Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:01 AM GMT

PDB ID	:	3KK3
Title	:	HIV-1 reverse transcriptase-DNA complex with GS-9148 terminated primer
Authors	:	Lansdon, E.B.
Deposited on	:	2009-11-04
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

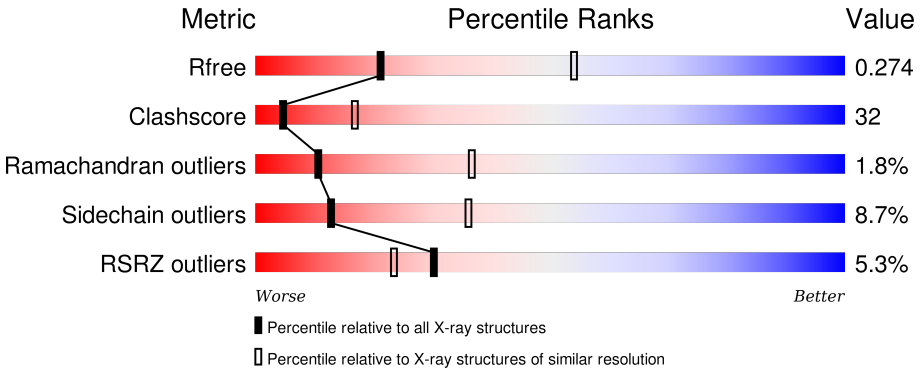
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	A	560	5%, 46%, 46%, 7%
2	B	452	5%, 38%, 47%, 5%, 10%
3	P	21	10%, 71%, 5%, 14%
4	T	27	4%, 11%, 74%, 15%

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
5	MG	A	601	-	-	-	X
6	SO4	P	3	-	-	-	X
6	SO4	T	2	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8752 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
1	A	555	Total	C	N	O	S	0	0	0
			4514	2917	753	836	8			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	407	Total	C	N	O	S	0	0	0
			3361	2191	555	609	6			

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	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*C*(URT))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	P	18	Total	C	F	N	O	P	0	0	0
			366	173	1	64	110	18			

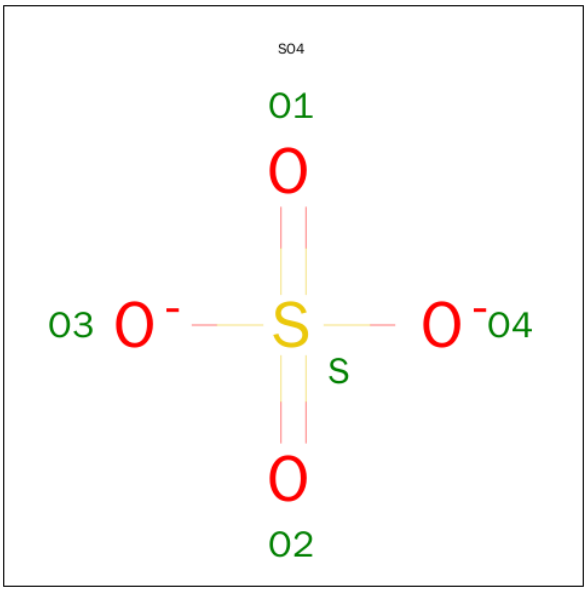
- Molecule 4 is a DNA chain called 5'-D(*AP*TP*GP*GP*TP*TP*GP*GP*CP*GP*CP*C P*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	T	23	Total	C	N	O	P	0	0	0
			478	224	94	137	23			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

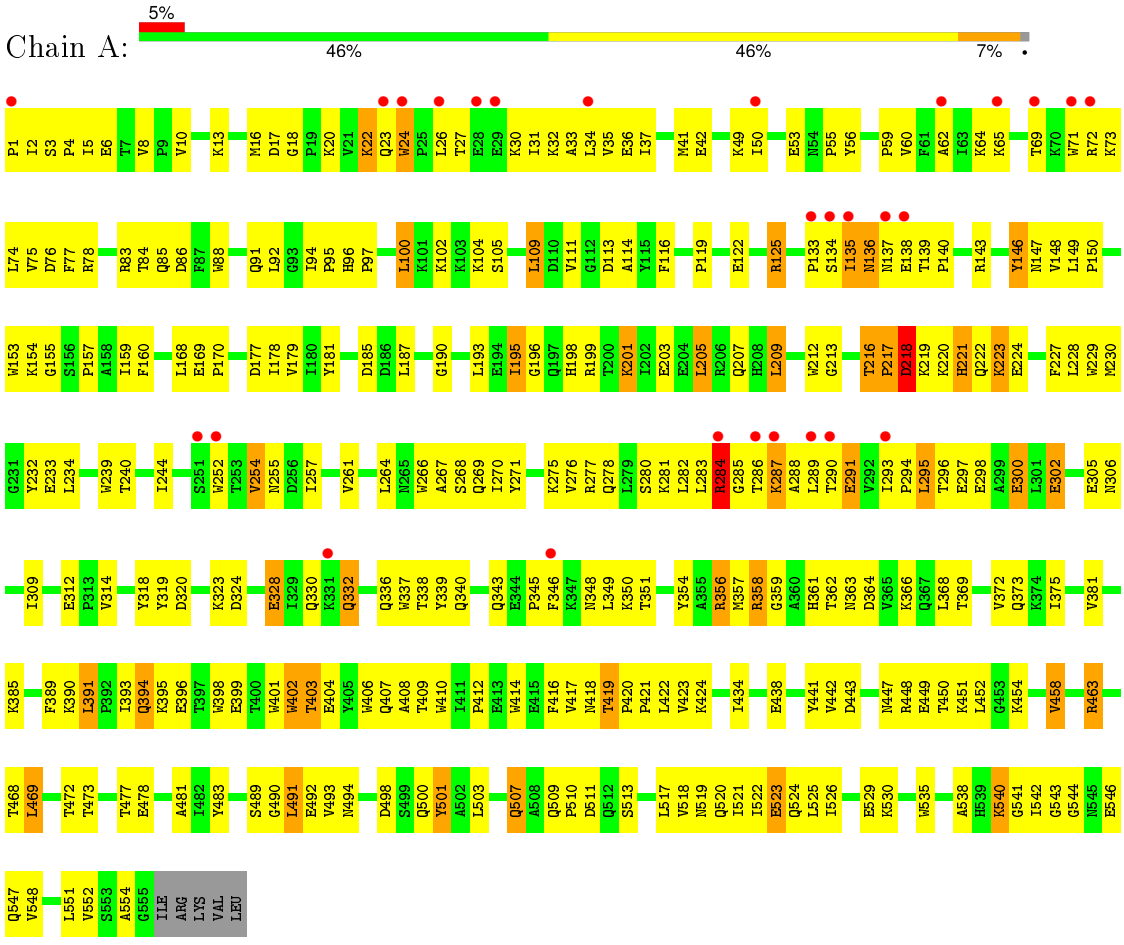
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	15	Total O 15 15	0	0
7	B	4	Total O 4 4	0	0
7	P	2	Total O 2 2	0	0
7	T	1	Total O 1 1	0	0

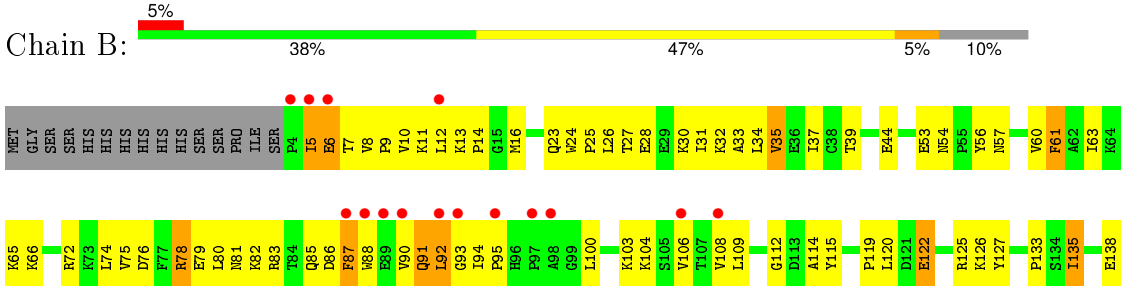
3 Residue-property plots (i)

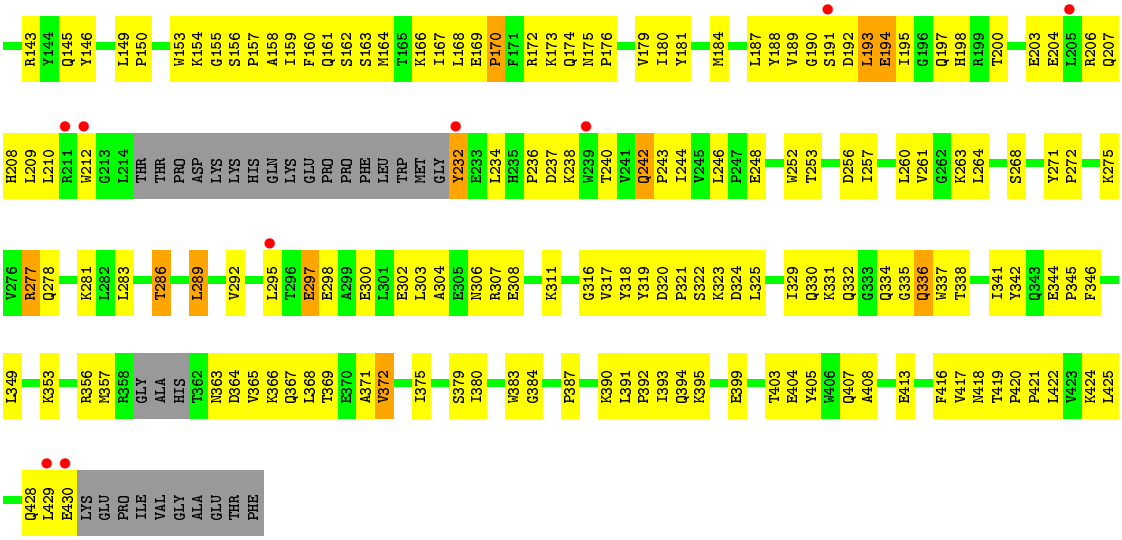
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Reverse transcriptase p66 subunit

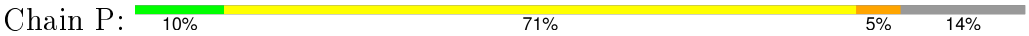


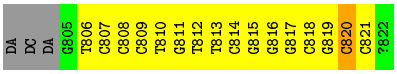
- Molecule 2: Reverse transcriptase p51 subunit



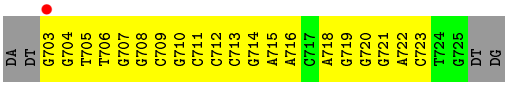


• Molecule 3: 5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*C*(URT))-3'





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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	167.00Å 169.07Å 96.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.90 48.20 – 2.79	Depositor EDS
% Data completeness (in resolution range)	89.1 (29.99-2.90) 84.3 (48.20-2.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.50 (at 2.77Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.223 , 0.287 0.209 , 0.274	Depositor DCC
R_{free} test set	1343 reflections (5.19%)	DCC
Wilson B-factor (Å^2)	68.9	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.5	EDS
Estimated twinning fraction	0.022 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 31422 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8752	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: URT, MG, 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	0/4631	0.59	0/6292
2	B	0.37	0/3455	0.54	0/4694
3	P	0.63	0/384	1.05	0/590
4	T	0.58	0/537	0.97	0/828
All	All	0.44	0/9007	0.64	0/12404

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	3
3	P	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	ASP	Peptide
1	A	286	THR	Peptide
1	A	287	LYS	Peptide
3	P	820	DC	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	4514	0	4563	297	0
2	B	3361	0	3393	222	1
3	P	366	0	200	26	0
4	T	478	0	257	32	0
5	A	1	0	0	0	0
6	P	5	0	0	0	0
6	T	5	0	0	0	0
7	A	15	0	0	1	0
7	B	4	0	0	1	0
7	P	2	0	0	0	0
7	T	1	0	0	0	0
All	All	8752	0	8413	546	1

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 32.

All (546) 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:336:GLN:HE22	2:B:353:LYS:HD2	1.26	1.00
1:A:125:ARG:HG2	1:A:146:TYR:O	1.63	0.98
2:B:5:ILE:HG23	2:B:6:GLU:H	1.30	0.96
1:A:195:ILE:H	1:A:195:ILE:HD13	1.29	0.96
1:A:255:ASN:HD22	1:A:289:LEU:HD22	1.28	0.96
3:P:820:DC:H2"	3:P:821:DC:H5'	1.48	0.92
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.53	0.90
2:B:35:VAL:O	2:B:39:THR:HG23	1.73	0.89
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.56	0.87
2:B:277:ARG:NH1	2:B:281:LYS:HD3	1.91	0.85
1:A:199:ARG:NH2	1:A:223:LYS:HB2	1.90	0.85
2:B:180:ILE:HG23	2:B:189:VAL:HG22	1.59	0.85
1:A:136:ASN:ND2	1:A:138:GLU:HB3	1.91	0.85
2:B:429:LEU:HD23	2:B:430:GLU:H	1.40	0.84
4:T:713:DC:H2'	4:T:714:DG:C8	2.13	0.83
1:A:518:VAL:O	1:A:522:ILE:HG13	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ASP:HA	2:B:88:TRP:CZ3	2.15	0.81
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.45	0.81
1:A:296:THR:HG22	1:A:298:GLU:H	1.45	0.80
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.62	0.80
1:A:297:GLU:HA	1:A:300:GLU:HB2	1.65	0.79
2:B:122:GLU:HA	2:B:125:ARG:HH11	1.48	0.78
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.66	0.78
1:A:224:GLU:O	1:A:224:GLU:HG2	1.81	0.77
2:B:420:PRO:HB2	2:B:422:LEU:HD23	1.67	0.77
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.67	0.76
2:B:103:LYS:HD2	2:B:191:SER:HA	1.68	0.75
3:P:813:DT:H2'	3:P:814:DC:C6	2.22	0.75
1:A:293:ILE:HD12	1:A:294:PRO:HD2	1.68	0.75
1:A:30:LYS:HG2	1:A:71:TRP:CZ3	2.22	0.75
1:A:109:LEU:HD12	1:A:187:LEU:HB2	1.68	0.75
2:B:345:PRO:O	2:B:346:PHE:HB2	1.86	0.75
1:A:295:LEU:HG	1:A:300:GLU:OE2	1.86	0.75
2:B:56:TYR:O	2:B:143:ARG:NH2	2.19	0.74
1:A:356:ARG:HD2	1:A:358:ARG:HG3	1.68	0.74
1:A:53:GLU:CD	1:A:53:GLU:H	1.91	0.74
2:B:115:TYR:OH	2:B:157:PRO:HB3	1.88	0.74
1:A:31:ILE:O	1:A:35:VAL:HG23	1.88	0.73
1:A:275:LYS:H	1:A:306:ASN:HD21	1.34	0.73
2:B:86:ASP:HA	2:B:88:TRP:HZ3	1.52	0.73
2:B:126:LYS:HA	2:B:145:GLN:OE1	1.87	0.73
2:B:65:LYS:O	2:B:66:LYS:HD2	1.88	0.73
1:A:138:GLU:HG2	1:A:139:THR:N	2.03	0.73
1:A:417:VAL:HG12	1:A:419:THR:HG22	1.70	0.72
2:B:10:VAL:HG12	2:B:11:LYS:H	1.54	0.72
1:A:26:LEU:HD12	1:A:133:PRO:HG3	1.70	0.72
1:A:358:ARG:HH11	1:A:358:ARG:HB3	1.53	0.72
1:A:363:ASN:HA	1:A:511:ASP:OD2	1.90	0.70
1:A:520:GLN:O	1:A:523:GLU:HG3	1.92	0.70
4:T:703:DG:H2"	4:T:704:DG:N2	2.07	0.70
1:A:2:ILE:CG2	1:A:119:PRO:HG3	2.23	0.69
2:B:79:GLU:HG3	2:B:83:ARG:HH11	1.57	0.69
1:A:8:VAL:HG21	1:A:159:ILE:HG23	1.75	0.68
1:A:97:PRO:O	1:A:100:LEU:HB2	1.94	0.68
2:B:200:THR:O	2:B:204:GLU:HG3	1.93	0.68
2:B:275:LYS:HE3	2:B:277:ARG:HB2	1.75	0.68
2:B:163:SER:O	2:B:167:ILE:HG13	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HB3	1:A:336:GLN:NE2	2.09	0.67
1:A:418:ASN:O	1:A:420:PRO:HD3	1.94	0.67
1:A:492:GLU:OE1	1:A:530:LYS:HD2	1.94	0.67
2:B:429:LEU:HD23	2:B:430:GLU:N	2.09	0.67
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.29	0.67
1:A:65:LYS:HG2	1:A:72:ARG:HE	1.58	0.67
2:B:82:LYS:HE2	2:B:413:GLU:OE2	1.94	0.67
4:T:704:DG:H2"	4:T:705:DT:OP1	1.94	0.67
4:T:713:DC:H2"	4:T:714:DG:O4'	1.94	0.67
2:B:5:ILE:HG23	2:B:6:GLU:N	2.08	0.67
1:A:255:ASN:ND2	1:A:289:LEU:HD22	2.05	0.67
2:B:336:GLN:NE2	2:B:353:LYS:HD2	2.05	0.66
2:B:275:LYS:HE3	2:B:277:ARG:CB	2.25	0.66
1:A:403:THR:HG22	1:A:404:GLU:N	2.11	0.66
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.79	0.65
2:B:31:ILE:HD12	2:B:135:ILE:HG22	1.79	0.65
2:B:278:GLN:HB2	2:B:302:GLU:OE1	1.96	0.65
1:A:122:GLU:HG2	1:A:125:ARG:NH2	2.11	0.65
2:B:13:LYS:HZ1	2:B:88:TRP:HH2	1.45	0.65
1:A:366:LYS:O	1:A:369:THR:HB	1.96	0.65
1:A:199:ARG:HH21	1:A:223:LYS:HB2	1.59	0.65
2:B:104:LYS:HB3	2:B:192:ASP:HA	1.78	0.65
4:T:707:DG:H2"	4:T:708:DG:H5'	1.79	0.65
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.77	0.65
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.79	0.65
1:A:478:GLU:OE1	1:A:478:GLU:HA	1.96	0.65
2:B:206:ARG:O	2:B:210:LEU:HD13	1.97	0.65
1:A:60:VAL:HG21	1:A:73:LYS:HE2	1.78	0.65
2:B:425:LEU:HD12	2:B:428:GLN:HG3	1.79	0.65
4:T:708:DG:H2'	4:T:709:DC:C6	2.33	0.64
2:B:109:LEU:HB3	2:B:187:LEU:HB3	1.79	0.64
1:A:22:LYS:HG2	1:A:22:LYS:O	1.98	0.64
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.32	0.64
1:A:195:ILE:HD13	1:A:195:ILE:N	2.10	0.63
2:B:122:GLU:HA	2:B:125:ARG:NH1	2.13	0.63
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.18	0.63
2:B:26:LEU:HD12	2:B:133:PRO:CG	2.28	0.63
4:T:718:DA:H2"	4:T:719:DG:OP1	1.97	0.63
2:B:88:TRP:O	2:B:92:LEU:HD12	1.97	0.63
2:B:33:ALA:O	2:B:37:ILE:HG13	1.98	0.63
1:A:27:THR:OG1	1:A:30:LYS:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:HE2	4:T:703:DG:H22	1.64	0.63
2:B:170:PRO:HB2	2:B:208:HIS:NE2	2.14	0.63
1:A:393:ILE:HG13	1:A:423:VAL:HB	1.80	0.63
2:B:337:TRP:HE1	2:B:367:GLN:HG2	1.64	0.63
1:A:33:ALA:O	1:A:37:ILE:HG13	1.98	0.63
2:B:172:ARG:NH2	2:B:180:ILE:HB	2.14	0.62
1:A:500:GLN:HE21	2:B:420:PRO:CB	2.12	0.62
1:A:143:ARG:HG3	1:A:143:ARG:NH1	2.14	0.62
2:B:277:ARG:HH11	2:B:281:LYS:HD3	1.65	0.62
2:B:81:ASN:O	2:B:154:LYS:HE3	2.00	0.62
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.82	0.62
1:A:94:ILE:CD1	4:T:709:DC:H1'	2.29	0.61
1:A:390:LYS:HB3	1:A:417:VAL:CG2	2.30	0.61
1:A:94:ILE:HD13	4:T:709:DC:H1'	1.82	0.61
2:B:109:LEU:HD23	2:B:187:LEU:HD23	1.82	0.61
4:T:714:DG:H2'	4:T:715:DA:C8	2.36	0.61
2:B:422:LEU:N	2:B:422:LEU:HD22	2.16	0.61
1:A:1:PRO:HG2	1:A:213:GLY:HA2	1.83	0.61
2:B:368:LEU:O	2:B:368:LEU:HD22	2.01	0.60
2:B:197:GLN:HA	2:B:200:THR:HG22	1.83	0.60
2:B:79:GLU:HG3	2:B:83:ARG:NH1	2.16	0.60
1:A:1:PRO:O	1:A:2:ILE:HD13	2.01	0.60
1:A:285:GLY:O	1:A:287:LYS:HB3	2.01	0.60
1:A:104:LYS:HD2	1:A:193:LEU:O	2.01	0.60
1:A:361:HIS:ND1	1:A:513:SER:HB2	2.16	0.60
1:A:399:GLU:HA	1:A:402:TRP:HD1	1.67	0.60
2:B:203:GLU:OE1	2:B:206:ARG:HD3	2.02	0.60
1:A:469:LEU:HB2	1:A:472:THR:HG21	1.83	0.60
2:B:244:ILE:N	2:B:244:ILE:HD12	2.16	0.60
1:A:222:GLN:O	1:A:223:LYS:C	2.38	0.60
2:B:316:GLY:HA2	2:B:318:TYR:CE2	2.37	0.60
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.83	0.60
1:A:23:GLN:NE2	1:A:59:PRO:HA	2.17	0.60
2:B:31:ILE:CD1	2:B:135:ILE:HG22	2.32	0.60
2:B:100:LEU:HD12	2:B:100:LEU:O	2.02	0.60
4:T:720:DG:H2'	4:T:721:DG:C8	2.37	0.60
1:A:458:VAL:HG13	2:B:286:THR:HG21	1.83	0.60
2:B:344:GLU:OE1	2:B:344:GLU:HA	2.01	0.60
1:A:254:VAL:O	1:A:257:ILE:HB	2.02	0.59
2:B:90:VAL:HG12	2:B:91:GLN:HE22	1.67	0.59
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:PHE:CZ	2:B:155:GLY:HA2	2.37	0.59
1:A:16:MET:HB3	1:A:83:ARG:NH1	2.17	0.59
1:A:23:GLN:HE22	1:A:59:PRO:HA	1.67	0.59
1:A:199:ARG:NH2	1:A:223:LYS:CB	2.62	0.59
2:B:257:ILE:O	2:B:261:VAL:HG23	2.03	0.59
1:A:320:ASP:OD2	1:A:323:LYS:HG3	2.03	0.59
3:P:817:DG:H2'	3:P:818:DC:C6	2.37	0.58
3:P:820:DC:H2"	3:P:821:DC:C5'	2.27	0.58
2:B:104:LYS:O	2:B:236:PRO:HD2	2.04	0.58
1:A:277:ARG:HB3	1:A:336:GLN:CD	2.23	0.58
1:A:543:GLY:HA3	2:B:283:LEU:O	2.03	0.58
2:B:421:PRO:O	2:B:424:LYS:HB3	2.03	0.58
2:B:335:GLY:HA2	2:B:367:GLN:NE2	2.18	0.58
2:B:5:ILE:HG12	2:B:6:GLU:HG3	1.84	0.58
1:A:64:LYS:HE3	1:A:71:TRP:CZ2	2.39	0.58
1:A:135:ILE:HG23	1:A:136:ASN:OD1	2.02	0.58
1:A:195:ILE:H	1:A:195:ILE:CD1	2.09	0.58
3:P:818:DC:H2"	3:P:819:DG:H5'	1.85	0.58
2:B:191:SER:H	2:B:198:HIS:HE1	1.52	0.58
1:A:60:VAL:O	1:A:60:VAL:HG13	2.03	0.58
1:A:295:LEU:HD12	1:A:296:THR:O	2.04	0.58
1:A:522:ILE:O	1:A:526:ILE:HG13	2.04	0.57
1:A:69:THR:HG22	1:A:69:THR:O	2.03	0.57
2:B:160:PHE:O	2:B:164:MET:HB2	2.04	0.57
2:B:191:SER:HB2	2:B:193:LEU:HD13	1.85	0.57
1:A:469:LEU:N	1:A:469:LEU:HD22	2.20	0.57
2:B:90:VAL:HG12	2:B:91:GLN:NE2	2.20	0.57
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.40	0.57
2:B:277:ARG:HD3	2:B:277:ARG:O	2.05	0.57
1:A:394:GLN:HB2	1:A:396:GLU:OE1	2.04	0.57
2:B:108:VAL:HG13	2:B:188:TYR:CE2	2.40	0.57
1:A:136:ASN:HD21	1:A:138:GLU:HB3	1.70	0.57
2:B:13:LYS:HB2	2:B:16:MET:HG3	1.85	0.57
1:A:139:THR:HG22	1:A:140:PRO:O	2.05	0.57
2:B:368:LEU:O	2:B:372:VAL:HG13	2.05	0.56
1:A:398:TRP:CH2	1:A:409:THR:HG23	2.39	0.56
2:B:390:LYS:HB3	2:B:417:VAL:HG21	1.86	0.56
2:B:92:LEU:HD22	2:B:94:ILE:HG13	1.86	0.56
1:A:473:THR:O	1:A:477:THR:HG23	2.04	0.56
1:A:94:ILE:HD12	1:A:94:ILE:N	2.20	0.56
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.40	0.56
1:A:85:GLN:HG3	1:A:86:ASP:O	2.05	0.56
1:A:135:ILE:HG23	1:A:136:ASN:CG	2.25	0.56
2:B:209:LEU:O	2:B:212:TRP:N	2.38	0.56
1:A:332:GLN:HG3	1:A:336:GLN:O	2.05	0.56
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.30	0.56
2:B:103:LYS:HE2	2:B:179:VAL:HG12	1.87	0.56
1:A:30:LYS:CE	4:T:703:DG:N2	2.68	0.56
3:P:810:DT:H2'	3:P:811:DG:C8	2.41	0.56
1:A:233:GLU:HB2	1:A:240:THR:HG23	1.87	0.56
2:B:356:ARG:HD2	2:B:367:GLN:HG3	1.87	0.56
1:A:136:ASN:HD22	1:A:138:GLU:HB3	1.71	0.55
1:A:216:THR:O	1:A:217:PRO:O	2.24	0.55
1:A:547:GLN:O	1:A:551:LEU:HD13	2.06	0.55
1:A:389:PHE:HB3	1:A:391:LEU:CD1	2.36	0.55
1:A:406:TRP:HA	2:B:331:LYS:HD2	1.88	0.55
2:B:88:TRP:HB3	2:B:154:LYS:HD2	1.89	0.55
2:B:194:GLU:HG2	2:B:195:ILE:N	2.22	0.55
3:P:813:DT:H2'	3:P:814:DC:H6	1.67	0.55
1:A:223:LYS:O	1:A:223:LYS:HG2	2.06	0.55
1:A:205:LEU:HD22	1:A:209:LEU:HD22	1.89	0.55
2:B:7:THR:HB	2:B:119:PRO:HB2	1.89	0.54
1:A:230:MET:HA	3:P:821:DC:O3'	2.07	0.54
2:B:308:GLU:O	2:B:311:LYS:HG3	2.08	0.54
1:A:30:LYS:HE2	4:T:703:DG:N2	2.22	0.54
4:T:715:DA:H2'	4:T:716:DA:C8	2.42	0.54
2:B:11:LYS:HB3	2:B:85:GLN:OE1	2.08	0.54
2:B:10:VAL:HG12	2:B:11:LYS:N	2.21	0.54
2:B:422:LEU:H	2:B:422:LEU:HD22	1.71	0.54
2:B:379:SER:HA	2:B:383:TRP:CE3	2.42	0.54
3:P:813:DT:H2"	3:P:814:DC:H5'	1.90	0.54
1:A:97:PRO:HA	1:A:100:LEU:HD22	1.90	0.54
1:A:257:ILE:HD12	1:A:293:ILE:HG21	1.89	0.53
1:A:37:ILE:HG22	1:A:41:MET:HE3	1.90	0.53
2:B:345:PRO:O	2:B:346:PHE:CB	2.55	0.53
1:A:31:ILE:HD13	1:A:135:ILE:HA	1.91	0.53
1:A:510:PRO:HB2	1:A:522:ILE:HD11	1.89	0.53
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.43	0.53
2:B:120:LEU:O	2:B:125:ARG:NH1	2.42	0.53
4:T:721:DG:H2"	4:T:722:DA:O5'	2.08	0.53
1:A:32:LYS:O	1:A:36:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLU:OE1	2:B:32:LYS:HE2	2.08	0.53
1:A:199:ARG:HH21	1:A:223:LYS:CB	2.20	0.53
2:B:87:PHE:HB2	2:B:91:GLN:HB2	1.89	0.53
1:A:73:LYS:HG3	1:A:74:LEU:N	2.24	0.53
2:B:61:PHE:HD1	2:B:61:PHE:H	1.56	0.53
1:A:178:ILE:HD11	1:A:201:LYS:HG2	1.90	0.53
2:B:112:GLY:C	2:B:114:ALA:H	2.10	0.52
1:A:37:ILE:HG22	1:A:41:MET:CE	2.39	0.52
1:A:320:ASP:HB3	1:A:323:LYS:HZ2	1.75	0.52
2:B:24:TRP:HB2	2:B:25:PRO:HD2	1.90	0.52
1:A:448:ARG:HH12	4:T:723:DC:H1'	1.74	0.52
1:A:135:ILE:HD13	1:A:135:ILE:O	2.10	0.52
2:B:395:LYS:HE2	2:B:399:GLU:OE1	2.10	0.52
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.90	0.52
1:A:134:SER:O	1:A:136:ASN:N	2.42	0.52
1:A:270:ILE:HG23	1:A:314:VAL:HG21	1.90	0.52
3:P:818:DC:H2'	3:P:819:DG:H8	1.73	0.52
1:A:420:PRO:HA	1:A:421:PRO:C	2.29	0.52
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.91	0.52
1:A:296:THR:HG22	1:A:298:GLU:N	2.20	0.52
2:B:194:GLU:HG2	2:B:195:ILE:H	1.75	0.51
1:A:233:GLU:HB2	1:A:240:THR:CG2	2.39	0.51
2:B:341:ILE:HD12	2:B:341:ILE:N	2.25	0.51
1:A:393:ILE:O	1:A:414:TRP:CH2	2.62	0.51
2:B:366:LYS:O	2:B:369:THR:HG22	2.10	0.51
1:A:434:ILE:HD12	1:A:493:VAL:O	2.11	0.51
1:A:283:LEU:O	1:A:285:GLY:N	2.40	0.51
1:A:222:GLN:O	1:A:224:GLU:HB2	2.11	0.51
2:B:191:SER:H	2:B:198:HIS:CE1	2.28	0.51
3:P:817:DG:H2"	3:P:818:DC:H5'	1.93	0.51
3:P:817:DG:H2'	3:P:818:DC:H6	1.75	0.51
1:A:255:ASN:HD22	1:A:289:LEU:CD2	2.14	0.51
1:A:277:ARG:H	1:A:336:GLN:NE2	2.09	0.51
2:B:371:ALA:O	2:B:375:ILE:HG13	2.11	0.51
1:A:403:THR:CG2	1:A:404:GLU:N	2.74	0.51
1:A:410:TRP:HB2	2:B:365:VAL:HG23	1.91	0.51
3:P:818:DC:H2'	3:P:819:DG:C8	2.46	0.51
3:P:819:DG:H2'	3:P:820:DC:C6	2.46	0.51
2:B:79:GLU:HB2	7:B:442:HOH:O	2.11	0.51
2:B:191:SER:CB	2:B:193:LEU:HD13	2.40	0.51
1:A:454:LYS:CE	1:A:554:ALA:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:VAL:HB	1:A:77:PHE:CE2	2.46	0.50
1:A:454:LYS:NZ	1:A:554:ALA:HB3	2.26	0.50
2:B:66:LYS:HG2	2:B:232:TYR:CE1	2.47	0.50
2:B:319:TYR:CZ	2:B:321:PRO:HA	2.47	0.50
1:A:350:LYS:NZ	1:A:351:THR:O	2.45	0.50
2:B:380:ILE:O	2:B:384:GLY:HA2	2.12	0.50
1:A:407:GLN:OE1	2:B:419:THR:HG22	2.12	0.50
1:A:222:GLN:O	1:A:224:GLU:CB	2.60	0.50
1:A:403:THR:HG22	1:A:404:GLU:HG3	1.92	0.50
2:B:334:GLN:HA	2:B:334:GLN:NE2	2.27	0.50
1:A:503:LEU:O	1:A:507:GLN:HB2	2.12	0.50
1:A:271:TYR:CE1	1:A:314:VAL:HG22	2.47	0.49
1:A:228:LEU:HD23	1:A:228:LEU:N	2.27	0.49
1:A:491:LEU:HG	1:A:529:GLU:HG3	1.94	0.49
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.95	0.49
1:A:278:GLN:HB2	1:A:302:GLU:OE1	2.13	0.49
1:A:179:VAL:HG12	1:A:190:GLY:O	2.12	0.49
2:B:275:LYS:HE3	2:B:277:ARG:HB3	1.94	0.49
1:A:218:ASP:N	1:A:218:ASP:OD1	2.46	0.49
2:B:252:TRP:O	2:B:292:VAL:HG13	2.12	0.49
2:B:253:THR:H	2:B:256:ASP:HB2	1.78	0.49
4:T:706:DT:H2'	4:T:707:DG:C8	2.47	0.49
1:A:297:GLU:CA	1:A:300:GLU:HB2	2.40	0.49
2:B:103:LYS:O	2:B:236:PRO:HG2	2.11	0.49
1:A:5:ILE:HG12	1:A:6:GLU:N	2.27	0.49
1:A:438:GLU:OE2	1:A:463:ARG:NH1	2.45	0.49
1:A:458:VAL:HG12	1:A:548:VAL:HG22	1.92	0.49
2:B:390:LYS:HB3	2:B:417:VAL:CG2	2.43	0.49
1:A:134:SER:CB	1:A:139:THR:HB	2.43	0.49
1:A:17:ASP:O	1:A:83:ARG:HD3	2.13	0.49
2:B:27:THR:OG1	2:B:30:LYS:HG3	2.13	0.49
1:A:229:TRP:HB3	1:A:234:LEU:HD11	1.95	0.49
1:A:220:LYS:HE3	1:A:222:GLN:HG3	1.95	0.48
1:A:509:GLN:N	1:A:510:PRO:HD3	2.28	0.48
1:A:389:PHE:HB3	1:A:391:LEU:HD13	1.95	0.48
1:A:354:TYR:OH	1:A:356:ARG:HB3	2.13	0.48
1:A:8:VAL:O	1:A:10:VAL:HG23	2.13	0.48
2:B:79:GLU:CG	2:B:83:ARG:NH1	2.76	0.48
1:A:410:TRP:CZ2	2:B:363:ASN:ND2	2.81	0.48
1:A:153:TRP:O	1:A:155:GLY:N	2.46	0.48
1:A:195:ILE:HG12	1:A:196:GLY:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:HG13	1:A:143:ARG:HB3	1.94	0.48
2:B:159:ILE:C	2:B:161:GLN:H	2.15	0.48
1:A:138:GLU:CG	1:A:139:THR:N	2.75	0.48
1:A:410:TRP:CZ2	1:A:412:PRO:HA	2.49	0.48
4:T:721:DG:C2'	4:T:722:DA:O5'	2.62	0.48
1:A:102:LYS:HE3	1:A:102:LYS:HB2	1.55	0.48
2:B:164:MET:HA	2:B:167:ILE:HD12	1.96	0.48
1:A:483:TYR:HB2	1:A:521:ILE:HG12	1.95	0.48
1:A:261:VAL:HG13	1:A:276:VAL:HG21	1.95	0.48
1:A:287:LYS:HE3	1:A:289:LEU:CD2	2.43	0.48
1:A:393:ILE:O	1:A:414:TRP:CZ3	2.67	0.48
1:A:359:GLY:HA2	3:P:811:DG:OP2	2.14	0.48
1:A:418:ASN:O	1:A:420:PRO:CD	2.62	0.48
1:A:320:ASP:OD2	1:A:323:LYS:HE3	2.14	0.48
1:A:372:VAL:HG13	1:A:389:PHE:CZ	2.49	0.48
1:A:280:SER:HB2	4:T:712:DC:H4'	1.96	0.48
3:P:813:DT:H2"	3:P:814:DC:C5'	2.43	0.47
2:B:66:LYS:HE2	2:B:232:TYR:HD1	1.78	0.47
1:A:517:LEU:HA	1:A:520:GLN:OE1	2.14	0.47
1:A:203:GLU:O	1:A:207:GLN:HG3	2.13	0.47
2:B:76:ASP:OD1	2:B:78:ARG:HB2	2.14	0.47
2:B:332:GLN:HB2	2:B:336:GLN:O	2.14	0.47
2:B:325:LEU:HB3	2:B:387:PRO:HA	1.95	0.47
1:A:324:ASP:O	1:A:343:GLN:HG2	2.14	0.47
3:P:809:DC:H2"	3:P:810:DT:O5'	2.15	0.47
1:A:447:ASN:O	1:A:449:GLU:N	2.46	0.47
2:B:166:LYS:O	2:B:168:LEU:N	2.46	0.47
1:A:26:LEU:HD12	1:A:133:PRO:CG	2.40	0.47
1:A:266:TRP:O	1:A:269:GLN:HG2	2.14	0.47
1:A:410:TRP:CB	2:B:365:VAL:HG23	2.45	0.47
2:B:106:VAL:HG23	2:B:236:PRO:HG3	1.97	0.47
3:P:816:DG:H2"	3:P:817:DG:O5'	2.14	0.47
2:B:12:LEU:O	2:B:13:LYS:C	2.53	0.47
2:B:106:VAL:HA	2:B:190:GLY:HA3	1.96	0.47
1:A:328:GLU:O	1:A:339:TYR:HA	2.15	0.47
4:T:704:DG:C2'	4:T:705:DT:OP1	2.63	0.47
2:B:31:ILE:O	2:B:35:VAL:HG13	2.15	0.47
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.97	0.46
1:A:27:THR:H	1:A:30:LYS:HD2	1.80	0.46
4:T:703:DG:H2"	4:T:704:DG:H22	1.80	0.46
2:B:316:GLY:HA2	2:B:318:TYR:HE2	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:PHE:HZ	2:B:155:GLY:HA2	1.80	0.46
1:A:289:LEU:CD1	3:P:817:DG:H4'	2.45	0.46
2:B:23:GLN:NE2	2:B:24:TRP:O	2.48	0.46
2:B:125:ARG:HG2	2:B:146:TYR:O	2.15	0.46
2:B:337:TRP:HE1	2:B:367:GLN:HE21	1.63	0.46
1:A:320:ASP:CB	1:A:323:LYS:NZ	2.78	0.46
1:A:501:TYR:CE1	3:P:809:DC:H4'	2.51	0.46
1:A:270:ILE:HG23	1:A:314:VAL:CG2	2.46	0.46
1:A:254:VAL:CG1	1:A:289:LEU:HA	2.46	0.46
2:B:393:ILE:HG12	2:B:394:GLN:N	2.30	0.46
2:B:236:PRO:C	2:B:238:LYS:H	2.18	0.46
2:B:244:ILE:HD12	2:B:244:ILE:H	1.80	0.46
1:A:95:PRO:HB2	1:A:229:TRP:CH2	2.51	0.46
2:B:297:GLU:HG3	2:B:298:GLU:OE2	2.16	0.46
1:A:199:ARG:O	1:A:203:GLU:HG2	2.15	0.46
2:B:87:PHE:CE2	2:B:158:ALA:HB3	2.51	0.46
1:A:221:HIS:CD2	1:A:228:LEU:H	2.34	0.46
3:P:806:DT:H2'	3:P:807:DC:C6	2.51	0.46
3:P:815:DG:H2'	3:P:816:DG:C8	2.51	0.46
2:B:66:LYS:HA	2:B:407:GLN:HE22	1.81	0.46
1:A:94:ILE:HG23	1:A:230:MET:CE	2.46	0.45
4:T:719:DG:H2'	4:T:720:DG:C8	2.51	0.45
1:A:116:PHE:HA	1:A:148:VAL:HG21	1.98	0.45
1:A:96:HIS:NE2	1:A:269:GLN:NE2	2.64	0.45
1:A:441:TYR:HB2	1:A:458:VAL:HG12	1.97	0.45
2:B:61:PHE:CD1	2:B:61:PHE:N	2.84	0.45
2:B:289:LEU:HD12	2:B:289:LEU:HA	1.60	0.45
1:A:41:MET:CE	1:A:73:LYS:HD3	2.46	0.45
1:A:76:ASP:OD2	1:A:78:ARG:NH2	2.49	0.45
1:A:177:ASP:HB2	7:A:564:HOH:O	2.15	0.45
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.52	0.45
1:A:493:VAL:HG22	1:A:494:ASN:N	2.32	0.45
2:B:172:ARG:CZ	2:B:180:ILE:HB	2.46	0.45
1:A:300:GLU:HA	1:A:300:GLU:OE1	2.16	0.45
1:A:84:THR:HG22	1:A:85:GLN:O	2.17	0.45
2:B:173:LYS:O	2:B:176:PRO:HD3	2.17	0.45
2:B:93:GLY:O	2:B:95:PRO:HD3	2.16	0.45
4:T:705:DT:H2"	4:T:706:DT:H5'	1.98	0.45
2:B:13:LYS:NZ	2:B:88:TRP:HH2	2.11	0.45
3:P:810:DT:H2'	3:P:811:DG:H8	1.82	0.45
2:B:88:TRP:CE3	2:B:154:LYS:HE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:CD	1:A:358:ARG:HG3	2.43	0.45
1:A:483:TYR:CE1	1:A:520:GLN:HB3	2.51	0.45
1:A:13:LYS:HG3	1:A:84:THR:O	2.17	0.45
1:A:17:ASP:O	1:A:83:ARG:NH1	2.50	0.45
2:B:94:ILE:HG21	2:B:181:TYR:HE1	1.82	0.45
1:A:281:LYS:C	1:A:283:LEU:N	2.70	0.44
4:T:706:DT:H2'	4:T:707:DG:H8	1.81	0.44
2:B:157:PRO:HG3	2:B:184:MET:HA	1.99	0.44
1:A:408:ALA:HB2	2:B:337:TRP:HH2	1.82	0.44
1:A:389:PHE:HB3	1:A:391:LEU:HD11	1.98	0.44
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.99	0.44
2:B:8:VAL:HA	2:B:9:PRO:HD3	1.73	0.44
4:T:710:DG:H2'	4:T:711:DC:C6	2.52	0.44
4:T:713:DC:C2'	4:T:714:DG:O4'	2.64	0.44
1:A:358:ARG:HH11	1:A:358:ARG:CB	2.28	0.44
2:B:112:GLY:C	2:B:114:ALA:N	2.71	0.44
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.99	0.44
2:B:281:LYS:NZ	2:B:281:LYS:CB	2.80	0.44
1:A:410:TRP:CE2	2:B:363:ASN:ND2	2.86	0.44
1:A:408:ALA:HB2	2:B:337:TRP:CH2	2.52	0.44
1:A:458:VAL:CG1	1:A:548:VAL:HG22	2.46	0.44
1:A:3:SER:C	1:A:5:ILE:H	2.20	0.44
2:B:30:LYS:O	2:B:34:LEU:HG	2.18	0.44
1:A:181:TYR:CD2	2:B:138:GLU:HA	2.52	0.44
2:B:115:TYR:O	2:B:149:LEU:HB2	2.17	0.44
1:A:381:VAL:HG22	2:B:25:PRO:HB3	2.00	0.44
2:B:63:ILE:HD11	2:B:408:ALA:O	2.17	0.44
1:A:401:TRP:C	1:A:403:THR:N	2.70	0.44
1:A:404:GLU:OE2	1:A:509:GLN:NE2	2.51	0.44
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.48	0.44
2:B:341:ILE:CG2	2:B:342:TYR:N	2.80	0.44
2:B:168:LEU:HB3	2:B:172:ARG:HG3	2.00	0.44
2:B:337:TRP:NE1	2:B:367:GLN:HG2	2.30	0.44
3:P:807:DC:H2'	3:P:808:DC:O4'	2.17	0.44
1:A:450:THR:O	1:A:452:LEU:HD13	2.17	0.44
1:A:122:GLU:O	1:A:125:ARG:HB2	2.18	0.44
1:A:500:GLN:HE21	2:B:420:PRO:HB2	1.81	0.44
1:A:232:TYR:HB3	1:A:240:THR:O	2.18	0.44
1:A:494:ASN:HB3	2:B:289:LEU:HD22	2.00	0.44
1:A:3:SER:HA	1:A:212:TRP:O	2.17	0.44
1:A:302:GLU:O	1:A:305:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:LYS:HB2	1:A:552:VAL:O	2.17	0.44
1:A:454:LYS:HE2	1:A:468:THR:HG22	1.99	0.44
1:A:312:GLU:HA	1:A:312:GLU:OE1	2.16	0.44
1:A:525:LEU:HA	1:A:525:LEU:HD23	1.77	0.44
2:B:248:GLU:HB3	2:B:307:ARG:HH12	1.83	0.44
1:A:3:SER:HA	1:A:4:PRO:HD3	1.82	0.44
1:A:401:TRP:C	1:A:403:THR:H	2.21	0.43
1:A:362:THR:HA	1:A:366:LYS:HE3	1.99	0.43
3:P:811:DG:H2"	3:P:812:DT:O5'	2.18	0.43
2:B:163:SER:O	2:B:166:LYS:HB2	2.18	0.43
2:B:100:LEU:HD13	2:B:179:VAL:HG13	1.99	0.43
2:B:194:GLU:HB3	2:B:197:GLN:HG2	2.00	0.43
1:A:49:LYS:HB2	1:A:49:LYS:NZ	2.33	0.43
1:A:337:TRP:CH2	1:A:368:LEU:HB2	2.53	0.43
1:A:348:ASN:O	1:A:349:LEU:C	2.57	0.43
1:A:227:PHE:C	1:A:228:LEU:HD23	2.38	0.43
1:A:2:ILE:HG22	1:A:119:PRO:HG3	1.97	0.43
2:B:175:ASN:N	2:B:176:PRO:HD3	2.33	0.43
2:B:260:LEU:HD12	2:B:260:LEU:HA	1.78	0.43
1:A:399:GLU:O	1:A:403:THR:HB	2.19	0.43
1:A:244:ILE:HD13	1:A:267:ALA:HB2	2.01	0.43
1:A:254:VAL:HG13	1:A:289:LEU:HA	2.01	0.43
1:A:56:TYR:O	1:A:143:ARG:NH2	2.51	0.43
4:T:722:DA:H2'	4:T:723:DC:H6	1.83	0.43
1:A:450:THR:O	1:A:451:LYS:HB2	2.19	0.43
2:B:170:PRO:O	2:B:174:GLN:HG2	2.18	0.43
1:A:361:HIS:ND1	1:A:513:SER:CB	2.82	0.43
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.54	0.43
1:A:5:ILE:HG12	1:A:6:GLU:H	1.83	0.43
2:B:329:ILE:HG22	2:B:330:GLN:N	2.33	0.42
1:A:195:ILE:HG12	1:A:196:GLY:N	2.34	0.42
1:A:281:LYS:O	1:A:284:ARG:HG2	2.19	0.42
1:A:136:ASN:N	1:A:136:ASN:ND2	2.67	0.42
2:B:112:GLY:HA2	2:B:115:TYR:HD1	1.84	0.42
2:B:126:LYS:HE2	2:B:127:TYR:CZ	2.54	0.42
1:A:338:THR:HG22	1:A:339:TYR:N	2.34	0.42
1:A:443:ASP:OD2	1:A:498:ASP:OD2	2.36	0.42
2:B:78:ARG:HB2	2:B:78:ARG:HE	1.70	0.42
2:B:180:ILE:HG23	2:B:189:VAL:CG2	2.40	0.42
2:B:207:GLN:C	2:B:209:LEU:N	2.72	0.42
2:B:81:ASN:OD1	2:B:153:TRP:HD1	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ASN:HB3	2:B:143:ARG:HH12	1.84	0.42
2:B:26:LEU:HD12	2:B:133:PRO:HG2	1.98	0.42
1:A:319:TYR:OH	1:A:385:LYS:HD3	2.19	0.42
1:A:541:GLY:HA2	1:A:546:GLU:HB2	2.01	0.42
2:B:422:LEU:H	2:B:422:LEU:CD2	2.31	0.42
2:B:303:LEU:HA	2:B:306:ASN:HB2	2.01	0.42
1:A:111:VAL:HB	1:A:185:ASP:HB2	2.02	0.42
2:B:271:TYR:HA	2:B:272:PRO:HD3	1.81	0.42
4:T:704:DG:OP2	4:T:704:DG:N2	2.51	0.42
1:A:17:ASP:CG	1:A:18:GLY:H	2.23	0.42
1:A:524:GLN:HA	1:A:524:GLN:OE1	2.19	0.42
2:B:61:PHE:CD2	2:B:403:THR:HB	2.55	0.42
2:B:112:GLY:HA2	2:B:115:TYR:CD1	2.54	0.42
2:B:341:ILE:HG22	2:B:342:TYR:N	2.35	0.42
1:A:91:GLN:O	4:T:708:DG:H4'	2.20	0.41
1:A:222:GLN:O	1:A:224:GLU:N	2.53	0.41
1:A:277:ARG:HH12	1:A:357:MET:HB2	1.84	0.41
1:A:288:ALA:O	1:A:291:GLU:HB3	2.20	0.41
1:A:88:TRP:CE2	2:B:57:ASN:HB2	2.55	0.41
1:A:30:LYS:HG2	1:A:71:TRP:HZ3	1.80	0.41
2:B:236:PRO:O	2:B:238:LYS:N	2.51	0.41
1:A:305:GLU:O	1:A:309:ILE:HG13	2.20	0.41
1:A:270:ILE:HA	1:A:270:ILE:HD12	1.82	0.41
2:B:391:LEU:HA	2:B:392:PRO:HD3	1.86	0.41
2:B:320:ASP:HB3	2:B:323:LYS:HB2	2.02	0.41
1:A:266:TRP:CE2	3:P:820:DC:H4'	2.55	0.41
2:B:164:MET:SD	2:B:167:ILE:HD12	2.60	0.41
2:B:80:LEU:O	2:B:80:LEU:HD12	2.19	0.41
2:B:332:GLN:CG	2:B:338:THR:HG23	2.50	0.41
1:A:34:LEU:CD2	1:A:62:ALA:HB2	2.43	0.41
2:B:10:VAL:HG13	2:B:85:GLN:NE2	2.35	0.41
1:A:513:SER:O	1:A:519:ASN:ND2	2.53	0.41
2:B:422:LEU:CD2	2:B:422:LEU:N	2.84	0.41
1:A:412:PRO:O	1:A:414:TRP:HD1	2.03	0.41
1:A:358:ARG:HB3	1:A:358:ARG:NH1	2.27	0.41
4:T:722:DA:H2"	4:T:723:DC:O5'	2.20	0.41
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.70	0.41
1:A:24:TRP:CH2	4:T:704:DG:C8	3.08	0.41
2:B:209:LEU:HG	2:B:210:LEU:N	2.36	0.41
1:A:219:LYS:HG2	1:A:219:LYS:H	1.73	0.41
1:A:293:ILE:O	1:A:293:ILE:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ILE:CD1	1:A:135:ILE:HA	2.50	0.41
2:B:92:LEU:CD2	2:B:94:ILE:HG13	2.49	0.41
1:A:282:LEU:HD21	1:A:296:THR:HB	2.02	0.41
2:B:331:LYS:HA	2:B:337:TRP:CE3	2.55	0.41
1:A:472:THR:OG1	1:A:473:THR:N	2.53	0.41
1:A:489:SER:HB2	1:A:493:VAL:HB	2.02	0.41
2:B:180:ILE:HG12	2:B:189:VAL:CG1	2.50	0.41
2:B:16:MET:HE2	2:B:83:ARG:HA	2.01	0.41
1:A:100:LEU:O	1:A:318:TYR:HB3	2.20	0.41
1:A:543:GLY:HA2	1:A:544:GLY:HA2	1.41	0.41
1:A:105:SER:HB3	1:A:198:HIS:CG	2.56	0.41
1:A:419:THR:HG23	1:A:419:THR:O	2.21	0.41
2:B:8:VAL:O	2:B:8:VAL:HG13	2.21	0.41
2:B:5:ILE:HG12	2:B:6:GLU:N	2.36	0.41
1:A:221:HIS:N	1:A:221:HIS:ND1	2.69	0.41
2:B:300:GLU:O	2:B:304:ALA:HB2	2.21	0.41
1:A:416:PHE:HZ	1:A:422:LEU:HD11	1.85	0.41
1:A:281:LYS:C	1:A:283:LEU:H	2.24	0.40
1:A:394:GLN:O	1:A:395:LYS:C	2.60	0.40
2:B:337:TRP:HE1	2:B:367:GLN:CG	2.33	0.40
1:A:239:TRP:HE3	1:A:240:THR:N	2.18	0.40
2:B:246:LEU:HD22	2:B:260:LEU:HD11	2.03	0.40
2:B:74:LEU:HD12	2:B:74:LEU:HA	1.96	0.40
1:A:424:LYS:HB3	1:A:424:LYS:HE3	1.78	0.40
1:A:345:PRO:HB2	1:A:346:PHE:HD1	1.86	0.40
2:B:162:SER:OG	2:B:163:SER:N	2.54	0.40
1:A:287:LYS:HE3	1:A:289:LEU:HG	2.01	0.40
1:A:205:LEU:HD22	1:A:209:LEU:CD2	2.51	0.40
2:B:263:LYS:HB2	2:B:263:LYS:HE3	1.79	0.40
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.87	0.40
2:B:242:GLN:HA	2:B:243:PRO:HD3	1.79	0.40
1:A:540:LYS:HB3	1:A:542:ILE:CD1	2.52	0.40
2:B:341:ILE:CD1	2:B:341:ILE:N	2.83	0.40
1:A:491:LEU:HG	1:A:529:GLU:CG	2.51	0.40
1:A:337:TRP:CZ3	1:A:368:LEU:HB2	2.57	0.40
1:A:134:SER:HB3	1:A:139:THR:HB	2.02	0.40
1:A:53:GLU:CD	1:A:53:GLU:N	2.65	0.40
2:B:302:GLU:HG2	2:B:306:ASN:ND2	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:LYS:NZ	2:B:173:LYS:NZ[3_656]	2.01	0.19

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	553/560 (99%)	501 (91%)	44 (8%)	8 (1%)	14 44
2	B	401/452 (89%)	355 (88%)	37 (9%)	9 (2%)	8 31
All	All	954/1012 (94%)	856 (90%)	81 (8%)	17 (2%)	11 37

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	LYS
2	B	5	ILE
2	B	193	LEU
1	A	217	PRO
1	A	291	GLU
2	B	240	THR
2	B	357	MET
1	A	223	LYS
1	A	284	ARG
2	B	170	PRO
2	B	14	PRO
2	B	87	PHE
1	A	419	THR
2	B	234	LEU
2	B	237	ASP
1	A	157	PRO
1	A	490	GLY

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	495/500 (99%)	447 (90%)	48 (10%)	10 30
2	B	369/411 (90%)	342 (93%)	27 (7%)	17 45
All	All	864/911 (95%)	789 (91%)	75 (9%)	13 36

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	24	TRP
1	A	42	GLU
1	A	92	LEU
1	A	100	LEU
1	A	109	LEU
1	A	113	ASP
1	A	125	ARG
1	A	135	ILE
1	A	136	ASN
1	A	137	ASN
1	A	146	TYR
1	A	168	LEU
1	A	195	ILE
1	A	201	LYS
1	A	205	LEU
1	A	209	LEU
1	A	216	THR
1	A	218	ASP
1	A	221	HIS
1	A	252	TRP
1	A	254	VAL
1	A	264	LEU
1	A	268	SER
1	A	284	ARG
1	A	290	THR
1	A	295	LEU

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Mol	Chain	Res	Type
1	A	300	GLU
1	A	302	GLU
1	A	328	GLU
1	A	330	GLN
1	A	332	GLN
1	A	340	GLN
1	A	356	ARG
1	A	358	ARG
1	A	373	GLN
1	A	391	LEU
1	A	394	GLN
1	A	402	TRP
1	A	403	THR
1	A	458	VAL
1	A	463	ARG
1	A	469	LEU
1	A	491	LEU
1	A	501	TYR
1	A	507	GLN
1	A	523	GLU
1	A	540	LYS
2	B	6	GLU
2	B	35	VAL
2	B	44	GLU
2	B	53	GLU
2	B	61	PHE
2	B	72	ARG
2	B	78	ARG
2	B	91	GLN
2	B	92	LEU
2	B	122	GLU
2	B	135	ILE
2	B	194	GLU
2	B	232	TYR
2	B	242	GLN
2	B	268	SER
2	B	277	ARG
2	B	286	THR
2	B	289	LEU
2	B	295	LEU
2	B	297	GLU
2	B	322	SER

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Mol	Chain	Res	Type
2	B	324	ASP
2	B	336	GLN
2	B	364	ASP
2	B	372	VAL
2	B	404	GLU
2	B	418	ASN

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

Mol	Chain	Res	Type
1	A	136	ASN
1	A	137	ASN
1	A	161	GLN
1	A	197	GLN
1	A	242	GLN
1	A	255	ASN
1	A	269	GLN
1	A	306	ASN
1	A	336	GLN
1	A	373	GLN
1	A	464	GLN
1	A	480	GLN
1	A	487	GLN
1	A	500	GLN
2	B	91	GLN
2	B	182	GLN
2	B	235	HIS
2	B	242	GLN
2	B	265	ASN
2	B	334	GLN
2	B	336	GLN
2	B	367	GLN
2	B	428	GLN

5.3.3 RNA

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	URT	P	822	3	11,23,24	1.43	2 (18%)	10,33,36	1.51	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	URT	P	822	3	-	0/1/21/22	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	822	URT	C8-N4	2.14	1.38	1.33
3	P	822	URT	C5-N3	2.45	1.39	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	P	822	URT	N3-C8-N4	-2.97	126.62	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
6	SO4	P	3	-	4,4,4	0.25	0	6,6,6	0.14	0
6	SO4	T	2	-	4,4,4	0.22	0	6,6,6	0.11	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
6	SO4	P	3	-	-	0/0/0/0	0/0/0/0
6	SO4	T	2	-	-	0/0/0/0	0/0/0/0

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	555/560 (99%)	0.11	28 (5%) 32 26	30, 59, 110, 135	0
2	B	407/452 (90%)	0.31	24 (5%) 26 19	40, 78, 133, 145	0
3	P	17/21 (80%)	-0.62	0 100 100	37, 65, 84, 95	0
4	T	23/27 (85%)	-0.29	1 (4%) 39 32	36, 76, 125, 160	0
All	All	1002/1060 (94%)	0.17	53 (5%) 30 23	30, 67, 124, 160	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	6.5
2	B	4	PRO	5.9
2	B	95	PRO	5.1
1	A	69	THR	4.8
1	A	65	LYS	4.8
1	A	286	THR	4.7
1	A	289	LEU	4.6
2	B	211	ARG	4.5
1	A	137	ASN	4.2
1	A	133	PRO	4.2
1	A	290	THR	3.8
2	B	6	GLU	3.7
1	A	135	ILE	3.6
2	B	89	GLU	3.5
2	B	232	TYR	3.4
1	A	252	TRP	3.3
1	A	28	GLU	3.3
2	B	92	LEU	3.2
1	A	62	ALA	3.1
2	B	87	PHE	3.1
1	A	1	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	191	SER	3.0
2	B	98	ALA	3.0
1	A	24	TRP	2.9
1	A	26	LEU	2.9
1	A	50	ILE	2.9
1	A	138	GLU	2.8
2	B	205	LEU	2.8
2	B	295	LEU	2.8
1	A	284	ARG	2.8
1	A	287	LYS	2.7
2	B	90	VAL	2.7
2	B	212	TRP	2.6
4	T	703	DG	2.6
2	B	5	ILE	2.6
2	B	106	VAL	2.3
2	B	108	VAL	2.3
1	A	134	SER	2.3
2	B	93	GLY	2.3
1	A	331	LYS	2.2
1	A	29	GLU	2.2
2	B	430	GLU	2.2
2	B	12	LEU	2.2
2	B	429	LEU	2.2
2	B	97	PRO	2.2
1	A	72	ARG	2.2
1	A	346	PHE	2.2
1	A	34	LEU	2.2
1	A	23	GLN	2.1
1	A	251	SER	2.1
1	A	71	TRP	2.1
2	B	239	TRP	2.1
1	A	293	ILE	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. 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	URT	P	822	21/22	0.96	0.16	-	45,49,51,52	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
6	SO4	T	2	5/5	0.84	0.27	7.06	102,102,103,103	0
6	SO4	P	3	5/5	0.94	0.30	5.42	110,111,111,112	0
5	MG	A	601	1/1	0.99	0.24	2.26	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.