Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2017 – 12:14 AM EST

PDB ID	:	1ZVV
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

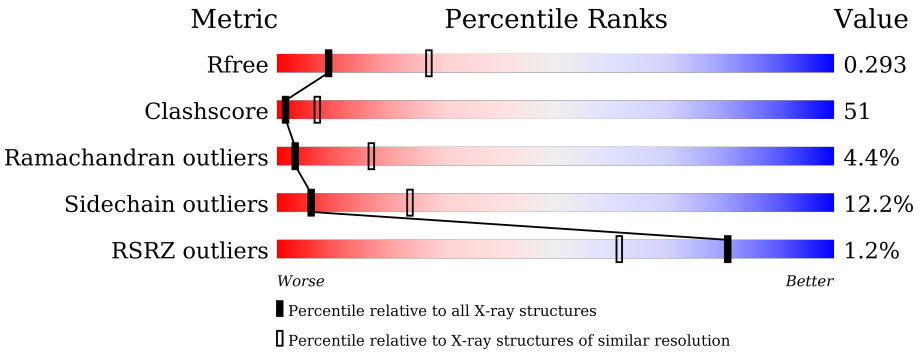
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	O	16	100%
1	R	16	6% 100%
1	T	16	100%
2	A	332	% 33% 56% 11%
2	B	332	% 32% 58% 10%
2	G	332	2% 35% 54% 10%

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Mol	Chain	Length	Quality of chain
3	J	85	35% 52% 11%
3	P	85	28% 60% 9%
3	W	85	2% 33% 53% 13%

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	414	-	-	-	X
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	C	N	O	P	S	0	0	0
			652	407	109	132	1	3			
3	P	84	Total	C	N	O	P	S	0	0	0
			652	407	109	132	1	3			
3	J	84	Total	C	N	O	P	S	0	0	0
			652	407	109	132	1	3			

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 (three-letter code: IOD) (formula: I).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	9	Total	O	0	0
			9	9		
5	G	12	Total	O	0	0
			12	12		

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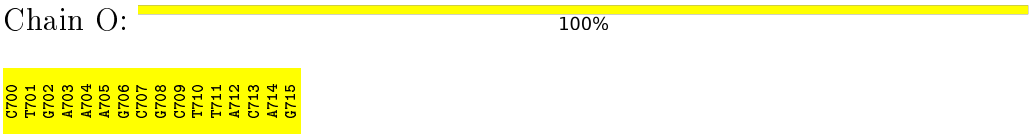
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	6	Total O 6 6	0	0
5	P	2	Total O 2 2	0	0
5	T	1	Total O 1 1	0	0
5	W	6	Total O 6 6	0	0

3 Residue-property plots (i)

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

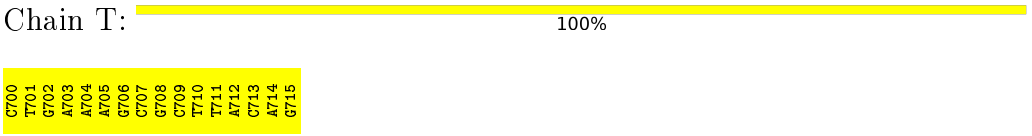
- Molecule 1: DNA recognition strand CRE

Chain O:



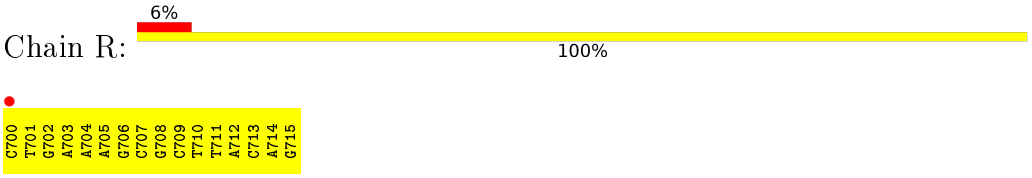
- Molecule 1: DNA recognition strand CRE

Chain T:



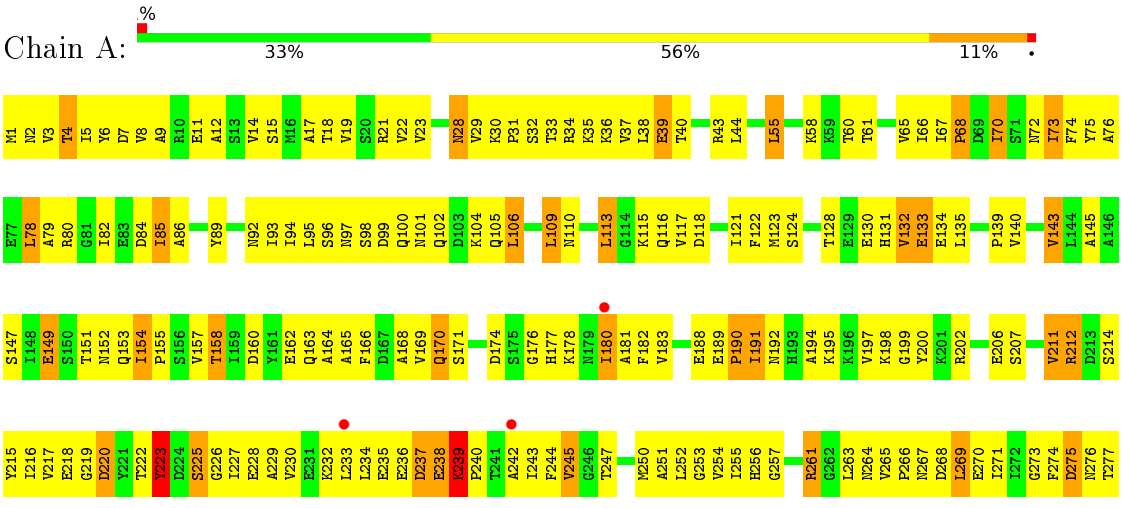
- Molecule 1: DNA recognition strand CRE

Chain R:



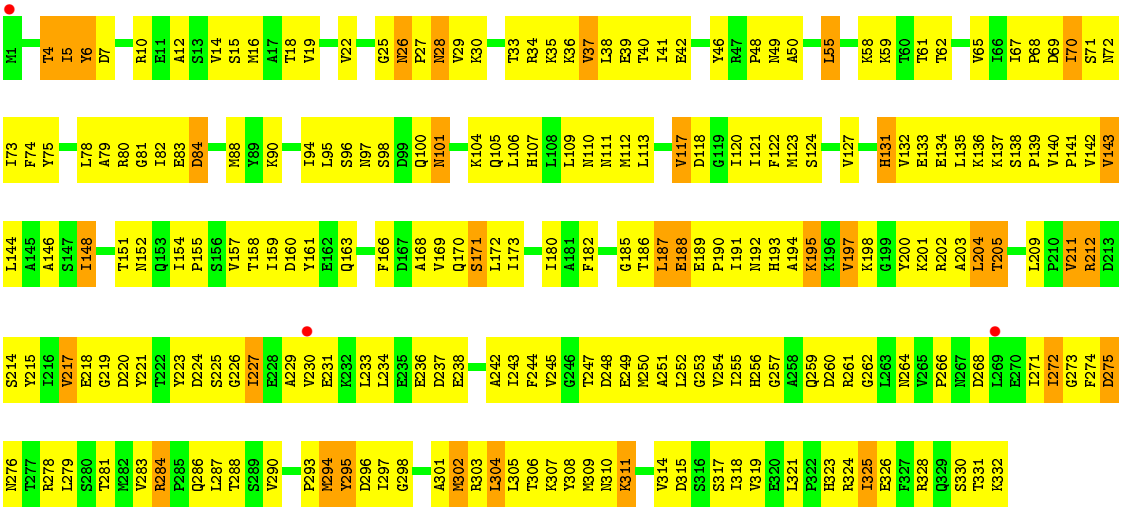
- Molecule 2: Glucose-resistance amylase regulator

Chain A:



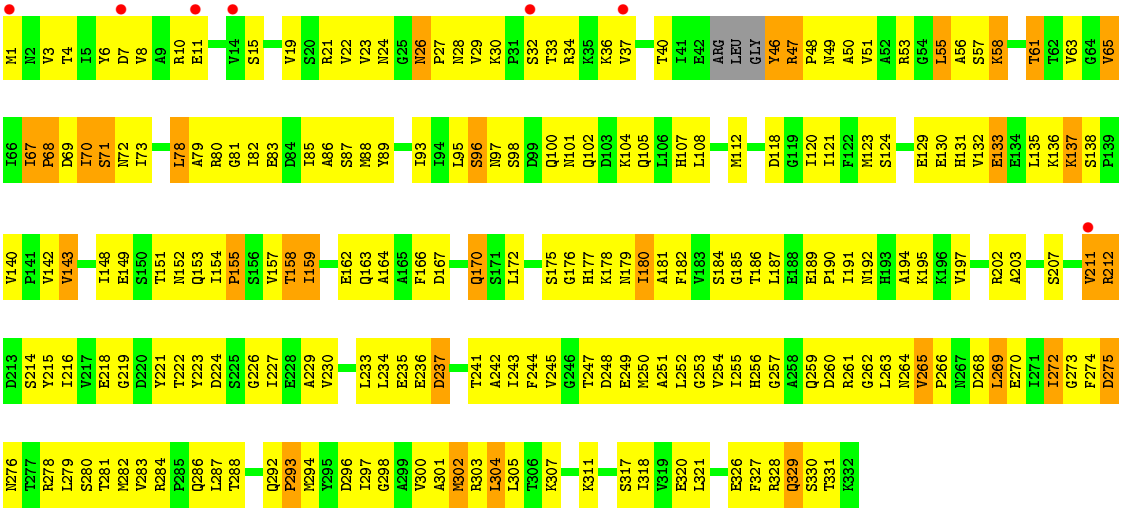
• Molecule 2: Glucose-resistance amylase regulator

Chain B:



• Molecule 2: Glucose-resistance amylase regulator

Chain G:

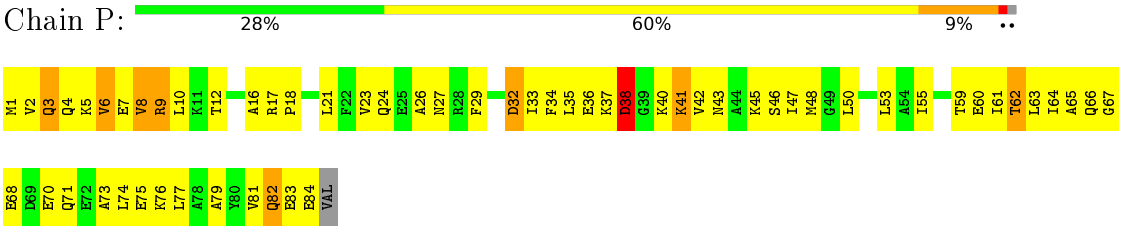


• Molecule 3: HPr-like protein crh

Chain W:

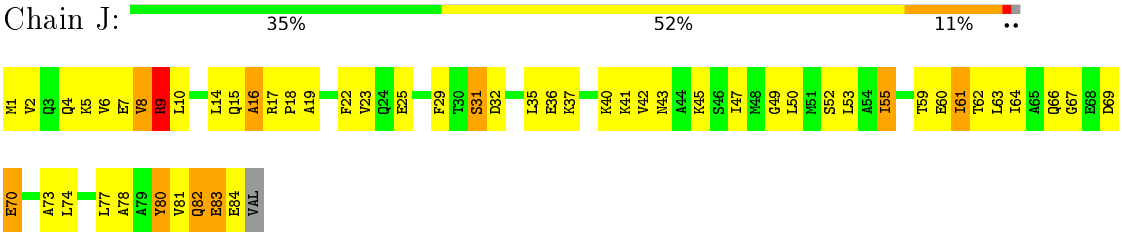
- Molecule 3: HPr-like protein crh

Chain P:



- Molecule 3: HPr-like protein crh

Chain J:



4 Data and refinement statistics (i)

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 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.2 (79.05-2.98) 91.6 (79.05-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.298 0.226 , 0.293	Depositor DCC
R_{free} test set	2450 reflections (8.74%)	DCC
Wilson B-factor (Å^2)	68.9	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 71.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	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.*

[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: 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	0.53	0/366	0.77	0/563
1	R	0.53	0/366	0.83	0/563
1	T	0.51	0/366	0.75	0/563
2	A	0.43	0/2596	0.70	0/3513
2	B	0.46	0/2610	0.76	1/3536 (0.0%)
2	G	0.46	0/2574	0.72	0/3484
3	J	0.54	0/645	0.75	0/863
3	P	0.44	0/645	0.72	0/863
3	W	0.57	0/645	0.83	1/863 (0.1%)
All	All	0.47	0/10813	0.74	2/14811 (0.0%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	W	63	LEU	CA-CB-CG	6.79	130.92	115.30
2	B	187	LEU	CA-CB-CG	5.15	127.14	115.30

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	277	0
2	B	2572	0	2602	259	0
2	G	2538	0	2557	249	0
3	J	652	0	668	72	0
3	P	652	0	668	86	0
3	W	652	0	668	80	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	1074	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 51.

All (1074) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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: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:H6	1:O:707:DC:H5'	1.40	0.85
2:B:68:PRO:HD3	2:B:123:MET:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	3:W:55:ILE:HD12	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
3:J:9:ARG:HD2	3:J:82:GLN:HE22	1.39	0.83
1:T:705:DA:H2"	1:T:706:DG:OP2	1.78	0.83
3:J:42:VAL:HG11	3:J:53:LEU:HD21	1.60	0.83
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
2:A:22:VAL:HG21	2:A:37:VAL:HG11	1.62	0.81
2:A:154:ILE:H	2:A:154:ILE:HD12	1.45	0.81
2:B:152:ASN:HD22	2:B:318:ILE:HG12	1.45	0.81
1:T:708:DG:H2"	1:T:709:DC:H5"	1.62	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
2:G:286:GLN:HB3	2:G:328:ARG:HB3	1.64	0.80
1:O:712:DA:H2"	1:O:713:DC:H5'	1.63	0.80
2:A:113:LEU:HD11	2:A:139:PRO:HD2	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: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:HA	2:B:137:LYS:HE2	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:B:187:LEU:HG	2:B:218:GLU:CD	2.04	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:181:ALA:HA	2:A:215:TYR:HB3	1.67	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
1:R:714:DA:H1'	1:R:715:DG:H5"	1.67	0.77
3:W:2:VAL:HG12	3:W:74:LEU:HD22	1.65	0.77
1:O:700:DC:H5"	2:A:28:ASN:C	2.05	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
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
2:A:239:LYS:HD2	2:A:239:LYS:H	1.51	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
3:P:63:LEU:C	3:P:64:ILE:HD12	2.07	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:HD2	2:A:212:ARG:H	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:G:85:ILE:HG21	2:G:302:MET:HB3	1.71	0.73
2:B:295:TYR:OH	3:P:17:ARG:HG3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:60:THR:O	2:A:61:THR:HB	1.89	0.72
2:B:250:MET:O	2:B:254:VAL:HG23	1.89	0.72
1:O:700:DC:H3'	2:A:29:VAL:HA	1.71	0.72
2:A:149:GLU:CG	2:A:154:ILE:HD11	2.18	0.72
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
3:W:82:GLN:C	3:W:84:GLU:H	1.93	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
2:G:260:ASP:C	2:G:262:GLY:H	1.95	0.70
2:B:276:ASN:OD1	2:B:328:ARG:NH2	2.24	0.70
2:G:85:ILE:CG2	2:G:302:MET:HB3	2.21	0.70
1:T:702:DG:H5'	1:T:702:DG:H8	1.56	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
3:P:63:LEU:O	3:P:64:ILE:HD12	1.91	0.70
2:G:65:VAL:HG11	2:G:93:ILE:HD11	1.73	0.70
1:R:708:DG:H1'	1:R:709:DC:H5"	1.72	0.70
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
2:G:176:GLY:O	2:G:178:LYS:HG3	1.91	0.69
3:P:66:GLN:HG3	3:P:66:GLN:O	1.92	0.69
3:P:42:VAL:HG12	3:P:43:ASN:H	1.58	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: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
2:G:4:THR:HG23	2:G:7:ASP:H	1.59	0.68
3:W:9:ARG:CG	3:W:9:ARG:HH11	2.06	0.68
2:B:245:VAL:HG21	2:B:254:VAL:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:46:TYR:OH	2:G:48:PRO:HA	1.92	0.68
3:W:9:ARG:HG3	3:W:9:ARG:HH11	1.58	0.68
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
3:J:7:GLU:HG3	3:J:8:VAL:N	2.08	0.68
3:W:61:ILE:HD12	3:W:61:ILE:O	1.93	0.67
2:G:63:VAL:HG21	2:G:302:MET:CE	2.24	0.67
3:W:4:GLN:HG2	3:W:6:VAL:HG22	1.76	0.67
2:A:166:PHE:CE1	2:A:170:GLN:HG3	2.30	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: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:G:4:THR:OG1	2:G:6:TYR:HB3	1.95	0.67
2:B:161:TYR:HB2	2:B:195:LYS:CB	2.23	0.67
2:B:41:ILE:HG23	2:B:46:TYR:HB3	1.74	0.67
2:A:157:VAL:CG1	2:A:301:ALA:HB2	2.24	0.67
2:A:61:THR:O	2:A:61:THR:HG22	1.95	0.67
3:J:37:LYS:HE2	3:J:59:THR:HG21	1.77	0.67
3:J:36:GLU:O	3:J:61:ILE:HB	1.95	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
2:G:98:SER:HB2	2:G:105:GLN:HG2	1.76	0.66
3:W:47:ILE:H	3:W:47:ILE:HD12	1.59	0.66
3:J:82:GLN:C	3:J:84:GLU:H	1.99	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:W:1:MET:HE1	3:W:3:GLN:HB2	1.77	0.66
2:G:21:ARG:HA	2:G:24:ASN:HB2	1.77	0.65
2:G:63:VAL:HG21	2:G:302:MET:HE3	1.78	0.65
2:G:96:SER:OG	2:G:108:LEU:HD22	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:10:LEU:HD23	3:P:83:GLU:HG2	1.76	0.65
3:J:4:GLN:OE1	3:J:74:LEU:HD21	1.97	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:T:701:DT:H2"	1:T:702:DG:H5'	1.78	0.65
2:B:318:ILE:N	2:B:318:ILE:HD12	2.11	0.65
1:O:703:DA:H1'	1:O:704:DA:H5'	1.77	0.65
2:A:245:VAL:CG2	2:A:251:ALA:HB2	2.23	0.65
2:A:230:VAL:HG21	2:A:254:VAL:HA	1.78	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
2:G:182:PHE:HE1	2:G:197:VAL:HG22	1.61	0.64
3:P:55:ILE:HD12	3:P:55:ILE:N	2.13	0.64
3:W:7:GLU:HG3	3:W:8:VAL:N	2.10	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:A:287:LEU:C	2:A:328:ARG:HD2	2.18	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: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
2:G:108:LEU:O	2:G:112:MET:HG2	1.98	0.63
1:T:703:DA:H1'	1:T:704:DA:H5'	1.81	0.63
2:A:180:ILE:H	2:A:180:ILE:HD13	1.62	0.63
2:A:70:ILE:CG2	2:A:97:ASN:HD21	2.11	0.63
2:B:310:ASN:C	2:B:311:LYS:HG3	2.18	0.63
1:O:710:DT:H6	1:O:710:DT:H5'	1.64	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:A:220:ASP:CG	2:A:225:SER:HB3	2.20	0.62
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: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: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: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
3:P:7:GLU:O	3:P:61:ILE:HD11	1.99	0.61
1:R:709:DC:H6	1:R:709:DC:H5'	1.64	0.61
2:A:130:GLU:O	2:A:133:GLU:HG2	2.00	0.61
2:A:85:ILE:HG12	2:A:299:ALA:HB1	1.83	0.61
2:B:161:TYR:CB	2:B:195:LYS:HB3	2.27	0.61
2:G:4:THR:C	2:G:6:TYR:H	2.02	0.61
2:A:95:LEU:HD23	2:A:96:SER:N	2.15	0.61
2:B:192:ASN:O	2:B:197:VAL:HG22	2.01	0.61
2:B:67:ILE:HD11	2:B:75:TYR:CB	2.27	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:G:4:THR:C	2:G:6:TYR:N	2.53	0.61
3:P:46:SEP:O2P	3:P:48:MET:HB2	2.00	0.61
2:B:70:ILE:O	2:B:70:ILE:HG12	2.01	0.61
2:G:157:VAL:HG22	2:G:297:ILE:HG23	1.83	0.61
2:B:29:VAL:HG11	2:B:34:ARG:HB2	1.83	0.60
2:G:241:THR:O	2:G:269:LEU:HA	2.01	0.60
2:G:70:ILE:H	2:G:97:ASN:HD21	1.48	0.60
2:A:151:THR:HB	2:A:153:GLN:HE21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:121:ILE:HD11	2:G:302:MET:HA	1.83	0.60
2:G:276:ASN:OD1	2:G:328:ARG:NH2	2.35	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:B:230:VAL:CG2	2:B:254:VAL:HG13	2.24	0.60
2:B:227:ILE:CG2	2:B:257:GLY:HA2	2.29	0.60
1:O:713:DC:H2"	1:O:714:DA:OP2	2.01	0.60
3:P:2:VAL:O	3:P:74:LEU:HD22	2.02	0.60
2:A:237:ASP:O	2:A:239:LYS:HD2	2.02	0.60
3:J:50:LEU:HD23	3:J:50:LEU:C	2.22	0.60
1:T:701:DT:H2"	1:T:702:DG:C8	2.37	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: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: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:G:180:ILE:HD13	2:G:180:ILE:H	1.68	0.59
2:G:157:VAL:HG13	2:G:297:ILE:HG22	1.85	0.59
3:P:29:PHE:CZ	3:P:73:ALA:HA	2.38	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: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
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
3:J:41:LYS:HG2	3:J:42:VAL:N	2.17	0.59
3:J:36:GLU:HG3	3:J:62:THR:HB	1.84	0.59
1:T:708:DG:C2'	1:T:709:DC:H5"	2.31	0.59
2:A:274:PHE:O	2:A:275:ASP:HB2	2.02	0.59
1:R:704:DA:H2"	1:R:705:DA:O5'	2.03	0.59
3:W:2:VAL:CG1	3:W:74:LEU:HD22	2.32	0.59
2:B:303:ARG:NH2	2:B:307:LYS:HE2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:700:DC:H2'	2:G:28:ASN:O	2.02	0.58
1:T:714:DA:H2"	1:T:715:DG:O5'	2.03	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:247:THR:HG22	2:A:250:MET:H	1.67	0.58
1:O:707:DC:H1'	2:A:55:LEU:HD22	1.85	0.58
2:G:26:ASN:C	2:G:28:ASN:H	2.07	0.58
3:J:17:ARG:HG2	3:J:17:ARG:HH11	1.68	0.58
3:P:4:GLN:O	3:P:62:THR:HG22	2.04	0.58
2:G:294:MET:CE	2:G:297:ILE:HD12	2.32	0.58
1:O:709:DC:C2'	1:O:710:DT:H5"	2.31	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: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
2:B:194:ALA:O	2:B:198:LYS:HE2	2.04	0.57
2:G:233:LEU:C	2:G:235:GLU:H	2.08	0.57
3:J:19:ALA:O	3:J:22:PHE:HB3	2.04	0.57
1:R:702:DG:H2"	1:R:703:DA:OP2	2.04	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:HG22	2:B:325:ILE:O	2.05	0.57
2:G:212:ARG:N	2:G:212:ARG:HD2	2.20	0.57
1:O:709:DC:H2"	1:O:710:DT:H5'	1.85	0.57
3:W:82:GLN:C	3:W:84:GLU:N	2.58	0.57
2:B:170:GLN:O	2:B:171:SER:C	2.43	0.57
2:G:259:GLN:HG2	2:G:260:ASP:N	2.18	0.57
2:G:30:LYS:HB2	2:G:30:LYS:NZ	2.19	0.57
3:J:9:ARG:CD	3:J:82:GLN:HE22	2.12	0.57
3:J:8:VAL:HG13	3:J:8:VAL:O	2.05	0.57
2:B:148:ILE:HD11	2:B:191:ILE:HG12	1.87	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:W:16:ALA:HB3	3:W:18:PRO:HD2	1.87	0.57
3:W:41:LYS:O	3:W:41:LYS:HG3	2.04	0.57
2:G:263:LEU:HD22	2:G:268:ASP:CG	2.25	0.56
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:A:230:VAL:CG2	2:A:254:VAL:HA	2.34	0.56
3:J:41:LYS:HE2	3:J:64:ILE:HD12	1.87	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
2:A:321:LEU:HD12	2:A:321:LEU:N	2.21	0.56
2:G:180:ILE:HD13	2:G:180:ILE:N	2.21	0.56
2:G:29:VAL:CG1	2:G:34:ARG:HB2	2.35	0.56
1:R:707:DC:C2	2:G:55:LEU:HD13	2.41	0.56
2:B:193:HIS:O	2:B:197:VAL:CG2	2.54	0.56
2:B:30:LYS:HB3	2:B:33:THR:CG2	2.35	0.56
2:B:201:LYS:O	2:B:204:LEU:HB2	2.05	0.56
1:O:715:DG:C2'	2:B:28:ASN:ND2	2.69	0.56
2:A:223:TYR:C	2:A:223:TYR:CD1	2.79	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
2:A:12:ALA:HA	2:A:36:LYS:NZ	2.19	0.56
1:O:702:DG:H2"	1:O:703:DA:C8	2.40	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
2:A:288:THR:HA	2:A:326:GLU:O	2.07	0.55
2:A:35:LYS:HD3	2:A:38:LEU:HD12	1.87	0.55
2:B:227:ILE:N	2:B:253:GLY:O	2.39	0.55
2:G:292:GLN:OE1	2:G:294:MET:HE3	2.04	0.55
3:P:42:VAL:HG12	3:P:43:ASN:N	2.21	0.55
2:A:270:GLU:CD	2:A:332:LYS:HG2	2.26	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
3:J:43:ASN:OD1	3:J:45:LYS:HB2	2.06	0.55
3:W:82:GLN:O	3:W:84:GLU:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:89:TYR:OH	2:G:303:ARG:NE	2.40	0.55
3:P:16:ALA:HB3	3:P:18:PRO:HD2	1.89	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:B:27:PRO:O	2:B:28:ASN:CG	2.44	0.55
2:G:82:ILE:CD1	2:G:121:ILE:HG21	2.37	0.55
2:G:158:THR:HG23	2:G:159:ILE:N	2.22	0.55
2:G:85:ILE:O	2:G:88:MET:N	2.40	0.55
2:A:223:TYR:C	2:A:223:TYR:HD1	2.11	0.55
2:B:304:LEU:HD22	2:B:308:TYR:CE2	2.41	0.55
3:W:53:LEU:HB2	3:W:55:ILE:HD11	1.89	0.55
3:W:8:VAL:HA	3:W:81:VAL:HG12	1.89	0.54
2:A:202:ARG:O	2:A:206:GLU:HB2	2.07	0.54
2:A:22:VAL:HG23	2:A:23:VAL:N	2.22	0.54
2:G:46:TYR:CD1	2:G:46:TYR:C	2.80	0.54
3:J:25:GLU:OE2	3:J:25:GLU:HA	2.07	0.54
2:B:220:ASP:O	2:B:221:TYR:HB2	2.08	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:144:LEU:HG	2:B:154:ILE:HG22	1.88	0.54
2:B:12:ALA:HA	2:B:36:LYS:HE3	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
2:A:117:VAL:O	2:A:140:VAL:HG11	2.07	0.54
2:A:307:LYS:HG2	2:A:307:LYS:O	2.08	0.54
2:B:110:ASN:O	2:B:111:ASN:C	2.43	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
1:T:710:DT:H4'	1:T:710:DT:OP1	2.07	0.54
2:A:163:GLN:OE1	2:A:163:GLN:HA	2.05	0.54
2:A:180:ILE:N	2:A:180:ILE:HD13	2.23	0.54
1:R:715:DG:H8	1:R:715:DG:H5'	1.73	0.54
3:W:6:VAL:CG1	3:W:82:GLN:HE21	2.19	0.54
2:G:260:ASP:C	2:G:262:GLY:N	2.61	0.54
2:A:102:GLN:CD	2:A:128:THR:HG21	2.29	0.54
2:A:329:GLN:O	2:A:329:GLN:HG2	2.08	0.54
2:A:34:ARG:O	2:A:37:VAL:HB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:143:VAL:HG11	2:G:305:LEU:HB2	1.89	0.54
2:G:329:GLN:C	2:G:331:THR:H	2.11	0.54
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:NH1	3:J:9:ARG:CG	2.59	0.53
1:O:715:DG:H2'	2:B:28:ASN:ND2	2.23	0.53
3:W:37:LYS:HD2	3:W:37:LYS:C	2.28	0.53
3:W:9:ARG:NH1	3:W:9:ARG:CG	2.67	0.53
2:B:26:ASN:HD22	2:B:27:PRO:HD2	1.73	0.53
2:B:305:LEU:HG	2:B:309:MET:HE2	1.89	0.53
2:G:269:LEU:HD23	2:G:269:LEU:H	1.72	0.53
3:P:50:LEU:HD13	3:P:50:LEU:C	2.28	0.53
2:G:95:LEU:CD2	2:G:96:SER:N	2.68	0.53
3:P:8:VAL:HG23	3:P:81:VAL:HG13	1.90	0.53
1:T:706:DG:H2"	1:T:707:DC:OP2	2.08	0.53
2:B:284:ARG:NH2	2:B:286:GLN:CG	2.68	0.53
2:B:22:VAL:HG21	2:B:37:VAL:CG1	2.38	0.53
3:P:1:MET:O	3:P:1:MET:HG3	2.07	0.53
2:A:307:LYS:HZ1	3:W:48:MET:CG	2.15	0.53
2:B:29:VAL:CB	2:B:34:ARG:HH21	2.20	0.53
3:J:35:LEU:HD21	3:J:55:ILE:HD11	1.90	0.53
1:O:710:DT:H2"	1:O:711:DT:C6	2.43	0.53
3:W:9:ARG:HB2	3:W:82:GLN:O	2.09	0.53
2:A:151:THR:CB	2:A:153:GLN:HE21	2.21	0.53
2:A:198:LYS:O	2:A:202:ARG:HB2	2.09	0.53
2:A:324:ARG:NH1	3:W:15:GLN:OE1	2.41	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
3:P:27:ASN:HA	3:P:45:LYS:HE2	1.89	0.53
3:P:10:LEU:HA	3:P:83:GLU:HG3	1.91	0.53
1:R:712:DA:H2"	1:R:713:DC:O5'	2.08	0.53
3:W:47:ILE:N	3:W:47:ILE:HD12	2.24	0.53
2:A:151:THR:O	2:A:152:ASN:HB2	2.09	0.53
2:B:193:HIS:O	2:B:197:VAL:HG23	2.09	0.53
2:G:3:VAL:O	2:G:3:VAL:HG23	2.08	0.53
3:W:37:LYS:HD3	3:W:38:ASP:OD1	2.09	0.53
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
2:A:5:ILE:HG13	2:A:19:VAL:HG11	1.90	0.52
2:G:272:ILE:C	2:G:272:ILE:HD13	2.29	0.52
3:P:66:GLN:HA	3:P:70:GLU:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:160:ASP:OD2	2:A:163:GLN:HB2	2.09	0.52
2:A:3:VAL:O	2:A:3:VAL:HG23	2.09	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:B:5:ILE:HD11	2:B:16:MET:O	2.10	0.52
2:A:197:VAL:O	2:A:200:TYR:HB3	2.09	0.52
2:A:78:LEU:HD12	2:A:78:LEU:O	2.10	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
2:B:157:VAL:O	2:B:157:VAL:HG13	2.09	0.52
3:J:82:GLN:O	3:J:84:GLU:N	2.42	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
3:P:26:ALA:O	3:P:45:LYS:HE3	2.10	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
2:G:256:HIS:C	2:G:259:GLN:HB3	2.30	0.52
2:G:65:VAL:CG1	2:G:93:ILE:HD11	2.39	0.52
1:O:707:DC:H2"	2:A:55:LEU:CD2	2.40	0.52
3:P:55:ILE:CD1	3:P:55:ILE:H	2.22	0.52
2:A:281:THR:HG22	2:A:328:ARG:NH1	2.24	0.52
1:R:701:DT:H1'	1:R:702:DG:H5'	1.92	0.52
3:W:8:VAL:C	3:W:10:LEU:H	2.12	0.52
3:P:17:ARG:N	3:P:18:PRO:CD	2.73	0.52
3:P:67:GLY:O	3:P:68:GLU:C	2.47	0.51
3:P:77:LEU:O	3:P:81:VAL:HG23	2.10	0.51
2:A:4:THR:CG2	2:A:6:TYR:HB3	2.40	0.51
1:O:712:DA:H4'	1:O:712:DA:OP1	2.09	0.51
2:A:227:ILE:HD13	2:A:253:GLY:O	2.10	0.51
2:A:30:LYS:HE2	2:A:32:SER:CB	2.39	0.51
2:A:44:LEU:N	2:A:44:LEU:HD12	2.24	0.51
2:B:170:GLN:NE2	2:B:170:GLN:HA	2.26	0.51
2:B:166:PHE:CD2	2:B:203:ALA:HB2	2.46	0.51
2:B:46:TYR:HE1	2:B:48:PRO:HG3	1.75	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
1:O:715:DG:C2'	2:B:28:ASN:HD22	2.24	0.51
3:P:9:ARG:HB3	3:P:83:GLU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:85:ILE:H	2:A:85:ILE:HD13	1.74	0.51
2:A:67:ILE:O	2:A:97:ASN:HA	2.10	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
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:CD1	3:P:55:ILE:N	2.74	0.51
2:B:243:ILE:HG22	2:B:244:PHE:N	2.26	0.51
2:G:233:LEU:C	2:G:235:GLU:N	2.63	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
3:J:29:PHE:CE2	3:J:73:ALA:HA	2.46	0.51
3:J:82:GLN:C	3:J:84:GLU:N	2.64	0.51
2:A:100:GLN:HB2	4:A:411:IOD:I	2.81	0.50
2:B:305:LEU:HG	2:B:309:MET:CE	2.42	0.50
2:B:82:ILE:HD13	2:B:298:GLY:O	2.11	0.50
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
2:G:294:MET:HE2	2:G:297:ILE:HD12	1.94	0.50
2:A:85:ILE:HG21	2:A:303:ARG:HB2	1.93	0.50
2:B:12:ALA:O	2:B:14:VAL:HG13	2.11	0.50
2:B:5:ILE:HD13	2:B:16:MET:HG3	1.92	0.50
2:G:292:GLN:HG2	2:G:294:MET:HE2	1.92	0.50
1:T:701:DT:H2"	1:T:702:DG:C5'	2.41	0.50
2:A:296:ASP:OD1	3:W:51:MET:HG2	2.11	0.50
1:O:707:DC:H2"	2:A:55:LEU:HD21	1.93	0.50
3:J:81:VAL:C	3:J:83:GLU:H	2.13	0.50
1:R:714:DA:H2"	1:R:715:DG:OP2	2.11	0.50
3:W:2:VAL:HG23	3:W:70:GLU:OE2	2.12	0.50
2:A:323:HIS:O	2:A:324:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:GLY:C	2:B:253:GLY:O	2.50	0.50
3:P:7:GLU:CG	3:P:8:VAL:N	2.75	0.50
1:T:703:DA:H2"	1:T:704:DA:O5'	2.12	0.50
2:A:78:LEU:HD22	2:A:294:MET:SD	2.51	0.50
2:G:88:MET:CE	3:J:47:ILE:HD13	2.41	0.50
2:B:245:VAL:HG11	2:B:251:ALA:N	2.27	0.49
2:B:276:ASN:ND2	2:B:276:ASN:O	2.44	0.49
2:B:81:GLY:O	2:B:82:ILE:C	2.50	0.49
2:B:82:ILE:HG23	2:B:302:MET:HG2	1.94	0.49
2:G:63:VAL:HG11	2:G:302:MET:HE1	1.94	0.49
3:J:17:ARG:N	3:J:18:PRO:CD	2.74	0.49
3:J:63:LEU:O	3:J:63:LEU:HD12	2.12	0.49
2:A:39:GLU:HG3	2:A:40:THR:N	2.26	0.49
2:G:157:VAL:HG13	2:G:297:ILE:CG2	2.42	0.49
2:G:19:VAL:C	2:G:21:ARG:H	2.15	0.49
2:G:4:THR:CG2	2:G:6:TYR:HB3	2.41	0.49
3:W:36:GLU:HB2	3:W:62:THR:HB	1.94	0.49
2:A:270:GLU:HB3	2:A:331:THR:HG22	1.92	0.49
2:A:12:ALA:C	2:A:36:LYS:HZ2	2.15	0.49
2:B:182:PHE:HB2	2:B:200:TYR:CE2	2.47	0.49
2:G:226:GLY:O	2:G:230:VAL:HG23	2.13	0.49
1:T:702:DG:H2"	1:T:703:DA:H8	1.74	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
2:G:81:GLY:O	2:G:82:ILE:C	2.51	0.49
2:G:61:THR:N	2:G:118:ASP:OD2	2.44	0.49
2:G:257:GLY:C	2:G:259:GLN:H	2.13	0.49
2:G:294:MET:HE1	2:G:297:ILE:HD12	1.93	0.49
3:P:79:ALA:O	3:P:84:GLU:O	2.31	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
2:A:180:ILE:CG2	2:A:242:ALA:HB3	2.34	0.49
2:B:185:GLY:H	2:B:192:ASN:HD21	1.61	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
1:O:710:DT:H5'	1:O:710:DT:C6	2.45	0.49
3:W:37:LYS:HD2	3:W:37:LYS:O	2.12	0.49
2:B:173:ILE:HD11	2:B:204:LEU:CD1	2.43	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
2:B:182:PHE:HE1	2:B:197:VAL:HG13	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:143:VAL:CG1	2:G:305:LEU:HD13	2.42	0.49
3:W:55:ILE:H	3:W:55:ILE:CD1	2.18	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
1:T:710:DT:H2"	1:T:711:DT:O5'	2.12	0.49
2:A:304:LEU:O	2:A:304:LEU:HD23	2.12	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
3:P:3:GLN:O	3:P:4:GLN:HB2	2.13	0.48
2:B:39:GLU:HG3	2:B:40:THR:N	2.27	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
2:G:249:GLU:HA	2:G:252:LEU:HD13	1.94	0.48
3:P:71:GLN:HE21	3:P:75:GLU:HG3	1.77	0.48
3:W:4:GLN:HG2	3:W:6:VAL:CG2	2.42	0.48
3:W:8:VAL:HG13	3:W:8:VAL:O	2.13	0.48
2:A:163:GLN:O	2:A:164:ALA:C	2.52	0.48
2:B:113:LEU:HD22	2:B:139:PRO:HD2	1.95	0.48
2:G:177:HIS:CE1	2:G:242:ALA:HB2	2.48	0.48
3:P:1:MET:CG	3:P:1:MET:O	2.60	0.48
3:P:9:ARG:HB3	3:P:83:GLU:CB	2.42	0.48
3:W:63:LEU:HD12	3:W:74:LEU:HD12	1.95	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:G:163:GLN:O	2:G:164:ALA:C	2.51	0.48
3:W:1:MET:CE	3:W:3:GLN:HB2	2.42	0.48
2:A:17:ALA:O	2:A:21:ARG:HG3	2.14	0.48
2:A:326:GLU:OE2	2:A:326:GLU:HA	2.13	0.48
2:B:274:PHE:O	2:B:275:ASP:CB	2.54	0.48
3:J:50:LEU:O	3:J:50:LEU:HD23	2.14	0.48
3:J:9:ARG:HB2	3:J:83:GLU:HB2	1.95	0.48
3:P:33:ILE:HA	3:P:64:ILE:O	2.13	0.48
3:W:57:THR:HG22	3:W:58:GLY:N	2.28	0.48
2:A:318:ILE:HG22	2:A:318:ILE:O	2.14	0.48
2:A:66:ILE:HB	2:A:122:PHE:CD2	2.47	0.48
2:G:224:ASP:O	2:G:227:ILE:N	2.46	0.48
2:G:223:TYR:O	2:G:227:ILE:HG13	2.14	0.48
2:G:264:ASN:OD1	2:G:266:PRO:HD2	2.14	0.48
2:G:97:ASN:O	2:G:108:LEU:HD11	2.13	0.48
3:W:42:VAL:HG21	3:W:49:GLY:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:68:PRO:HD3	2:A:123:MET:O	2.13	0.48
2:B:65:VAL:O	2:B:112:MET:HE3	2.13	0.48
2:G:280:SER:HA	2:G:287:LEU:HB3	1.95	0.48
2:B:26:ASN:HD22	2:B:27:PRO:CD	2.26	0.48
2:A:194:ALA:O	2:A:195:LYS:HD2	2.14	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
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: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
2:B:65:VAL:O	2:B:112:MET:CE	2.62	0.47
2:G:32:SER:OG	2:G:33:THR:N	2.47	0.47
2:G:63:VAL:HG21	2:G:302:MET:HE1	1.95	0.47
1:O:708:DG:H2"	1:O:709:DC:O5'	2.14	0.47
1:T:700:DC:O5'	1:T:700:DC:H6	1.97	0.47
3:W:9:ARG:HB2	3:W:83:GLU:HB3	1.96	0.47
2:B:190:PRO:HA	2:B:193:HIS:ND1	2.27	0.47
2:B:67:ILE:HA	2:B:123:MET:HG3	1.96	0.47
3:W:79:ALA:O	3:W:82:GLN:HB2	2.14	0.47
2:A:165:ALA:O	2:A:169:VAL:HG23	2.15	0.47
2:A:78:LEU:HD23	2:A:294:MET:SD	2.55	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
2:A:98:SER:C	2:A:100:GLN:N	2.66	0.47
3:P:35:LEU:HD13	3:P:50:LEU:HD21	1.96	0.47
2:A:226:GLY:O	2:A:254:VAL:HG22	2.14	0.47
2:B:101:ASN:O	2:B:105:GLN:HG3	2.15	0.47
2:B:247:THR:O	2:B:250:MET:N	2.47	0.47
2:G:19:VAL:HA	2:G:22:VAL:CG1	2.43	0.47
1:R:700:DC:H2'	1:R:700:DC:H6	1.55	0.47
2:B:163:GLN:HA	2:B:163:GLN:NE2	2.30	0.47
2:B:230:VAL:HG12	2:B:234:LEU:HG	1.97	0.47
2:B:326:GLU:HB3	2:B:328:ARG:NH1	2.29	0.47
2:G:82:ILE:O	2:G:302:MET:HG3	2.15	0.47
3:J:35:LEU:C	3:J:35:LEU:HD23	2.35	0.47
1:O:700:DC:H5"	2:A:29:VAL:CA	2.45	0.47
3:W:17:ARG:N	3:W:18:PRO:CD	2.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:300:VAL:HG21	2:G:321:LEU:HD21	1.97	0.47
2:G:72:ASN:C	2:G:72:ASN:OD1	2.53	0.47
3:P:37:LYS:NZ	3:P:59:THR:HG21	2.30	0.47
3:W:5:LYS:NZ	3:W:60:GLU:OE1	2.48	0.47
2:A:162:GLU:HG3	2:A:199:GLY:CA	2.45	0.47
2:B:70:ILE:HG22	2:B:97:ASN:ND2	2.19	0.47
2:G:148:ILE:CD1	2:G:148:ILE:O	2.59	0.47
3:W:35:LEU:HD23	3:W:35:LEU:C	2.35	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:78:LEU:HD23	2:G:294:MET:SD	2.55	0.46
2:A:307:LYS:NZ	3:W:48:MET:CE	2.76	0.46
2:B:138:SER:HA	2:B:139:PRO:HD3	1.77	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
2:G:257:GLY:C	2:G:259:GLN:N	2.68	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
3:W:1:MET:C	3:W:1:MET:HE3	2.36	0.46
2:A:30:LYS:CE	2:A:32:SER:HB3	2.44	0.46
2:B:62:THR:HG21	2:B:94:ILE:HG13	1.97	0.46
2:G:247:THR:HG22	2:G:248:ASP:N	2.29	0.46
3:P:2:VAL:HG12	3:P:74:LEU:CD2	2.46	0.46
1:T:701:DT:H2"	1:T:702:DG:H8	1.78	0.46
3:W:76:LYS:O	3:W:79:ALA:HB3	2.16	0.46
2:A:106:LEU:HD11	2:A:134:GLU:OE1	2.14	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:B:223:TYR:HH	2:B:256:HIS:CG	2.34	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
1:R:711:DT:H2"	1:R:712:DA:C8	2.51	0.46
2:A:68:PRO:HD3	2:A:123:MET:HG3	1.96	0.46
2:A:132:VAL:C	2:A:134:GLU:H	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:80:TYR:HD2	3:J:81:VAL:N	2.13	0.46
3:J:8:VAL:C	3:J:10:LEU:H	2.18	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
2:G:218:GLU:HG2	2:G:219:GLY:N	2.29	0.46
3:P:23:VAL:HG11	3:P:47:ILE:HD12	1.97	0.46
2:A:217:VAL:HG22	2:A:218:GLU:N	2.31	0.46
2:A:305:LEU:HG	2:A:309:MET:HE2	1.97	0.46
2:B:112:MET:O	2:B:117:VAL:HG22	2.15	0.46
2:A:145:ALA:C	2:A:147:SER:H	2.19	0.46
2:B:273:GLY:O	2:B:290:VAL:HG23	2.16	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
3:P:3:GLN:HG3	3:P:64:ILE:HG13	1.97	0.46
2:A:160:ASP:OD2	2:A:163:GLN:CB	2.64	0.46
2:G:252:LEU:HD12	2:G:252:LEU:N	2.31	0.46
3:W:8:VAL:O	3:W:10:LEU:N	2.49	0.46
2:B:61:THR:N	2:B:118:ASP:OD2	2.43	0.46
2:B:27:PRO:O	2:B:27:PRO:HG2	2.16	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
2:A:212:ARG:CD	2:A:212:ARG:H	2.20	0.45
2:A:238:GLU:O	2:A:239:LYS:C	2.54	0.45
2:A:295:TYR:CE2	3:W:17:ARG:HB2	2.52	0.45
1:O:715:DG:H3'	2:B:28:ASN:ND2	2.31	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: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
3:W:35:LEU:O	3:W:35:LEU:HD23	2.16	0.45
2:A:264:ASN:O	2:A:268:ASP:HB2	2.16	0.45
2:A:95:LEU:HD23	2:A:95:LEU:C	2.36	0.45
2:G:8:VAL:HG13	2:G:40:THR:OG1	2.15	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
2:G:19:VAL:C	2:G:21:ARG:N	2.70	0.45
2:G:252:LEU:HG	2:G:283:VAL:CG2	2.44	0.45
3:P:66:GLN:CG	3:P:66:GLN:O	2.62	0.45
3:W:19:ALA:O	3:W:22:PHE:HB3	2.17	0.45
2:A:98:SER:C	2:A:100:GLN:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:130:GLU:O	2:A:133:GLU:CG	2.65	0.45
2:A:8:VAL:HG12	2:A:19:VAL:HG22	1.98	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
2:A:211:VAL:HG23	2:A:211:VAL:O	2.16	0.45
1:R:705:DA:H2"	1:R:706:DG:O5'	2.16	0.45
1:T:702:DG:C2'	1:T:703:DA:C8	2.98	0.45
2:A:277:THR:C	2:A:279:LEU:N	2.69	0.45
2:G:78:LEU:HG	2:G:123:MET:CE	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
1:R:709:DC:H5'	1:R:709:DC:C6	2.47	0.45
2:A:22:VAL:CG2	2:A:23:VAL:N	2.80	0.45
2:G:10:ARG:NE	2:G:10:ARG:HA	2.31	0.45
2:G:278:ARG:C	2:G:280:SER:H	2.19	0.45
3:P:53:LEU:HB3	3:P:55:ILE:HD11	1.98	0.45
3:W:82:GLN:O	3:W:83:GLU:HB3	2.16	0.45
2:A:60:THR:H	2:A:118:ASP:CG	2.21	0.45
2:B:137:LYS:CA	2:B:137:LYS:HE2	2.42	0.45
2:B:201:LYS:HD2	2:B:211:VAL:HG11	1.98	0.45
2:G:243:ILE:HG22	2:G:244:PHE:N	2.31	0.45
2:A:235:GLU:HG2	2:A:261:ARG:NH2	2.33	0.44
2:A:85:ILE:HG12	2:A:299:ALA:CB	2.46	0.44
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: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
2:B:39:GLU:O	2:B:42:GLU:N	2.49	0.44
2:G:179:ASN:HB2	2:G:241:THR:HG23	1.99	0.44
2:G:69:ASP:OD1	2:G:71:SER:HB2	2.17	0.44
2:A:60:THR:N	2:A:118:ASP:OD2	2.46	0.44
2:B:26:ASN:C	2:B:26:ASN:HD22	2.20	0.44
2:B:69:ASP:O	2:B:71:SER:N	2.50	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
2:G:151:THR:O	2:G:152:ASN:C	2.54	0.44
3:P:8:VAL:HG12	3:P:59:THR:O	2.17	0.44
2:A:85:ILE:H	2:A:85:ILE:CD1	2.30	0.44
2:B:105:GLN:HE22	2:B:124:SER:HB3	1.80	0.44
2:B:15:SER:O	2:B:18:THR:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:LYS:HD2	2:B:211:VAL:CG1	2.48	0.44
1:O:700:DC:H3'	2:A:29:VAL:CA	2.43	0.44
2:B:307:LYS:HD2	3:P:48:MET:HE2	2.00	0.44
2:A:76:ALA:O	2:A:79:ALA:HB3	2.18	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
3:J:74:LEU:HD23	3:J:74:LEU:C	2.36	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:216:ILE:O	2:A:216:ILE:HG23	2.18	0.44
2:A:215:TYR:CZ	2:A:238:GLU:HB3	2.53	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
2:B:132:VAL:HG13	2:B:154:ILE:CG1	2.48	0.44
2:B:212:ARG:C	2:B:214:SER:H	2.21	0.44
2:B:4:THR:OG1	2:B:5:ILE:N	2.50	0.44
3:P:1:MET:HA	3:P:65:ALA:O	2.17	0.44
1:R:709:DC:H2"	1:R:710:DT:O5'	2.18	0.44
1:T:707:DC:H2'	1:T:707:DC:H6	1.67	0.44
3:W:23:VAL:O	3:W:27:ASN:ND2	2.51	0.44
2:B:40:THR:HG22	2:B:40:THR:O	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:A:149:GLU:OE2	2:A:149:GLU:C	2.56	0.44
2:B:81:GLY:HA2	2:B:295:TYR:CE1	2.53	0.44
2:G:96:SER:OG	2:G:108:LEU:HD13	2.18	0.44
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:B:25:GLY:O	2:B:26:ASN:C	2.56	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
3:J:32:ASP:N	3:J:66:GLN:O	2.50	0.43
1:R:714:DA:C1'	1:R:715:DG:H5"	2.45	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
2:A:6:TYR:O	2:A:9:ALA:HB3	2.17	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:B:42:GLU:OE2	2:B:42:GLU:HA	2.18	0.43
3:J:7:GLU:OE2	3:J:60:GLU:CG	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:704:DA:H2"	1:O:705:DA:OP2	2.18	0.43
3:W:50:LEU:HD22	3:W:50:LEU:O	2.19	0.43
2:A:132:VAL:O	2:A:134:GLU:N	2.51	0.43
2:A:191:ILE:HG22	2:A:191:ILE:O	2.18	0.43
2:A:189:GLU:O	2:A:191:ILE:N	2.51	0.43
2:B:101:ASN:C	2:B:101:ASN:OD1	2.56	0.43
2:G:158:THR:HG22	2:G:320:GLU:HG2	2.00	0.43
2:G:4:THR:HG22	2:G:7:ASP:OD2	2.18	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:283:VAL:CG1	2:G:284:ARG:N	2.80	0.43
2:G:296:ASP:C	2:G:298:GLY:N	2.71	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:G:211:VAL:O	2:G:211:VAL:HG23	2.18	0.43
2:G:234:LEU:HD21	2:G:269:LEU:HD13	2.00	0.43
2:B:5:ILE:HG12	2:B:19:VAL:HG11	2.00	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
2:G:85:ILE:O	2:G:86:ALA:C	2.57	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
2:G:79:ALA:O	2:G:80:ARG:C	2.56	0.43
1:O:715:DG:C3'	2:B:28:ASN:ND2	2.82	0.43
3:P:32:ASP:OD1	3:P:32:ASP:N	2.51	0.43
2:A:149:GLU:HG2	2:A:154:ILE:CD1	2.41	0.43
2:A:149:GLU:O	2:A:149:GLU:CG	2.66	0.43
2:A:256:HIS:O	2:A:257:GLY:C	2.57	0.43
2:B:243:ILE:CG2	2:B:244:PHE:N	2.82	0.43
2:G:88:MET:HE1	3:J:47:ILE:HD13	1.99	0.43
3:J:4:GLN:CG	3:J:5:LYS:N	2.82	0.43
3:P:41:LYS:HD2	3:P:41:LYS:O	2.18	0.43
2:A:105:GLN:HE22	2:A:124:SER:CB	2.29	0.43
2:A:12:ALA:HA	2:A:36:LYS:HZ2	1.83	0.43
2:A:218:GLU:HG2	2:A:219:GLY:N	2.34	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
2:A:287:LEU:HD12	2:A:288:THR:N	2.34	0.43
2:B:143:VAL:HG22	2:B:143:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:THR:O	2:B:19:VAL:C	2.57	0.43
2:G:96:SER:HG	2:G:108:LEU:HD22	1.84	0.43
2:G:33:THR:HA	2:G:36:LYS:HE3	2.01	0.43
2:B:245:VAL:HG11	2:B:251:ALA:CA	2.48	0.42
2:B:72:ASN:O	2:B:74:PHE:N	2.52	0.42
2:G:47:ARG:O	2:G:47:ARG:HD2	2.19	0.42
3:J:82:GLN:OE1	3:J:82:GLN:HA	2.18	0.42
3:P:37:LYS:O	3:P:38:ASP:O	2.37	0.42
1:R:705:DA:H8	1:R:705:DA:H5"	1.84	0.42
3:W:31:SER:O	3:W:32:ASP:C	2.58	0.42
2:A:22:VAL:HG21	2:A:37:VAL:HG12	1.98	0.42
2:G:236:GLU:O	2:G:237:ASP:C	2.57	0.42
3:J:9:ARG:HB2	3:J:83:GLU:CB	2.50	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:A:268:ASP:O	2:A:269:LEU:HB3	2.19	0.42
2:B:260:ASP:C	2:B:262:GLY:H	2.22	0.42
2:B:157:VAL:HG23	2:B:319:VAL:HG12	2.01	0.42
2:G:227:ILE:N	2:G:253:GLY:O	2.52	0.42
2:G:34:ARG:O	2:G:37:VAL:HB	2.19	0.42
3:W:17:ARG:O	3:W:18:PRO:C	2.57	0.42
2:B:170:GLN:HA	2:B:170:GLN:HE21	1.84	0.42
2:B:79:ALA:O	2:B:80:ARG:C	2.56	0.42
2:G:227:ILE:HA	2:G:230:VAL:HG23	2.00	0.42
2:G:184:SER:C	2:G:250:MET:HE1	2.40	0.42
2:G:252:LEU:H	2:G:252:LEU:HD12	1.84	0.42
3:P:38:ASP:OD1	3:P:38:ASP:N	2.51	0.42
3:P:8:VAL:HG13	3:P:8:VAL:O	2.18	0.42
2:A:145:ALA:C	2:A:147:SER:N	2.73	0.42
2:B:36:LYS:O	2:B:39:GLU:HG2	2.20	0.42
2:B:69:ASP:C	2:B:71:SER:H	2.23	0.42
2:G:33:THR:O	2:G:36:LYS:HB3	2.20	0.42
3:P:82:GLN:C	3:P:84:GLU:H	2.22	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:HE3	2:A:232:LYS:HB2	1.84	0.42
2:B:157:VAL:HA	2:B:319:VAL:HB	2.01	0.42
2:B:170:GLN:O	2:B:172:LEU:N	2.52	0.42
2:B:244:PHE:HA	2:B:272:ILE:O	2.20	0.42
2:G:19:VAL:HG13	2:G:22:VAL:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7:GLU:CG	3:P:8:VAL:H	2.33	0.42
2:A:78:LEU:HG	2:A:123:MET:SD	2.60	0.42
2:B:113:LEU:CD2	2:B:139:PRO:HD2	2.49	0.42
2:B:84:ASP:N	2:B:84:ASP:OD1	2.52	0.42
2:G:265:VAL:O	2:G:266:PRO:C	2.57	0.42
2:G:82:ILE:HG23	2:G:302:MET:HG2	2.01	0.42
2:A:264:ASN:H	2:A:268:ASP:CG	2.23	0.42
2:B:195:LYS:HE3	2:B:198:LYS:NZ	2.34	0.42
2:B:35:LYS:O	2:B:36:LYS:C	2.58	0.42
2:G:212:ARG:H	2:G:212:ARG:CD	2.25	0.42
2:G:255:ILE:C	2:G:257:GLY:N	2.72	0.42
2:B:88:MET:HE2	3:P:24:GLN:HG3	2.02	0.42
1:T:712:DA:C2'	1:T:713:DC:O5'	2.63	0.42
2:A:132:VAL:C	2:A:134:GLU:N	2.73	0.42
2:A:230:VAL:HG22	2:A:254:VAL:CG1	2.36	0.42
2:B:133:GLU:O	2:B:137:LYS:HG2	2.20	0.42
1:T:702:DG:OP2	2:B:15:SER:HB3	2.20	0.42
2:B:170:GLN:CA	2:B:170:GLN:HE21	2.33	0.42
2:G:129:GLU:O	2:G:130:GLU:C	2.58	0.42
2:G:46:TYR:HH	2:G:48:PRO:HA	1.83	0.42
2:G:4:THR:HG22	2:G:7:ASP:CG	2.40	0.42
3:J:80:TYR:CD2	3:J:81:VAL:N	2.88	0.42
3:P:41:LYS:HE3	3:P:41:LYS:HB3	1.77	0.42
3:W:27:ASN:N	3:W:27:ASN:HD22	2.17	0.42
3:W:7:GLU:CG	3:W:8:VAL:H	2.19	0.42
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
2:A:60:THR:O	2:A:61:THR:CB	2.62	0.41
2:B:6:TYR:O	2:B:10:ARG:HG2	2.20	0.41
2:B:5:ILE:CG2	2:B:6:TYR:N	2.83	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
1:O:702:DG:H5"	2:A:15:SER:HB2	2.00	0.41
3:P:36:GLU:N	3:P:62:THR:O	2.46	0.41
1:R:715:DG:C8	1:R:715:DG:H5'	2.53	0.41
3:W:29:PHE:CE2	3:W:73:ALA:HA	2.55	0.41
2:B:157:VAL:HG23	2:B:319:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:26:ASN:C	2:G:28:ASN:N	2.72	0.41
2:G:274:PHE:O	2:G:275:ASP:CB	2.66	0.41
3:J:36:GLU:HB3	3:J:41:LYS:HA	2.02	0.41
3:W:29:PHE:CZ	3:W:73:ALA:HA	2.55	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: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
2:B:49:ASN:O	2:B:50:ALA:C	2.59	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
1:R:700:DC:H6	2:G:28:ASN:O	2.03	0.41
2:A:266:PRO:O	2:A:267:ASN:C	2.58	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:G:329:GLN:C	2:G:331:THR:N	2.73	0.41
2:A:222:THR:O	2:A:223:TYR:C	2.59	0.41
2:A:296:ASP:CG	3:W:51:MET:HG2	2.40	0.41
2:B:217:VAL:HG13	2:B:233:LEU:HD21	2.01	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:22:VAL:HG23	2:G:23:VAL:HG23	2.03	0.41
2:G:245:VAL:HG11	2:G:251:ALA:CA	2.51	0.41
2:G:286:GLN:HB3	2:G:328:ARG:CB	2.43	0.41
2:A:304:LEU:C	2:A:304:LEU:CD2	2.88	0.41
2:A:78:LEU:HD12	2:A:78:LEU:C	2.41	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
3:J:15:GLN:O	3:J:16:ALA:C	2.59	0.41
3:P:76:LYS:O	3:P:77:LEU:C	2.59	0.41
1:R:702:DG:N2	1:R:703:DA:C2	2.89	0.41
3:W:36:GLU:HG2	3:W:41:LYS:CB	2.39	0.41
3:W:50:LEU:C	3:W:50:LEU:CD2	2.89	0.41
3:W:78:ALA:O	3:W:82:GLN:HG2	2.20	0.41
2:A:65:VAL:HG23	2:A:65:VAL:O	2.19	0.41
2:B:295:TYR:C	2:B:295:TYR:CD1	2.94	0.41
2:G:245:VAL:HG21	2:G:251:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:701:DT:H1'	1:O:702:DG:N7	2.35	0.41
3:P:37:LYS:O	3:P:38:ASP:C	2.59	0.41
2:B:144:LEU:HG	2:B:154:ILE:CG2	2.51	0.41
2:B:209:LEU:HD23	2:B:209:LEU:HA	1.91	0.41
2:G:189:GLU:C	2:G:191:ILE:N	2.73	0.41
2:G:226:GLY:O	2:G:229:ALA:HB3	2.21	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
3:W:8:VAL:C	3:W:10:LEU:N	2.73	0.41
2:A:200:TYR:CD1	2:A:200:TYR:C	2.93	0.41
2:A:265:VAL:HG13	2:A:269:LEU:O	2.20	0.41
2:A:277:THR:C	2:A:279:LEU:H	2.24	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:G:137:LYS:HA	2:G:137:LYS:HD3	1.76	0.41
3:J:23:VAL:HG11	3:J:47:ILE:HD12	2.02	0.41
2:B:141:PRO:HB2	2:B:305:LEU:CD1	2.50	0.41
2:B:223:TYR:CD1	2:B:223:TYR:C	2.95	0.41
2:A:163:GLN:O	2:A:166:PHE:N	2.54	0.40
2:A:190:PRO:C	2:A:192:ASN:H	2.24	0.40
2:A:296:ASP:HB3	2:A:321:LEU:CD2	2.51	0.40
2:G:133:GLU:OE1	2:G:133:GLU:O	2.38	0.40
2:G:293:PRO:O	2:G:294:MET:C	2.57	0.40
2:G:1:MET:HG3	2:G:47:ARG:HH22	1.86	0.40
2:A:295:TYR:CZ	3:W:17:ARG:HA	2.56	0.40
2:A:229:ALA:O	2:A:230:VAL:C	2.58	0.40
2:A:30:LYS:O	2:A:34:ARG:N	2.42	0.40
2:G:68:PRO:HD3	2:G:123:MET:HG3	2.02	0.40
3:J:1:MET:N	3:J:70:GLU:OE1	2.50	0.40
2:A:166:PHE:CD1	2:A:166:PHE:C	2.94	0.40
2:A:283:VAL:HG12	2:A:284:ARG:H	1.86	0.40
2:A:72:ASN:ND2	2:A:74:PHE:HB3	2.37	0.40
2:B:180:ILE:HG13	2:B:180:ILE:O	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:162:GLU:O	2:A:163:GLN:C	2.58	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: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:217:VAL:CG2	2:B:229:ALA:HB1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:TYR:HA	2:B:249:GLU:O	2.22	0.40
2:G:320:GLU:O	2:G:321:LEU:C	2.59	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
3:P:36:GLU:HG3	3:P:40:LYS:O	2.22	0.40
1:R:705:DA:H2"	1:R:706:DG:O4'	2.21	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%)	3 16
2	B	330/332 (99%)	257 (78%)	61 (18%)	12 (4%)	4 22
2	G	325/332 (98%)	242 (74%)	69 (21%)	14 (4%)	3 18
3	J	81/85 (95%)	56 (69%)	19 (24%)	6 (7%)	1 6
3	P	81/85 (95%)	54 (67%)	23 (28%)	4 (5%)	3 15
3	W	81/85 (95%)	65 (80%)	13 (16%)	3 (4%)	4 21
All	All	1228/1251 (98%)	935 (76%)	239 (20%)	54 (4%)	3 17

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (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
2	A	285/289 (99%)	249 (87%)	36 (13%)	5 22
2	B	289/289 (100%)	256 (89%)	33 (11%)	7 27
2	G	284/289 (98%)	248 (87%)	36 (13%)	5 22
3	J	68/69 (99%)	60 (88%)	8 (12%)	6 25
3	P	68/69 (99%)	61 (90%)	7 (10%)	9 31
3	W	68/69 (99%)	58 (85%)	10 (15%)	4 16
All	All	1062/1074 (99%)	932 (88%)	130 (12%)	6 24

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	ASN
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	73	ILE
2	A	78	LEU
2	A	85	ILE
2	A	92	ASN
2	A	106	LEU

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Mol	Chain	Res	Type
2	A	113	LEU
2	A	143	VAL
2	A	149	GLU
2	A	154	ILE
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	223	TYR
2	A	237	ASP
2	A	238	GLU
2	A	239	LYS
2	A	245	VAL
2	A	261	ARG
2	A	269	LEU
2	A	279	LEU
2	A	282	MET
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	30	THR
3	W	32	ASP
3	W	37	LYS
3	W	38	ASP
3	W	50	LEU
3	W	51	MET
3	W	55	ILE
3	W	56	SER
3	W	71	GLN
2	B	4	THR
2	B	5	ILE
2	B	6	TYR
2	B	26	ASN
2	B	38	LEU
2	B	55	LEU
2	B	78	LEU
2	B	84	ASP

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Mol	Chain	Res	Type
2	B	100	GLN
2	B	101	ASN
2	B	117	VAL
2	B	131	HIS
2	B	143	VAL
2	B	148	ILE
2	B	188	GLU
2	B	195	LYS
2	B	197	VAL
2	B	204	LEU
2	B	205	THR
2	B	212	ARG
2	B	215	TYR
2	B	217	VAL
2	B	224	ASP
2	B	227	ILE
2	B	259	GLN
2	B	272	ILE
2	B	284	ARG
2	B	294	MET
2	B	295	TYR
2	B	302	MET
2	B	304	LEU
2	B	311	LYS
2	B	315	ASP
3	P	6	VAL
3	P	21	LEU
3	P	32	ASP
3	P	38	ASP
3	P	41	LYS
3	P	62	THR
3	P	82	GLN
2	G	11	GLU
2	G	47	ARG
2	G	55	LEU
2	G	58	LYS
2	G	61	THR
2	G	65	VAL
2	G	67	ILE
2	G	70	ILE
2	G	71	SER
2	G	73	ILE

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Mol	Chain	Res	Type
2	G	78	LEU
2	G	83	GLU
2	G	87	SER
2	G	96	SER
2	G	100	GLN
2	G	102	GLN
2	G	133	GLU
2	G	140	VAL
2	G	143	VAL
2	G	149	GLU
2	G	155	PRO
2	G	158	THR
2	G	159	ILE
2	G	170	GLN
2	G	180	ILE
2	G	186	THR
2	G	207	SER
2	G	212	ARG
2	G	214	SER
2	G	269	LEU
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	61	ILE
3	J	70	GLU
3	J	82	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) 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

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Mol	Chain	Res	Type
2	A	110	ASN
2	A	170	GLN
2	A	193	HIS
2	A	256	HIS
2	A	267	ASN
3	W	3	GLN
3	W	27	ASN
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	3	GLN
3	P	24	GLN
3	P	71	GLN
2	G	24	ASN
2	G	97	ASN
2	G	105	GLN
2	G	107	HIS
2	G	110	ASN
2	G	152	ASN
2	G	170	GLN
3	J	3	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	J	46	3	7,9,10	1.12	0	8,12,14	2.10	2 (25%)
3	SEP	P	46	3	7,9,10	1.04	0	8,12,14	2.32	3 (37%)
3	SEP	W	46	3	7,9,10	1.07	1 (14%)	8,12,14	1.95	4 (50%)

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	J	46	3	-	0/5/8/10	0/0/0/0
3	SEP	P	46	3	-	0/5/8/10	0/0/0/0
3	SEP	W	46	3	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	W	46	SEP	P-O3P	-2.12	1.47	1.54

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	46	SEP	O2P-P-O1P	-2.32	103.06	110.63
3	W	46	SEP	O-C-CA	-2.15	119.96	125.72
3	W	46	SEP	O2P-P-O1P	-2.00	104.09	110.63
3	W	46	SEP	OG-CB-CA	2.39	110.35	108.26
3	W	46	SEP	O3P-P-O1P	3.58	122.32	110.63
3	J	46	SEP	O3P-P-O1P	3.59	122.34	110.63
3	P	46	SEP	O3P-P-O1P	3.81	123.05	110.63
3	J	46	SEP	OG-CB-CA	4.04	111.78	108.26
3	P	46	SEP	OG-CB-CA	4.26	111.97	108.26

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates 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, 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	O	16/16 (100%)	-0.66	0 100 100	33, 82, 107, 108	0
1	R	16/16 (100%)	-0.36	1 (6%) 23 11	32, 78, 135, 151	0
1	T	16/16 (100%)	-0.63	0 100 100	50, 72, 119, 137	0
2	A	332/332 (100%)	-0.35	3 (0%) 85 69	25, 72, 106, 137	0
2	B	332/332 (100%)	-0.23	3 (0%) 85 69	25, 63, 100, 125	0
2	G	329/332 (99%)	-0.20	7 (2%) 67 44	15, 63, 117, 144	0
3	J	83/85 (97%)	-0.34	0 100 100	23, 60, 80, 115	0
3	P	83/85 (97%)	-0.39	0 100 100	38, 72, 92, 119	0
3	W	83/85 (97%)	-0.49	2 (2%) 62 39	32, 58, 77, 110	0
All	All	1290/1299 (99%)	-0.30	16 (1%) 81 61	15, 65, 107, 151	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	11	GLU	4.2
2	G	32	SER	4.1
2	B	1	MET	3.7
2	G	7	ASP	3.5
2	G	211	VAL	3.4
3	W	84	GLU	3.1
1	R	700	DC	2.8
2	G	37	VAL	2.7
2	G	1	MET	2.6
3	W	2	VAL	2.5
2	B	269	LEU	2.4
2	A	233	LEU	2.2
2	A	242	ALA	2.2
2	A	180	ILE	2.2
2	B	230	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	G	14	VAL	2.2

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	SEP	J	46	10/11	0.98	0.13	-	22,33,37,40	0
3	SEP	P	46	10/11	0.97	0.12	-	49,56,58,59	0
3	SEP	W	46	10/11	0.98	0.13	-	23,39,49,49	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
4	IOD	G	414	1/1	0.98	0.23	2.91	45,45,45,45	1
4	IOD	B	420	1/1	0.92	0.12	-1.15	110,110,110,110	1
4	IOD	B	419	1/1	0.96	0.11	-2.05	109,109,109,109	1
4	IOD	A	411	1/1	0.88	0.07	-	120,120,120,120	1
4	IOD	A	410	1/1	0.90	0.07	-	77,77,77,77	1
4	IOD	B	422	1/1	0.88	0.07	-	114,114,114,114	1
4	IOD	A	413	1/1	0.99	0.05	-	66,66,66,66	1
4	IOD	A	412	1/1	0.91	0.09	-	95,95,95,95	1
4	IOD	P	421	1/1	0.96	0.09	-	99,99,99,99	1
4	IOD	O	415	1/1	0.87	0.06	-	111,111,111,111	1
4	IOD	G	418	1/1	0.97	0.13	-	98,98,98,98	1

6.5 Other polymers (i)

There are no such residues in this entry.