Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 05:35 PM EDT

PDB ID	:	4PWD
Title	:	Crystal structure of HIV-1 reverse transcriptase in complex with bulge-RNA/DNA and Nevirapine
Authors	:	Das, K.; Martinez, S.E.; Arnold, E.
Deposited on	:	2014-03-19
Resolution	:	3.00 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:

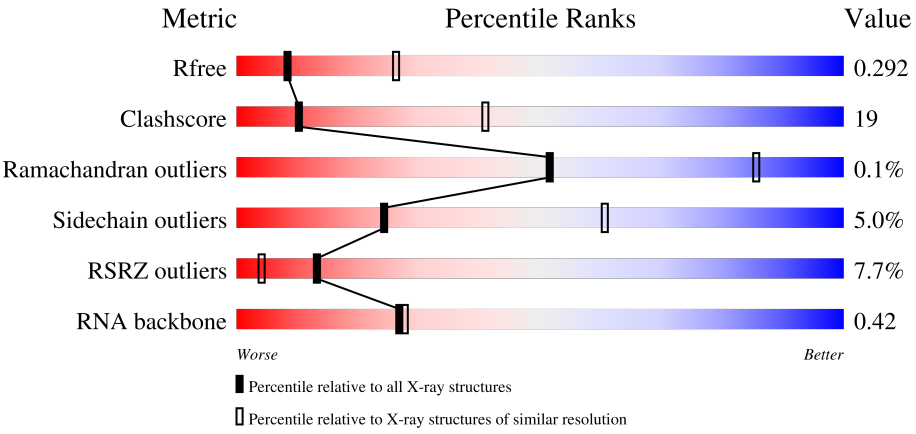
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 <=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	556	10% 59% 38%
1	C	556	12% 64% 34%
2	B	428	2% 57% 38%
2	D	428	2% 57% 36%

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Mol	Chain	Length	Quality of chain
3	E	27	19% 11% 15% 37% 11% 26%
3	T	27	15% 19% 30% 22% 7% 22%
4	F	21	24% 43% 38% 10% 10%
4	P	21	10% 24% 43% 24% 10%

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
7	SO4	B	501	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17508 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 HIV-1 Reverse Transcriptase, P66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4506	2917	748	833	8			
1	C	555	Total	C	N	O	S	0	0	0
			4506	2917	748	833	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	498	ASN	ASP	engineered mutation	UNP P03366
C	-1	MET	-	expression tag	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	258	CYS	GLN	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366
C	498	ASN	ASP	engineered mutation	UNP P03366

- Molecule 2 is a protein called HIV-1 Reverse Transcriptase, P51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			
2	D	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

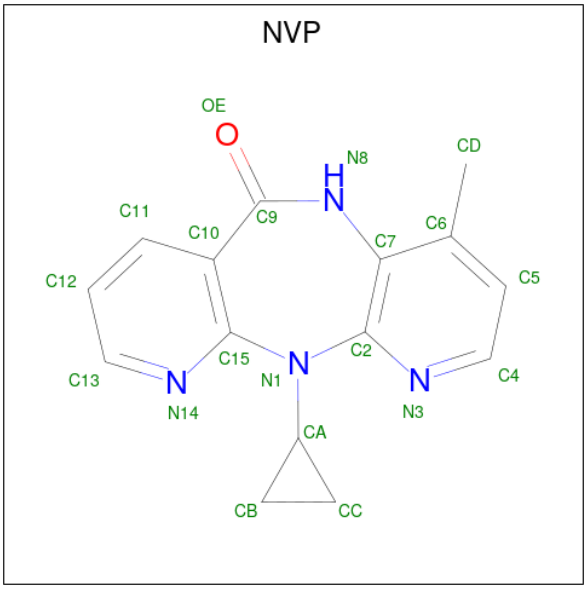
- Molecule 3 is a RNA chain called 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	21	Total	C	N	O	P	0	0	0
			454	202	88	143	21			
3	E	20	Total	C	N	O	P	0	0	0
			431	192	83	136	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	19	Total	C	N	O	P	0	0	0
			382	182	67	115	18			
4	F	19	Total	C	N	O	P	0	0	0
			382	182	67	115	18			

- Molecule 5 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: $C_{15}H_{14}N_4O$).

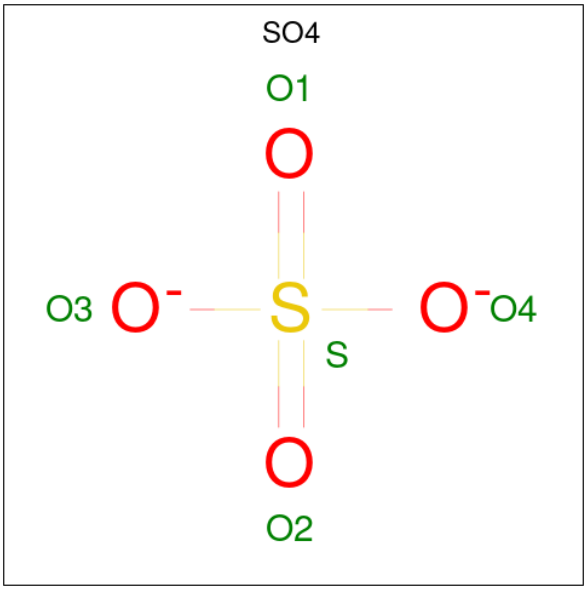


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	15	4	1		
5	C	1	Total	C	N	O	0	0
			20	15	4	1		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Ca 1 1	0	0
6	C	1	Total Ca 1 1	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



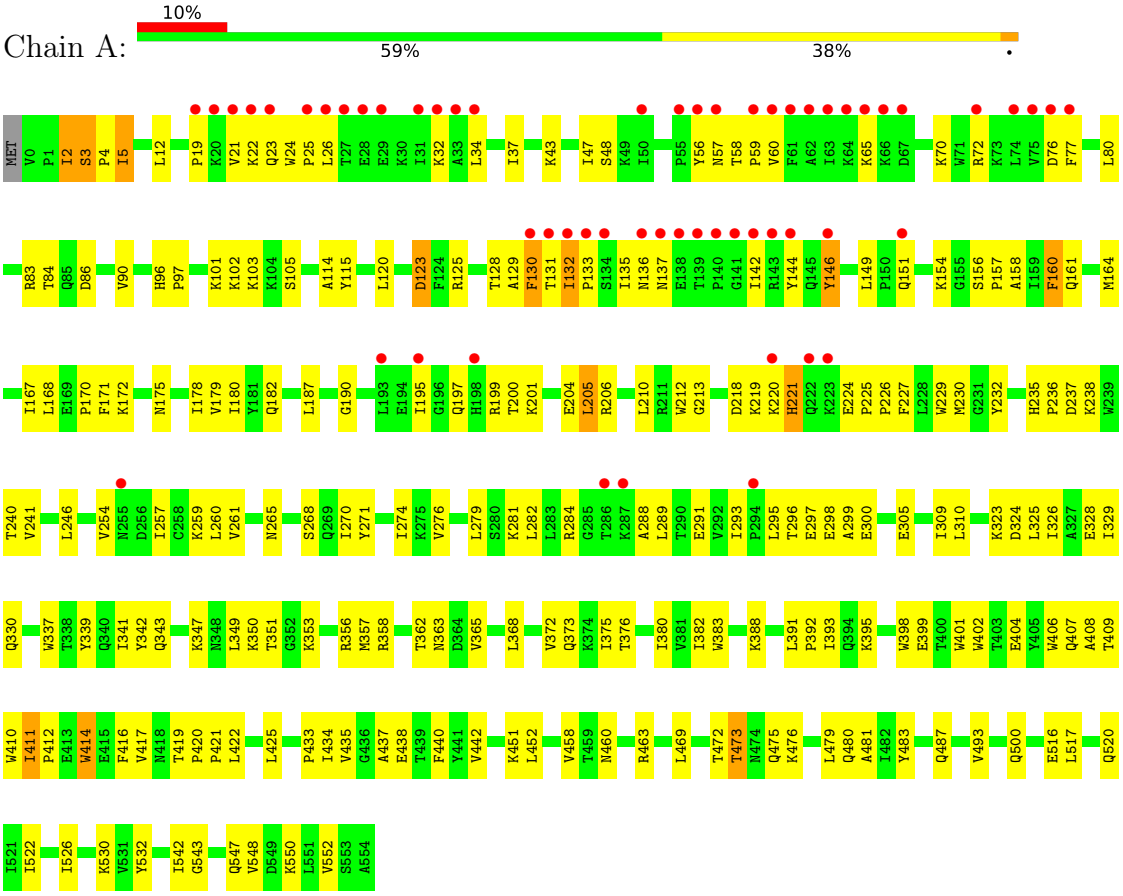
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total O S 5 4 1	0	0

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.

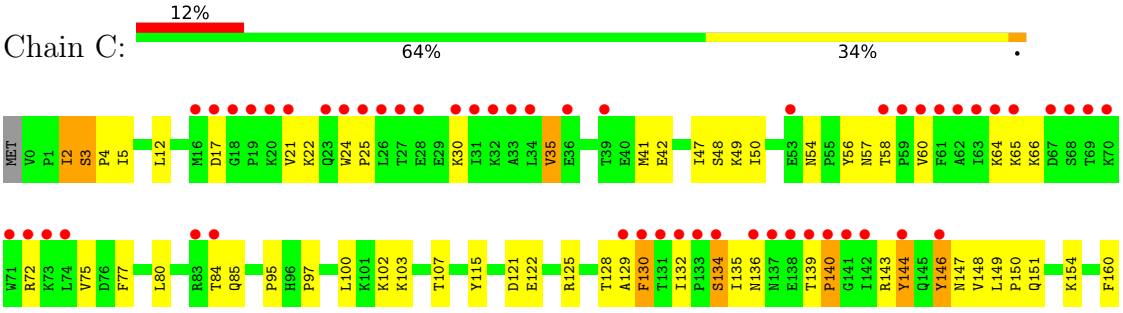
• Molecule 1: HIV-1 Reverse Transcriptase, P66 subunit

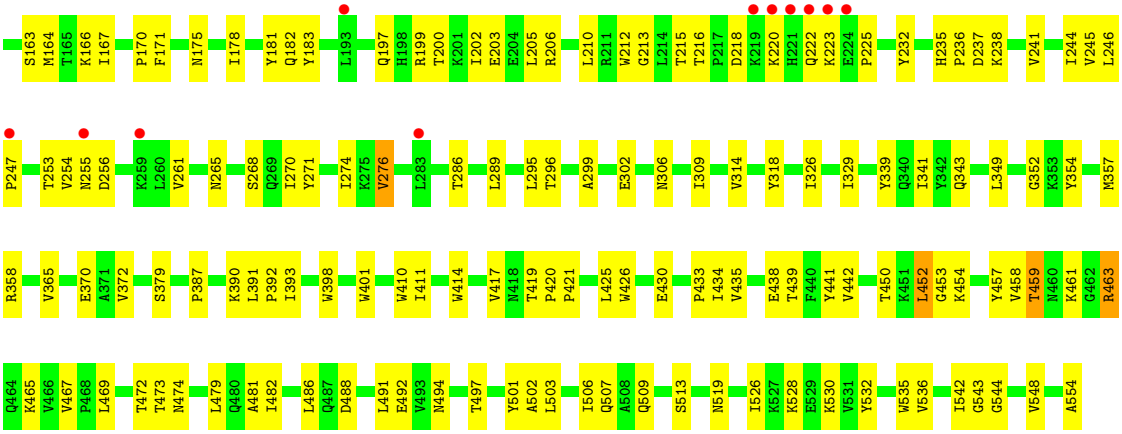
Chain A:



• Molecule 1: HIV-1 Reverse Transcriptase, P66 subunit

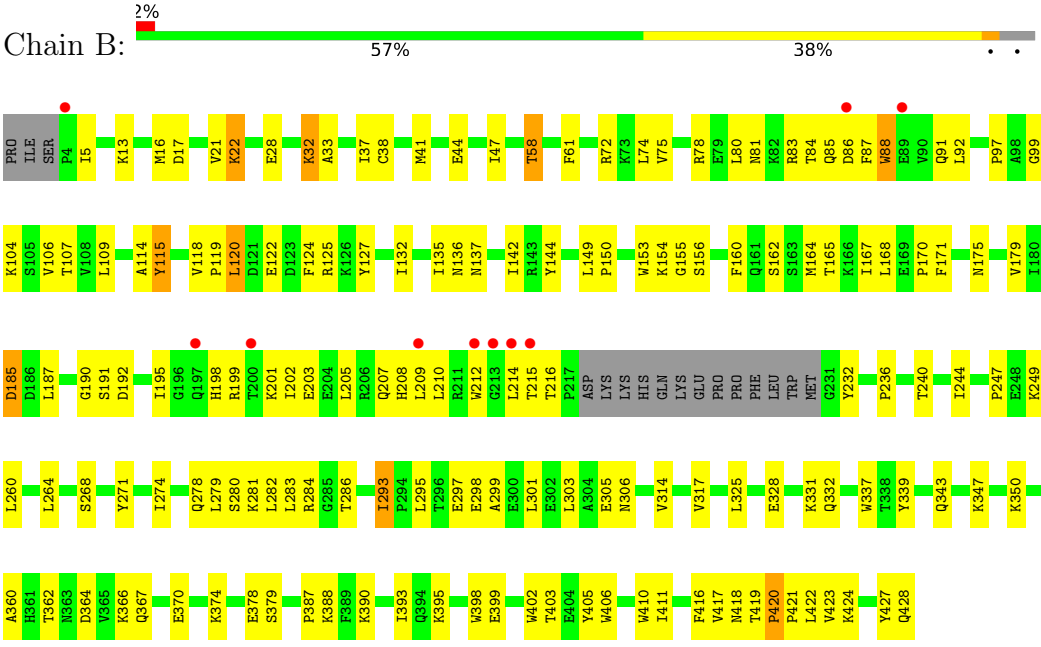
Chain C:





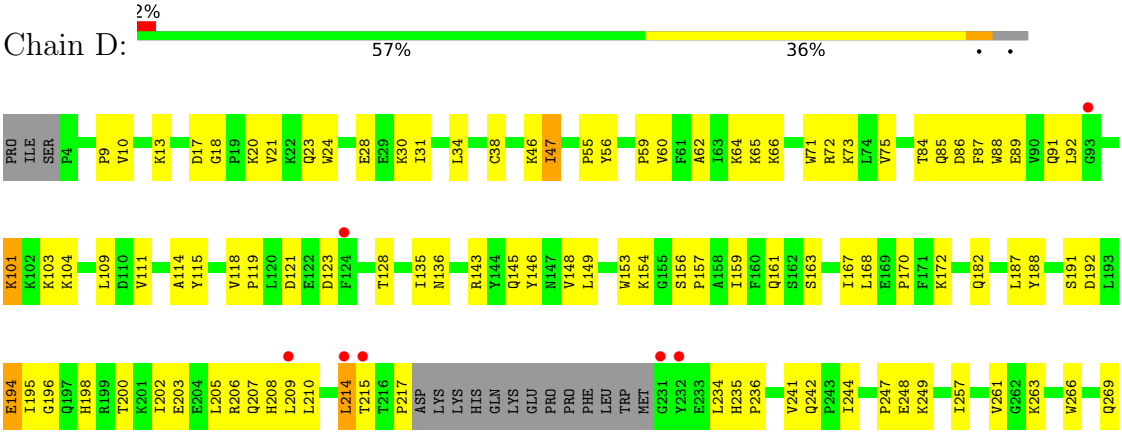
• Molecule 2: HIV-1 Reverse Transcriptase, P51 subunit

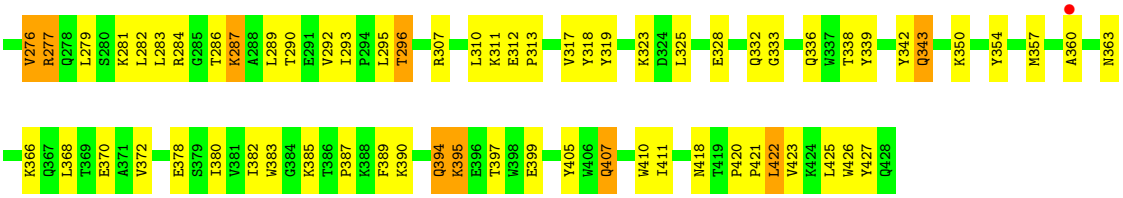
Chain B:



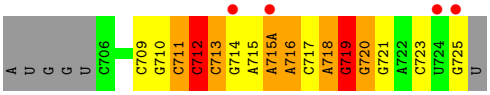
• Molecule 2: HIV-1 Reverse Transcriptase, P51 subunit

Chain D:

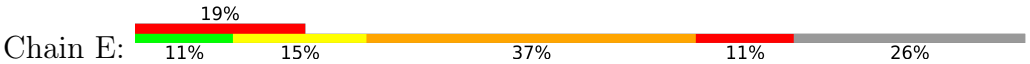


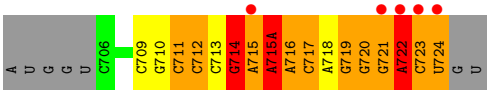


• Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*AP*C P*AP*GP*GP*GP*AP*CP*UP*GP*U)-3'

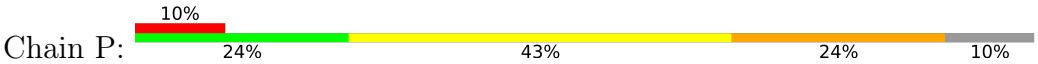


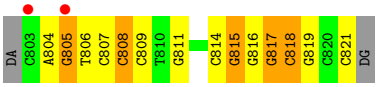
• Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*AP*C P*AP*GP*GP*GP*AP*CP*UP*GP*U)-3'



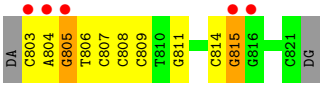


• Molecule 4: 5'-D(*A*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP *CP*CP*G)-3'





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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.68Å 130.76Å 141.87Å 90.00° 100.75° 90.00°	Depositor
Resolution (Å)	44.68 – 3.00 47.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (44.68-3.00) 96.1 (47.68-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.221 , 0.291 0.226 , 0.292	Depositor DCC
R_{free} test set	1841 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å^2)	63.8	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 77.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17508	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.72	1/4624 (0.0%)	0.80	1/6283 (0.0%)
1	C	0.68	0/4624	0.79	4/6283 (0.1%)
2	B	0.73	0/3497	0.80	3/4751 (0.1%)
2	D	0.70	0/3497	0.80	2/4751 (0.0%)
3	E	0.73	2/482 (0.4%)	1.37	10/750 (1.3%)
3	T	0.91	2/508 (0.4%)	1.46	3/791 (0.4%)
4	F	1.13	2/426 (0.5%)	1.08	1/655 (0.2%)
4	P	1.28	4/426 (0.9%)	1.20	3/655 (0.5%)
All	All	0.75	11/18084 (0.1%)	0.87	27/24919 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	811	DG	C3'-C2'	8.67	1.62	1.52
4	P	815	DG	C3'-C2'	7.44	1.61	1.52
4	P	818	DC	C3'-C2'	-7.28	1.43	1.52
4	P	805	DG	C3'-C2'	6.88	1.60	1.52
3	T	712	C	C3'-C2'	-6.20	1.46	1.52
3	E	714	G	C3'-C2'	-6.07	1.46	1.52
4	F	815	DG	C3'-C2'	6.00	1.59	1.52
3	E	724	U	C3'-C2'	5.95	1.59	1.52
1	A	414	TRP	CB-CG	5.94	1.60	1.50
4	P	808	DC	P-O5'	5.48	1.65	1.59
3	T	713	C	C3'-C2'	-5.34	1.46	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	817	DG	O4'-C4'-C3'	-8.44	100.94	106.00
3	E	717	C	C6-N1-C2	-7.45	117.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	364	ASP	CB-CG-OD1	6.98	124.58	118.30
3	E	723	C	C6-N1-C1'	-6.96	112.44	120.80
3	E	722	A	O4'-C1'-N9	6.62	113.50	108.20
1	C	463	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	411	ILE	CG1-CB-CG2	-6.44	97.24	111.40
1	C	463	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	C	4	PRO	N-CA-C	5.96	127.60	112.10
1	C	491	LEU	CA-CB-CG	5.79	128.61	115.30
2	D	214	LEU	CA-CB-CG	5.77	128.58	115.30
3	T	719	G	N7-C8-N9	5.75	115.98	113.10
4	F	805	DG	C1'-O4'-C4'	-5.72	104.38	110.10
3	T	719	G	C8-N9-C4	-5.68	104.13	106.40
2	B	88	TRP	CA-CB-CG	5.54	124.22	113.70
3	E	723	C	C2-N1-C1'	5.50	124.86	118.80
3	E	714	G	C2'-C3'-O3'	5.47	122.45	113.70
3	T	718	A	C5-C6-N6	-5.44	119.34	123.70
2	B	420	PRO	C-N-CD	5.44	139.82	128.40
3	E	723	C	N3-C4-C5	5.43	124.07	121.90
4	P	811	DG	O5'-P-OP1	-5.40	100.84	105.70
2	D	420	PRO	C-N-CD	5.33	139.60	128.40
3	E	723	C	C6-N1-C2	5.31	122.42	120.30
3	E	723	C	N1-C2-O2	5.25	122.05	118.90
3	E	715(A)	A	C3'-C2'-C1'	5.25	105.70	101.50
3	E	722	A	O5'-P-OP1	-5.17	101.05	105.70
4	P	817	DG	O4'-C1'-N9	5.02	111.52	108.00

There are no chirality outliers.

There are no planarity outliers.

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	4506	0	4560	171	0
1	C	4506	0	4560	154	0
2	B	3400	0	3433	144	0
2	D	3400	0	3433	120	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	431	0	220	20	0
3	T	454	0	231	20	0
4	F	382	0	215	9	0
4	P	382	0	215	23	0
5	A	20	0	14	1	0
5	C	20	0	14	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	B	5	0	0	2	0
All	All	17508	0	16895	638	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 19.

All (638) 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:D:282:LEU:HD21	2:D:296:THR:HG22	1.25	1.19
2:B:332:GLN:HE21	2:B:427:TYR:HB3	1.14	1.08
2:D:277:ARG:HD2	2:D:277:ARG:H	1.25	1.01
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.45	0.98
3:T:712:C:H2'	3:T:713:C:C6	2.03	0.93
1:C:21:VAL:H	1:C:57:ASN:HB2	1.32	0.92
3:T:712:C:H2'	3:T:713:C:H6	1.34	0.91
2:B:332:GLN:NE2	2:B:427:TYR:HB3	1.87	0.91
2:B:421:PRO:HB3	2:B:424:LYS:HG3	1.52	0.90
2:D:423:VAL:HG13	2:D:426:TRP:HD1	1.35	0.89
3:T:711:C:H2'	3:T:712:C:C6	2.07	0.88
2:B:115:TYR:HD2	2:B:156:SER:HB3	1.39	0.86
2:D:282:LEU:CD2	2:D:296:THR:HG22	2.05	0.85
4:P:807:DC:H2"	4:P:808:DC:H5'	1.59	0.84
1:A:5:ILE:HG22	1:A:212:TRP:HD1	1.41	0.83
1:C:5:ILE:HG22	1:C:212:TRP:HD1	1.44	0.83
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.12	0.82
1:A:281:LYS:HG2	1:A:284:ARG:HH21	1.42	0.81
1:C:372:VAL:HG11	1:C:411:ILE:HG23	1.59	0.81
2:D:276:VAL:H	2:D:277:ARG:NH1	1.77	0.81
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.63	0.80
1:A:195:ILE:HG22	1:A:199:ARG:HH12	1.44	0.80
3:E:713:C:H2'	3:E:714:G:C8	2.16	0.79
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:711:C:H2'	3:E:712:C:C6	2.18	0.78
4:P:807:DC:H2"	4:P:808:DC:C5'	2.13	0.77
2:D:13:LYS:HD3	2:D:85:GLN:HB3	1.67	0.77
1:C:435:VAL:HG13	2:D:290:THR:HG21	1.66	0.77
1:A:24:TRP:CD2	1:A:25:PRO:HD2	2.20	0.76
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.68	0.75
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.21	0.74
2:B:191:SER:HG	2:B:198:HIS:HD1	1.33	0.74
2:D:17:ASP:OD1	2:D:18:GLY:N	2.18	0.74
2:D:423:VAL:CG1	2:D:426:TRP:HD1	1.99	0.74
1:C:56:TYR:HB2	1:C:129:ALA:HB3	1.70	0.74
1:C:503:LEU:HD11	1:C:507:GLN:HE21	1.50	0.74
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.70	0.74
1:A:261:VAL:HG13	1:A:276:VAL:HG21	1.68	0.74
1:C:434:ILE:HD13	1:C:530:LYS:HB3	1.69	0.74
4:P:817:DG:H2'	4:P:818:DC:H6	1.52	0.73
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.71	0.73
2:B:195:ILE:HD11	2:B:199:ARG:HE	1.54	0.73
4:P:804:DA:C2	4:P:805:DG:C4	2.76	0.72
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.71	0.72
3:E:713:C:H2'	3:E:714:G:H8	1.53	0.71
2:B:13:LYS:HD2	2:B:86:ASP:H	1.56	0.71
1:A:5:ILE:HG22	1:A:212:TRP:CD1	2.24	0.71
1:C:175:ASN:HB3	1:C:178:ILE:HD13	1.72	0.71
2:D:421:PRO:HB2	2:D:423:VAL:H	1.56	0.71
1:C:542:ILE:HG23	2:D:283:LEU:HD13	1.74	0.70
1:A:86:ASP:OD1	1:A:154:LYS:NZ	2.22	0.70
1:A:206:ARG:HH11	1:A:220:LYS:HZ3	1.37	0.70
2:D:56:TYR:O	2:D:143:ARG:NH2	2.25	0.70
2:D:423:VAL:HG13	2:D:426:TRP:CD1	2.24	0.70
1:C:41:MET:SD	1:C:47:ILE:HD11	2.33	0.69
2:D:328:GLU:HG3	2:D:342:TYR:HE1	1.58	0.69
2:B:358:ARG:NE	2:B:370:GLU:OE1	2.24	0.68
1:C:35:VAL:HG23	1:C:134:SER:HB3	1.74	0.68
1:A:172:LYS:HE2	1:A:180:ILE:HD12	1.75	0.68
2:B:109:LEU:HD11	2:B:202:ILE:HG23	1.75	0.68
1:C:77:PHE:CD2	1:C:80:LEU:HB3	2.29	0.68
1:C:97:PRO:HG2	1:C:232:TYR:CE2	2.28	0.67
1:C:223:LYS:O	1:C:225:PRO:HD3	1.95	0.67
4:P:817:DG:H2'	4:P:818:DC:C6	2.29	0.67
3:T:711:C:H2'	3:T:712:C:H6	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:LYS:NZ	2:B:378:GLU:OE2	2.23	0.66
1:A:548:VAL:O	1:A:552:VAL:HG22	1.94	0.66
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.76	0.66
2:D:357:MET:O	2:D:360:ALA:HB2	1.95	0.66
2:D:423:VAL:HG12	2:D:423:VAL:O	1.95	0.66
2:B:28:GLU:HG2	2:B:32:LYS:HE2	1.76	0.66
1:C:97:PRO:HG2	1:C:232:TYR:CD2	2.31	0.66
1:A:288:ALA:HB3	1:A:291:GLU:HG3	1.78	0.65
1:A:438:GLU:HB3	1:A:440:PHE:HE1	1.60	0.65
1:C:220:LYS:HG3	1:C:222:GLN:HG2	1.78	0.65
2:D:422:LEU:C	2:D:422:LEU:HD23	2.16	0.65
2:B:171:PHE:HD2	2:B:205:LEU:HD13	1.60	0.65
1:A:123:ASP:OD1	1:A:123:ASP:N	2.29	0.65
3:T:718:A:H2'	3:T:719:G:C8	2.31	0.65
2:D:86:ASP:OD1	2:D:87:PHE:N	2.30	0.65
2:B:393:ILE:HG21	2:B:398:TRP:HB2	1.77	0.64
1:A:543:GLY:HA2	2:B:283:LEU:O	1.97	0.64
2:B:207:GLN:HA	2:B:210:LEU:HB3	1.79	0.64
2:D:338:THR:HG21	2:D:427:TYR:HB2	1.79	0.64
2:D:85:GLN:NE2	2:D:89:GLU:OE1	2.31	0.64
2:B:370:GLU:HG3	2:B:374:LYS:HD2	1.79	0.64
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.80	0.64
2:D:244:ILE:HB	2:D:310:LEU:HD22	1.79	0.64
2:B:252:TRP:NE1	2:B:295:LEU:HD11	2.13	0.64
2:B:332:GLN:HE21	2:B:427:TYR:CB	2.03	0.64
3:E:715:A:N3	3:E:716:A:N6	2.45	0.63
1:A:419:THR:H	1:A:422:LEU:HD21	1.63	0.63
1:C:503:LEU:O	1:C:507:GLN:HG3	1.98	0.63
2:B:80:LEU:HD23	2:B:153:TRP:CD1	2.34	0.63
4:F:807:DC:H2"	4:F:808:DC:C5'	2.29	0.63
3:T:718:A:H2'	3:T:719:G:H8	1.64	0.63
1:A:225:PRO:HA	1:A:226:PRO:C	2.20	0.62
2:B:393:ILE:HD13	2:B:398:TRP:HB2	1.81	0.62
1:A:65:LYS:HD3	1:A:72:ARG:HH21	1.63	0.62
1:C:210:LEU:O	1:C:213:GLY:N	2.24	0.62
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.35	0.62
1:C:494:ASN:HB3	2:D:289:LEU:HD12	1.81	0.62
4:F:803:DC:H2'	4:F:804:DA:C8	2.34	0.62
2:B:191:SER:OG	2:B:198:HIS:ND1	2.28	0.62
1:C:434:ILE:CD1	1:C:530:LYS:HB3	2.30	0.62
1:A:323:LYS:O	1:A:343:GLN:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:277:ARG:HD2	2:D:277:ARG:N	2.07	0.61
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.35	0.61
1:C:181:TYR:CE2	1:C:183:TYR:HB2	2.36	0.61
1:A:34:LEU:HA	1:A:37:ILE:HB	1.83	0.61
1:C:454:LYS:NZ	1:C:554:ALA:O	2.20	0.61
1:A:132:ILE:HG12	1:A:133:PRO:HD2	1.82	0.60
2:D:170:PRO:HB2	2:D:208:HIS:HE1	1.67	0.60
4:P:804:DA:C2	4:P:805:DG:C5	2.89	0.60
4:F:807:DC:H2"	4:F:808:DC:H5'	1.82	0.60
1:A:2:ILE:HG22	1:A:3:SER:H	1.66	0.60
1:A:167:ILE:O	1:A:170:PRO:HD2	2.01	0.60
3:T:709:C:H2'	3:T:710:G:C8	2.37	0.60
1:A:372:VAL:HG11	1:A:411:ILE:CG2	2.32	0.60
2:D:87:PHE:O	2:D:91:GLN:HB3	2.00	0.60
4:P:804:DA:N3	4:P:805:DG:C8	2.70	0.60
1:A:201:LYS:HA	1:A:204:GLU:HB3	1.83	0.60
2:B:209:LEU:HD23	2:B:214:LEU:HD23	1.82	0.60
2:D:163:SER:O	2:D:167:ILE:HG22	2.01	0.60
2:D:191:SER:OG	2:D:198:HIS:ND1	2.35	0.60
1:A:210:LEU:O	1:A:213:GLY:N	2.25	0.60
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.84	0.60
2:D:88:TRP:CG	2:D:154:LYS:HG2	2.37	0.60
1:C:65:LYS:HB3	1:C:72:ARG:NH1	2.17	0.59
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.36	0.59
2:B:247:PRO:HA	2:B:428:GLN:HE22	1.67	0.59
2:B:87:PHE:O	2:B:91:GLN:HB3	2.01	0.59
2:B:214:LEU:HD12	2:B:215:THR:H	1.67	0.59
1:C:21:VAL:HG12	1:C:22:LYS:H	1.67	0.59
1:C:139:THR:HB	1:C:140:PRO:HD2	1.85	0.59
1:C:163:SER:HA	1:C:166:LYS:HE3	1.84	0.59
1:C:339:TYR:CE2	1:C:341:ILE:HD11	2.38	0.59
1:C:543:GLY:HA3	2:D:283:LEU:O	2.03	0.59
2:B:84:THR:O	2:B:87:PHE:HB3	2.03	0.59
3:E:717:C:H2'	3:E:718:A:C8	2.38	0.59
1:A:473:THR:HG23	1:A:476:LYS:HG3	1.84	0.59
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.38	0.59
1:C:58:THR:H	1:C:130:PHE:HB2	1.68	0.59
2:D:247:PRO:O	2:D:307:ARG:NH2	2.36	0.59
1:C:12:LEU:HD22	1:C:84:THR:HA	1.85	0.58
1:C:30:LYS:HZ1	1:C:64:LYS:HD2	1.68	0.58
2:D:203:GLU:HA	2:D:206:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:111:VAL:HG23	2:D:115:TYR:HE2	1.69	0.58
3:T:713:C:H2'	3:T:714:G:C8	2.38	0.58
4:P:807:DC:H2"	4:P:808:DC:O5'	2.02	0.58
1:A:324:ASP:O	1:A:343:GLN:HG2	2.03	0.58
2:D:182:GLN:HB2	2:D:187:LEU:HD12	1.85	0.58
3:T:719:G:H2'	3:T:720:G:C8	2.39	0.58
1:A:26:LEU:HD22	1:A:60:VAL:HG11	1.85	0.58
2:D:257:ILE:O	2:D:261:VAL:HG23	2.03	0.58
2:B:91:GLN:HG3	2:B:92:LEU:HG	1.86	0.58
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.39	0.58
1:A:547:GLN:O	1:A:550:LYS:HG2	2.03	0.58
2:B:423:VAL:HG12	2:B:423:VAL:O	2.03	0.57
1:C:503:LEU:HD22	1:C:535:TRP:HB2	1.86	0.57
2:D:366:LYS:HG3	2:D:405:TYR:CD1	2.39	0.57
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.87	0.57
1:A:97:PRO:HG2	1:A:232:TYR:CE1	2.39	0.57
2:D:87:PHE:HZ	2:D:159:ILE:HG13	1.69	0.57
1:A:103:LYS:O	1:A:236:PRO:HB3	2.04	0.57
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.70	0.57
2:B:282:LEU:HB3	2:B:293:ILE:HD11	1.85	0.57
2:D:88:TRP:CD2	2:D:154:LYS:HG2	2.39	0.57
1:A:175:ASN:OD1	1:A:201:LYS:NZ	2.32	0.57
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.40	0.57
2:B:281:LYS:O	2:B:284:ARG:HG2	2.05	0.57
2:D:114:ALA:HB2	2:D:214:LEU:HD22	1.86	0.57
1:C:102:LYS:HG3	1:C:237:ASP:HA	1.85	0.57
1:C:218:ASP:OD2	1:C:222:GLN:NE2	2.37	0.57
1:C:339:TYR:HE2	1:C:341:ILE:HD11	1.69	0.57
3:E:719:G:H2'	3:E:720:G:C8	2.39	0.57
1:C:129:ALA:HB1	1:C:143:ARG:HD2	1.86	0.56
1:C:255:ASN:HB2	1:C:289:LEU:HG	1.86	0.56
1:A:339:TYR:CD2	1:A:375:ILE:HG12	2.40	0.56
1:A:12:LEU:HD22	1:A:83:ARG:O	2.05	0.56
2:B:297:GLU:O	2:B:301:LEU:HG	2.04	0.56
2:D:64:LYS:HG3	2:D:71:TRP:CE3	2.40	0.56
1:A:365:VAL:HG11	1:A:401:TRP:CD1	2.40	0.56
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.40	0.56
1:C:261:VAL:HG13	1:C:276:VAL:HG21	1.86	0.56
1:C:235:HIS:CE1	1:C:238:LYS:HE3	2.40	0.56
1:C:450:THR:OG1	1:C:452:LEU:HB2	2.06	0.56
2:D:206:ARG:NH2	2:D:217:PRO:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:TYR:HB2	1:A:129:ALA:HB3	1.88	0.56
2:B:120:LEU:HD12	2:B:149:LEU:HD23	1.86	0.56
3:E:711:C:H2'	3:E:712:C:H6	1.66	0.56
4:P:817:DG:C6	4:P:818:DC:C4	2.95	0.56
1:C:2:ILE:HG22	1:C:3:SER:H	1.71	0.55
1:C:241:VAL:HG21	1:C:244:ILE:HD11	1.88	0.55
2:D:382:ILE:HG22	2:D:383:TRP:CD2	2.41	0.55
1:A:60:VAL:HG21	1:A:132:ILE:HD12	1.86	0.55
2:B:325:LEU:HD23	2:B:343:GLN:HG2	1.89	0.55
1:C:75:VAL:HG12	1:C:77:PHE:HD1	1.71	0.55
4:F:805:DG:C8	4:F:806:DT:H71	2.41	0.55
1:A:96:HIS:HB3	1:A:382:ILE:HD13	1.89	0.55
1:A:475:GLN:NE2	4:P:809:DC:H5'	2.22	0.55
2:B:28:GLU:CB	2:B:135:ILE:HD11	2.36	0.55
2:B:354:TYR:OH	2:B:378:GLU:OE1	2.24	0.55
1:A:218:ASP:HA	1:A:220:LYS:HG2	1.88	0.55
1:A:229:TRP:CD1	1:A:230:MET:HG3	2.41	0.55
3:T:713:C:H2'	3:T:714:G:H8	1.72	0.55
1:C:197:GLN:O	1:C:200:THR:HB	2.07	0.55
1:A:438:GLU:HB3	1:A:440:PHE:CE1	2.41	0.55
2:B:107:THR:HG23	2:B:232:TYR:HB2	1.88	0.55
4:P:817:DG:C4	4:P:818:DC:C5	2.95	0.55
2:B:195:ILE:HD11	2:B:199:ARG:NE	2.19	0.54
1:C:398:TRP:CZ2	1:C:411:ILE:HG13	2.42	0.54
1:C:502:ALA:O	1:C:506:ILE:HG13	2.07	0.54
1:A:522:ILE:O	1:A:526:ILE:HG13	2.07	0.54
2:B:81:ASN:HB3	2:B:154:LYS:HG3	1.89	0.54
1:C:57:ASN:HA	1:C:130:PHE:HA	1.88	0.54
1:A:120:LEU:HD23	1:A:125:ARG:HA	1.89	0.54
2:B:41:MET:HA	2:B:44:GLU:OE2	2.08	0.54
1:C:513:SER:O	1:C:519:ASN:ND2	2.41	0.54
2:D:276:VAL:HG23	2:D:277:ARG:NH1	2.23	0.54
2:D:368:LEU:O	2:D:372:VAL:HG23	2.08	0.54
1:A:32:LYS:HD3	1:A:135:ILE:HB	1.88	0.54
2:B:17:ASP:O	2:B:83:ARG:HD3	2.07	0.54
2:B:120:LEU:HD13	2:B:150:PRO:HD3	1.90	0.54
1:C:122:GLU:H	1:C:122:GLU:CD	2.11	0.54
1:A:77:PHE:O	1:A:80:LEU:N	2.41	0.54
1:A:135:ILE:HG23	1:A:136:ASN:H	1.72	0.54
2:B:374:LYS:O	2:B:378:GLU:HG3	2.07	0.54
1:A:105:SER:O	1:A:190:GLY:HA2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LYS:HG2	1:A:284:ARG:NH2	2.19	0.54
2:D:85:GLN:HA	2:D:88:TRP:NE1	2.23	0.54
2:D:115:TYR:O	2:D:149:LEU:HB2	2.08	0.54
1:A:382:ILE:HA	2:B:136:ASN:OD1	2.08	0.54
2:D:114:ALA:N	2:D:214:LEU:HD13	2.23	0.53
3:T:715(A):A:H2'	3:T:715(A):A:N3	2.22	0.53
1:A:516:GLU:O	1:A:520:GLN:HG3	2.09	0.53
2:B:399:GLU:HG3	7:B:501:SO4:O3	2.08	0.53
3:T:715(A):A:OP2	3:T:715(A):A:H3'	2.09	0.53
1:A:268:SER:O	1:A:351:THR:OG1	2.27	0.53
1:A:416:PHE:CD1	1:A:417:VAL:N	2.77	0.53
1:C:150:PRO:O	1:C:151:GLN:NE2	2.42	0.53
2:D:357:MET:HB3	2:D:370:GLU:OE1	2.08	0.53
3:T:711:C:HO2'	3:T:712:C:P	2.31	0.53
1:C:48:SER:O	1:C:144:TYR:HB2	2.09	0.53
1:A:24:TRP:CG	1:A:25:PRO:HD2	2.43	0.53
1:A:408:ALA:HB3	2:B:393:ILE:HG13	1.91	0.53
1:C:235:HIS:ND1	1:C:238:LYS:HE3	2.24	0.53
2:B:170:PRO:HB2	2:B:208:HIS:NE2	2.23	0.53
1:A:224:GLU:N	1:A:225:PRO:HD2	2.23	0.53
2:B:162:SER:O	2:B:165:THR:HG22	2.08	0.53
2:B:421:PRO:HB3	2:B:424:LYS:CG	2.33	0.53
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.43	0.52
1:C:296:THR:HB	1:C:299:ALA:HB3	1.89	0.52
1:A:339:TYR:CE2	1:A:375:ILE:HG12	2.44	0.52
1:C:425:LEU:HD22	1:C:509:GLN:OE1	2.10	0.52
2:D:276:VAL:HG23	2:D:277:ARG:HH12	1.73	0.52
3:E:710:G:O2'	3:E:711:C:H5'	2.09	0.52
1:A:257:ILE:O	1:A:260:LEU:HB3	2.09	0.52
1:C:42:GLU:N	1:C:42:GLU:OE1	2.42	0.52
1:C:65:LYS:HB3	1:C:72:ARG:HH12	1.73	0.52
3:T:709:C:H2'	3:T:710:G:H8	1.74	0.52
4:F:803:DC:H2'	4:F:804:DA:H8	1.74	0.52
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.91	0.52
1:A:420:PRO:HA	1:A:421:PRO:C	2.29	0.52
2:D:72:ARG:HD3	2:D:73:LYS:O	2.10	0.52
2:D:115:TYR:CD1	2:D:156:SER:HB3	2.45	0.52
2:D:188:TYR:CE2	2:D:380:ILE:HG21	2.45	0.52
1:A:404:GLU:HA	1:A:404:GLU:OE1	2.10	0.52
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.44	0.52
1:C:474:ASN:ND2	3:E:722:A:O2'	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:VAL:HG13	2:D:87:PHE:CD1	2.45	0.51
2:D:281:LYS:HA	2:D:284:ARG:HG3	1.92	0.51
1:A:259:LYS:HG3	4:P:819:DG:OP1	2.11	0.51
1:C:171:PHE:CG	1:C:205:LEU:HD13	2.46	0.51
2:B:278:GLN:HB3	2:B:299:ALA:HB2	1.92	0.51
1:C:65:LYS:HG2	1:C:66:LYS:O	2.11	0.51
2:D:168:LEU:HD13	2:D:172:LYS:HE3	1.92	0.51
2:D:276:VAL:CG2	2:D:277:ARG:HH12	2.23	0.51
1:A:433:PRO:HD3	1:A:532:TYR:CZ	2.45	0.51
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.91	0.51
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.91	0.51
1:C:536:VAL:HB	1:C:542:ILE:HD12	1.93	0.51
2:D:194:GLU:CD	2:D:195:ILE:H	2.13	0.51
1:A:476:LYS:O	1:A:480:GLN:HB2	2.11	0.51
2:B:167:ILE:HG23	2:B:212:TRP:CD1	2.45	0.51
1:A:433:PRO:HD3	1:A:532:TYR:CE2	2.45	0.51
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.45	0.51
1:A:175:ASN:HB3	1:A:178:ILE:CG1	2.39	0.51
1:A:221:HIS:CG	1:A:224:GLU:HB2	2.46	0.50
2:D:354:TYR:OH	2:D:378:GLU:OE1	2.27	0.50
1:A:305:GLU:O	1:A:309:ILE:HG13	2.11	0.50
2:B:427:TYR:O	2:B:428:GLN:OXT	2.29	0.50
2:B:13:LYS:HG3	2:B:16:MET:CE	2.41	0.50
2:B:164:MET:HE2	2:B:168:LEU:HD11	1.93	0.50
1:C:103:LYS:O	1:C:236:PRO:HB3	2.11	0.50
1:C:107:THR:HG23	1:C:222:GLN:O	2.10	0.50
1:A:417:VAL:HG22	1:A:419:THR:OG1	2.11	0.50
2:B:103:LYS:HE2	2:B:179:VAL:HG23	1.92	0.50
2:D:263:LYS:HA	2:D:425:LEU:HD13	1.94	0.50
3:E:712:C:H3'	3:E:713:C:C6	2.47	0.50
1:A:295:LEU:HD13	1:A:300:GLU:HG2	1.93	0.50
1:C:199:ARG:HH22	1:C:223:LYS:HD3	1.76	0.50
1:C:220:LYS:HE2	1:C:222:GLN:HA	1.93	0.50
1:A:171:PHE:CD2	1:A:205:LEU:HD12	2.47	0.50
1:A:398:TRP:CZ2	1:A:411:ILE:HG13	2.47	0.50
2:B:114:ALA:N	2:B:214:LEU:HD13	2.26	0.50
1:C:441:TYR:CG	1:C:544:GLY:HA3	2.47	0.50
4:P:817:DG:C2	4:P:818:DC:C2	2.99	0.50
1:C:365:VAL:HG11	1:C:401:TRP:CD1	2.46	0.50
1:A:21:VAL:O	1:A:57:ASN:ND2	2.45	0.49
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TRP:HB2	1:A:409:THR:HG23	1.93	0.49
1:A:460:ASN:HA	2:B:286:THR:O	2.12	0.49
4:P:814:DC:H2'	4:P:815:DG:C8	2.48	0.49
1:C:115:TYR:HD2	1:C:151:GLN:HE22	1.59	0.49
1:C:306:ASN:O	1:C:309:ILE:HG12	2.11	0.49
2:D:196:GLY:O	2:D:200:THR:OG1	2.26	0.49
2:D:279:LEU:O	2:D:282:LEU:HB2	2.12	0.49
1:A:115:TYR:CE1	1:A:160:PHE:HD2	2.31	0.49
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.47	0.49
1:C:245:VAL:O	1:C:247:PRO:HD3	2.12	0.49
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.95	0.49
1:A:398:TRP:CE2	1:A:402:TRP:CD1	3.00	0.49
2:B:249:LYS:HB2	2:B:252:TRP:CZ2	2.47	0.49
1:C:379:SER:CB	1:C:387:PRO:HD3	2.42	0.49
2:D:241:VAL:HG12	2:D:350:LYS:HG3	1.94	0.49
1:A:160:PHE:CD1	1:A:160:PHE:C	2.85	0.49
3:T:714:G:O2'	3:T:715:A:H5'	2.12	0.49
1:C:181:TYR:HE2	1:C:183:TYR:HB2	1.74	0.49
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.48	0.49
2:B:78:ARG:HD3	2:B:411:ILE:O	2.13	0.49
1:A:362:THR:OG1	1:A:363:ASN:N	2.45	0.49
1:C:453:GLY:O	1:C:469:LEU:N	2.46	0.49
1:C:457:TYR:C	1:C:457:TYR:CD1	2.85	0.49
2:D:292:VAL:O	2:D:293:ILE:HD13	2.13	0.49
2:B:244:ILE:HD12	2:B:271:TYR:HE1	1.78	0.49
2:B:331:LYS:O	2:B:424:LYS:HE2	2.13	0.49
3:E:720:G:O2'	3:E:721:G:OP1	2.26	0.49
2:B:249:LYS:HG3	2:B:252:TRP:CH2	2.47	0.48
1:C:49:LYS:O	1:C:50:ILE:HD12	2.13	0.48
1:C:457:TYR:HA	1:C:548:VAL:HG21	1.95	0.48
2:D:323:LYS:HB2	2:D:343:GLN:HG2	1.94	0.48
2:D:332:GLN:HG3	2:D:338:THR:HG23	1.95	0.48
1:A:347:LYS:HE3	1:A:347:LYS:HB2	1.65	0.48
2:B:106:VAL:HG22	2:B:190:GLY:HA3	1.95	0.48
1:C:60:VAL:HG21	1:C:132:ILE:HD13	1.94	0.48
1:C:254:VAL:HG21	1:C:286:THR:HG21	1.96	0.48
2:B:118:VAL:HG12	2:B:119:PRO:O	2.12	0.48
2:B:182:GLN:HG3	2:B:187:LEU:HD12	1.95	0.48
1:C:171:PHE:CD2	1:C:205:LEU:HD13	2.47	0.48
4:F:805:DG:C8	4:F:806:DT:C7	2.96	0.48
1:A:47:ILE:HG23	1:A:144:TYR:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:HB3	1:A:151:GLN:HE22	1.78	0.48
1:A:195:ILE:HG22	1:A:199:ARG:NH1	2.23	0.48
2:B:115:TYR:O	2:B:149:LEU:HB2	2.12	0.48
2:B:171:PHE:HE2	2:B:205:LEU:HB2	1.79	0.48
2:B:402:TRP:HZ3	2:B:406:TRP:CD2	2.32	0.48
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.94	0.48
2:B:175:ASN:OD1	2:B:201:LYS:NZ	2.36	0.48
2:D:366:LYS:O	2:D:370:GLU:HG3	2.14	0.48
3:E:714:G:O2'	3:E:715:A:OP1	2.29	0.48
3:E:722:A:H2'	3:E:723:C:O4'	2.14	0.48
2:B:214:LEU:HD12	2:B:215:THR:N	2.29	0.48
1:C:47:ILE:HG22	1:C:48:SER:H	1.78	0.48
1:A:337:TRP:CZ3	1:A:368:LEU:HD13	2.49	0.48
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.42	0.48
1:A:168:LEU:HD21	1:A:187:LEU:HD13	1.96	0.47
1:A:225:PRO:HD3	1:A:227:PHE:CE1	2.49	0.47
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.95	0.47
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.29	0.47
2:B:279:LEU:HA	2:B:279:LEU:HD23	1.65	0.47
1:C:135:ILE:HG12	1:C:136:ASN:OD1	2.14	0.47
1:C:420:PRO:HA	1:C:421:PRO:C	2.34	0.47
1:C:459:THR:HG23	1:C:461:LYS:H	1.78	0.47
2:D:394:GLN:NE2	2:D:418:ASN:OD1	2.48	0.47
1:C:329:ILE:O	1:C:392:PRO:HD3	2.14	0.47
2:D:84:THR:HG21	2:D:153:TRP:CZ2	2.49	0.47
1:A:406:TRP:CH2	2:B:418:ASN:CA	2.94	0.47
2:B:402:TRP:HZ3	2:B:406:TRP:CG	2.32	0.47
2:D:205:LEU:HD12	2:D:205:LEU:HA	1.80	0.47
4:P:817:DG:C5	4:P:818:DC:C5	3.02	0.47
2:D:333:GLY:O	2:D:336:GLN:HB2	2.13	0.47
3:T:715(A):A:H3'	3:T:715(A):A:P	2.54	0.47
1:A:325:LEU:HD11	1:A:383:TRP:CG	2.50	0.47
1:A:356:ARG:HH21	1:A:358:ARG:HG3	1.80	0.47
1:C:77:PHE:HD2	1:C:80:LEU:HB3	1.78	0.47
1:C:326:ILE:O	1:C:341:ILE:HA	2.14	0.47
2:D:84:THR:HG21	2:D:153:TRP:HZ2	1.80	0.47
2:D:115:TYR:HE1	2:D:157:PRO:HA	1.78	0.47
1:A:22:LYS:HG2	1:A:23:GLN:N	2.30	0.47
1:A:59:PRO:O	1:A:76:ASP:HB3	2.15	0.47
1:A:197:GLN:O	1:A:200:THR:HB	2.15	0.47
1:C:148:VAL:O	1:C:150:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:OG1	1:A:130:PHE:HB2	2.15	0.47
1:A:230:MET:HG2	4:P:821:DC:H4'	1.97	0.47
2:D:101:LYS:O	2:D:236:PRO:HB2	2.14	0.47
1:A:164:MET:O	1:A:168:LEU:HD13	2.15	0.46
1:A:171:PHE:CE2	1:A:205:LEU:HD12	2.51	0.46
1:A:296:THR:OG1	1:A:298:GLU:OE1	2.32	0.46
1:A:398:TRP:CH2	1:A:411:ILE:HG13	2.50	0.46
2:B:264:LEU:HD23	2:B:274:ILE:HD13	1.96	0.46
2:B:282:LEU:HD23	2:B:282:LEU:HA	1.74	0.46
1:C:270:ILE:HG23	1:C:271:TYR:N	2.30	0.46
1:C:458:VAL:HG12	2:D:286:THR:HG21	1.97	0.46
2:D:167:ILE:O	2:D:208:HIS:NE2	2.34	0.46
3:E:718:A:H2'	3:E:719:G:C8	2.50	0.46
4:P:804:DA:H2"	4:P:805:DG:H8	1.79	0.46
1:A:350:LYS:HB2	1:A:350:LYS:HE3	1.56	0.46
1:A:376:THR:O	1:A:380:ILE:HG13	2.15	0.46
2:B:142:ILE:HG22	2:B:144:TYR:CE1	2.50	0.46
2:B:317:VAL:HG12	2:B:347:LYS:HB3	1.97	0.46
1:C:95:PRO:HA	2:D:136:ASN:OD1	2.16	0.46
2:B:97:PRO:HD2	2:B:181:TYR:CD1	2.50	0.46
1:C:125:ARG:O	1:C:128:THR:OG1	2.31	0.46
1:A:2:ILE:N	1:A:2:ILE:HD12	2.30	0.46
1:A:398:TRP:CE2	1:A:402:TRP:HD1	2.34	0.46
2:B:22:LYS:HB2	2:B:22:LYS:HE3	1.75	0.46
4:F:814:DC:H2"	4:F:815:DG:C8	2.50	0.46
1:A:90:VAL:HG11	1:A:161:GLN:HB3	1.96	0.46
1:A:326:ILE:HD13	1:A:388:LYS:HB3	1.97	0.46
2:B:154:LYS:HG2	2:B:184:MET:HE1	1.97	0.46
1:C:54:ASN:HB3	1:C:56:TYR:CE2	2.51	0.46
1:C:65:LYS:HD3	1:C:72:ARG:HH22	1.80	0.46
1:C:438:GLU:OE1	1:C:461:LYS:HD2	2.15	0.46
1:C:486:LEU:O	1:C:528:LYS:NZ	2.34	0.46
1:C:100:LEU:O	1:C:318:TYR:HB3	2.15	0.46
1:C:482:ILE:O	1:C:486:LEU:HG	2.16	0.46
2:D:65:LYS:HA	2:D:407:GLN:HG2	1.97	0.46
4:F:805:DG:N7	4:F:806:DT:H73	2.30	0.46
2:B:360:ALA:HA	2:B:367:GLN:OE1	2.16	0.46
1:C:206:ARG:HG2	1:C:216:THR:OG1	2.16	0.46
1:C:417:VAL:HG22	1:C:419:THR:OG1	2.16	0.46
2:D:311:LYS:HZ3	2:D:311:LYS:HG3	1.49	0.46
1:A:220:LYS:O	1:A:220:LYS:HG3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:LYS:HB3	1:C:102:LYS:HE2	1.76	0.46
1:A:479:LEU:HD23	1:A:479:LEU:HA	1.80	0.46
1:C:203:GLU:OE1	1:C:206:ARG:HD2	2.15	0.46
1:C:410:TRP:CE2	2:D:363:ASN:ND2	2.83	0.46
2:D:423:VAL:CG1	2:D:423:VAL:O	2.63	0.46
3:T:711:C:C2	3:T:712:C:C5	3.03	0.46
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.51	0.45
2:B:185:ASP:N	2:B:185:ASP:OD1	2.48	0.45
2:D:312:GLU:HB3	2:D:313:PRO:HD2	1.98	0.45
1:C:84:THR:HG22	1:C:85:GLN:N	2.32	0.45
1:C:274:ILE:HA	1:C:306:ASN:OD1	2.16	0.45
2:B:314:VAL:O	2:B:317:VAL:HG22	2.15	0.45
1:C:254:VAL:HG12	1:C:289:LEU:HD12	1.99	0.45
1:A:406:TRP:CH2	2:B:418:ASN:CB	3.00	0.45
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.51	0.45
1:C:121:ASP:O	1:C:125:ARG:HG3	2.17	0.45
1:C:171:PHE:CE2	1:C:205:LEU:HB2	2.51	0.45
2:D:167:ILE:HD11	2:D:209:LEU:HA	1.98	0.45
4:P:805:DG:N2	4:P:806:DT:C2	2.84	0.45
2:B:101:LYS:O	2:B:236:PRO:HB2	2.16	0.45
2:B:274:ILE:HG12	2:B:306:ASN:OD1	2.16	0.45
2:B:160:PHE:O	2:B:160:PHE:CD1	2.69	0.45
1:A:48:SER:O	1:A:144:TYR:HB2	2.15	0.45
1:A:160:PHE:C	1:A:160:PHE:HD1	2.20	0.45
2:D:118:VAL:HG12	2:D:119:PRO:O	2.17	0.45
1:A:410:TRP:CZ2	1:A:412:PRO:HA	2.51	0.45
1:A:296:THR:HG23	1:A:299:ALA:H	1.82	0.45
1:A:329:ILE:O	1:A:392:PRO:HD3	2.17	0.45
2:D:28:GLU:HA	2:D:135:ILE:HD11	1.99	0.45
1:A:142:ILE:HD12	1:A:142:ILE:HA	1.78	0.44
1:C:149:LEU:HA	1:C:150:PRO:HD3	1.80	0.44
1:A:90:VAL:HG23	1:A:158:ALA:HA	2.00	0.44
2:B:183:TYR:CE1	2:B:184:MET:HG2	2.53	0.44
2:D:66:LYS:HG3	2:D:407:GLN:CD	2.38	0.44
2:D:20:LYS:HE2	2:D:55:PRO:HB2	1.98	0.44
4:P:805:DG:C2	4:P:806:DT:C2	3.06	0.44
2:B:109:LEU:HD22	2:B:216:THR:HG21	2.00	0.44
1:C:139:THR:HB	1:C:140:PRO:CD	2.47	0.44
1:C:465:LYS:HD3	1:C:467:VAL:HG23	1.99	0.44
3:T:716:A:H2'	3:T:717:C:H6	1.81	0.44
2:B:136:ASN:O	2:B:137:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:ILE:O	2:B:293:ILE:HG12	2.18	0.44
1:C:343:GLN:HG3	1:C:349:LEU:HD11	2.00	0.44
2:D:257:ILE:HB	2:D:283:LEU:HD21	2.00	0.44
3:T:715(A):A:O2'	3:T:716:A:O5'	2.36	0.44
1:A:271:TYR:O	1:A:274:ILE:HD13	2.17	0.44
2:B:160:PHE:CD1	2:B:164:MET:HB2	2.53	0.44
1:C:160:PHE:C	1:C:160:PHE:CD1	2.90	0.44
1:C:160:PHE:CE1	1:C:164:MET:HB2	2.53	0.44
1:C:391:LEU:HD12	1:C:414:TRP:CE3	2.53	0.44
1:C:473:THR:HG21	4:F:809:DC:OP1	2.18	0.44
2:B:181:TYR:HE2	2:B:183:TYR:HB2	1.83	0.44
1:C:35:VAL:HB	1:C:135:ILE:HB	1.99	0.44
1:C:459:THR:CG2	1:C:461:LYS:H	2.31	0.44
1:C:128:THR:CB	1:C:146:TYR:HB2	2.48	0.44
1:A:221:HIS:CG	1:A:224:GLU:HG3	2.52	0.43
1:A:254:VAL:HG23	1:A:289:LEU:O	2.18	0.43
2:B:58:THR:CG2	2:B:75:VAL:HG12	2.48	0.43
2:D:60:VAL:HG23	2:D:75:VAL:HG22	2.00	0.43
2:D:207:GLN:HA	2:D:210:LEU:HB3	2.00	0.43
1:C:463:ARG:HE	1:C:463:ARG:HB2	1.52	0.43
2:D:214:LEU:HD12	2:D:215:THR:H	1.83	0.43
1:A:440:PHE:N	1:A:440:PHE:CD1	2.85	0.43
2:D:423:VAL:O	2:D:426:TRP:HB2	2.18	0.43
3:E:720:G:HO2'	3:E:721:G:P	2.39	0.43
1:C:439:THR:HG22	1:C:441:TYR:CE1	2.53	0.43
3:E:709:C:H2'	3:E:710:G:O4'	2.18	0.43
1:A:114:ALA:HB1	1:A:160:PHE:HE2	1.83	0.43
1:A:500:GLN:HG2	2:B:422:LEU:HD12	2.00	0.43
2:B:317:VAL:HG23	2:B:317:VAL:O	2.19	0.43
1:C:220:LYS:CG	1:C:222:GLN:HG2	2.47	0.43
2:D:34:LEU:O	2:D:38:CYS:HB2	2.18	0.43
2:D:266:TRP:O	2:D:269:GLN:HG3	2.19	0.43
1:C:430:GLU:HB2	1:C:532:TYR:HB2	2.00	0.43
2:D:55:PRO:HG2	2:D:56:TYR:CE1	2.53	0.43
1:A:102:LYS:HG2	1:A:236:PRO:O	2.19	0.43
1:A:221:HIS:ND1	1:A:224:GLU:HG3	2.34	0.43
2:B:99:GLY:O	2:B:102:LYS:N	2.42	0.43
2:D:92:LEU:HD21	2:D:161:GLN:OE1	2.18	0.43
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.54	0.43
1:A:326:ILE:O	1:A:341:ILE:HA	2.19	0.43
2:B:317:VAL:HG12	2:B:347:LYS:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ASN:HB3	1:C:56:TYR:HE2	1.84	0.43
2:D:202:ILE:HA	2:D:202:ILE:HD13	1.76	0.43
1:A:179:VAL:HG12	5:A:901:NVP:HCC2	2.00	0.43
2:B:390:LYS:HB3	2:B:417:VAL:HG11	2.00	0.43
2:B:209:LEU:HB3	2:B:214:LEU:HD23	2.01	0.42
1:C:125:ARG:HE	1:C:147:ASN:HA	1.83	0.42
1:C:488:ASP:N	1:C:488:ASP:OD1	2.52	0.42
2:D:23:GLN:HG3	2:D:24:TRP:O	2.19	0.42
2:D:319:TYR:CG	2:D:383:TRP:CD1	3.07	0.42
3:E:717:C:H2'	3:E:718:A:H8	1.84	0.42
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.34	0.42
2:D:21:VAL:HG12	2:D:59:PRO:HG3	2.01	0.42
1:A:22:LYS:HE3	1:A:23:GLN:O	2.19	0.42
1:A:451:LYS:O	1:A:452:LEU:HD12	2.18	0.42
2:B:379:SER:CB	2:B:387:PRO:HD3	2.49	0.42
1:C:398:TRP:CZ3	1:C:411:ILE:HD11	2.55	0.42
2:D:9:PRO:HA	2:D:121:ASP:OD2	2.19	0.42
2:D:31:ILE:HD13	2:D:135:ILE:HG13	2.01	0.42
2:D:46:LYS:HA	2:D:148:VAL:HG13	2.02	0.42
1:A:328:GLU:HG2	1:A:330:GLN:NE2	2.33	0.42
2:B:114:ALA:HB2	2:B:214:LEU:HD13	2.01	0.42
2:D:287:LYS:HZ2	2:D:287:LYS:HG2	1.67	0.42
2:D:339:TYR:CE1	2:D:354:TYR:CE2	3.08	0.42
4:P:817:DG:C6	4:P:818:DC:N4	2.88	0.42
1:A:483:TYR:O	1:A:487:GLN:HG3	2.20	0.42
1:A:517:LEU:HD12	1:A:517:LEU:HA	1.68	0.42
2:B:5:ILE:HD11	2:B:119:PRO:HD2	2.02	0.42
2:B:328:GLU:O	2:B:339:TYR:HA	2.20	0.42
1:C:246:LEU:HA	1:C:247:PRO:HD3	1.84	0.42
3:E:715:A:H5'	3:E:715(A):A:N7	2.34	0.42
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.59	0.42
2:D:30:LYS:HD3	2:D:62:ALA:O	2.19	0.42
2:D:47:ILE:HG22	2:D:145:GLN:O	2.20	0.42
2:B:203:GLU:O	2:B:207:GLN:HG2	2.20	0.42
2:B:358:ARG:HG3	2:B:366:LYS:HD3	2.01	0.42
2:D:34:LEU:HD23	2:D:34:LEU:HA	1.76	0.42
1:A:70:LYS:HE2	1:A:70:LYS:HB3	1.82	0.42
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.85	0.42
1:C:302:GLU:O	1:C:306:ASN:N	2.49	0.42
1:C:339:TYR:CE1	1:C:352:GLY:HA3	2.55	0.42
1:C:457:TYR:HE1	1:C:463:ARG:HG2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:THR:OG1	2:D:146:TYR:HB2	2.20	0.42
1:A:240:THR:HG23	1:A:241:VAL:O	2.20	0.42
1:A:437:ALA:HB1	1:A:493:VAL:HA	2.01	0.42
1:C:85:GLN:C	1:C:154:LYS:HZ1	2.20	0.42
2:D:209:LEU:HB3	2:D:214:LEU:HD23	2.00	0.42
4:P:815:DG:H2'	4:P:816:DG:C8	2.55	0.42
1:A:5:ILE:CG2	1:A:212:TRP:HD1	2.23	0.41
1:A:417:VAL:O	1:A:417:VAL:HG13	2.18	0.41
1:C:58:THR:N	1:C:130:PHE:HB2	2.33	0.41
2:D:242:GLN:O	2:D:242:GLN:HG3	2.20	0.41
3:E:714:G:HO2'	3:E:715:A:P	2.42	0.41
1:A:19:PRO:O	1:A:56:TYR:HA	2.20	0.41
1:A:219:LYS:HA	1:A:219:LYS:HD2	1.91	0.41
1:C:296:THR:HB	1:C:299:ALA:CB	2.49	0.41
1:C:391:LEU:HD12	1:C:414:TRP:CD2	2.54	0.41
1:C:426:TRP:HB3	1:C:526:ILE:HD13	2.03	0.41
3:T:719:G:H2'	3:T:720:G:H8	1.84	0.41
2:B:419:THR:HG22	2:B:420:PRO:O	2.20	0.41
1:C:164:MET:HA	1:C:167:ILE:HD12	2.02	0.41
1:C:167:ILE:O	1:C:170:PRO:HD2	2.21	0.41
1:C:391:LEU:O	1:C:393:ILE:N	2.45	0.41
1:A:265:ASN:OD1	1:A:353:LYS:HD3	2.20	0.41
2:B:33:ALA:O	2:B:37:ILE:HD12	2.20	0.41
2:D:395:LYS:HE3	2:D:399:GLU:OE2	2.20	0.41
1:A:226:PRO:HB3	1:A:235:HIS:CE1	2.55	0.41
1:A:237:ASP:OD2	1:A:238:LYS:HE2	2.21	0.41
1:C:24:TRP:HA	1:C:25:PRO:HD3	1.60	0.41
2:D:372:VAL:HG13	2:D:389:PHE:CE2	2.55	0.41
1:A:32:LYS:CD	1:A:135:ILE:HB	2.51	0.41
2:B:80:LEU:O	2:B:83:ARG:N	2.53	0.41
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.54	0.41
1:C:199:ARG:HA	1:C:202:ILE:HB	2.03	0.41
1:C:253:THR:HG23	1:C:256:ASP:H	1.85	0.41
1:C:433:PRO:HG3	1:C:532:TYR:CE2	2.55	0.41
4:P:807:DC:H2'	4:P:808:DC:C6	2.56	0.41
1:A:43:LYS:HA	1:A:43:LYS:HD3	1.70	0.41
1:A:342:TYR:HA	1:A:349:LEU:HD12	2.01	0.41
2:B:41:MET:HE2	2:B:47:ILE:HD13	2.02	0.41
2:B:103:LYS:HA	2:B:103:LYS:HD3	1.92	0.41
1:C:265:ASN:O	1:C:268:SER:OG	2.35	0.41
1:C:479:LEU:HD11	1:C:501:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:LYS:HD2	2:D:192:ASP:HB3	2.03	0.41
1:A:342:TYR:CD1	1:A:342:TYR:C	2.95	0.41
1:A:483:TYR:CZ	1:A:487:GLN:OE1	2.74	0.41
2:B:104:LYS:HG3	2:B:192:ASP:OD2	2.21	0.41
2:B:279:LEU:HD11	2:B:303:LEU:HB2	2.03	0.41
1:C:41:MET:HG2	1:C:47:ILE:HG13	2.03	0.41
1:C:103:LYS:HA	1:C:103:LYS:HD3	1.84	0.41
2:D:88:TRP:CD1	2:D:154:LYS:HB3	2.56	0.41
2:D:103:LYS:HD2	2:D:191:SER:HA	2.03	0.41
2:D:325:LEU:HB2	2:D:387:PRO:HA	2.03	0.41
2:D:332:GLN:NE2	2:D:427:TYR:HB3	2.36	0.41
4:P:817:DG:C4	4:P:818:DC:C6	3.08	0.41
1:A:241:VAL:HG22	1:A:270:ILE:HG21	2.03	0.41
2:B:149:LEU:HA	2:B:150:PRO:HD3	1.77	0.41
1:C:21:VAL:N	1:C:57:ASN:HB2	2.15	0.41
1:C:30:LYS:HD2	1:C:30:LYS:N	2.36	0.41
2:D:411:ILE:HD13	2:D:411:ILE:HG21	1.81	0.41
2:B:13:LYS:HG3	2:B:16:MET:HE1	2.02	0.40
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.21	0.40
1:C:295:LEU:HG	1:C:296:THR:H	1.86	0.40
1:A:96:HIS:N	2:B:136:ASN:HD21	2.18	0.40
1:A:326:ILE:HB	1:A:342:TYR:CE1	2.56	0.40
1:A:391:LEU:O	1:A:393:ILE:N	2.47	0.40
2:B:78:ARG:CZ	2:B:411:ILE:HG21	2.51	0.40
2:B:85:GLN:HG3	2:B:88:TRP:CZ2	2.56	0.40
2:B:422:LEU:HA	2:B:422:LEU:HD23	1.78	0.40
1:C:430:GLU:HG3	1:C:434:ILE:HD11	2.03	0.40
2:D:235:HIS:N	2:D:236:PRO:HD3	2.36	0.40
2:B:103:LYS:HE2	2:B:179:VAL:CG2	2.51	0.40
2:B:124:PHE:CD1	2:B:127:TYR:HD2	2.39	0.40
2:B:183:TYR:CD1	2:B:184:MET:HG2	2.56	0.40
2:B:399:GLU:HG3	7:B:501:SO4:S	2.62	0.40
1:C:354:TYR:OH	1:C:370:GLU:HB3	2.21	0.40
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.56	0.40
1:C:302:GLU:O	1:C:306:ASN:HB2	2.21	0.40
2:D:276:VAL:CG2	2:D:277:ARG:NH1	2.82	0.40
1:A:128:THR:HB	1:A:146:TYR:HB2	2.03	0.40
1:A:149:LEU:HD13	1:A:156:SER:HA	2.04	0.40
2:B:278:GLN:OE1	2:B:298:GLU:HB2	2.21	0.40
3:E:718:A:H2'	3:E:719:G:H8	1.85	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	553/556 (100%)	525 (95%)	27 (5%)	1 (0%)	47 82
1	C	553/556 (100%)	520 (94%)	33 (6%)	0	100 100
2	B	408/428 (95%)	396 (97%)	12 (3%)	0	100 100
2	D	408/428 (95%)	396 (97%)	12 (3%)	0	100 100
All	All	1922/1968 (98%)	1837 (96%)	84 (4%)	1 (0%)	51 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	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	494/497 (99%)	470 (95%)	24 (5%)	25 61
1	C	494/497 (99%)	474 (96%)	20 (4%)	31 68
2	B	374/390 (96%)	356 (95%)	18 (5%)	25 62
2	D	374/390 (96%)	350 (94%)	24 (6%)	17 51
All	All	1736/1774 (98%)	1650 (95%)	86 (5%)	24 60

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	3	SER
1	A	5	ILE
1	A	84	THR
1	A	101	LYS
1	A	123	ASP
1	A	130	PHE
1	A	131	THR
1	A	132	ILE
1	A	137	ASN
1	A	146	TYR
1	A	160	PHE
1	A	182	GLN
1	A	205	LEU
1	A	221	HIS
1	A	297	GLU
1	A	357	MET
1	A	373	GLN
1	A	399	GLU
1	A	435	VAL
1	A	463	ARG
1	A	469	LEU
1	A	472	THR
1	A	473	THR
2	B	21	VAL
2	B	22	LYS
2	B	32	LYS
2	B	58	THR
2	B	72	ARG
2	B	115	TYR
2	B	120	LEU
2	B	185	ASP
2	B	240	THR
2	B	250	ASP
2	B	268	SER
2	B	280	SER
2	B	293	ILE
2	B	305	GLU
2	B	362	THR
2	B	388	LYS
2	B	403	THR
2	B	410	TRP
1	C	2	ILE

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Mol	Chain	Res	Type
1	C	3	SER
1	C	17	ASP
1	C	35	VAL
1	C	130	PHE
1	C	134	SER
1	C	140	PRO
1	C	144	TYR
1	C	146	TYR
1	C	182	GLN
1	C	215	THR
1	C	276	VAL
1	C	314	VAL
1	C	357	MET
1	C	358	ARG
1	C	390	LYS
1	C	452	LEU
1	C	459	THR
1	C	472	THR
1	C	497	THR
2	D	47	ILE
2	D	101	LYS
2	D	109	LEU
2	D	123	ASP
2	D	194	GLU
2	D	234	LEU
2	D	248	GLU
2	D	249	LYS
2	D	276	VAL
2	D	277	ARG
2	D	287	LYS
2	D	295	LEU
2	D	296	THR
2	D	317	VAL
2	D	318	TYR
2	D	343	GLN
2	D	385	LYS
2	D	390	LYS
2	D	394	GLN
2	D	395	LYS
2	D	397	THR
2	D	407	GLN
2	D	410	TRP

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Mol	Chain	Res	Type
2	D	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	340	GLN
1	A	373	GLN
2	B	151	GLN
2	B	428	GLN
1	C	151	GLN
1	C	161	GLN
1	C	182	GLN
1	C	474	ASN
1	C	487	GLN
1	C	507	GLN
2	D	278	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	19/27 (70%)	8 (42%)	6 (31%)
3	T	20/27 (74%)	7 (35%)	4 (20%)
All	All	39/54 (72%)	15 (38%)	10 (25%)

All (15) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	712	C
3	T	715(A)	A
3	T	716	A
3	T	720	G
3	T	721	G
3	T	723	C
3	T	725	G
3	E	712	C
3	E	715	A
3	E	715(A)	A
3	E	716	A
3	E	720	G
3	E	721	G

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Mol	Chain	Res	Type
3	E	722	A
3	E	724	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	T	711	C
3	T	715(A)	A
3	T	719	G
3	T	720	G
3	E	711	C
3	E	714	G
3	E	715(A)	A
3	E	719	G
3	E	720	G
3	E	722	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
7	SO4	B	501	-	4,4,4	0.35	0	6,6,6	0.77	0
5	NVP	A	901	-	23,23,23	1.73	6 (26%)	34,34,34	3.74	17 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NVP	C	901	-	23,23,23	1.62	8 (34%)	34,34,34	4.69	17 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NVP	A	901	-	-	1/4/6/6	0/4/4/4
5	NVP	C	901	-	-	0/4/6/6	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	NVP	C2-N3	3.80	1.41	1.34
5	C	901	NVP	C15-N14	3.04	1.40	1.34
5	A	901	NVP	C4-N3	2.96	1.40	1.34
5	A	901	NVP	C15-N14	2.91	1.40	1.34
5	A	901	NVP	C15-N1	-2.87	1.40	1.42
5	C	901	NVP	C2-N1	-2.80	1.40	1.42
5	C	901	NVP	C2-N3	2.65	1.39	1.34
5	A	901	NVP	C10-C15	-2.57	1.37	1.40
5	A	901	NVP	C13-N14	2.53	1.39	1.34
5	C	901	NVP	C4-N3	2.50	1.39	1.34
5	C	901	NVP	C15-N1	-2.50	1.40	1.42
5	C	901	NVP	C13-N14	2.27	1.39	1.34
5	C	901	NVP	C10-C15	-2.18	1.37	1.40
5	C	901	NVP	C9-N8	-2.02	1.33	1.35

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	901	NVP	C7-C2-N1	18.07	127.07	120.09
5	A	901	NVP	C7-C2-N1	13.71	125.38	120.09
5	A	901	NVP	C7-N8-C9	-8.96	120.80	128.40
5	C	901	NVP	OE-C9-N8	-7.18	114.11	120.51
5	C	901	NVP	C6-C7-N8	-6.82	113.55	119.04
5	C	901	NVP	N3-C2-N1	-6.79	111.50	116.62
5	C	901	NVP	C7-N8-C9	-6.58	122.82	128.40
5	C	901	NVP	C10-C9-N8	6.40	125.83	120.16
5	C	901	NVP	C10-C15-N1	5.89	125.38	120.72
5	A	901	NVP	C10-C15-N1	5.26	124.88	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	901	NVP	C15-C10-C9	5.08	127.64	123.85
5	C	901	NVP	CC-CA-N1	-5.02	113.04	116.10
5	C	901	NVP	C2-C7-N8	4.99	125.88	121.69
5	A	901	NVP	OE-C9-N8	-4.88	116.16	120.51
5	A	901	NVP	C10-C9-N8	4.72	124.35	120.16
5	A	901	NVP	C15-C10-C9	4.25	127.02	123.85
5	C	901	NVP	N14-C15-N1	-4.16	113.48	116.62
5	A	901	NVP	N14-C15-N1	-3.77	113.77	116.62
5	C	901	NVP	C15-N1-C2	3.61	118.71	115.06
5	A	901	NVP	C15-N1-CA	3.48	119.15	116.29
5	A	901	NVP	C2-N1-CA	3.29	119.00	116.29
5	A	901	NVP	C11-C10-C15	3.17	120.47	117.34
5	A	901	NVP	C6-C7-N8	-3.07	116.57	119.04
5	C	901	NVP	C15-N1-CA	3.05	118.80	116.29
5	A	901	NVP	N3-C2-N1	-2.85	114.47	116.62
5	A	901	NVP	C6-C7-C2	2.82	121.35	118.95
5	C	901	NVP	C11-C10-C15	2.64	119.95	117.34
5	A	901	NVP	C12-C13-N14	-2.63	119.12	123.43
5	C	901	NVP	C12-C13-N14	-2.61	119.16	123.43
5	C	901	NVP	C11-C10-C9	-2.58	112.40	116.86
5	A	901	NVP	C11-C10-C9	-2.51	112.52	116.86
5	A	901	NVP	CD-C6-C7	2.49	124.64	121.44
5	C	901	NVP	C5-C4-N3	-2.28	121.13	123.96
5	A	901	NVP	C15-N1-C2	2.04	117.13	115.06

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	901	NVP	CC-CA-N1-C15

There are no ring outliers.

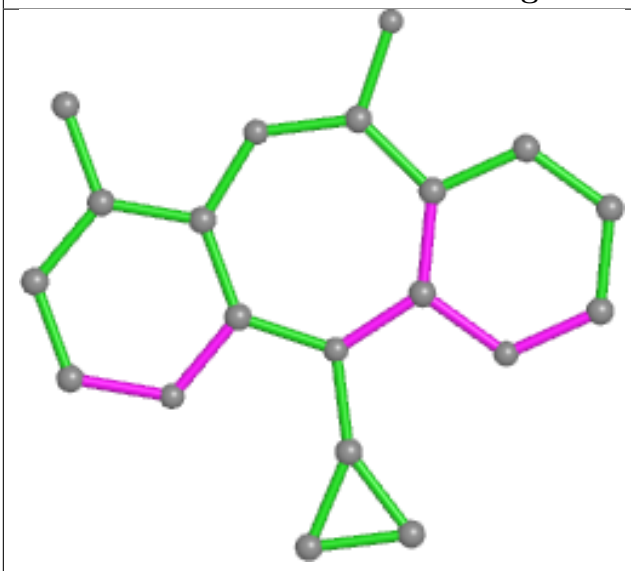
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	501	SO4	2	0
5	A	901	NVP	1	0

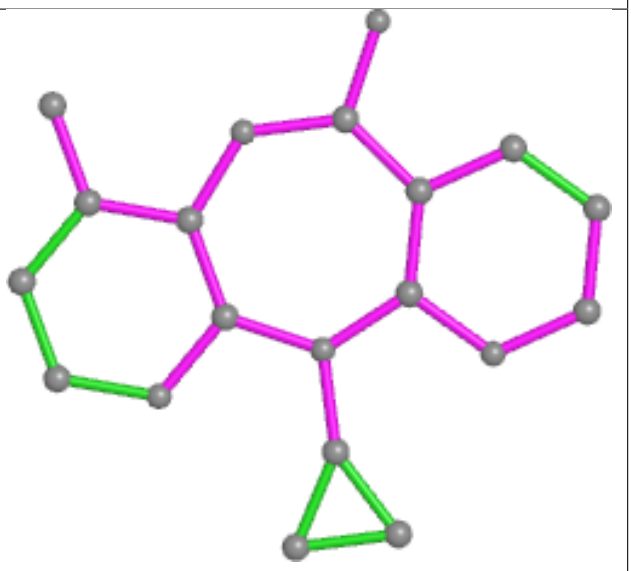
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

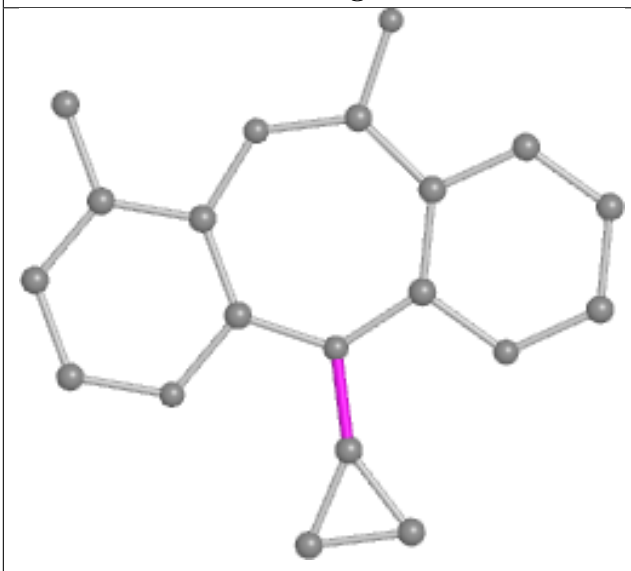
Ligand NVP A 901



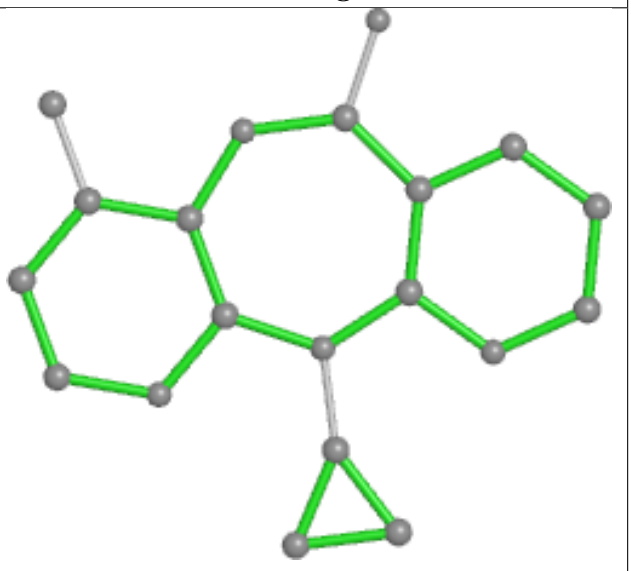
Bond lengths



Bond angles

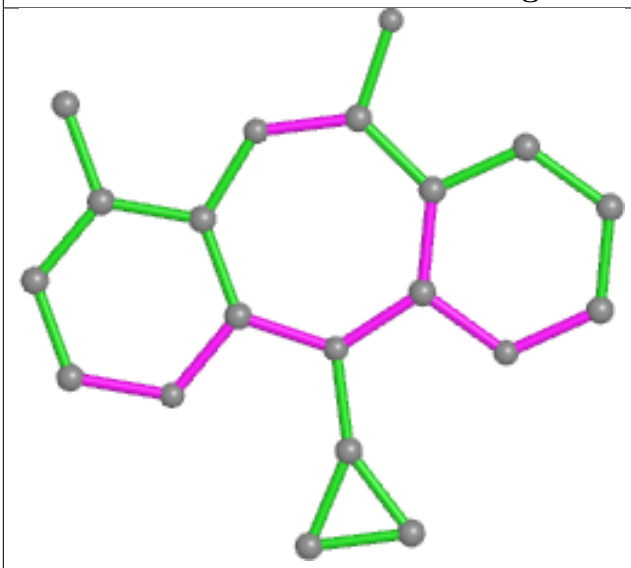


Torsions

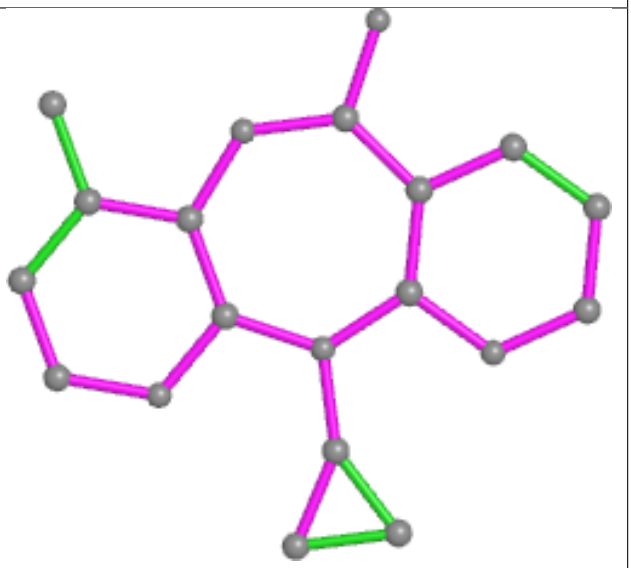


Rings

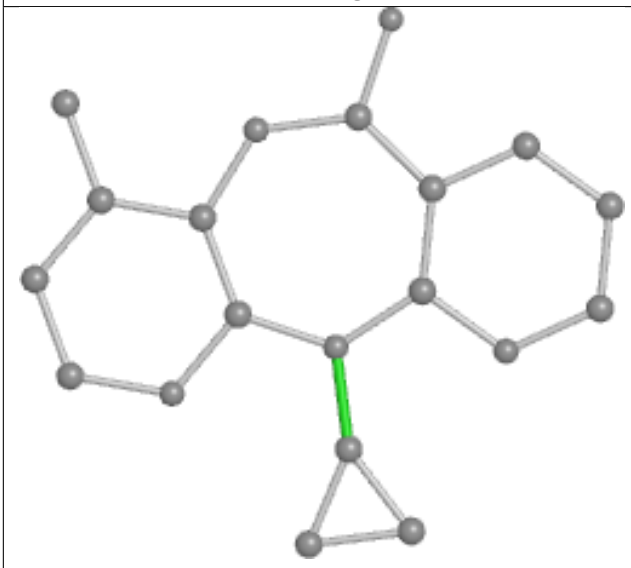
Ligand NVP C 901



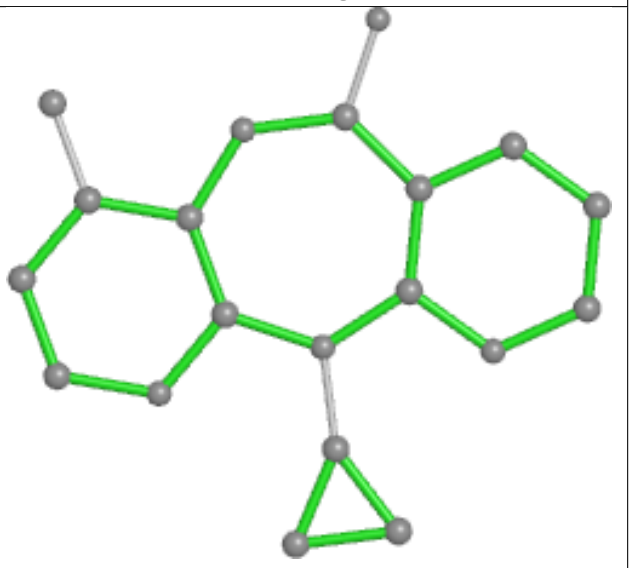
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	555/556 (99%)	0.35	58 (10%) 6 2	17, 78, 180, 206	0
1	C	555/556 (99%)	0.47	64 (11%) 4 1	14, 83, 188, 209	0
2	B	412/428 (96%)	-0.16	10 (2%) 59 30	22, 60, 106, 131	0
2	D	412/428 (96%)	-0.09	8 (1%) 66 37	21, 64, 116, 141	0
3	E	20/27 (74%)	1.42	5 (25%) 0 0	126, 143, 174, 194	0
3	T	21/27 (77%)	0.68	4 (19%) 1 0	81, 105, 147, 174	0
4	F	19/21 (90%)	1.30	5 (26%) 0 0	83, 126, 184, 188	0
4	P	19/21 (90%)	0.29	2 (10%) 6 2	60, 105, 147, 159	0
All	All	2013/2064 (97%)	0.21	156 (7%) 13 4	14, 71, 167, 209	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	62	ALA	15.4
1	A	133	PRO	14.6
1	A	62	ALA	12.9
1	C	33	ALA	11.2
1	C	59	PRO	9.9
1	C	31	ILE	9.8
1	A	65	LYS	8.5
1	A	60	VAL	8.3
1	C	61	PHE	7.4
1	A	137	ASN	7.3
1	C	136	ASN	6.8
1	C	69	THR	6.8
1	A	27	THR	6.5
1	A	26	LEU	6.3
2	D	215	THR	6.2
1	C	140	PRO	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	34	LEU	6.2
1	C	132	ILE	5.9
1	A	222	GLN	5.8
1	A	29	GLU	5.8
1	C	223	LYS	5.8
3	T	725	G	5.8
1	C	131	THR	5.7
2	D	214	LEU	5.7
1	C	68	SER	5.7
1	A	59	PRO	5.6
1	A	132	ILE	5.6
1	C	32	LYS	5.6
1	A	31	ILE	5.5
1	C	26	LEU	5.5
2	B	214	LEU	5.4
1	C	137	ASN	5.4
1	A	61	PHE	5.2
1	A	19	PRO	5.1
1	C	71	TRP	5.0
1	A	223	LYS	5.0
1	A	63	ILE	5.0
1	C	222	GLN	4.9
1	C	27	THR	4.9
1	A	25	PRO	4.8
1	A	67	ASP	4.7
1	C	129	ALA	4.7
1	A	34	LEU	4.6
1	A	21	VAL	4.5
1	A	66	LYS	4.5
1	C	19	PRO	4.4
1	C	139	THR	4.4
1	A	75	VAL	4.4
3	E	724	U	4.3
1	A	23	GLN	4.3
1	C	130	PHE	4.3
1	C	74	LEU	4.3
1	A	130	PHE	4.3
1	C	133	PRO	4.2
4	F	804	DA	4.2
1	A	56	TYR	4.2
1	C	25	PRO	4.2
1	A	138	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	24	TRP	4.1
1	C	58	THR	4.1
1	A	22	LYS	4.0
1	A	33	ALA	3.9
1	C	64	LYS	3.9
1	A	74	LEU	3.9
1	A	193	LEU	3.8
1	A	140	PRO	3.8
1	A	131	THR	3.8
1	A	64	LYS	3.7
1	C	146	TYR	3.7
1	C	30	LYS	3.7
1	C	21	VAL	3.7
1	C	134	SER	3.5
3	E	715	A	3.4
1	C	28	GLU	3.4
3	E	721	G	3.3
1	A	28	GLU	3.3
1	C	84	THR	3.3
1	A	144	TYR	3.3
4	F	803	DC	3.3
1	C	18	GLY	3.2
1	A	139	THR	3.2
1	A	20	LYS	3.2
2	D	93	GLY	3.2
1	A	72	ARG	3.1
1	C	141	GLY	3.1
1	C	138	GLU	3.1
3	E	723	C	3.1
1	A	151	GLN	3.1
1	C	72	ARG	3.1
1	C	20	LYS	3.0
1	C	144	TYR	3.0
1	A	198	HIS	2.9
1	A	50	ILE	2.9
1	A	77	PHE	2.9
1	C	220	LYS	2.9
1	A	136	ASN	2.9
2	B	215	THR	2.8
1	C	63	ILE	2.8
1	C	219	LYS	2.8
4	F	816	DG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	255	ASN	2.7
1	C	70	LYS	2.7
2	B	200	THR	2.7
2	B	212	TRP	2.6
1	A	141	GLY	2.6
2	B	86	ASP	2.6
1	A	142	ILE	2.6
2	D	209	LEU	2.6
1	C	224	GLU	2.6
1	C	142	ILE	2.6
2	B	197	GLN	2.6
1	C	255	ASN	2.6
1	A	32	LYS	2.5
2	D	231	GLY	2.5
1	A	57	ASN	2.5
4	F	805	DG	2.5
1	A	134	SER	2.5
1	C	17	ASP	2.5
1	C	221	HIS	2.5
1	A	55	PRO	2.4
2	D	360	ALA	2.4
1	A	195	ILE	2.4
2	B	89	GLU	2.4
2	B	209	LEU	2.4
1	A	146	TYR	2.4
1	C	73	LYS	2.4
1	C	283	LEU	2.4
2	B	213	GLY	2.3
2	D	124	PHE	2.3
1	C	23	GLN	2.3
1	C	60	VAL	2.3
3	T	724	U	2.3
2	D	232	TYR	2.3
1	A	220	LYS	2.3
1	C	39	THR	2.3
3	T	715(A)	A	2.3
1	C	193	LEU	2.2
4	F	815	DG	2.2
1	A	294	PRO	2.2
3	T	714	G	2.2
1	C	53	GLU	2.2
2	B	4	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	76	ASP	2.1
1	C	67	ASP	2.1
4	P	803	DC	2.1
1	C	16	MET	2.1
3	E	722	A	2.1
1	C	259	LYS	2.1
1	A	286	THR	2.1
1	A	143	ARG	2.1
1	A	287	LYS	2.1
1	C	65	LYS	2.1
1	C	247	PRO	2.1
1	C	36	GLU	2.0
4	P	805	DG	2.0
1	C	83	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

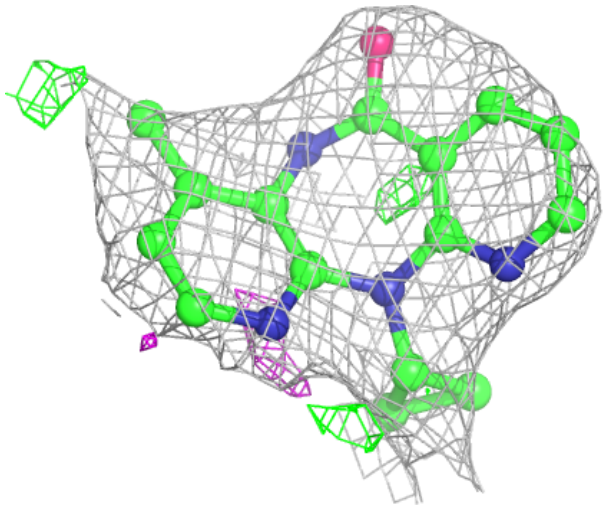
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

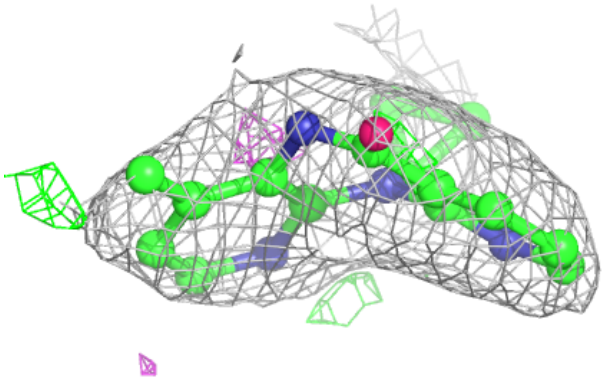
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NVP	A	901	20/20	0.93	0.27	59,68,72,79	0
6	CA	C	902	1/1	0.95	0.08	73,73,73,73	0
7	SO4	B	501	5/5	0.95	0.16	42,48,54,71	0
5	NVP	C	901	20/20	0.96	0.26	61,66,74,76	0
6	CA	A	902	1/1	0.96	0.08	73,73,73,73	0

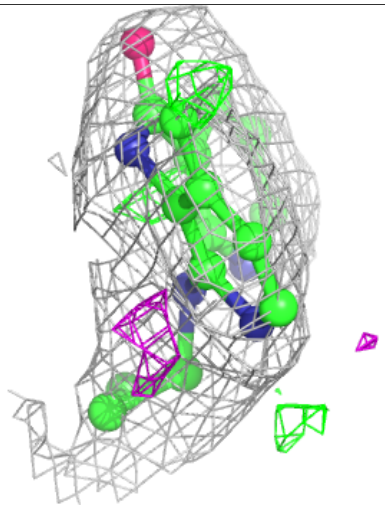
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NVP A 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

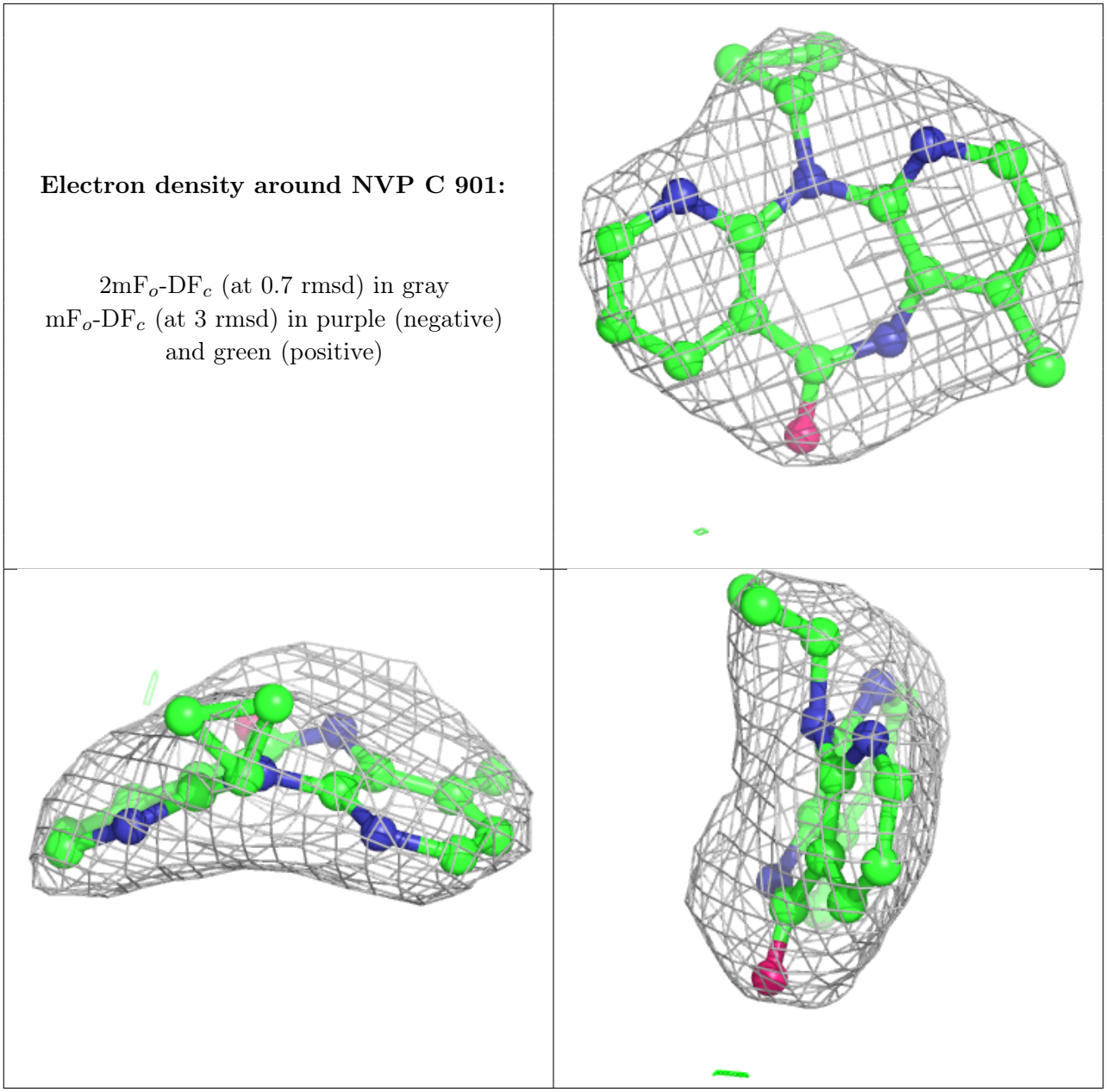






Electron density around NVP C 901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.