Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 01:56 PM EDT

PDB ID	:	3KJV
Title	:	HIV-1 reverse transcriptase in complex with DNA
Authors	:	Lansdon, E.B.
Deposited on	:	2009-11-03
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

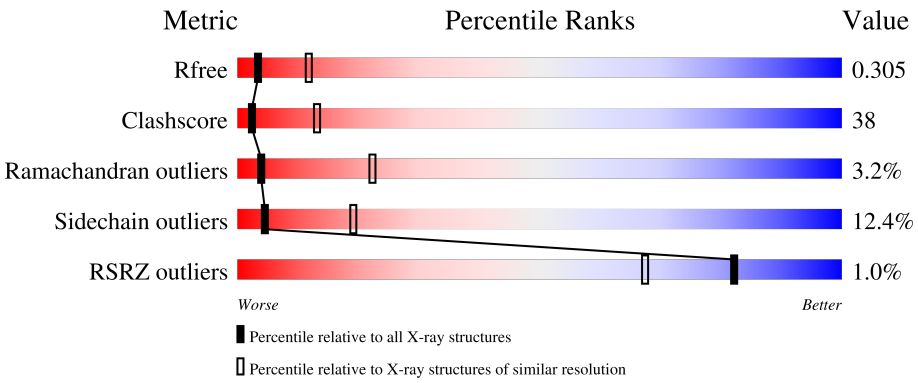
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	560	.% 35% 52% 9% • •
2	B	452	37% 44% 7% 12%
3	P	21	10% 76% 14%
4	T	27	22% 59% • 15%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8653 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Reverse transcriptase p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	4449	2872	744	825	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	CYS	GLN	engineered mutation	UNP P04585
A	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 2 is a protein called Reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	400	3298	2141	551	600	6	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	expression tag	UNP P04585
B	-10	GLY	-	expression tag	UNP P04585
B	-9	SER	-	expression tag	UNP P04585
B	-8	SER	-	expression tag	UNP P04585
B	-7	HIS	-	expression tag	UNP P04585
B	-6	HIS	-	expression tag	UNP P04585
B	-5	HIS	-	expression tag	UNP P04585
B	-4	HIS	-	expression tag	UNP P04585
B	-3	HIS	-	expression tag	UNP P04585
B	-2	HIS	-	expression tag	UNP P04585
B	-1	SER	-	expression tag	UNP P04585
B	0	SER	-	expression tag	UNP P04585
B	280	SER	CYS	engineered mutation	UNP P04585

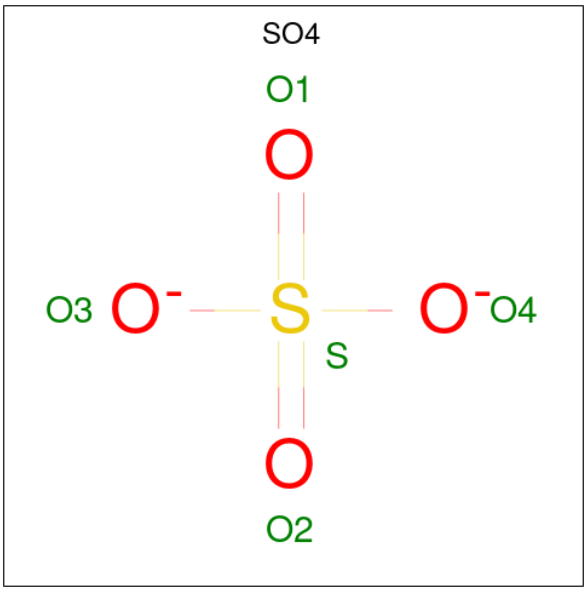
- Molecule 3 is a DNA chain called 5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*(DOC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	18	363	172	62	111	18	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	T	23	480	224	97	136	23	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
5	P	1	5	4	1	0	0
5	T	1	5	4	1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0

- Molecule 7 is water.

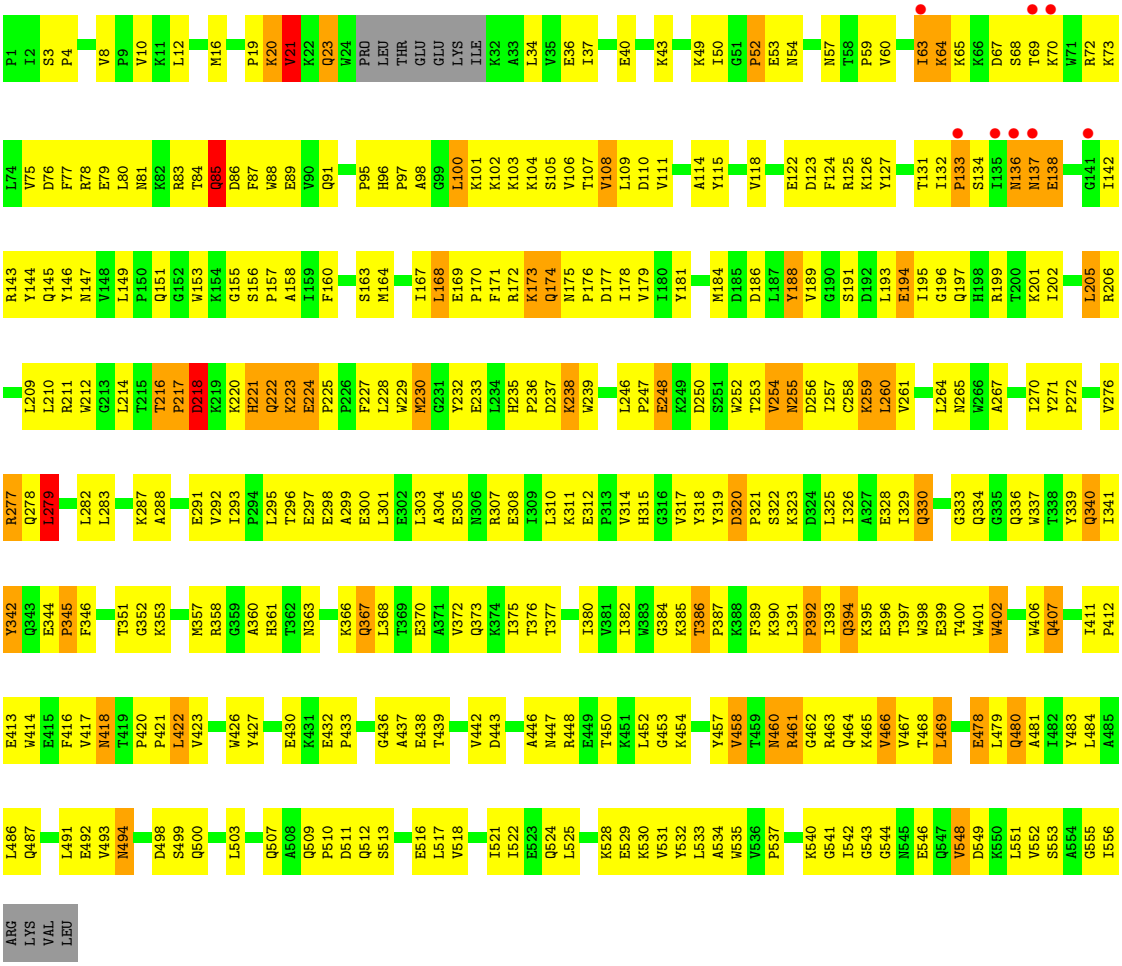
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	19	19	19	0	0
			Total	O		
7	B	21	21	21	0	0
			Total	O		
7	P	4	4	4	0	0
			Total	O		
7	T	3	3	3	0	0

3 Residue-property plots (i)

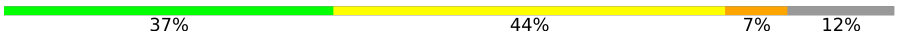
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

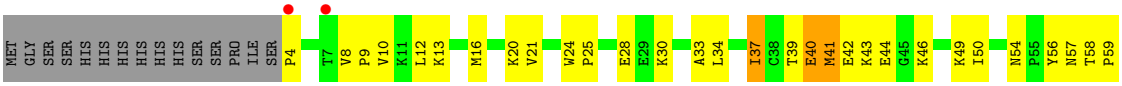
- Molecule 1: Reverse transcriptase p66 subunit

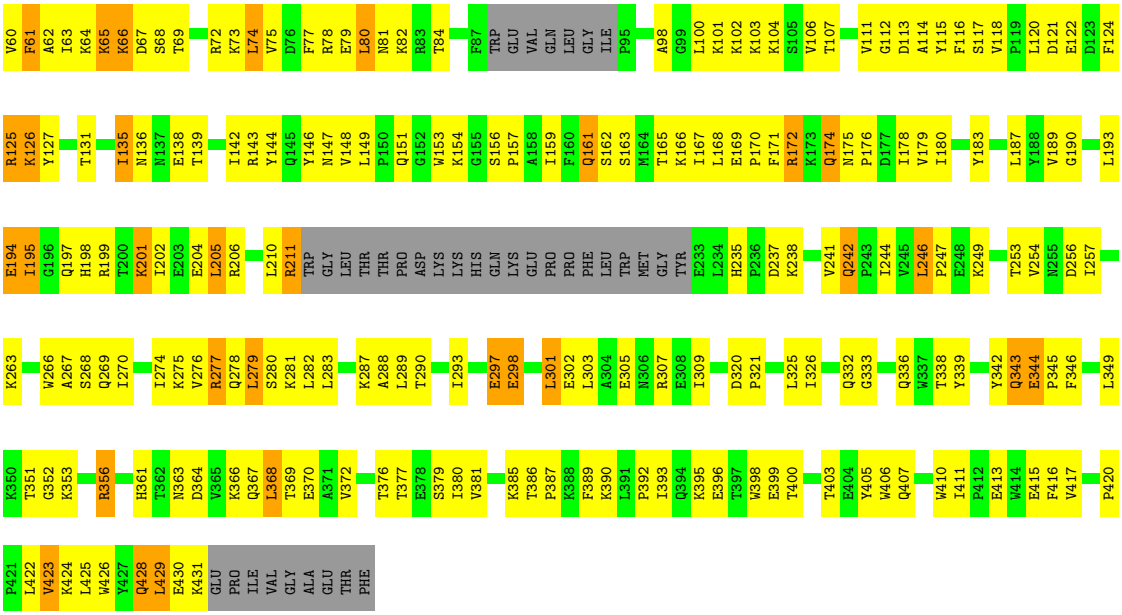
Chain A:



- Molecule 2: Reverse transcriptase p51 subunit

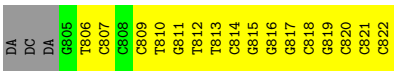
Chain B: 





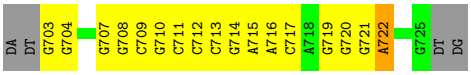
• Molecule 3: 5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*(DOC))-3'

Chain P: 10% 76% 14%



• Molecule 4: 5'-D(*AP*TP*GP*GP*TP*GP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3'

Chain T: 22% 59% • 15%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	165.42Å 171.97Å 103.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.10 47.98 – 3.08	Depositor EDS
% Data completeness (in resolution range)	94.4 (29.84-3.10) 93.4 (47.98-3.08)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 3.07Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.239 , 0.321 0.225 , 0.305	Depositor DCC
R_{free} test set	1294 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 50.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8653	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DOC, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.45	0/4562	0.63	0/6197
2	B	0.41	0/3387	0.57	1/4595 (0.0%)
3	P	0.63	0/384	1.10	1/590 (0.2%)
4	T	0.59	0/540	0.98	0/833
All	All	0.45	0/8873	0.67	2/12215 (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
1	A	0	4
4	T	0	1
All	All	0	5

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	P	809	DC	N1-C1'-C2'	6.13	124.25	112.60
2	B	4	PRO	N-CA-CB	5.68	110.11	103.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ASN	Peptide
1	A	218	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	A	279	LEU	Peptide
1	A	344	GLU	Peptide
4	T	722	DA	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4449	0	4484	388	0
2	B	3298	0	3333	231	0
3	P	363	0	203	20	0
4	T	480	0	256	26	0
5	A	5	0	0	0	0
5	P	5	0	0	0	0
5	T	5	0	0	0	0
6	A	1	0	0	0	0
7	A	19	0	0	3	0
7	B	21	0	0	1	0
7	P	4	0	0	0	0
7	T	3	0	0	0	0
All	All	8653	0	8276	641	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 38.

All (641) 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:B:172:ARG:HG3	2:B:172:ARG:HH11	1.13	1.12
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.32	1.10
1:A:50:ILE:HG21	1:A:145:GLN:HG3	1.28	1.08
2:B:135:ILE:HD12	2:B:135:ILE:H	1.27	1.00
2:B:125:ARG:HE	2:B:147:ASN:HA	1.29	0.98
1:A:389:PHE:HB3	1:A:391:LEU:HD21	1.46	0.95
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.03	0.93
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:GLN:OE1	1:A:60:VAL:HG22	1.72	0.88
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.38	0.87
2:B:172:ARG:HG3	2:B:172:ARG:NH1	1.85	0.87
1:A:111:VAL:HG11	1:A:214:LEU:HD12	1.57	0.87
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.53	0.87
1:A:63:ILE:HG13	1:A:64:LYS:H	1.35	0.86
1:A:49:LYS:HD3	1:A:142:ILE:HD11	1.58	0.86
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.11	0.85
2:B:118:VAL:HB	2:B:149:LEU:HD12	1.56	0.85
2:B:149:LEU:HD21	2:B:159:ILE:HD12	1.55	0.85
2:B:135:ILE:HD12	2:B:135:ILE:N	1.92	0.85
1:A:50:ILE:HG12	1:A:143:ARG:O	1.76	0.85
1:A:390:LYS:HB3	1:A:417:VAL:HG13	1.58	0.85
2:B:125:ARG:NE	2:B:147:ASN:HA	1.93	0.84
2:B:66:LYS:HD2	2:B:68:SER:HB3	1.58	0.83
1:A:97:PRO:HA	1:A:100:LEU:HD22	1.58	0.83
1:A:175:ASN:HB3	1:A:178:ILE:HG13	1.62	0.82
4:T:704:DG:N3	4:T:704:DG:H2'	1.94	0.82
1:A:178:ILE:HD11	1:A:201:LYS:HE2	1.60	0.82
1:A:78:ARG:NH2	4:T:704:DG:H4'	1.95	0.81
1:A:390:LYS:HB3	1:A:417:VAL:CG1	2.08	0.81
1:A:50:ILE:CG2	1:A:145:GLN:HG3	2.10	0.81
1:A:317:VAL:HG12	1:A:318:TYR:H	1.44	0.81
1:A:52:PRO:HA	1:A:143:ARG:NH1	1.96	0.80
2:B:395:LYS:HE2	2:B:396:GLU:OE1	1.82	0.80
1:A:277:ARG:HA	1:A:277:ARG:HH11	1.45	0.79
1:A:503:LEU:O	1:A:507:GLN:HG3	1.81	0.79
4:T:708:DG:H2'	4:T:709:DC:C6	2.18	0.79
1:A:65:LYS:HD2	1:A:70:LYS:HG2	1.65	0.79
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.48	0.79
4:T:716:DA:H2'	4:T:717:DC:O4'	1.84	0.78
3:P:821:DC:H2'	3:P:822:DOC:H6	1.65	0.78
1:A:49:LYS:HG2	1:A:144:TYR:CE1	2.18	0.78
1:A:108:VAL:HG11	1:A:227:PHE:HB3	1.66	0.77
1:A:518:VAL:O	1:A:522:ILE:HG13	1.85	0.77
1:A:12:LEU:HD11	1:A:127:TYR:CE2	2.20	0.77
1:A:454:LYS:HE3	1:A:468:THR:HG22	1.65	0.76
1:A:491:LEU:HB3	1:A:529:GLU:HG3	1.65	0.76
1:A:199:ARG:HH22	1:A:223:LYS:HB2	1.50	0.76
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.66	0.76
2:B:172:ARG:HH11	2:B:172:ARG:CG	1.96	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:703:DG:H2'	4:T:704:DG:C5	2.21	0.75
2:B:125:ARG:HH21	2:B:147:ASN:HB3	1.53	0.74
1:A:12:LEU:HD12	1:A:12:LEU:N	2.03	0.74
1:A:297:GLU:O	1:A:301:LEU:HG	1.88	0.74
1:A:317:VAL:HG12	1:A:318:TYR:N	2.02	0.74
2:B:117:SER:HA	7:B:457:HOH:O	1.86	0.74
1:A:265:ASN:OD1	1:A:353:LYS:HE2	1.87	0.73
1:A:427:TYR:CE2	1:A:525:LEU:HD13	2.23	0.73
2:B:66:LYS:HG2	2:B:67:ASP:H	1.53	0.73
2:B:277:ARG:O	2:B:281:LYS:HG3	1.88	0.73
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.69	0.73
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.09	0.73
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.52	0.73
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.03	0.73
2:B:363:ASN:ND2	2:B:366:LYS:HB2	2.03	0.73
3:P:815:DG:H2"	3:P:816:DG:O5'	1.89	0.73
1:A:460:ASN:OD1	1:A:460:ASN:N	2.18	0.72
1:A:478:GLU:HG2	1:A:499:SER:CB	2.14	0.72
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.04	0.72
2:B:332:GLN:OE1	2:B:428:GLN:HG2	1.88	0.72
1:A:437:ALA:HB1	1:A:493:VAL:HA	1.71	0.72
2:B:135:ILE:H	2:B:135:ILE:CD1	1.88	0.72
2:B:122:GLU:HA	2:B:125:ARG:HH11	1.55	0.72
1:A:320:ASP:N	1:A:320:ASP:OD1	2.23	0.72
4:T:713:DC:H2'	4:T:714:DG:C8	2.25	0.72
1:A:109:LEU:HD23	1:A:109:LEU:H	1.53	0.71
1:A:448:ARG:HH21	3:P:807:DC:H1'	1.54	0.71
1:A:503:LEU:HG	1:A:507:GLN:HE21	1.55	0.71
1:A:108:VAL:O	1:A:108:VAL:HG22	1.90	0.71
1:A:253:THR:HG22	1:A:292:VAL:HA	1.72	0.71
1:A:260:LEU:HD22	1:A:264:LEU:HD13	1.72	0.71
2:B:377:THR:O	2:B:381:VAL:HG23	1.90	0.71
1:A:500:GLN:HG2	2:B:422:LEU:HD22	1.72	0.71
3:P:818:DC:H2'	3:P:819:DG:H8	1.54	0.71
2:B:246:LEU:HD12	2:B:247:PRO:HD2	1.72	0.70
1:A:503:LEU:CG	1:A:507:GLN:HE21	2.04	0.70
1:A:511:ASP:OD1	1:A:512:GLN:HG2	1.91	0.70
1:A:278:GLN:O	1:A:282:LEU:HD13	1.91	0.70
1:A:418:ASN:O	1:A:420:PRO:HD3	1.92	0.70
1:A:261:VAL:HG22	1:A:265:ASN:HD21	1.56	0.70
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ILE:O	2:B:41:MET:HG3	1.92	0.69
1:A:361:HIS:ND1	1:A:513:SER:HB2	2.07	0.69
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.74	0.69
2:B:120:LEU:H	2:B:148:VAL:HA	1.55	0.69
1:A:80:LEU:O	1:A:84:THR:HG23	1.91	0.69
1:A:105:SER:HB2	1:A:191:SER:OG	1.93	0.69
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.28	0.69
1:A:277:ARG:HA	1:A:277:ARG:NH1	2.07	0.69
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.22	0.69
3:P:821:DC:H2'	3:P:822:DOC:C6	2.23	0.68
2:B:162:SER:O	2:B:165:THR:HG22	1.93	0.68
1:A:239:TRP:CH2	1:A:270:ILE:HD13	2.28	0.68
1:A:136:ASN:N	1:A:136:ASN:HD22	1.91	0.68
2:B:122:GLU:O	2:B:125:ARG:HG2	1.94	0.68
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.75	0.68
1:A:111:VAL:HG21	1:A:164:MET:CE	2.25	0.67
2:B:103:LYS:HE2	2:B:179:VAL:HG12	1.73	0.67
1:A:102:LYS:HB2	1:A:318:TYR:HD2	1.59	0.67
1:A:457:TYR:OH	1:A:465:LYS:HG3	1.93	0.67
2:B:12:LEU:N	2:B:12:LEU:HD12	2.08	0.67
2:B:78:ARG:HH11	2:B:411:ILE:HG22	1.60	0.67
1:A:271:TYR:CE1	1:A:314:VAL:HG12	2.30	0.67
2:B:126:LYS:HD3	2:B:127:TYR:CE2	2.30	0.67
1:A:136:ASN:HD22	1:A:136:ASN:H	1.41	0.66
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.09	0.66
2:B:287:LYS:HD3	2:B:293:ILE:HD11	1.77	0.66
2:B:298:GLU:CD	2:B:298:GLU:H	1.98	0.66
1:A:380:ILE:O	1:A:384:GLY:HA2	1.95	0.66
1:A:246:LEU:HD12	1:A:260:LEU:HD21	1.76	0.66
1:A:382:ILE:O	2:B:136:ASN:HB2	1.95	0.66
3:P:817:DG:H2'	3:P:818:DC:C6	2.30	0.66
1:A:197:GLN:O	1:A:201:LYS:HB2	1.96	0.66
1:A:254:VAL:O	1:A:257:ILE:N	2.24	0.66
1:A:111:VAL:HG21	1:A:164:MET:HE3	1.79	0.65
1:A:368:LEU:O	1:A:372:VAL:HG23	1.96	0.65
1:A:549:ASP:O	1:A:553:SER:HB2	1.96	0.65
1:A:466:VAL:O	1:A:466:VAL:HG13	1.97	0.65
2:B:356:ARG:HG2	2:B:367:GLN:HG2	1.79	0.65
1:A:438:GLU:HG2	1:A:461:ARG:NH1	2.12	0.65
1:A:223:LYS:HE3	1:A:223:LYS:O	1.96	0.65
2:B:24:TRP:HB2	2:B:25:PRO:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:818:DC:H2'	3:P:819:DG:C8	2.32	0.65
3:P:819:DG:H2'	3:P:820:DC:C6	2.32	0.64
4:T:709:DC:H2'	4:T:710:DG:H8	1.60	0.64
4:T:707:DG:H2"	4:T:708:DG:H5'	1.78	0.64
1:A:221:HIS:CE1	1:A:228:LEU:HB2	2.32	0.64
1:A:199:ARG:NH2	1:A:223:LYS:HB2	2.12	0.64
1:A:402:TRP:HZ3	2:B:364:ASP:CG	2.01	0.64
2:B:201:LYS:NZ	2:B:201:LYS:HB3	2.13	0.64
3:P:810:DT:H2'	3:P:811:DG:C8	2.31	0.64
1:A:136:ASN:N	1:A:136:ASN:ND2	2.46	0.64
1:A:261:VAL:HG22	1:A:265:ASN:ND2	2.12	0.64
2:B:420:PRO:HG2	2:B:423:VAL:HG12	1.78	0.64
1:A:173:LYS:O	1:A:176:PRO:HD3	1.97	0.64
2:B:30:LYS:HE3	2:B:62:ALA:O	1.98	0.64
1:A:137:ASN:O	1:A:138:GLU:HB2	1.96	0.64
4:T:712:DC:H2'	4:T:713:DC:C6	2.33	0.63
1:A:376:THR:HG23	1:A:386:THR:HG22	1.78	0.63
2:B:112:GLY:C	2:B:114:ALA:H	2.01	0.63
2:B:263:LYS:HE3	2:B:426:TRP:O	1.98	0.63
1:A:131:THR:CG2	1:A:143:ARG:HG2	2.29	0.63
2:B:235:HIS:HB3	2:B:238:LYS:HD3	1.81	0.63
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.34	0.63
2:B:195:ILE:CD1	2:B:199:ARG:HE	2.10	0.62
1:A:20:LYS:HA	1:A:57:ASN:O	1.99	0.62
2:B:50:ILE:HD12	2:B:143:ARG:HE	1.63	0.62
2:B:65:LYS:HA	2:B:407:GLN:HE22	1.64	0.62
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.80	0.62
2:B:149:LEU:HD22	2:B:156:SER:HA	1.82	0.62
1:A:376:THR:O	1:A:380:ILE:HD12	1.99	0.62
1:A:21:VAL:HG23	1:A:59:PRO:HD3	1.82	0.61
1:A:337:TRP:CZ3	1:A:368:LEU:HD23	2.35	0.61
1:A:314:VAL:HG22	1:A:315:HIS:N	2.15	0.61
1:A:458:VAL:HG22	1:A:464:GLN:HG2	1.83	0.61
2:B:201:LYS:HB3	2:B:201:LYS:HZ2	1.62	0.61
2:B:193:LEU:HD13	2:B:201:LYS:HG3	1.81	0.61
1:A:78:ARG:HH21	4:T:704:DG:H4'	1.63	0.61
1:A:328:GLU:HG2	1:A:330:GLN:NE2	2.15	0.61
2:B:125:ARG:HE	2:B:147:ASN:CA	2.09	0.61
1:A:34:LEU:HD12	1:A:34:LEU:O	2.00	0.61
1:A:277:ARG:HH21	1:A:357:MET:CG	2.12	0.61
1:A:163:SER:O	1:A:167:ILE:HG13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.83	0.61
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.36	0.60
3:P:813:DT:H2"	3:P:814:DC:H5'	1.82	0.60
1:A:34:LEU:HD21	1:A:134:SER:O	2.01	0.60
2:B:420:PRO:HG2	2:B:423:VAL:CG1	2.31	0.60
2:B:66:LYS:HD2	2:B:68:SER:CB	2.28	0.60
2:B:112:GLY:C	2:B:151:GLN:HE21	2.04	0.60
2:B:275:LYS:HE3	2:B:305:GLU:OE1	2.01	0.60
1:A:34:LEU:HD22	1:A:132:ILE:HG22	1.82	0.60
1:A:40:GLU:OE2	1:A:43:LYS:HE2	2.01	0.60
2:B:368:LEU:HD11	2:B:392:PRO:HD2	1.82	0.60
4:T:714:DG:H2'	4:T:715:DA:C8	2.37	0.60
1:A:224:GLU:O	1:A:224:GLU:HG2	2.02	0.60
1:A:279:LEU:O	1:A:282:LEU:HD22	2.01	0.60
1:A:167:ILE:C	1:A:169:GLU:H	2.05	0.60
1:A:479:LEU:O	1:A:521:ILE:HD11	2.01	0.60
2:B:21:VAL:O	2:B:57:ASN:ND2	2.33	0.60
1:A:340:GLN:HG3	1:A:340:GLN:O	2.00	0.60
1:A:277:ARG:HH11	1:A:277:ARG:CA	2.13	0.59
1:A:317:VAL:CG1	1:A:318:TYR:H	2.14	0.59
2:B:429:LEU:HD23	2:B:430:GLU:H	1.67	0.59
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.83	0.59
1:A:118:VAL:CG2	1:A:149:LEU:HG	2.32	0.59
1:A:555:GLY:O	1:A:556:ILE:CB	2.50	0.59
1:A:10:VAL:HG23	1:A:124:PHE:CD1	2.38	0.59
2:B:423:VAL:O	2:B:423:VAL:HG22	2.01	0.59
1:A:254:VAL:HG13	1:A:283:LEU:HD11	1.83	0.59
2:B:279:LEU:HB2	2:B:302:GLU:OE1	2.03	0.59
1:A:416:PHE:HZ	1:A:422:LEU:HD11	1.66	0.59
2:B:163:SER:O	2:B:167:ILE:HG13	2.02	0.59
1:A:4:PRO:HG2	1:A:212:TRP:CE3	2.38	0.59
1:A:270:ILE:O	1:A:272:PRO:HD3	2.01	0.59
2:B:118:VAL:HB	2:B:149:LEU:CD1	2.31	0.58
1:A:377:THR:HG23	7:A:574:HOH:O	2.02	0.58
2:B:210:LEU:O	2:B:211:ARG:NE	2.36	0.58
1:A:277:ARG:HD3	1:A:334:GLN:HB2	1.85	0.58
1:A:532:TYR:CE1	1:A:534:ALA:HB2	2.37	0.58
2:B:69:THR:HG22	2:B:69:THR:O	2.02	0.58
1:A:36:GLU:OE2	1:A:36:GLU:HA	2.02	0.58
1:A:50:ILE:HG21	1:A:145:GLN:CG	2.18	0.58
1:A:272:PRO:HG3	1:A:351:THR:HG21	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LYS:HB3	1:A:417:VAL:HG11	1.86	0.58
1:A:486:LEU:O	1:A:528:LYS:NZ	2.28	0.58
1:A:510:PRO:HB2	1:A:522:ILE:HD11	1.85	0.58
1:A:430:GLU:HB2	1:A:531:VAL:O	2.04	0.58
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.39	0.58
1:A:77:PHE:CD1	1:A:80:LEU:HD23	2.39	0.58
1:A:178:ILE:CD1	1:A:201:LYS:HE2	2.34	0.58
1:A:97:PRO:HD3	1:A:232:TYR:CE2	2.38	0.57
2:B:287:LYS:CD	2:B:293:ILE:HD11	2.34	0.57
2:B:344:GLU:HG3	2:B:345:PRO:HD2	1.86	0.57
1:A:111:VAL:CG1	1:A:214:LEU:HD12	2.32	0.57
1:A:172:ARG:NH2	2:B:139:THR:HG22	2.20	0.57
1:A:380:ILE:HD11	1:A:386:THR:HG23	1.85	0.57
1:A:453:GLY:O	1:A:454:LYS:HD2	2.05	0.57
2:B:178:ILE:HG23	2:B:190:GLY:O	2.05	0.57
2:B:395:LYS:O	2:B:399:GLU:HG3	2.04	0.57
3:P:812:DT:H2'	3:P:813:DT:C6	2.39	0.57
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.86	0.57
2:B:206:ARG:HB2	2:B:206:ARG:NH1	2.19	0.57
1:A:63:ILE:HG13	1:A:64:LYS:N	2.13	0.57
1:A:97:PRO:HA	1:A:100:LEU:CD2	2.32	0.57
1:A:395:LYS:HD2	1:A:414:TRP:CZ2	2.40	0.57
1:A:438:GLU:HG2	1:A:461:ARG:HH11	1.68	0.57
1:A:175:ASN:HD21	1:A:201:LYS:NZ	2.02	0.57
1:A:360:ALA:O	1:A:513:SER:HA	2.04	0.57
2:B:54:ASN:HB3	2:B:143:ARG:HH21	1.68	0.57
2:B:242:GLN:HG3	2:B:353:LYS:HE2	1.86	0.57
1:A:443:ASP:OD1	1:A:498:ASP:OD2	2.23	0.56
1:A:108:VAL:O	1:A:221:HIS:HB2	2.05	0.56
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.05	0.56
1:A:326:ILE:HD12	1:A:342:TYR:HE2	1.71	0.56
1:A:341:ILE:N	1:A:341:ILE:HD12	2.21	0.56
2:B:65:LYS:HD2	2:B:65:LYS:O	2.05	0.56
3:P:813:DT:H2"	3:P:814:DC:C5'	2.34	0.56
4:T:721:DG:H2"	4:T:722:DA:O5'	2.03	0.56
1:A:102:LYS:HD3	1:A:236:PRO:O	2.05	0.56
1:A:454:LYS:HE3	1:A:468:THR:CG2	2.33	0.56
1:A:320:ASP:OD2	1:A:323:LYS:HD3	2.05	0.56
1:A:420:PRO:HA	1:A:421:PRO:C	2.25	0.56
1:A:52:PRO:HA	1:A:143:ARG:HH11	1.68	0.56
2:B:349:LEU:HD23	2:B:349:LEU:N	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LEU:HD23	1:A:109:LEU:N	2.21	0.56
1:A:447:ASN:ND2	1:A:450:THR:HG23	2.21	0.56
1:A:109:LEU:HD12	1:A:216:THR:HG21	1.89	0.55
2:B:274:ILE:HG23	2:B:275:LYS:N	2.20	0.55
1:A:171:PHE:CE2	1:A:205:LEU:HG	2.41	0.55
1:A:376:THR:HG23	1:A:386:THR:CG2	2.37	0.55
1:A:469:LEU:N	1:A:469:LEU:HD13	2.22	0.55
4:T:710:DG:H2"	4:T:711:DC:H5'	1.87	0.55
1:A:64:LYS:HG3	1:A:65:LYS:N	2.21	0.55
1:A:205:LEU:HD22	1:A:209:LEU:CD2	2.36	0.55
1:A:246:LEU:HD12	1:A:260:LEU:CD2	2.37	0.55
2:B:122:GLU:HA	2:B:125:ARG:NH1	2.21	0.55
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.89	0.54
1:A:450:THR:HB	1:A:452:LEU:HD23	1.90	0.54
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.88	0.54
1:A:457:TYR:CZ	1:A:465:LYS:HG3	2.43	0.54
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.88	0.54
2:B:298:GLU:CD	2:B:298:GLU:N	2.61	0.54
1:A:224:GLU:O	1:A:225:PRO:C	2.45	0.54
1:A:458:VAL:HA	1:A:463:ARG:O	2.08	0.53
2:B:80:LEU:O	2:B:80:LEU:HD22	2.08	0.53
2:B:326:ILE:HB	2:B:342:TYR:O	2.07	0.53
1:A:220:LYS:O	1:A:220:LYS:HG2	2.08	0.53
2:B:33:ALA:O	2:B:37:ILE:HG12	2.09	0.53
3:P:819:DG:H2'	3:P:820:DC:H6	1.70	0.53
2:B:235:HIS:CB	2:B:238:LYS:HD3	2.39	0.53
1:A:104:LYS:HE3	1:A:194:GLU:HA	1.91	0.53
2:B:50:ILE:CD1	2:B:143:ARG:HE	2.21	0.53
2:B:78:ARG:HH11	2:B:411:ILE:CG2	2.22	0.53
4:T:703:DG:H5"	4:T:704:DG:N1	2.23	0.53
1:A:20:LYS:O	1:A:21:VAL:HG13	2.08	0.53
1:A:70:LYS:HE3	1:A:72:ARG:NE	2.23	0.53
1:A:402:TRP:HZ3	2:B:364:ASP:OD2	1.92	0.53
1:A:307:ARG:O	1:A:311:LYS:HG3	2.09	0.53
1:A:389:PHE:HB3	1:A:391:LEU:CD2	2.29	0.53
1:A:491:LEU:O	1:A:529:GLU:HB2	2.09	0.53
2:B:39:THR:O	2:B:43:LYS:HG3	2.09	0.53
2:B:201:LYS:NZ	2:B:201:LYS:CB	2.72	0.53
1:A:96:HIS:CD2	1:A:97:PRO:HD2	2.43	0.52
1:A:254:VAL:O	1:A:256:ASP:N	2.41	0.52
1:A:366:LYS:HD2	1:A:401:TRP:CH2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:CE	1:A:367:GLN:HE22	2.21	0.52
1:A:516:GLU:OE2	1:A:516:GLU:HA	2.09	0.52
2:B:195:ILE:HD11	2:B:199:ARG:CZ	2.38	0.52
1:A:450:THR:O	1:A:452:LEU:HD22	2.10	0.52
4:T:709:DC:H2'	4:T:710:DG:C8	2.43	0.52
1:A:52:PRO:HA	1:A:143:ARG:HH12	1.73	0.52
1:A:88:TRP:CD1	2:B:143:ARG:NH1	2.78	0.52
1:A:503:LEU:CD1	1:A:507:GLN:HE21	2.22	0.52
1:A:108:VAL:O	1:A:108:VAL:CG2	2.57	0.52
2:B:46:LYS:HG2	2:B:116:PHE:HB3	1.92	0.52
1:A:205:LEU:HD22	1:A:209:LEU:HD21	1.91	0.52
2:B:244:ILE:HD13	2:B:266:TRP:CZ3	2.44	0.52
2:B:277:ARG:HG3	2:B:278:GLN:N	2.24	0.52
1:A:107:THR:HG22	1:A:108:VAL:N	2.25	0.52
3:P:820:DC:H2"	3:P:821:DC:H5'	1.92	0.52
1:A:279:LEU:H	1:A:279:LEU:HD22	1.75	0.51
1:A:345:PRO:HB2	1:A:346:PHE:HD1	1.75	0.51
1:A:402:TRP:CZ3	2:B:364:ASP:CG	2.83	0.51
2:B:339:TYR:CE1	2:B:352:GLY:HA3	2.45	0.51
1:A:254:VAL:HG12	1:A:255:ASN:N	2.25	0.51
1:A:288:ALA:HB3	1:A:291:GLU:HB2	1.92	0.51
2:B:194:GLU:HG3	2:B:197:GLN:HB2	1.92	0.51
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.25	0.51
1:A:49:LYS:HG2	1:A:144:TYR:HE1	1.71	0.51
1:A:101:LYS:HD2	1:A:321:PRO:HD3	1.92	0.51
1:A:229:TRP:CD2	1:A:230:MET:HB2	2.46	0.51
1:A:49:LYS:HG2	1:A:144:TYR:CD1	2.46	0.51
1:A:483:TYR:O	1:A:487:GLN:HG2	2.11	0.51
1:A:510:PRO:O	1:A:522:ILE:HD13	2.10	0.51
2:B:268:SER:O	2:B:270:ILE:N	2.44	0.51
1:A:57:ASN:OD1	1:A:131:THR:HG23	2.12	0.50
1:A:460:ASN:C	1:A:462:GLY:H	2.15	0.50
2:B:103:LYS:HD2	2:B:190:GLY:C	2.31	0.50
2:B:122:GLU:CA	2:B:125:ARG:HH11	2.22	0.50
1:A:131:THR:HG22	1:A:143:ARG:HG2	1.93	0.50
1:A:167:ILE:O	1:A:170:PRO:HD2	2.12	0.50
1:A:224:GLU:N	1:A:225:PRO:CD	2.74	0.50
2:B:171:PHE:CE1	2:B:205:LEU:HG	2.45	0.50
1:A:12:LEU:N	1:A:12:LEU:CD1	2.72	0.50
1:A:340:GLN:HA	1:A:351:THR:HA	1.94	0.50
2:B:77:PHE:CD1	2:B:80:LEU:HD12	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:303:LEU:HD11	2:B:307:ARG:NH2	2.27	0.50
2:B:65:LYS:CA	2:B:407:GLN:HE22	2.23	0.50
2:B:333:GLY:O	2:B:336:GLN:HB2	2.12	0.50
2:B:396:GLU:O	2:B:400:THR:OG1	2.30	0.50
1:A:63:ILE:HG21	4:T:704:DG:H22	1.76	0.50
1:A:393:ILE:HG13	1:A:423:VAL:HB	1.94	0.50
1:A:436:GLY:O	1:A:461:ARG:NH2	2.39	0.50
1:A:500:GLN:CG	2:B:422:LEU:HD22	2.39	0.50
2:B:125:ARG:NH2	2:B:147:ASN:HB3	2.25	0.50
2:B:163:SER:HA	2:B:166:LYS:HE3	1.94	0.50
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.42	0.50
2:B:195:ILE:HD13	2:B:195:ILE:C	2.31	0.50
1:A:63:ILE:HG21	4:T:704:DG:N2	2.27	0.49
1:A:111:VAL:HG21	1:A:164:MET:HE1	1.94	0.49
2:B:34:LEU:HG	2:B:62:ALA:HB2	1.93	0.49
2:B:63:ILE:HD11	2:B:406:TRP:O	2.11	0.49
2:B:66:LYS:HB3	2:B:68:SER:H	1.76	0.49
1:A:101:LYS:HD3	1:A:319:TYR:CD2	2.47	0.49
1:A:156:SER:CB	1:A:157:PRO:HD3	2.40	0.49
1:A:457:TYR:CE2	1:A:465:LYS:HB2	2.47	0.49
1:A:458:VAL:CG2	1:A:551:LEU:HD11	2.42	0.49
2:B:122:GLU:HA	2:B:125:ARG:CG	2.42	0.49
2:B:376:THR:O	2:B:380:ILE:HG13	2.13	0.49
1:A:199:ARG:NH2	1:A:222:GLN:HG2	2.28	0.49
1:A:277:ARG:HD2	1:A:336:GLN:HG3	1.94	0.49
2:B:13:LYS:HD2	2:B:16:MET:SD	2.52	0.49
1:A:81:ASN:OD1	1:A:153:TRP:HA	2.13	0.49
1:A:288:ALA:CB	1:A:291:GLU:HB2	2.42	0.49
1:A:295:LEU:HG	1:A:300:GLU:HB2	1.95	0.49
1:A:446:ALA:HA	1:A:453:GLY:HA2	1.93	0.49
1:A:458:VAL:HG12	1:A:458:VAL:O	2.11	0.49
1:A:131:THR:HG21	1:A:143:ARG:HE	1.77	0.49
1:A:271:TYR:CG	1:A:310:LEU:HD23	2.47	0.49
1:A:433:PRO:HB3	2:B:289:LEU:HD23	1.94	0.49
2:B:142:ILE:N	2:B:142:ILE:HD12	2.28	0.49
3:P:813:DT:H2'	3:P:814:DC:C6	2.47	0.49
1:A:194:GLU:OE1	1:A:197:GLN:N	2.45	0.49
2:B:66:LYS:HG2	2:B:67:ASP:N	2.25	0.49
1:A:458:VAL:HG23	1:A:551:LEU:HD11	1.95	0.49
1:A:106:VAL:HB	1:A:227:PHE:HE1	1.78	0.49
1:A:253:THR:HG22	1:A:292:VAL:CA	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:GLY:HA2	1:A:546:GLU:HG2	1.95	0.49
2:B:122:GLU:HG2	2:B:125:ARG:NH1	2.28	0.49
1:A:491:LEU:HD23	1:A:529:GLU:HG3	1.95	0.49
2:B:254:VAL:HG21	2:B:287:LYS:HB3	1.95	0.49
1:A:218:ASP:HA	1:A:220:LYS:N	2.28	0.48
1:A:339:TYR:CE1	1:A:352:GLY:HA3	2.45	0.48
1:A:411:ILE:HG23	1:A:412:PRO:HD2	1.93	0.48
2:B:398:TRP:CD1	2:B:416:PHE:HE1	2.31	0.48
1:A:326:ILE:O	1:A:341:ILE:HA	2.13	0.48
1:A:363:ASN:HB3	1:A:509:GLN:O	2.13	0.48
2:B:8:VAL:HG13	2:B:8:VAL:O	2.13	0.48
1:A:75:VAL:HB	1:A:77:PHE:CE2	2.49	0.48
1:A:167:ILE:C	1:A:169:GLU:N	2.66	0.48
2:B:175:ASN:OD1	2:B:201:LYS:HE3	2.12	0.48
2:B:100:LEU:HD13	2:B:179:VAL:HG13	1.96	0.48
2:B:107:THR:HG21	2:B:202:ILE:HG21	1.95	0.48
2:B:420:PRO:O	2:B:423:VAL:HG12	2.14	0.48
1:A:138:GLU:HA	1:A:138:GLU:OE2	2.13	0.48
2:B:65:LYS:C	2:B:407:GLN:HE22	2.17	0.48
4:T:710:DG:H2'	4:T:711:DC:C6	2.49	0.48
1:A:65:LYS:CD	1:A:70:LYS:HE2	2.43	0.48
1:A:108:VAL:HG13	1:A:221:HIS:HB3	1.94	0.48
2:B:253:THR:H	2:B:256:ASP:HB2	1.79	0.48
1:A:132:ILE:CG2	1:A:133:PRO:HD2	2.44	0.47
1:A:305:GLU:O	1:A:308:GLU:HB2	2.14	0.47
2:B:112:GLY:O	2:B:114:ALA:N	2.47	0.47
1:A:125:ARG:HD3	1:A:146:TYR:O	2.13	0.47
1:A:132:ILE:HG22	1:A:133:PRO:HD2	1.95	0.47
1:A:443:ASP:O	1:A:552:VAL:HG11	2.14	0.47
2:B:98:ALA:O	2:B:101:LYS:HE2	2.14	0.47
2:B:195:ILE:CD1	2:B:199:ARG:HH21	2.23	0.47
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.49	0.47
1:A:380:ILE:HD12	1:A:380:ILE:H	1.79	0.47
2:B:249:LYS:HE2	2:B:249:LYS:HB3	1.74	0.47
1:A:21:VAL:O	1:A:57:ASN:ND2	2.46	0.47
1:A:535:TRP:CH2	1:A:537:PRO:HA	2.50	0.47
2:B:424:LYS:HD2	2:B:425:LEU:HD12	1.96	0.47
1:A:76:ASP:C	1:A:78:ARG:H	2.18	0.47
1:A:85:GLN:NE2	1:A:86:ASP:O	2.44	0.47
1:A:254:VAL:O	1:A:257:ILE:HG22	2.14	0.47
1:A:426:TRP:O	1:A:427:TYR:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:THR:O	2:B:154:LYS:NZ	2.46	0.47
3:P:810:DT:H2'	3:P:811:DG:H8	1.77	0.47
1:A:151:GLN:HG3	1:A:151:GLN:O	2.15	0.47
1:A:220:LYS:O	1:A:221:HIS:C	2.53	0.47
1:A:397:THR:O	1:A:400:THR:HB	2.15	0.47
1:A:406:TRP:CH2	1:A:507:GLN:HB2	2.50	0.47
3:P:811:DG:H2"	3:P:812:DT:H5'	1.96	0.47
1:A:168:LEU:HD21	1:A:209:LEU:HD11	1.97	0.47
1:A:248:GLU:H	1:A:248:GLU:HG3	1.45	0.47
1:A:260:LEU:HD11	1:A:303:LEU:HD13	1.97	0.47
2:B:390:LYS:HE2	2:B:415:GLU:OE2	2.15	0.47
1:A:95:PRO:HA	2:B:136:ASN:O	2.15	0.47
1:A:460:ASN:C	1:A:462:GLY:N	2.69	0.47
1:A:65:LYS:HE3	1:A:70:LYS:HE2	1.95	0.46
1:A:254:VAL:O	1:A:255:ASN:C	2.53	0.46
1:A:254:VAL:HG13	1:A:283:LEU:CD1	2.46	0.46
1:A:277:ARG:HH11	1:A:277:ARG:CB	2.29	0.46
1:A:548:VAL:O	1:A:551:LEU:HB2	2.15	0.46
2:B:42:GLU:HG3	2:B:43:LYS:N	2.30	0.46
2:B:64:LYS:HD2	2:B:68:SER:O	2.15	0.46
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.50	0.46
2:B:154:LYS:O	2:B:154:LYS:HG2	2.15	0.46
1:A:328:GLU:HG2	1:A:330:GLN:HE21	1.80	0.46
2:B:61:PHE:N	2:B:61:PHE:CD1	2.83	0.46
2:B:339:TYR:CZ	2:B:352:GLY:HA3	2.50	0.46
1:A:65:LYS:HD2	1:A:70:LYS:HE2	1.97	0.46
1:A:103:LYS:NZ	1:A:179:VAL:HG21	2.30	0.46
1:A:394:GLN:H	1:A:394:GLN:HG2	1.34	0.46
1:A:503:LEU:HG	1:A:507:GLN:NE2	2.26	0.46
2:B:106:VAL:HG13	2:B:189:VAL:O	2.15	0.46
1:A:64:LYS:HG3	1:A:65:LYS:H	1.78	0.46
1:A:279:LEU:O	1:A:282:LEU:HB2	2.16	0.46
1:A:118:VAL:HG22	1:A:149:LEU:HG	1.96	0.46
1:A:406:TRP:CD1	1:A:407:GLN:NE2	2.83	0.46
1:A:246:LEU:N	1:A:246:LEU:HD22	2.31	0.46
1:A:467:VAL:HG22	1:A:484:LEU:HD11	1.98	0.46
1:A:50:ILE:HG12	1:A:143:ARG:C	2.36	0.46
1:A:101:LYS:HD3	1:A:319:TYR:HD2	1.81	0.46
1:A:541:GLY:HA2	1:A:546:GLU:CG	2.46	0.46
2:B:241:VAL:HG13	2:B:351:THR:O	2.15	0.46
2:B:325:LEU:HB3	2:B:387:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:GLN:NE2	2:B:338:THR:OG1	2.44	0.46
1:A:16:MET:HB3	1:A:83:ARG:NH1	2.31	0.46
2:B:112:GLY:C	2:B:114:ALA:N	2.67	0.46
1:A:34:LEU:HD11	1:A:134:SER:O	2.16	0.46
1:A:256:ASP:O	1:A:259:LYS:HB2	2.15	0.46
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.98	0.46
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.50	0.46
1:A:181:TYR:CE1	2:B:138:GLU:HB2	2.49	0.45
1:A:503:LEU:HD11	1:A:507:GLN:HE21	1.81	0.45
2:B:135:ILE:N	2:B:135:ILE:CD1	2.59	0.45
2:B:325:LEU:HD23	2:B:387:PRO:HB3	1.96	0.45
2:B:345:PRO:O	2:B:346:PHE:HB2	2.16	0.45
2:B:366:LYS:O	2:B:369:THR:HB	2.16	0.45
1:A:65:LYS:HD3	1:A:67:ASP:O	2.16	0.45
1:A:188:TYR:CD2	1:A:188:TYR:C	2.90	0.45
1:A:329:ILE:HD11	1:A:375:ILE:CD1	2.43	0.45
1:A:480:GLN:HG2	1:A:517:LEU:HD21	1.98	0.45
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.98	0.45
1:A:193:LEU:N	1:A:193:LEU:HD12	2.31	0.45
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.99	0.45
2:B:148:VAL:O	2:B:149:LEU:C	2.54	0.45
4:T:704:DG:N3	4:T:704:DG:C2'	2.75	0.45
2:B:56:TYR:O	2:B:57:ASN:HB2	2.16	0.45
2:B:367:GLN:O	2:B:370:GLU:N	2.49	0.45
4:T:719:DG:H2'	4:T:720:DG:C8	2.51	0.45
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.36	0.45
1:A:317:VAL:CG1	1:A:318:TYR:N	2.71	0.45
2:B:111:VAL:HG23	2:B:111:VAL:O	2.17	0.45
2:B:320:ASP:OD1	2:B:320:ASP:C	2.55	0.45
4:T:716:DA:H2'	4:T:717:DC:C1'	2.46	0.45
1:A:398:TRP:CH2	1:A:411:ILE:HG13	2.51	0.45
1:A:463:ARG:C	1:A:464:GLN:HG3	2.37	0.45
2:B:12:LEU:N	2:B:12:LEU:CD1	2.78	0.45
2:B:193:LEU:CD1	2:B:201:LYS:HG3	2.45	0.45
3:P:806:DT:H2'	3:P:807:DC:C6	2.52	0.45
1:A:87:PHE:CE1	1:A:155:GLY:HA2	2.52	0.45
1:A:108:VAL:HG13	1:A:221:HIS:CB	2.46	0.45
2:B:74:LEU:HD12	2:B:74:LEU:H	1.81	0.45
1:A:189:VAL:HG11	1:A:202:ILE:CD1	2.47	0.45
1:A:288:ALA:HB3	1:A:291:GLU:CB	2.47	0.45
1:A:160:PHE:HE1	1:A:184:MET:O	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HD22	1:A:132:ILE:CG2	2.47	0.44
1:A:396:GLU:O	1:A:397:THR:C	2.55	0.44
1:A:402:TRP:CZ3	2:B:364:ASP:OD2	2.70	0.44
2:B:49:LYS:HD3	2:B:144:TYR:CE1	2.51	0.44
1:A:102:LYS:HB3	1:A:102:LYS:HE3	1.72	0.44
1:A:224:GLU:N	1:A:225:PRO:HD3	2.33	0.44
1:A:314:VAL:CG2	1:A:315:HIS:N	2.79	0.44
1:A:104:LYS:HE3	1:A:194:GLU:CA	2.48	0.44
2:B:9:PRO:HA	2:B:121:ASP:OD2	2.17	0.44
2:B:65:LYS:O	2:B:407:GLN:NE2	2.51	0.44
2:B:77:PHE:HD1	2:B:80:LEU:HB3	1.82	0.44
2:B:79:GLU:OE2	2:B:79:GLU:HA	2.17	0.44
2:B:282:LEU:HB3	2:B:293:ILE:HG21	1.98	0.44
1:A:8:VAL:N	7:A:562:HOH:O	2.41	0.44
1:A:107:THR:CG2	1:A:108:VAL:N	2.80	0.44
1:A:264:LEU:HD23	1:A:276:VAL:HG12	2.00	0.44
2:B:303:LEU:HD11	2:B:307:ARG:HH22	1.83	0.44
1:A:110:ASP:O	1:A:216:THR:HG22	2.17	0.44
1:A:216:THR:HA	1:A:217:PRO:HD2	1.83	0.44
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.17	0.44
2:B:178:ILE:HD11	2:B:201:LYS:HD3	1.99	0.44
1:A:122:GLU:C	1:A:124:PHE:H	2.20	0.44
2:B:72:ARG:HH12	2:B:151:GLN:CD	2.21	0.44
2:B:121:ASP:OD1	2:B:121:ASP:C	2.56	0.44
4:T:715:DA:H2'	4:T:716:DA:C8	2.52	0.44
1:A:67:ASP:O	1:A:69:THR:N	2.50	0.44
1:A:202:ILE:O	1:A:206:ARG:HG3	2.18	0.44
1:A:296:THR:O	1:A:299:ALA:HB3	2.17	0.44
1:A:531:VAL:CG1	1:A:532:TYR:N	2.81	0.44
1:A:376:THR:O	1:A:380:ILE:CD1	2.64	0.44
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	3.05	0.44
1:A:106:VAL:CG2	1:A:227:PHE:HE1	2.30	0.43
1:A:264:LEU:O	1:A:267:ALA:HB3	2.17	0.43
1:A:492:GLU:OE2	1:A:530:LYS:HD3	2.18	0.43
1:A:531:VAL:HG12	1:A:532:TYR:N	2.34	0.43
2:B:390:LYS:HE3	2:B:390:LYS:HB2	1.91	0.43
1:A:329:ILE:HG22	1:A:330:GLN:N	2.32	0.43
2:B:81:ASN:OD1	2:B:153:TRP:HA	2.18	0.43
2:B:125:ARG:HB3	2:B:146:TYR:O	2.19	0.43
1:A:394:GLN:O	1:A:396:GLU:N	2.52	0.43
1:A:19:PRO:O	1:A:20:LYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:PRO:C	1:A:522:ILE:HD13	2.38	0.43
2:B:368:LEU:O	2:B:372:VAL:HG22	2.19	0.43
1:A:480:GLN:O	1:A:483:TYR:HB3	2.18	0.43
2:B:201:LYS:O	2:B:204:GLU:HB3	2.19	0.43
1:A:278:GLN:O	1:A:282:LEU:CD1	2.64	0.43
1:A:312:GLU:H	1:A:312:GLU:HG2	1.55	0.43
1:A:89:GLU:OE1	1:A:158:ALA:HB2	2.18	0.43
1:A:258:CYS:HA	1:A:261:VAL:HG12	2.01	0.43
2:B:376:THR:OG1	2:B:389:PHE:HE1	2.02	0.43
4:T:708:DG:H2'	4:T:709:DC:C5	2.53	0.43
1:A:384:GLY:O	2:B:28:GLU:HG3	2.19	0.43
1:A:416:PHE:CZ	1:A:422:LEU:HD11	2.50	0.43
1:A:437:ALA:O	1:A:438:GLU:C	2.57	0.43
2:B:111:VAL:HA	2:B:112:GLY:HA3	1.52	0.43
2:B:183:TYR:OH	2:B:386:THR:HB	2.19	0.43
1:A:131:THR:CG2	1:A:143:ARG:HE	2.32	0.42
1:A:173:LYS:C	1:A:175:ASN:N	2.71	0.42
1:A:325:LEU:HD12	1:A:385:LYS:CG	2.49	0.42
1:A:326:ILE:HD12	1:A:342:TYR:CE2	2.51	0.42
2:B:367:GLN:O	2:B:368:LEU:C	2.55	0.42
4:T:703:DG:H2'	4:T:704:DG:C4	2.52	0.42
1:A:170:PRO:O	1:A:174:GLN:HB3	2.19	0.42
1:A:292:VAL:O	1:A:293:ILE:HD13	2.19	0.42
1:A:390:LYS:HE3	7:A:580:HOH:O	2.18	0.42
1:A:524:GLN:HE22	1:A:528:LYS:HZ2	1.66	0.42
1:A:88:TRP:HZ3	2:B:20:LYS:HB3	1.83	0.42
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.42
2:B:268:SER:C	2:B:270:ILE:H	2.23	0.42
2:B:353:LYS:NZ	2:B:429:LEU:HD11	2.34	0.42
2:B:390:LYS:HG2	2:B:417:VAL:HB	2.02	0.42
1:A:304:ALA:O	1:A:308:GLU:HG2	2.18	0.42
2:B:122:GLU:HA	2:B:125:ARG:HG2	2.02	0.42
2:B:305:GLU:O	2:B:309:ILE:HG12	2.19	0.42
2:B:325:LEU:HD12	2:B:343:GLN:OE1	2.19	0.42
1:A:491:LEU:HD23	1:A:529:GLU:CG	2.49	0.42
2:B:301:LEU:HA	2:B:301:LEU:HD22	1.81	0.42
1:A:439:THR:HG23	1:A:494:ASN:HB2	2.00	0.42
2:B:161:GLN:O	2:B:162:SER:C	2.57	0.42
2:B:278:GLN:HE21	2:B:298:GLU:HG3	1.84	0.42
4:T:707:DG:H2"	4:T:708:DG:C5'	2.48	0.42
1:A:325:LEU:HD12	1:A:385:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:SER:OG	1:A:4:PRO:HD2	2.20	0.42
1:A:257:ILE:O	1:A:260:LEU:N	2.52	0.42
2:B:422:LEU:C	2:B:424:LYS:H	2.23	0.42
1:A:107:THR:CG2	1:A:109:LEU:HD22	2.50	0.42
2:B:320:ASP:HA	2:B:321:PRO:HD3	1.84	0.42
2:B:376:THR:HG1	2:B:389:PHE:HE1	1.68	0.42
1:A:64:LYS:CG	1:A:65:LYS:N	2.83	0.41
1:A:224:GLU:H	1:A:225:PRO:HD3	1.85	0.41
1:A:542:ILE:N	1:A:546:GLU:HG3	2.35	0.41
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.74	0.41
2:B:148:VAL:O	2:B:148:VAL:HG23	2.19	0.41
4:T:703:DG:H5"	4:T:704:DG:C2	2.55	0.41
1:A:65:LYS:CE	1:A:70:LYS:HE2	2.49	0.41
1:A:115:TYR:O	1:A:149:LEU:HB2	2.20	0.41
1:A:196:GLY:HA2	1:A:199:ARG:HB2	2.02	0.41
1:A:296:THR:CG2	1:A:297:GLU:N	2.82	0.41
1:A:79:GLU:OE1	1:A:79:GLU:HA	2.20	0.41
1:A:170:PRO:O	1:A:174:GLN:CB	2.68	0.41
1:A:254:VAL:C	1:A:256:ASP:N	2.71	0.41
1:A:386:THR:HA	1:A:387:PRO:HD3	1.73	0.41
2:B:40:GLU:O	2:B:44:GLU:HG3	2.19	0.41
2:B:61:PHE:CD2	2:B:403:THR:HG22	2.55	0.41
2:B:268:SER:C	2:B:270:ILE:N	2.73	0.41
2:B:10:VAL:HG23	2:B:124:PHE:CD1	2.54	0.41
1:A:37:ILE:HD13	1:A:37:ILE:HA	1.91	0.41
2:B:168:LEU:O	2:B:169:GLU:C	2.59	0.41
2:B:297:GLU:HB3	2:B:298:GLU:OE1	2.20	0.41
1:A:279:LEU:H	1:A:279:LEU:CD2	2.33	0.41
2:B:363:ASN:ND2	2:B:405:TYR:CZ	2.89	0.41
1:A:184:MET:HB3	3:P:822:DOC:H2"	2.03	0.41
1:A:209:LEU:HD22	1:A:209:LEU:H	1.85	0.41
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.51	0.41
1:A:427:TYR:HE2	1:A:525:LEU:HD13	1.83	0.41
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.21	0.41
2:B:121:ASP:OD1	2:B:122:GLU:N	2.54	0.41
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.94	0.41
3:P:815:DG:H2'	3:P:816:DG:C8	2.56	0.41
2:B:198:HIS:O	2:B:201:LYS:HB2	2.21	0.41
2:B:366:LYS:HG3	2:B:405:TYR:CG	2.56	0.41
2:B:379:SER:CB	2:B:387:PRO:HD3	2.51	0.41
1:A:132:ILE:HB	1:A:142:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:O	1:A:256:ASP:HB3	2.21	0.40
1:A:458:VAL:HG23	1:A:551:LEU:CD1	2.51	0.40
1:A:106:VAL:CG2	1:A:227:PHE:CE1	3.04	0.40
1:A:296:THR:HG22	1:A:297:GLU:N	2.37	0.40
1:A:543:GLY:HA2	1:A:544:GLY:HA2	1.42	0.40
2:B:267:ALA:O	2:B:268:SER:C	2.58	0.40
1:A:110:ASP:OD1	1:A:186:ASP:OD2	2.39	0.40
2:B:12:LEU:O	2:B:13:LYS:C	2.59	0.40
2:B:28:GLU:HG3	2:B:28:GLU:H	1.69	0.40
2:B:34:LEU:HD23	2:B:34:LEU:HA	1.89	0.40
1:A:326:ILE:CD1	1:A:342:TYR:HE2	2.33	0.40
1:A:452:LEU:HD13	1:A:452:LEU:HA	1.90	0.40
1:A:238:LYS:HB3	1:A:315:HIS:HD2	1.87	0.40
1:A:339:TYR:CE1	1:A:353:LYS:N	2.89	0.40
1:A:366:LYS:O	1:A:370:GLU:HG3	2.21	0.40
1:A:391:LEU:HA	1:A:392:PRO:HD3	1.76	0.40
2:B:174:GLN:O	2:B:176:PRO:HD3	2.20	0.40
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	545/560 (97%)	448 (82%)	71 (13%)	26 (5%)	2 14
2	B	394/452 (87%)	338 (86%)	52 (13%)	4 (1%)	15 49
All	All	939/1012 (93%)	786 (84%)	123 (13%)	30 (3%)	4 22

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	254	VAL
1	A	466	VAL
1	A	64	LYS
1	A	68	SER
1	A	138	GLU
1	A	333	GLY
1	A	340	GLN
1	A	461	ARG
2	B	113	ASP
1	A	20	LYS
1	A	133	PRO
1	A	217	PRO
1	A	413	GLU
1	A	458	VAL
1	A	63	ILE
1	A	85	GLN
1	A	98	ALA
1	A	168	LEU
1	A	221	HIS
2	B	269	GLN
2	B	428	GLN
1	A	247	PRO
1	A	255	ASN
1	A	392	PRO
1	A	52	PRO
1	A	224	GLU
1	A	21	VAL
1	A	345	PRO
1	A	195	ILE
2	B	423	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	486/500 (97%)	426 (88%)	60 (12%)	4 19
2	B	362/411 (88%)	317 (88%)	45 (12%)	4 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	848/911 (93%)	743 (88%)	105 (12%)	4 19

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	23	GLN
1	A	53	GLU
1	A	54	ASN
1	A	73	LYS
1	A	85	GLN
1	A	91	GLN
1	A	100	LEU
1	A	108	VAL
1	A	123	ASP
1	A	126	LYS
1	A	136	ASN
1	A	173	LYS
1	A	174	GLN
1	A	177	ASP
1	A	188	TYR
1	A	194	GLU
1	A	205	LEU
1	A	210	LEU
1	A	211	ARG
1	A	216	THR
1	A	218	ASP
1	A	222	GLN
1	A	223	LYS
1	A	230	MET
1	A	233	GLU
1	A	237	ASP
1	A	238	LYS
1	A	248	GLU
1	A	250	ASP
1	A	252	TRP
1	A	259	LYS
1	A	260	LEU
1	A	277	ARG
1	A	279	LEU
1	A	287	LYS
1	A	298	GLU

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Mol	Chain	Res	Type
1	A	320	ASP
1	A	322	SER
1	A	330	GLN
1	A	342	TYR
1	A	358	ARG
1	A	367	GLN
1	A	373	GLN
1	A	386	THR
1	A	394	GLN
1	A	399	GLU
1	A	402	TRP
1	A	407	GLN
1	A	418	ASN
1	A	422	LEU
1	A	432	GLU
1	A	460	ASN
1	A	469	LEU
1	A	478	GLU
1	A	480	GLN
1	A	494	ASN
1	A	533	LEU
1	A	540	LYS
1	A	548	VAL
2	B	37	ILE
2	B	40	GLU
2	B	41	MET
2	B	58	THR
2	B	61	PHE
2	B	65	LYS
2	B	66	LYS
2	B	73	LYS
2	B	74	LEU
2	B	80	LEU
2	B	82	LYS
2	B	102	LYS
2	B	104	LYS
2	B	125	ARG
2	B	126	LYS
2	B	135	ILE
2	B	161	GLN
2	B	172	ARG
2	B	174	GLN

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Mol	Chain	Res	Type
2	B	194	GLU
2	B	195	ILE
2	B	201	LYS
2	B	205	LEU
2	B	211	ARG
2	B	237	ASP
2	B	242	GLN
2	B	246	LEU
2	B	276	VAL
2	B	277	ARG
2	B	279	LEU
2	B	280	SER
2	B	290	THR
2	B	297	GLU
2	B	298	GLU
2	B	301	LEU
2	B	343	GLN
2	B	344	GLU
2	B	356	ARG
2	B	361	HIS
2	B	368	LEU
2	B	385	LYS
2	B	410	TRP
2	B	413	GLU
2	B	429	LEU
2	B	431	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	145	GLN
1	A	175	ASN
1	A	197	GLN
1	A	278	GLN
1	A	306	ASN
1	A	330	GLN
1	A	340	GLN
1	A	367	GLN
1	A	480	GLN
1	A	507	GLN
1	A	520	GLN

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Mol	Chain	Res	Type
1	A	524	GLN
1	A	545	ASN
2	B	151	GLN
2	B	174	GLN
2	B	394	GLN
2	B	407	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	DOC	P	822	3,4	16,19,20	0.40	0	20,26,29	0.64	0

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	DOC	P	822	3,4	-	0/7/18/19	0/2/2/2

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	822	DOC	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	$\#\|Z\| > 2$
5	SO4	T	2	-	4,4,4	0.26	0	6,6,6	0.10	0
5	SO4	P	3	-	4,4,4	0.27	0	6,6,6	0.07	0
5	SO4	A	561	-	4,4,4	0.46	0	6,6,6	0.67	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	549/560 (98%)	-0.37	8 (1%)	73	54	15, 49, 102, 123	0
2	B	400/452 (88%)	-0.48	2 (0%)	91	81	20, 50, 80, 116	0
3	P	17/21 (80%)	-0.83	0	100	100	33, 47, 68, 70	0
4	T	23/27 (85%)	-0.55	0	100	100	30, 59, 100, 154	0
All	All	989/1060 (93%)	-0.43	10 (1%)	82	67	15, 50, 93, 154	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	LYS	3.3
1	A	137	ASN	3.2
1	A	69	THR	2.5
1	A	63	ILE	2.5
1	A	135	ILE	2.5
1	A	136	ASN	2.4
2	B	4	PRO	2.2
2	B	7	THR	2.1
1	A	141	GLY	2.1
1	A	133	PRO	2.0

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	DOC	P	822	18/19	0.97	0.15	30,33,36,37	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	SO4	P	3	5/5	0.89	0.22	116,116,117,117	0
5	SO4	A	561	5/5	0.92	0.18	84,85,86,87	0
5	SO4	T	2	5/5	0.92	0.20	97,97,98,98	0
6	MG	A	601	1/1	0.98	0.18	1,1,1,1	0

6.5 Other polymers (i)

There are no such residues in this entry.