



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 10:55 PM EDT

PDB ID : 3KK1
Title : HIV-1 reverse transcriptase-DNA complex with nucleotide inhibitor GS-9148-diphosphate bound in nucleotide site
Authors : Lansdon, E.B.
Deposited on : 2009-11-04
Resolution : 2.70 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
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

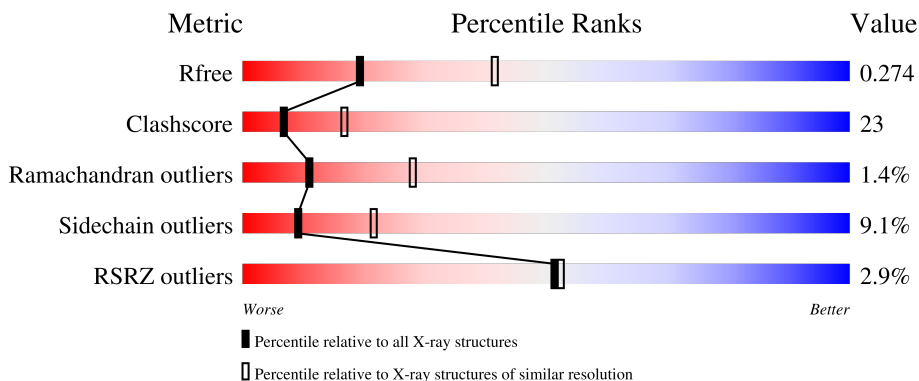
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	560	 2% 55% 37% 6% ..
2	B	452	 3% 51% 35% 9%
3	P	21	 10% 71% 5% 14%
4	T	27	 4% 81% 11%

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8968 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	555	4514	2917	753	836	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	412	3396	2210	565	614	7	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

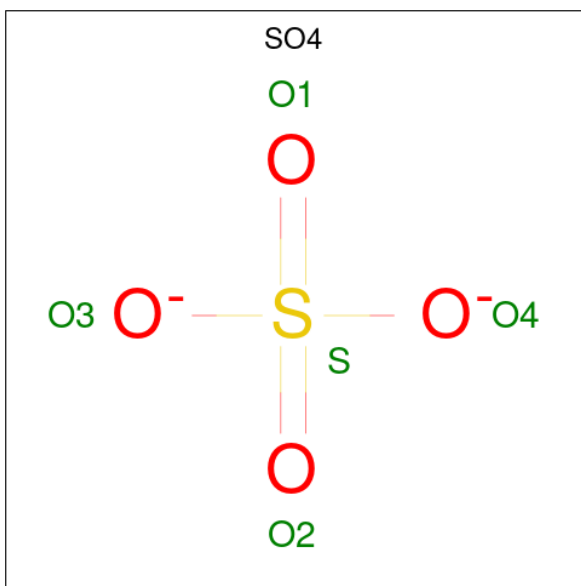
- Molecule 3 is a DNA chain called 5'-D(*AP*CP*A*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*(DOC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	18	360	172	62	109	17	0	0	0

- Molecule 4 is a DNA chain called 5'-D(*A*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	24	497	234	99	141	23	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

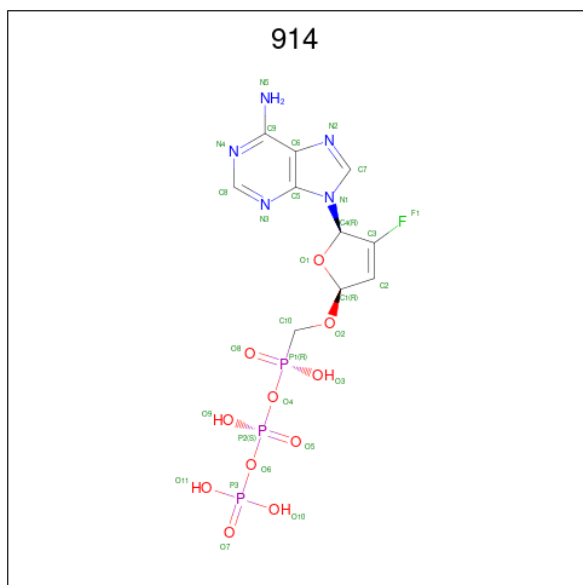


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
5	A	1	5	4	1	0	0
5	P	1	5	4	1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Mg 2 2	0	0

- Molecule 7 is [(2R,5R)-5-(6-aminopurin-9-yl)-4-fluoro-2,5-dihydrofuran-2-yl]oxymethyl-hydroxy(phosphonoxy)phosphoryl]oxy-phosphinic acid (three-letter code: 914) (formula: C₁₀H₁₃FN₅O₁₁P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			P
7	A	1	30	10	1	5	11	3	0	0

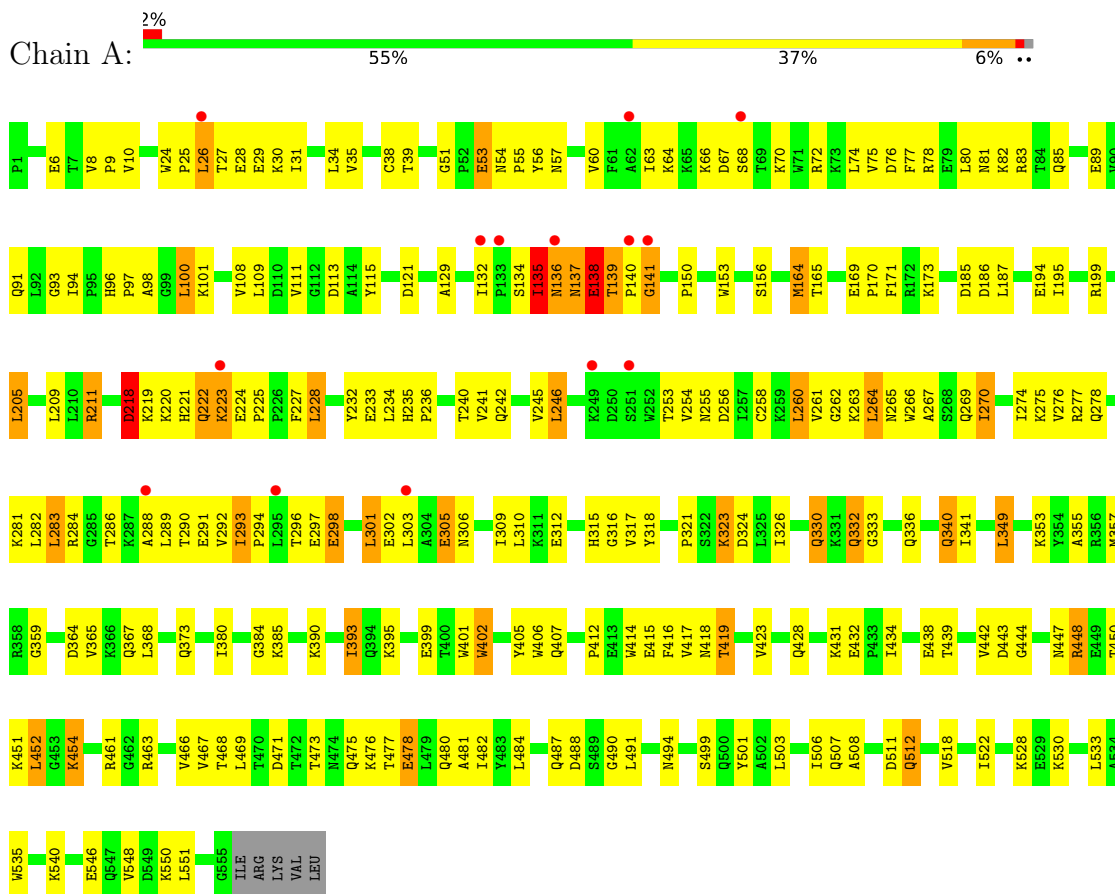
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	76	Total O 76 76	0	0
8	B	54	Total O 54 54	0	0
8	P	10	Total O 10 10	0	0
8	T	14	Total O 14 14	0	0

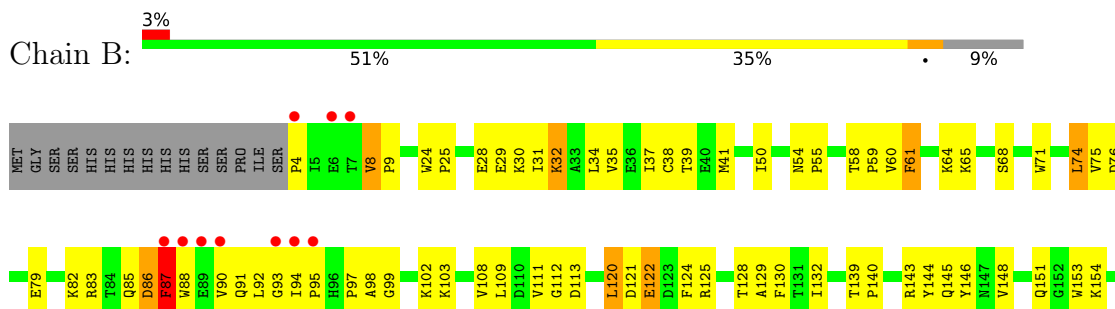
3 Residue-property plots

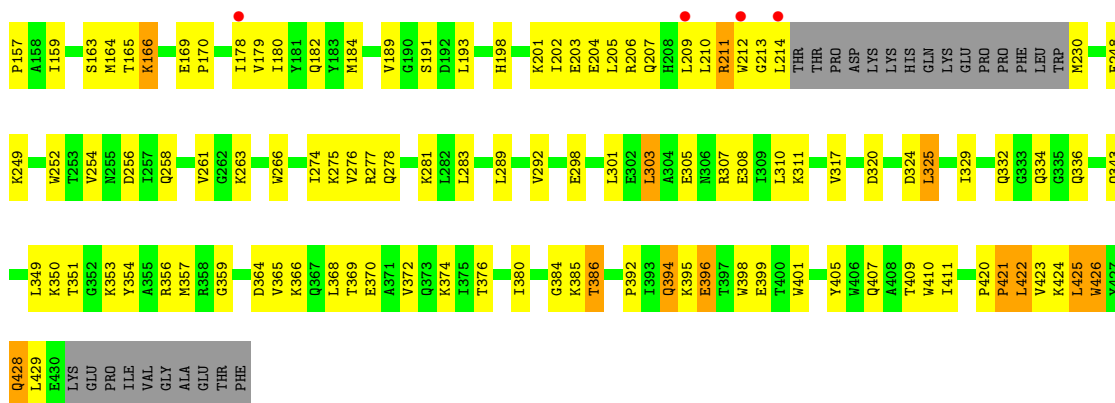
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Reverse transcriptase p66 subunit



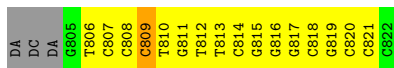
• Molecule 2: Reverse transcriptase p51 subunit





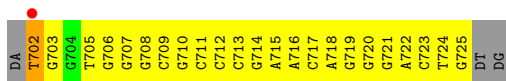
● Molecule 3: 5'-D(*AP*CP*A*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*(DOC))-3'

Chain P: 10% 71% 5% 14%



● Molecule 4: 5'-D(*A*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: 4% 81% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	165.75Å 169.24Å 103.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.71 – 2.70 47.41 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.71-2.70) 91.7 (47.41-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.32 (at 2.69Å)	Xtrriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.204 , 0.274 0.203 , 0.274	Depositor DCC
R_{free} test set	1837 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtrriage
Anisotropy	0.160	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.020 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8968	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 914, DOC, MG

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	0.40	1/4631 (0.0%)	0.55	1/6292 (0.0%)
2	B	0.35	0/3491	0.52	1/4742 (0.0%)
3	P	0.46	0/381	1.10	1/586 (0.2%)
4	T	0.58	1/559 (0.2%)	1.08	4/863 (0.5%)
All	All	0.40	2/9062 (0.0%)	0.63	7/12483 (0.1%)

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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	702	DT	C3'-O3'	-6.08	1.36	1.44
1	A	138	GLU	CD-OE1	5.71	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	702	DT	O4'-C4'-C3'	-11.83	98.90	106.00
4	T	702	DT	OP1-P-O3'	-5.78	92.49	105.20
4	T	702	DT	O3'-P-O5'	5.71	114.85	104.00
4	T	702	DT	C4'-C3'-O3'	5.42	123.26	109.70
2	B	4	PRO	N-CA-CB	5.30	109.66	103.30
3	P	809	DC	N1-C1'-C2'	5.12	122.32	112.60
1	A	219	LYS	N-CA-C	5.01	124.53	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	ILE	Peptide
1	A	218	ASP	Peptide

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	208	0
2	B	3396	0	3426	159	0
3	P	360	0	204	20	0
4	T	497	0	269	31	0
5	A	10	0	0	0	0
5	P	5	0	0	0	0
6	A	2	0	0	0	0
7	A	30	0	9	1	0
8	A	76	0	0	1	0
8	B	54	0	0	1	0
8	P	10	0	0	0	0
8	T	14	0	0	0	0
All	All	8968	0	8471	403	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 23.

All (403) 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:425:LEU:HD22	2:B:428:GLN:HG3	1.46	0.96
1:A:511:ASP:OD1	1:A:512:GLN:HG3	1.69	0.91
1:A:288:ALA:HB3	1:A:291:GLU:HG3	1.56	0.88
1:A:135:ILE:HG21	1:A:138:GLU:OE2	1.74	0.87
1:A:246:LEU:H	1:A:246:LEU:HD12	1.41	0.86
1:A:275:LYS:H	1:A:306:ASN:HD21	1.23	0.85
2:B:334:GLN:H	2:B:334:GLN:HE21	1.23	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:VAL:HG12	1:A:265:ASN:ND2	1.91	0.84
2:B:320:ASP:H	2:B:343:GLN:HE22	1.24	0.84
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.17	0.84
1:A:253:THR:HG22	1:A:292:VAL:HG12	1.61	0.82
1:A:97:PRO:HA	1:A:100:LEU:HD22	1.61	0.82
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.62	0.81
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.60	0.81
1:A:140:PRO:N	1:A:141:GLY:HA2	1.97	0.79
2:B:139:THR:HG22	2:B:140:PRO:O	1.83	0.79
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.63	0.78
1:A:218:ASP:HA	1:A:220:LYS:H	1.49	0.78
2:B:35:VAL:O	2:B:39:THR:HG23	1.84	0.77
2:B:365:VAL:O	2:B:369:THR:HG23	1.86	0.76
1:A:546:GLU:HG2	1:A:550:LYS:HE2	1.66	0.76
1:A:218:ASP:HA	1:A:220:LYS:N	2.01	0.75
1:A:260:LEU:HD11	1:A:303:LEU:HD13	1.69	0.75
1:A:139:THR:HG23	1:A:141:GLY:HA3	1.68	0.75
1:A:138:GLU:O	1:A:139:THR:HB	1.87	0.74
4:T:705:DT:H2''	4:T:706:DG:H5'	1.70	0.74
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.70	0.73
1:A:478:GLU:HG2	1:A:499:SER:CB	2.19	0.73
1:A:454:LYS:HE2	1:A:468:THR:HG22	1.70	0.72
2:B:394:GLN:OE1	2:B:396:GLU:HG2	1.90	0.71
1:A:96:HIS:HD1	1:A:98:ALA:H	1.39	0.71
1:A:241:VAL:HG12	1:A:242:GLN:O	1.91	0.70
1:A:297:GLU:O	1:A:301:LEU:HB2	1.92	0.70
2:B:369:THR:HA	2:B:372:VAL:HG22	1.73	0.70
4:T:702:DT:H2'	4:T:703:DG:C5'	2.22	0.69
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.57	0.69
1:A:274:ILE:HA	1:A:306:ASN:ND2	2.07	0.69
2:B:74:LEU:HD12	2:B:411:ILE:HD11	1.74	0.69
1:A:77:PHE:CD1	1:A:80:LEU:HD23	2.28	0.68
1:A:306:ASN:O	1:A:309:ILE:HG22	1.93	0.68
2:B:88:TRP:HH2	2:B:385:LYS:HE3	1.57	0.68
2:B:92:LEU:HD13	2:B:94:ILE:HD12	1.75	0.68
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.29	0.68
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.76	0.67
2:B:203:GLU:O	2:B:207:GLN:HG2	1.94	0.67
1:A:135:ILE:CG2	1:A:138:GLU:OE2	2.42	0.67
1:A:194:GLU:N	1:A:194:GLU:CD	2.47	0.67
1:A:218:ASP:OD1	1:A:218:ASP:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:708:DG:H2'	4:T:709:DC:C6	2.30	0.66
1:A:261:VAL:HG12	1:A:265:ASN:HD21	1.61	0.66
1:A:293:ILE:HG12	1:A:294:PRO:HD2	1.77	0.66
4:T:714:DG:H2'	4:T:715:DA:C8	2.30	0.66
2:B:24:TRP:HB2	2:B:25:PRO:HD2	1.76	0.66
2:B:86:ASP:O	2:B:90:VAL:HG12	1.96	0.66
2:B:99:GLY:HA2	2:B:102:LYS:HD2	1.78	0.65
2:B:357:MET:HG2	2:B:359:GLY:H	1.61	0.65
1:A:134:SER:HB3	1:A:139:THR:HG23	1.79	0.65
3:P:816:DG:H2'	3:P:817:DG:C8	2.32	0.65
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.79	0.64
1:A:258:CYS:SG	1:A:283:LEU:HD11	2.37	0.64
1:A:35:VAL:O	1:A:39:THR:HG23	1.97	0.64
1:A:450:THR:HB	1:A:452:LEU:HD22	1.78	0.64
2:B:143:ARG:HG2	2:B:143:ARG:HH11	1.61	0.64
2:B:334:GLN:H	2:B:334:GLN:NE2	1.94	0.64
2:B:125:ARG:HD3	2:B:146:TYR:O	1.98	0.64
2:B:356:ARG:HG3	2:B:357:MET:H	1.63	0.64
1:A:223:LYS:HE3	1:A:223:LYS:O	1.98	0.64
1:A:194:GLU:CD	1:A:194:GLU:H	2.01	0.63
1:A:246:LEU:HD11	1:A:310:LEU:CD1	2.29	0.63
1:A:270:ILE:HD11	1:A:315:HIS:C	2.19	0.63
1:A:78:ARG:NH1	4:T:705:DT:H5''	2.14	0.63
1:A:27:THR:O	1:A:31:ILE:HG13	1.98	0.63
1:A:281:LYS:O	1:A:284:ARG:HG2	1.97	0.63
1:A:109:LEU:HD23	1:A:220:LYS:HG3	1.81	0.63
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.80	0.62
1:A:245:VAL:O	1:A:263:LYS:HE2	1.99	0.62
1:A:246:LEU:HD12	1:A:246:LEU:N	2.12	0.62
4:T:712:DC:H2'	4:T:713:DC:C6	2.34	0.62
2:B:58:THR:HG23	2:B:76:ASP:O	1.99	0.62
1:A:254:VAL:HG12	1:A:289:LEU:HD12	1.82	0.62
1:A:255:ASN:HD22	1:A:289:LEU:HD21	1.65	0.62
1:A:390:LYS:HB3	1:A:417:VAL:HG21	1.82	0.61
1:A:317:VAL:HG23	1:A:349:LEU:HD13	1.81	0.61
4:T:714:DG:H2'	4:T:715:DA:H8	1.64	0.61
1:A:27:THR:HG22	1:A:29:GLU:H	1.65	0.61
1:A:278:GLN:O	1:A:282:LEU:HD13	2.01	0.61
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.82	0.61
1:A:8:VAL:O	1:A:10:VAL:HG23	2.01	0.61
2:B:201:LYS:O	2:B:204:GLU:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:LYS:HD3	2:B:429:LEU:CD1	2.31	0.61
2:B:65:LYS:HA	2:B:407:GLN:HE22	1.66	0.60
2:B:90:VAL:HG13	2:B:91:GLN:N	2.15	0.60
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.36	0.60
1:A:450:THR:O	1:A:451:LYS:HB2	2.00	0.60
2:B:178:ILE:HD11	2:B:201:LYS:HG2	1.83	0.60
3:P:816:DG:H2'	3:P:817:DG:H8	1.67	0.60
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.84	0.59
1:A:431:LYS:HE2	1:A:432:GLU:HG2	1.83	0.59
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.67	0.59
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.16	0.59
3:P:806:DT:H2'	3:P:807:DC:C6	2.38	0.59
4:T:702:DT:H2'	4:T:703:DG:H5'	1.84	0.59
1:A:78:ARG:HH11	4:T:705:DT:H5''	1.68	0.59
3:P:817:DG:H2'	3:P:818:DC:C6	2.38	0.59
2:B:254:VAL:O	2:B:258:GLN:HG3	2.03	0.59
1:A:473:THR:O	1:A:477:THR:HG23	2.02	0.59
2:B:334:GLN:HE21	2:B:334:GLN:N	1.97	0.59
1:A:108:VAL:HB	1:A:221:HIS:HB2	1.85	0.58
1:A:399:GLU:O	1:A:402:TRP:HD1	1.86	0.58
2:B:424:LYS:O	2:B:428:GLN:HG2	2.04	0.58
2:B:103:LYS:HE2	2:B:179:VAL:HG12	1.85	0.58
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.39	0.58
2:B:205:LEU:HD23	2:B:205:LEU:O	2.04	0.57
1:A:134:SER:HB3	1:A:139:THR:CG2	2.34	0.57
3:P:813:DT:H2''	3:P:814:DC:H5'	1.86	0.57
1:A:9:PRO:HA	1:A:121:ASP:OD2	2.04	0.57
2:B:65:LYS:HE2	2:B:230:MET:N	2.19	0.57
1:A:293:ILE:HD13	1:A:294:PRO:N	2.20	0.57
1:A:253:THR:HA	1:A:292:VAL:HA	1.85	0.57
2:B:298:GLU:CD	2:B:298:GLU:H	2.07	0.57
1:A:277:ARG:H	1:A:336:GLN:NE2	2.03	0.56
2:B:88:TRP:CH2	2:B:385:LYS:HE3	2.40	0.56
2:B:369:THR:HA	2:B:372:VAL:CG2	2.36	0.56
1:A:292:VAL:O	1:A:293:ILE:HB	2.05	0.56
2:B:425:LEU:HA	2:B:428:GLN:CG	2.35	0.56
4:T:709:DC:H2'	4:T:710:DG:H8	1.71	0.56
4:T:711:DC:H2'	4:T:712:DC:C6	2.40	0.56
3:P:813:DT:H2''	3:P:814:DC:C5'	2.36	0.56
1:A:246:LEU:HD11	1:A:310:LEU:HD13	1.86	0.56
1:A:195:ILE:O	1:A:199:ARG:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:LYS:HE2	2:B:68:SER:O	2.07	0.55
2:B:85:GLN:C	2:B:87:PHE:H	2.09	0.55
1:A:136:ASN:N	1:A:136:ASN:OD1	2.39	0.55
1:A:431:LYS:HE2	1:A:432:GLU:CG	2.37	0.55
1:A:27:THR:HG22	1:A:28:GLU:N	2.21	0.55
1:A:274:ILE:HA	1:A:306:ASN:HD22	1.70	0.55
2:B:8:VAL:HG13	2:B:159:ILE:HD12	1.88	0.55
4:T:716:DA:H2'	4:T:717:DC:C6	2.42	0.55
2:B:93:GLY:O	2:B:95:PRO:HD3	2.07	0.55
2:B:281:LYS:HB2	2:B:281:LYS:NZ	2.22	0.55
3:P:820:DC:H2''	3:P:821:DC:H5'	1.89	0.55
1:A:270:ILE:HD11	1:A:316:GLY:N	2.22	0.54
1:A:138:GLU:O	1:A:139:THR:CB	2.55	0.54
1:A:140:PRO:N	1:A:141:GLY:CA	2.70	0.54
2:B:274:ILE:HD11	2:B:310:LEU:HD21	1.88	0.54
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.42	0.54
2:B:98:ALA:O	2:B:102:LYS:HE2	2.06	0.54
1:A:165:THR:OG1	2:B:140:PRO:HG2	2.08	0.54
1:A:417:VAL:HG12	1:A:419:THR:HG22	1.88	0.54
4:T:716:DA:H2'	4:T:717:DC:O4'	2.08	0.54
1:A:275:LYS:HD3	1:A:332:GLN:HG2	1.90	0.54
2:B:8:VAL:CG1	2:B:159:ILE:HD12	2.38	0.54
1:A:518:VAL:O	1:A:522:ILE:HG13	2.07	0.54
2:B:278:GLN:OE1	2:B:298:GLU:HG3	2.08	0.54
2:B:332:GLN:HB2	2:B:336:GLN:HB2	1.89	0.54
1:A:443:ASP:OD2	1:A:444:GLY:N	2.41	0.53
2:B:120:LEU:HD22	2:B:121:ASP:H	1.72	0.53
4:T:706:DG:H2'	4:T:707:DG:C8	2.43	0.53
2:B:163:SER:HA	2:B:166:LYS:HD3	1.91	0.53
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.43	0.53
4:T:721:DG:H2''	4:T:722:DA:O5'	2.09	0.53
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.91	0.53
1:A:31:ILE:O	1:A:35:VAL:HG22	2.09	0.53
4:T:713:DC:H2'	4:T:714:DG:C8	2.44	0.52
1:A:63:ILE:HG12	1:A:74:LEU:HD21	1.92	0.52
1:A:275:LYS:CD	1:A:332:GLN:HG2	2.38	0.52
2:B:422:LEU:HG	2:B:426:TRP:CZ2	2.44	0.52
1:A:264:LEU:O	1:A:267:ALA:HB3	2.09	0.52
2:B:366:LYS:HE3	2:B:370:GLU:OE2	2.09	0.52
2:B:420:PRO:C	2:B:422:LEU:H	2.13	0.52
1:A:140:PRO:CD	1:A:141:GLY:HA2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:LYS:O	2:B:68:SER:HB2	2.10	0.52
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.40	0.52
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.40	0.52
2:B:308:GLU:HA	2:B:311:LYS:HG3	1.90	0.52
1:A:270:ILE:HG12	1:A:270:ILE:O	2.09	0.52
1:A:364:ASP:CB	1:A:423:VAL:HG13	2.38	0.52
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.45	0.52
1:A:302:GLU:HA	1:A:305:GLU:CG	2.40	0.51
2:B:92:LEU:HD22	2:B:94:ILE:HD11	1.93	0.51
2:B:275:LYS:HE2	2:B:305:GLU:OE1	2.11	0.51
2:B:281:LYS:HB2	2:B:281:LYS:HZ3	1.74	0.51
2:B:425:LEU:HA	2:B:428:GLN:HG2	1.93	0.51
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.46	0.51
1:A:475:GLN:CD	1:A:475:GLN:H	2.14	0.51
2:B:32:LYS:N	2:B:32:LYS:HD2	2.26	0.51
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.93	0.51
1:A:82:LYS:HD2	1:A:82:LYS:O	2.11	0.50
1:A:246:LEU:H	1:A:246:LEU:CD1	2.18	0.50
4:T:719:DG:H2'	4:T:720:DG:C8	2.47	0.50
2:B:308:GLU:O	2:B:311:LYS:N	2.44	0.50
2:B:320:ASP:OD1	2:B:320:ASP:C	2.49	0.50
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.47	0.50
1:A:330:GLN:HE22	1:A:340:GLN:CD	2.15	0.50
1:A:283:LEU:HD23	1:A:283:LEU:O	2.12	0.50
2:B:61:PHE:N	2:B:61:PHE:CD1	2.79	0.50
2:B:143:ARG:HG2	2:B:143:ARG:NH1	2.25	0.50
4:T:702:DT:H2'	4:T:703:DG:O5'	2.10	0.50
2:B:206:ARG:O	2:B:210:LEU:HG	2.12	0.50
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.47	0.50
1:A:64:LYS:HD3	1:A:68:SER:O	2.11	0.50
1:A:253:THR:HB	1:A:290:THR:O	2.12	0.50
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.93	0.50
2:B:376:THR:HG21	2:B:410:TRP:CZ3	2.46	0.50
1:A:218:ASP:CA	1:A:220:LYS:H	2.21	0.50
1:A:293:ILE:HD13	1:A:294:PRO:O	2.12	0.50
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.46	0.50
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.46	0.50
2:B:122:GLU:HA	2:B:125:ARG:HG3	1.94	0.50
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.93	0.49
4:T:709:DC:H2'	4:T:710:DG:C8	2.47	0.49
4:T:711:DC:H2'	4:T:712:DC:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ARG:HG2	1:A:74:LEU:CD2	2.41	0.49
1:A:67:ASP:OD2	1:A:68:SER:N	2.46	0.49
1:A:139:THR:CG2	1:A:141:GLY:HA3	2.41	0.49
1:A:96:HIS:NE2	1:A:269:GLN:NE2	2.61	0.49
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.47	0.49
3:P:813:DT:H2'	3:P:814:DC:C6	2.48	0.49
1:A:330:GLN:HE22	1:A:340:GLN:NE2	2.10	0.49
1:A:511:ASP:OD1	1:A:512:GLN:CG	2.54	0.49
2:B:120:LEU:HD22	2:B:121:ASP:N	2.26	0.49
2:B:85:GLN:O	2:B:87:PHE:N	2.46	0.49
1:A:380:ILE:O	1:A:384:GLY:HA2	2.13	0.48
1:A:72:ARG:HD3	1:A:74:LEU:HD11	1.95	0.48
4:T:709:DC:H2''	4:T:710:DG:H5'	1.94	0.48
1:A:276:VAL:HA	1:A:302:GLU:OE1	2.13	0.48
1:A:359:GLY:HA2	3:P:811:DG:OP2	2.12	0.48
3:P:808:DC:H2'	3:P:809:DC:C6	2.47	0.48
1:A:30:LYS:O	1:A:34:LEU:HG	2.14	0.48
1:A:233:GLU:HG3	1:A:240:THR:HG22	1.95	0.48
2:B:129:ALA:HA	2:B:144:TYR:O	2.14	0.48
2:B:354:TYR:OH	2:B:356:ARG:NH2	2.45	0.48
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.13	0.48
4:T:722:DA:H2'	4:T:723:DC:H6	1.79	0.48
2:B:28:GLU:HG3	2:B:32:LYS:HD3	1.96	0.48
2:B:54:ASN:HA	2:B:55:PRO:HD3	1.67	0.48
2:B:108:VAL:C	2:B:109:LEU:HD12	2.34	0.48
2:B:92:LEU:HB3	2:B:94:ILE:HG13	1.95	0.47
3:P:810:DT:H2'	3:P:811:DG:C8	2.50	0.47
4:T:720:DG:H2'	4:T:721:DG:C8	2.49	0.47
1:A:55:PRO:HG2	1:A:56:TYR:CE2	2.49	0.47
1:A:57:ASN:HA	1:A:129:ALA:O	2.14	0.47
1:A:277:ARG:HH22	1:A:357:MET:HE3	1.79	0.47
1:A:417:VAL:CG1	1:A:419:THR:HG22	2.44	0.47
1:A:473:THR:HG23	1:A:476:LYS:HD2	1.97	0.47
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.96	0.47
1:A:293:ILE:CG1	1:A:294:PRO:HD2	2.44	0.47
2:B:90:VAL:CG1	2:B:91:GLN:N	2.77	0.47
1:A:302:GLU:O	1:A:305:GLU:HG2	2.14	0.47
1:A:478:GLU:HG2	1:A:499:SER:HB3	1.92	0.47
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.96	0.47
2:B:50:ILE:HD13	2:B:145:GLN:HB3	1.97	0.47
2:B:164:MET:HG2	2:B:182:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:GLN:O	2:B:281:LYS:HG2	2.14	0.47
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.96	0.47
1:A:77:PHE:HE2	1:A:150:PRO:HB2	1.80	0.47
1:A:227:PHE:O	1:A:233:GLU:HA	2.15	0.47
2:B:31:ILE:O	2:B:35:VAL:HG23	2.15	0.47
1:A:365:VAL:HG11	1:A:401:TRP:CD1	2.50	0.46
1:A:275:LYS:N	1:A:306:ASN:HD21	2.03	0.46
2:B:249:LYS:HE3	2:B:256:ASP:CG	2.36	0.46
2:B:261:VAL:HG13	2:B:276:VAL:CG2	2.44	0.46
2:B:425:LEU:HD13	2:B:425:LEU:O	2.15	0.46
1:A:137:ASN:N	1:A:137:ASN:ND2	2.63	0.46
1:A:109:LEU:CD2	1:A:220:LYS:HG3	2.44	0.46
1:A:302:GLU:HA	1:A:305:GLU:HG3	1.96	0.46
2:B:157:PRO:HB3	2:B:182:GLN:HE21	1.80	0.46
2:B:90:VAL:HG13	2:B:91:GLN:HG2	1.97	0.46
1:A:211:ARG:HD3	1:A:211:ARG:C	2.35	0.46
1:A:234:LEU:HB3	1:A:318:TYR:OH	2.16	0.46
2:B:65:LYS:HA	2:B:407:GLN:NE2	2.31	0.45
1:A:326:ILE:O	1:A:341:ILE:HA	2.16	0.45
4:T:721:DG:H2'	4:T:722:DA:C8	2.51	0.45
1:A:490:GLY:O	1:A:528:LYS:NZ	2.33	0.45
2:B:99:GLY:HA2	2:B:102:LYS:CD	2.46	0.45
3:P:814:DC:H2'	3:P:815:DG:C8	2.51	0.45
1:A:171:PHE:CD1	1:A:205:LEU:HD23	2.51	0.45
1:A:475:GLN:NE2	3:P:808:DC:O3'	2.49	0.45
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.51	0.45
4:T:722:DA:H2'	4:T:723:DC:C6	2.52	0.45
1:A:332:GLN:HB3	1:A:333:GLY:H	1.64	0.45
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.17	0.45
1:A:74:LEU:HD22	1:A:74:LEU:N	2.32	0.45
1:A:261:VAL:CG1	1:A:265:ASN:HD21	2.29	0.45
1:A:306:ASN:HA	1:A:309:ILE:HG22	1.99	0.44
1:A:220:LYS:HZ2	1:A:220:LYS:HG2	1.54	0.44
2:B:165:THR:O	2:B:169:GLU:HB2	2.17	0.44
2:B:209:LEU:HD23	2:B:209:LEU:HA	1.77	0.44
1:A:466:VAL:HG21	1:A:551:LEU:HG	1.99	0.44
1:A:416:PHE:CD1	1:A:417:VAL:N	2.85	0.44
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	3.05	0.44
3:P:812:DT:H2'	3:P:813:DT:C6	2.52	0.44
1:A:221:HIS:NE2	1:A:228:LEU:HB2	2.32	0.44
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PRO:O	1:A:414:TRP:HD1	2.00	0.44
1:A:266:TRP:CE2	3:P:820:DC:H4'	2.53	0.44
2:B:193:LEU:HD12	2:B:198:HIS:HA	2.00	0.44
1:A:340:GLN:HE21	1:A:340:GLN:HB2	1.53	0.44
2:B:125:ARG:CD	2:B:146:TYR:O	2.64	0.44
1:A:253:THR:H	1:A:256:ASP:HB2	1.82	0.44
2:B:356:ARG:CG	2:B:357:MET:H	2.27	0.44
7:A:825:914:O9	7:A:825:914:H10A	2.17	0.44
2:B:88:TRP:HB2	2:B:154:LYS:HD2	2.00	0.44
2:B:356:ARG:HA	2:B:356:ARG:HD3	1.75	0.44
2:B:103:LYS:HD2	2:B:191:SER:CA	2.48	0.43
1:A:60:VAL:HG12	1:A:75:VAL:HG22	2.00	0.43
1:A:199:ARG:NH2	1:A:223:LYS:HB2	2.32	0.43
2:B:74:LEU:HD21	2:B:409:THR:HA	1.99	0.43
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.32	0.43
1:A:448:ARG:H	1:A:448:ARG:HG2	1.64	0.43
2:B:76:ASP:OD1	2:B:76:ASP:C	2.57	0.43
2:B:350:LYS:HD3	2:B:351:THR:N	2.34	0.43
2:B:37:ILE:O	2:B:41:MET:HG3	2.18	0.43
2:B:120:LEU:HB2	2:B:148:VAL:O	2.17	0.43
2:B:189:VAL:HG11	2:B:202:ILE:CD1	2.49	0.43
3:P:818:DC:H2'	3:P:819:DG:H8	1.84	0.43
1:A:89:GLU:HG3	4:T:708:DG:OP1	2.19	0.43
1:A:503:LEU:CD1	1:A:507:GLN:HG3	2.49	0.43
2:B:60:VAL:HG11	2:B:130:PHE:CD2	2.54	0.43
2:B:354:TYR:HE1	2:B:374:LYS:HD3	1.82	0.43
1:A:393:ILE:HG13	1:A:423:VAL:HB	2.00	0.43
1:A:406:TRP:CH2	1:A:508:ALA:HB2	2.54	0.43
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.19	0.43
2:B:202:ILE:HD13	2:B:202:ILE:HA	1.85	0.43
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.49	0.43
2:B:8:VAL:HA	2:B:9:PRO:HD3	1.93	0.43
1:A:402:TRP:HZ3	2:B:364:ASP:OD2	2.02	0.43
1:A:467:VAL:CG2	1:A:484:LEU:HD11	2.48	0.43
1:A:186:ASP:O	1:A:187:LEU:HD23	2.19	0.43
2:B:205:LEU:HD23	2:B:205:LEU:C	2.39	0.43
2:B:303:LEU:HD22	2:B:307:ARG:NH1	2.34	0.43
2:B:334:GLN:NE2	2:B:334:GLN:N	2.62	0.43
4:T:715:DA:H2'	4:T:716:DA:C8	2.54	0.43
1:A:111:VAL:HG21	1:A:164:MET:CE	2.49	0.42
1:A:135:ILE:HG22	1:A:138:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:N	1:A:225:PRO:HD3	2.34	0.42
1:A:390:LYS:HE3	1:A:415:GLU:OE2	2.18	0.42
1:A:222:GLN:HB3	1:A:223:LYS:H	1.67	0.42
1:A:93:GLY:C	1:A:94:ILE:HD13	2.39	0.42
1:A:296:THR:C	1:A:298:GLU:N	2.70	0.42
2:B:211:ARG:HB3	2:B:212:TRP:CE3	2.54	0.42
1:A:262:GLY:HA3	3:P:819:DG:O4'	2.20	0.42
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.50	0.42
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.94	0.42
1:A:24:TRP:HB2	1:A:25:PRO:CD	2.43	0.42
2:B:65:LYS:O	2:B:68:SER:CB	2.67	0.42
2:B:395:LYS:O	2:B:399:GLU:HG3	2.19	0.42
1:A:91:GLN:O	4:T:708:DG:H4'	2.20	0.42
1:A:111:VAL:HB	1:A:185:ASP:HB2	2.01	0.42
1:A:482:ILE:HD13	1:A:506:ILE:HD12	2.00	0.42
2:B:34:LEU:HA	2:B:34:LEU:HD23	1.73	0.42
2:B:85:GLN:C	2:B:87:PHE:N	2.73	0.42
2:B:109:LEU:HD12	2:B:109:LEU:N	2.34	0.42
2:B:184:MET:HB2	8:B:476:HOH:O	2.18	0.42
2:B:325:LEU:HD12	2:B:325:LEU:HA	1.93	0.42
2:B:353:LYS:HD3	2:B:429:LEU:HD11	2.00	0.42
1:A:323:LYS:N	1:A:323:LYS:CD	2.83	0.42
1:A:349:LEU:HD12	1:A:349:LEU:HA	1.63	0.42
2:B:112:GLY:HA3	2:B:151:GLN:OE1	2.19	0.42
2:B:266:TRP:CH2	2:B:426:TRP:HB3	2.54	0.42
2:B:254:VAL:HG13	2:B:283:LEU:HD22	2.00	0.42
2:B:394:GLN:HE22	2:B:396:GLU:CG	2.33	0.42
1:A:255:ASN:HB2	1:A:289:LEU:CG	2.41	0.42
2:B:99:GLY:HA2	2:B:102:LYS:CE	2.49	0.42
1:A:51:GLY:HA3	1:A:53:GLU:OE2	2.20	0.42
1:A:438:GLU:OE2	1:A:461:ARG:HB2	2.20	0.42
2:B:128:THR:OG1	2:B:146:TYR:HB2	2.20	0.42
1:A:278:GLN:OE1	1:A:298:GLU:HB2	2.20	0.41
1:A:463:ARG:NH2	1:A:488:ASP:HB3	2.35	0.41
2:B:380:ILE:O	2:B:384:GLY:N	2.51	0.41
2:B:385:LYS:HG2	2:B:386:THR:N	2.35	0.41
3:P:815:DG:H2'	3:P:816:DG:C8	2.55	0.41
2:B:169:GLU:HB3	2:B:170:PRO:CD	2.41	0.41
1:A:135:ILE:CG2	1:A:138:GLU:CD	2.89	0.41
2:B:410:TRP:C	2:B:411:ILE:HG13	2.39	0.41
2:B:79:GLU:OE2	2:B:79:GLU:HA	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PRO:HG3	1:A:232:TYR:CD1	2.56	0.41
1:A:302:GLU:HA	1:A:305:GLU:HG2	2.02	0.41
3:P:815:DG:H2''	3:P:816:DG:O5'	2.21	0.41
3:P:818:DC:H2''	3:P:819:DG:H5'	2.02	0.41
1:A:81:ASN:ND2	4:T:706:DG:H5''	2.35	0.41
1:A:367:GLN:HE22	1:A:512:GLN:HE22	1.67	0.41
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.83	0.41
1:A:111:VAL:HG21	1:A:164:MET:HE1	2.03	0.41
1:A:317:VAL:O	1:A:349:LEU:HD12	2.21	0.41
4:T:724:DT:H2'	4:T:725:DG:O4'	2.19	0.41
1:A:169:GLU:N	1:A:170:PRO:CD	2.84	0.41
1:A:416:PHE:CZ	1:A:418:ASN:HA	2.56	0.41
2:B:29:GLU:HG3	2:B:71:TRP:CH2	2.56	0.41
2:B:29:GLU:HG2	2:B:30:LYS:N	2.35	0.41
2:B:180:ILE:HD13	2:B:205:LEU:HD11	2.03	0.41
2:B:263:LYS:HE3	2:B:426:TRP:O	2.21	0.41
2:B:425:LEU:HA	2:B:428:GLN:HG3	2.01	0.41
1:A:26:LEU:CD1	1:A:30:LYS:HB2	2.51	0.41
4:T:718:DA:H2'	4:T:719:DG:O4'	2.21	0.41
1:A:27:THR:CG2	1:A:28:GLU:N	2.82	0.40
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.61	0.40
2:B:292:VAL:O	2:B:292:VAL:HG23	2.20	0.40
2:B:422:LEU:HA	2:B:422:LEU:HD12	1.78	0.40
2:B:329:ILE:O	2:B:392:PRO:HG3	2.21	0.40
1:A:195:ILE:HG12	8:A:640:HOH:O	2.21	0.40
1:A:277:ARG:H	1:A:336:GLN:HE22	1.69	0.40
2:B:213:GLY:HA2	2:B:214:LEU:HA	1.90	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	553/560 (99%)	508 (92%)	37 (7%)	8 (1%)	11	28
2	B	408/452 (90%)	373 (91%)	30 (7%)	5 (1%)	13	32
All	All	961/1012 (95%)	881 (92%)	67 (7%)	13 (1%)	11	28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	THR
2	B	87	PHE
1	A	85	GLN
1	A	286	THR
1	A	355	ALA
2	B	86	ASP
1	A	113	ASP
2	B	97	PRO
1	A	141	GLY
1	A	270	ILE
2	B	111	VAL
1	A	135	ILE
2	B	421	PRO

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%)	441 (89%)	54 (11%)	6	14
2	B	371/411 (90%)	346 (93%)	25 (7%)	16	37
All	All	866/911 (95%)	787 (91%)	79 (9%)	9	21

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	26	LEU
1	A	53	GLU

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Mol	Chain	Res	Type
1	A	54	ASN
1	A	66	LYS
1	A	70	LYS
1	A	83	ARG
1	A	100	LEU
1	A	136	ASN
1	A	137	ASN
1	A	138	GLU
1	A	164	MET
1	A	173	LYS
1	A	205	LEU
1	A	209	LEU
1	A	211	ARG
1	A	218	ASP
1	A	222	GLN
1	A	223	LYS
1	A	228	LEU
1	A	246	LEU
1	A	260	LEU
1	A	264	LEU
1	A	283	LEU
1	A	293	ILE
1	A	298	GLU
1	A	301	LEU
1	A	305	GLU
1	A	312	GLU
1	A	323	LYS
1	A	324	ASP
1	A	330	GLN
1	A	332	GLN
1	A	340	GLN
1	A	349	LEU
1	A	353	LYS
1	A	368	LEU
1	A	373	GLN
1	A	385	LYS
1	A	393	ILE
1	A	402	TRP
1	A	419	THR
1	A	428	GLN
1	A	448	ARG
1	A	452	LEU

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Mol	Chain	Res	Type
1	A	454	LYS
1	A	471	ASP
1	A	478	GLU
1	A	487	GLN
1	A	491	LEU
1	A	512	GLN
1	A	533	LEU
1	A	540	LYS
1	A	548	VAL
2	B	8	VAL
2	B	32	LYS
2	B	61	PHE
2	B	74	LEU
2	B	82	LYS
2	B	87	PHE
2	B	113	ASP
2	B	120	LEU
2	B	122	GLU
2	B	166	LYS
2	B	211	ARG
2	B	248	GLU
2	B	277	ARG
2	B	301	LEU
2	B	303	LEU
2	B	324	ASP
2	B	325	LEU
2	B	368	LEU
2	B	386	THR
2	B	394	GLN
2	B	396	GLU
2	B	422	LEU
2	B	425	LEU
2	B	426	TRP
2	B	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	137	ASN
1	A	197	GLN
1	A	222	GLN

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Mol	Chain	Res	Type
1	A	242	GLN
1	A	255	ASN
1	A	265	ASN
1	A	269	GLN
1	A	306	ASN
1	A	330	GLN
1	A	332	GLN
1	A	340	GLN
1	A	407	GLN
1	A	418	ASN
1	A	428	GLN
1	A	464	GLN
1	A	475	GLN
1	A	480	GLN
1	A	487	GLN
1	A	507	GLN
1	A	512	GLN
1	A	520	GLN
2	B	174	GLN
2	B	197	GLN
2	B	334	GLN
2	B	343	GLN
2	B	407	GLN
2	B	428	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	4,3	16,19,20	0.40	0	20,26,29	0.54	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	4,3	-	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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	A	561	-	4,4,4	0.27	0	6,6,6	0.07	0
5	SO4	P	2	-	4,4,4	0.27	0	6,6,6	0.11	0
5	SO4	A	562	-	4,4,4	0.29	0	6,6,6	0.07	0
7	914	A	825	6	26,32,32	2.34	9 (34%)	24,50,50	1.63	5 (20%)

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
7	914	A	825	6	-	7/13/34/34	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	825	914	P1-O4	6.25	1.65	1.58
7	A	825	914	O2-C10	-4.03	1.37	1.42
7	A	825	914	F1-C3	-3.82	1.32	1.36
7	A	825	914	C5-N3	3.56	1.40	1.35
7	A	825	914	O2-C1	-3.22	1.36	1.42
7	A	825	914	P1-O3	-2.88	1.49	1.56
7	A	825	914	C8-N3	2.85	1.36	1.32
7	A	825	914	C7-N2	-2.68	1.29	1.34
7	A	825	914	O1-C4	-2.16	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	825	914	C4-O1-C1	3.56	114.43	106.81
7	A	825	914	P2-O6-P3	3.39	144.45	132.83
7	A	825	914	C3-C4-N1	-2.81	110.43	113.44
7	A	825	914	O3-P1-O8	2.75	119.25	110.07
7	A	825	914	C1-C2-C3	-2.33	107.83	110.22

There are no chirality outliers.

All (7) torsion outliers are listed below:

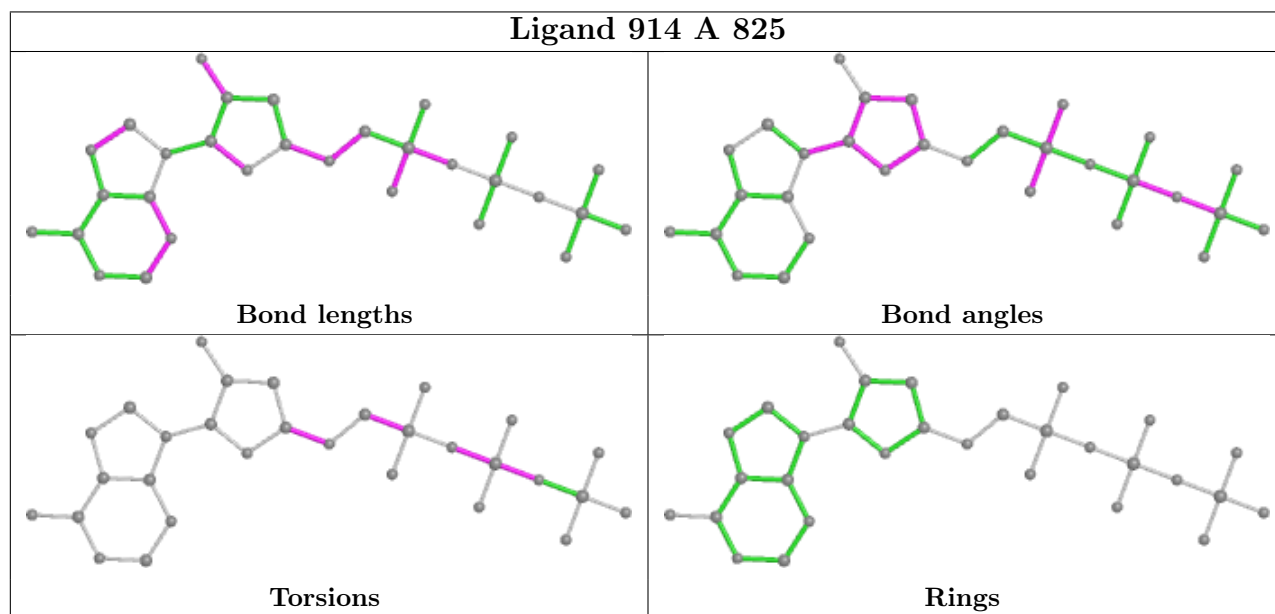
Mol	Chain	Res	Type	Atoms
7	A	825	914	O1-C1-O2-C10
7	A	825	914	O2-C10-P1-O8
7	A	825	914	O2-C10-P1-O3
7	A	825	914	P3-O6-P2-O4
7	A	825	914	O2-C10-P1-O4
7	A	825	914	P1-O4-P2-O9
7	A	825	914	P3-O6-P2-O9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	825	914	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	555/560 (99%)	-0.01	14 (2%) 57 59	22, 47, 89, 109	0
2	B	412/452 (91%)	0.00	14 (3%) 45 45	27, 57, 94, 121	0
3	P	17/21 (80%)	-0.78	0 100 100	38, 60, 78, 80	0
4	T	24/27 (88%)	-0.23	1 (4%) 36 35	37, 75, 95, 120	0
All	All	1008/1060 (95%)	-0.02	29 (2%) 51 52	22, 52, 91, 121	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	6.9
2	B	4	PRO	6.3
2	B	89	GLU	5.4
2	B	87	PHE	5.4
1	A	288	ALA	4.0
1	A	62	ALA	3.6
2	B	90	VAL	3.5
1	A	140	PRO	3.1
1	A	136	ASN	3.0
1	A	295	LEU	3.0
2	B	95	PRO	2.9
1	A	251	SER	2.9
2	B	93	GLY	2.8
2	B	94	ILE	2.6
2	B	178	ILE	2.6
1	A	132	ILE	2.6
1	A	68	SER	2.6
1	A	249	LYS	2.5
1	A	141	GLY	2.5
1	A	303	LEU	2.5
1	A	223	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	2.4
2	B	7	THR	2.4
1	A	26	LEU	2.3
2	B	6	GLU	2.3
4	T	702	DT	2.2
2	B	212	TRP	2.2
2	B	209	LEU	2.1
2	B	214	LEU	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	0.98	0.14	35,39,40,41	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

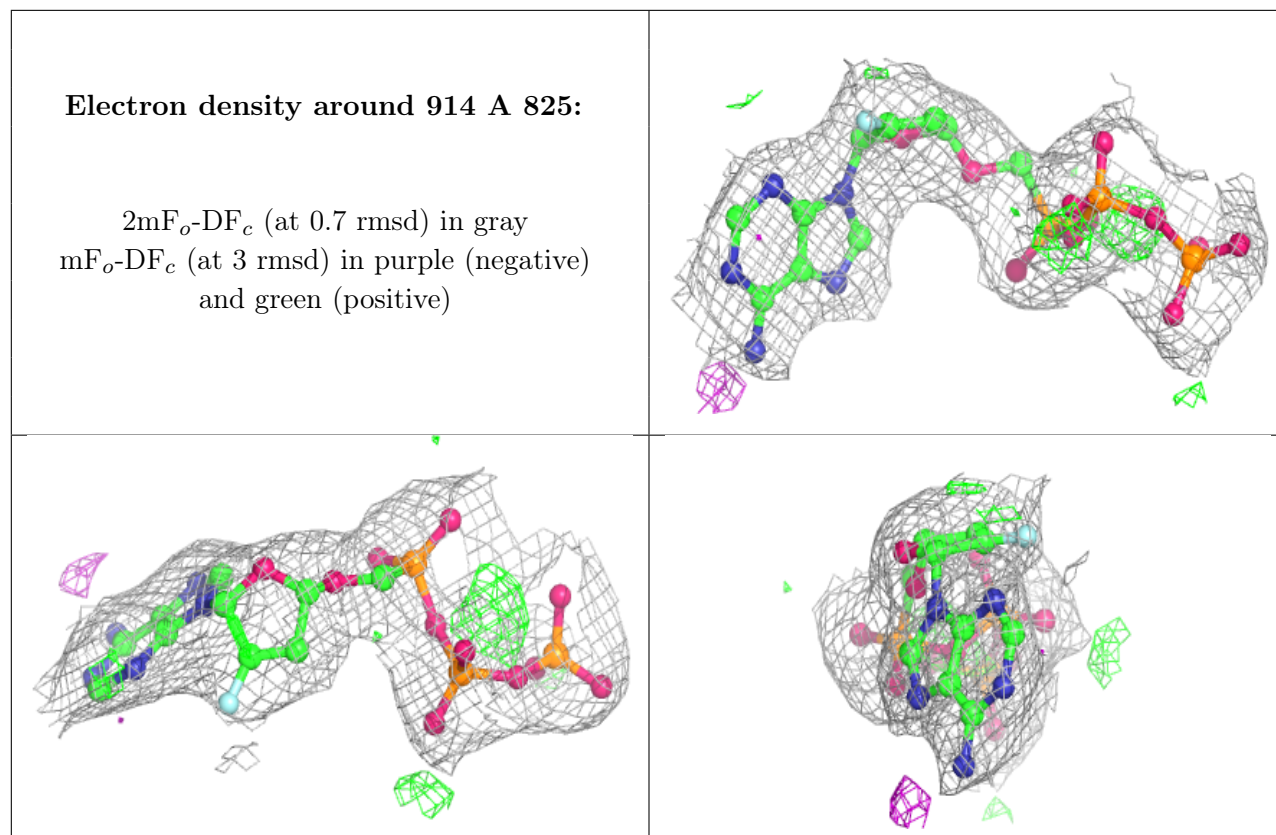
6.4 Ligands [i](#)

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	A	562	5/5	0.86	0.18	115,116,117,117	0
5	SO4	P	2	5/5	0.88	0.19	115,115,116,116	0
6	MG	A	601	1/1	0.95	0.23	13,13,13,13	0
7	914	A	825	30/30	0.96	0.17	46,51,53,56	0
5	SO4	A	561	5/5	0.98	0.12	66,67,67,67	0
6	MG	A	600	1/1	0.99	0.21	15,15,15,15	0

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

orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.