%)	54 (4%)	2	10

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	28	ASN
2	B	28	ASN
2	B	275	ASP
3	P	38	ASP
2	G	27	PRO
3	J	16	ALA
2	A	211	VAL
2	A	275	ASP
3	W	9	ARG
2	B	70	ILE
3	P	3	GLN
3	P	9	ARG
2	G	137	LYS
2	G	261	ARG
2	G	275	ASP
2	G	329	GLN
3	J	9	ARG
3	J	83	GLU
2	A	109	LEU
2	A	133	GLU
2	B	73	ILE
2	B	90	LYS
2	B	261	ARG
2	G	50	ALA
3	J	8	VAL
3	J	80	TYR

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Mol	Chain	Res	Type
3	W	8	VAL
3	W	73	ALA
2	G	167	ASP
2	G	211	VAL
2	G	279	LEU
2	G	318	ILE
3	J	55	ILE
2	A	99	ASP
2	A	220	ASP
2	A	223	TYR
2	A	225	SER
2	B	151	THR
2	B	294	MET
2	G	26	ASN
2	G	237	ASP
2	B	171	SER
2	A	132	VAL
2	A	190	PRO
2	B	37	VAL
2	B	325	ILE
2	G	265	VAL
2	A	70	ILE
2	A	191	ILE
2	A	68	PRO
2	A	239	LYS
2	G	68	PRO
2	B	211	VAL
3	P	8	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	285/289 (99%)	247 (87%)	38 (13%)	4	17
2	B	289/289 (100%)	257 (89%)	32 (11%)	6	23
2	G	284/289 (98%)	243 (86%)	41 (14%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	68/69 (99%)	58 (85%)	10 (15%)	3	14
3	P	68/69 (99%)	59 (87%)	9 (13%)	4	17
3	W	68/69 (99%)	56 (82%)	12 (18%)	2	9
All	All	1062/1074 (99%)	920 (87%)	142 (13%)	4	16

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	4	THR
2	A	11	GLU
2	A	18	THR
2	A	39	GLU
2	A	55	LEU
2	A	58	LYS
2	A	72	ASN
2	A	73	ILE
2	A	78	LEU
2	A	85	ILE
2	A	92	ASN
2	A	94	ILE
2	A	106	LEU
2	A	112	MET
2	A	113	LEU
2	A	143	VAL
2	A	149	GLU
2	A	154	ILE
2	A	157	VAL
2	A	158	THR
2	A	170	GLN
2	A	174	ASP
2	A	180	ILE
2	A	207	SER
2	A	212	ARG
2	A	237	ASP
2	A	238	GLU
2	A	239	LYS
2	A	245	VAL
2	A	247	THR
2	A	261	ARG
2	A	279	LEU
2	A	282	MET

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Mol	Chain	Res	Type
2	A	283	VAL
2	A	304	LEU
2	A	308	TYR
2	A	315	ASP
2	A	332	LYS
3	W	1	MET
3	W	6	VAL
3	W	9	ARG
3	W	30	THR
3	W	37	LYS
3	W	50	LEU
3	W	51	MET
3	W	55	ILE
3	W	56	SER
3	W	71	GLN
3	W	74	LEU
3	W	77	LEU
2	B	4	THR
2	B	5	ILE
2	B	22	VAL
2	B	38	LEU
2	B	55	LEU
2	B	68	PRO
2	B	78	LEU
2	B	100	GLN
2	B	101	ASN
2	B	117	VAL
2	B	143	VAL
2	B	148	ILE
2	B	151	THR
2	B	188	GLU
2	B	195	LYS
2	B	197	VAL
2	B	204	LEU
2	B	205	THR
2	B	215	TYR
2	B	217	VAL
2	B	224	ASP
2	B	227	ILE
2	B	248	ASP
2	B	259	GLN
2	B	272	ILE

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Mol	Chain	Res	Type
2	B	284	ARG
2	B	287	LEU
2	B	294	MET
2	B	302	MET
2	B	304	LEU
2	B	311	LYS
2	B	315	ASP
3	P	5	LYS
3	P	6	VAL
3	P	21	LEU
3	P	38	ASP
3	P	42	VAL
3	P	55	ILE
3	P	62	THR
3	P	76	LYS
3	P	82	GLN
2	G	11	GLU
2	G	30	LYS
2	G	47	ARG
2	G	55	LEU
2	G	58	LYS
2	G	61	THR
2	G	63	VAL
2	G	65	VAL
2	G	67	ILE
2	G	70	ILE
2	G	71	SER
2	G	73	ILE
2	G	78	LEU
2	G	85	ILE
2	G	87	SER
2	G	92	ASN
2	G	94	ILE
2	G	96	SER
2	G	102	GLN
2	G	122	PHE
2	G	133	GLU
2	G	140	VAL
2	G	143	VAL
2	G	148	ILE
2	G	149	GLU
2	G	155	PRO

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Mol	Chain	Res	Type
2	G	158	THR
2	G	159	ILE
2	G	170	GLN
2	G	174	ASP
2	G	180	ILE
2	G	186	THR
2	G	188	GLU
2	G	207	SER
2	G	214	SER
2	G	272	ILE
2	G	293	PRO
2	G	302	MET
2	G	304	LEU
2	G	311	LYS
2	G	326	GLU
3	J	2	VAL
3	J	6	VAL
3	J	9	ARG
3	J	31	SER
3	J	40	LYS
3	J	47	ILE
3	J	61	ILE
3	J	70	GLU
3	J	81	VAL
3	J	82	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	2	ASN
2	A	24	ASN
2	A	97	ASN
2	A	105	GLN
2	A	110	ASN
2	A	126	ASN
2	A	170	GLN
2	A	193	HIS
2	A	256	HIS
2	A	267	ASN
2	A	329	GLN
3	W	3	GLN
3	W	27	ASN

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Mol	Chain	Res	Type
3	W	82	GLN
2	B	2	ASN
2	B	26	ASN
2	B	28	ASN
2	B	97	ASN
2	B	105	GLN
2	B	152	ASN
2	B	163	GLN
2	B	170	GLN
2	B	192	ASN
2	B	193	HIS
2	B	310	ASN
3	P	24	GLN
3	P	27	ASN
3	P	71	GLN
2	G	24	ASN
2	G	97	ASN
2	G	101	ASN
2	G	105	GLN
2	G	107	HIS
2	G	110	ASN
2	G	152	ASN
2	G	170	GLN
2	G	329	GLN
3	J	3	GLN
3	J	24	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SEP	W	46	3	8,9,10	1.03	0	7,12,14	1.72	2 (28%)
3	SEP	J	46	3	8,9,10	1.08	0	7,12,14	1.94	2 (28%)
3	SEP	P	46	3	8,9,10	0.95	0	7,12,14	2.12	2 (28%)

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
3	SEP	W	46	3	-	6/6/8/10	-
3	SEP	J	46	3	-	5/6/8/10	-
3	SEP	P	46	3	-	5/6/8/10	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	46	SEP	OG-CB-CA	3.94	111.97	108.14
3	J	46	SEP	OG-CB-CA	3.74	111.78	108.14
3	P	46	SEP	O3P-P-O1P	3.13	123.05	110.83
3	J	46	SEP	O3P-P-O1P	2.95	122.34	110.83
3	W	46	SEP	O3P-P-O1P	2.95	122.32	110.83
3	W	46	SEP	OG-CB-CA	2.26	110.35	108.14

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	W	46	SEP	C-CA-CB-OG
3	W	46	SEP	CA-CB-OG-P
3	W	46	SEP	CB-OG-P-O1P
3	W	46	SEP	CB-OG-P-O2P
3	W	46	SEP	CB-OG-P-O3P
3	P	46	SEP	N-CA-CB-OG
3	P	46	SEP	C-CA-CB-OG
3	P	46	SEP	CB-OG-P-O2P
3	P	46	SEP	CB-OG-P-O3P
3	J	46	SEP	N-CA-CB-OG
3	J	46	SEP	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
3	J	46	SEP	CB-OG-P-O2P
3	J	46	SEP	CB-OG-P-O3P
3	P	46	SEP	CA-CB-OG-P
3	W	46	SEP	N-CA-CB-OG
3	J	46	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	46	SEP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	O	16/16 (100%)	-0.08	0 100 100	33, 82, 107, 108	0
1	R	16/16 (100%)	0.24	1 (6%) 26 16	32, 78, 135, 151	0
1	T	16/16 (100%)	-0.03	0 100 100	50, 72, 119, 137	0
2	A	332/332 (100%)	0.01	4 (1%) 76 59	25, 72, 106, 137	0
2	B	332/332 (100%)	0.04	5 (1%) 72 53	25, 63, 100, 125	0
2	G	329/332 (99%)	-0.03	5 (1%) 72 53	15, 63, 117, 144	0
3	J	83/85 (97%)	-0.09	3 (3%) 46 29	23, 60, 80, 115	0
3	P	83/85 (97%)	-0.13	0 100 100	38, 72, 92, 119	0
3	W	83/85 (97%)	-0.41	0 100 100	32, 58, 77, 110	0
All	All	1290/1299 (99%)	-0.03	18 (1%) 73 55	15, 65, 107, 151	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	7	ASP	3.1
2	G	211	VAL	3.0
2	B	269	LEU	2.8
1	R	700	DC	2.7
2	A	110	ASN	2.7
2	G	41	ILE	2.6
3	J	12	THR	2.6
2	B	230	VAL	2.5
2	A	164	ALA	2.5
2	B	215	TYR	2.4
3	J	81	VAL	2.4
2	G	37	VAL	2.4
2	G	209	LEU	2.4
2	A	6	TYR	2.3
3	J	8	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	234	LEU	2.3
2	B	205	THR	2.3
2	B	181	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SEP	P	46	10/11	0.97	0.05	49,56,58,59	0
3	SEP	W	46	10/11	0.98	0.04	23,39,49,49	0
3	SEP	J	46	10/11	0.98	0.05	22,33,37,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	IOD	O	415	1/1	0.88	0.08	111,111,111,111	1
4	IOD	B	422	1/1	0.93	0.06	114,114,114,114	1
4	IOD	P	421	1/1	0.94	0.10	99,99,99,99	1
4	IOD	A	410	1/1	0.95	0.06	77,77,77,77	1
4	IOD	B	420	1/1	0.95	0.11	110,110,110,110	1
4	IOD	A	411	1/1	0.95	0.07	120,120,120,120	1
4	IOD	G	418	1/1	0.95	0.06	98,98,98,98	1
4	IOD	B	419	1/1	0.97	0.06	109,109,109,109	1
4	IOD	A	412	1/1	0.97	0.07	95,95,95,95	1
4	IOD	A	413	1/1	0.98	0.04	66,66,66,66	1
4	IOD	G	414	1/1	0.99	0.12	45,45,45,45	1

6.5 Other polymers [i](#)

There are no such residues in this entry.