



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:12 PM UTC

PDB ID : 4Q0B / pdb_00004q0b
Title : Crystal structure of HIV-1 reverse transcriptase in complex with gap-RNA/DNA and Nevirapine
Authors : Das, K.; Martinez, S.E.; Arnold, E.
Deposited on : 2014-04-01
Resolution : 3.30 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

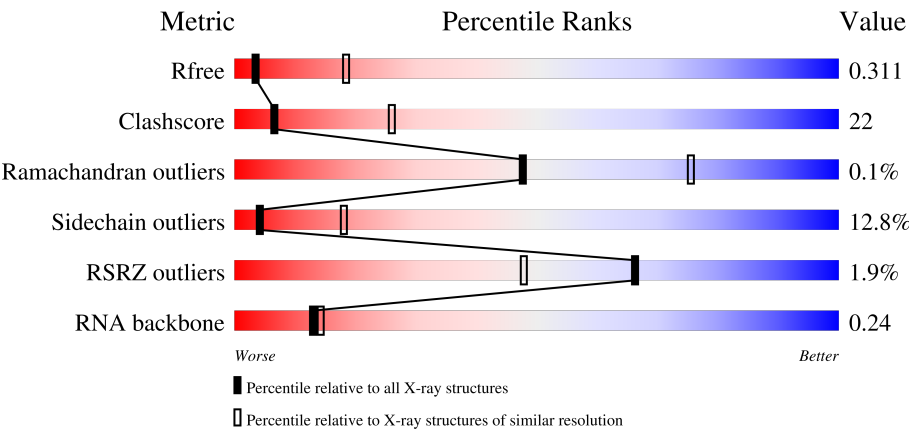
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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	556	
1	C	556	
2	B	428	
2	D	428	

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Mol	Chain	Length	Quality of chain
3	E	14	21%14%29%36%
3	T	14	7%29%29%36%
4	e	12	25%17%25%8%25%
4	t	12	25%17%42%17%
5	F	21	38%43%10%10%
5	P	21	48%38%5%10%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17428 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
			4512	2920	751	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*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	9	Total	C	N	O	P	0	0	0
			192	85	35	63	9			
3	E	9	Total	C	N	O	P	0	0	0
			192	85	35	63	9			

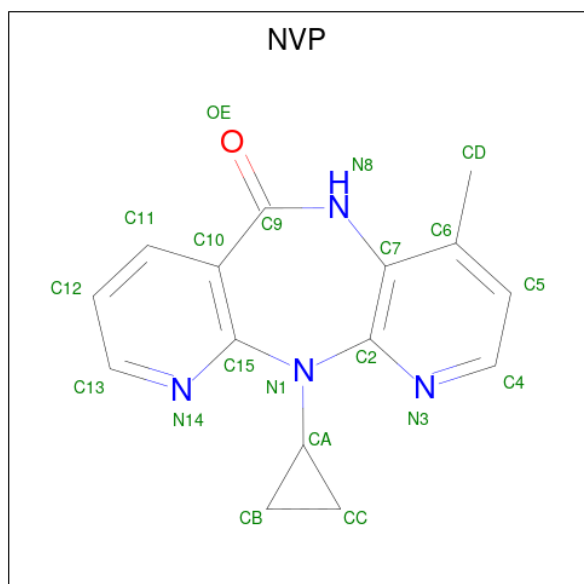
- Molecule 4 is a RNA chain called 5'-R(P*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	t	10	Total	C	N	O	P	0	0	0
			219	97	43	69	10			
4	e	9	Total	C	N	O	P	0	0	0
			196	87	38	62	9			

- Molecule 5 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
5	P	19	Total	C	N	O	P	0	0	0
			382	182	67	115	18			
5	F	19	Total	C	N	O	P	0	0	0
			382	182	67	115	18			

- Molecule 6 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (CCD ID: NVP) (formula: C₁₅H₁₄N₄O).

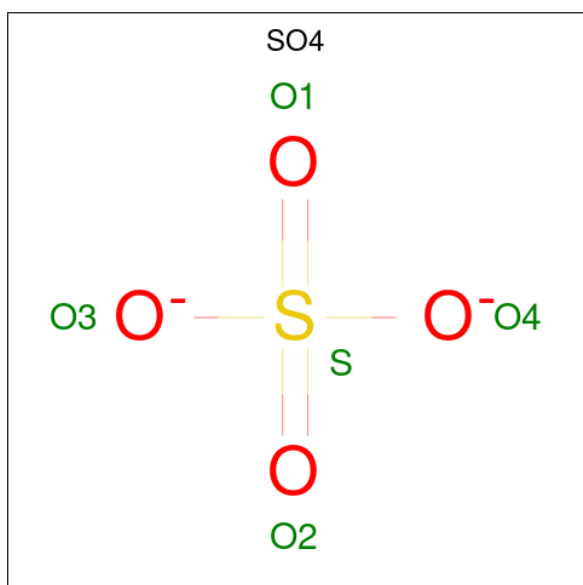


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			20	15	4	1		
6	C	1	Total	C	N	O	0	0
			20	15	4	1		

- Molecule 7 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Mn	0	0
			1	1		
7	C	1	Total	Mn	0	0
			1	1		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

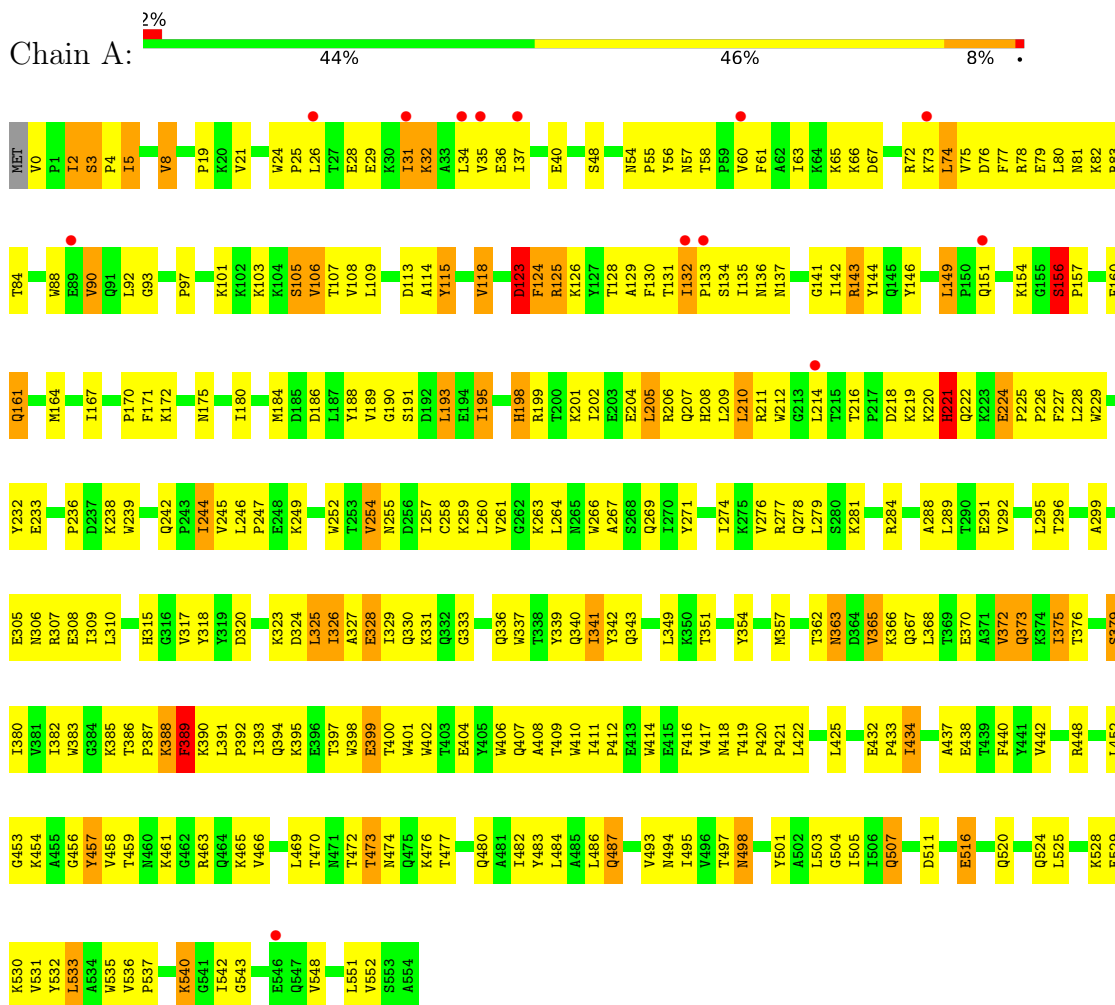


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	e	1	Total	O	S	0	0
			5	4	1		

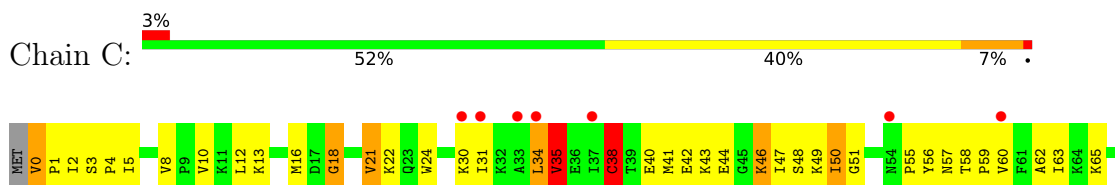
3 Residue-property plots

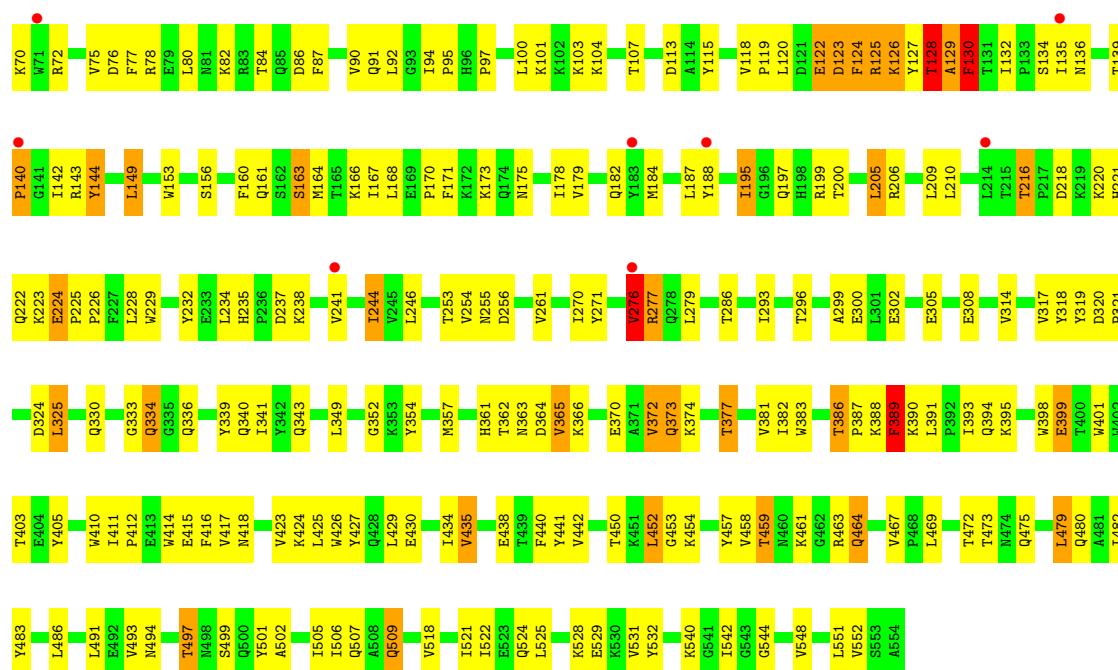
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HIV-1 reverse transcriptase, p66 subunit

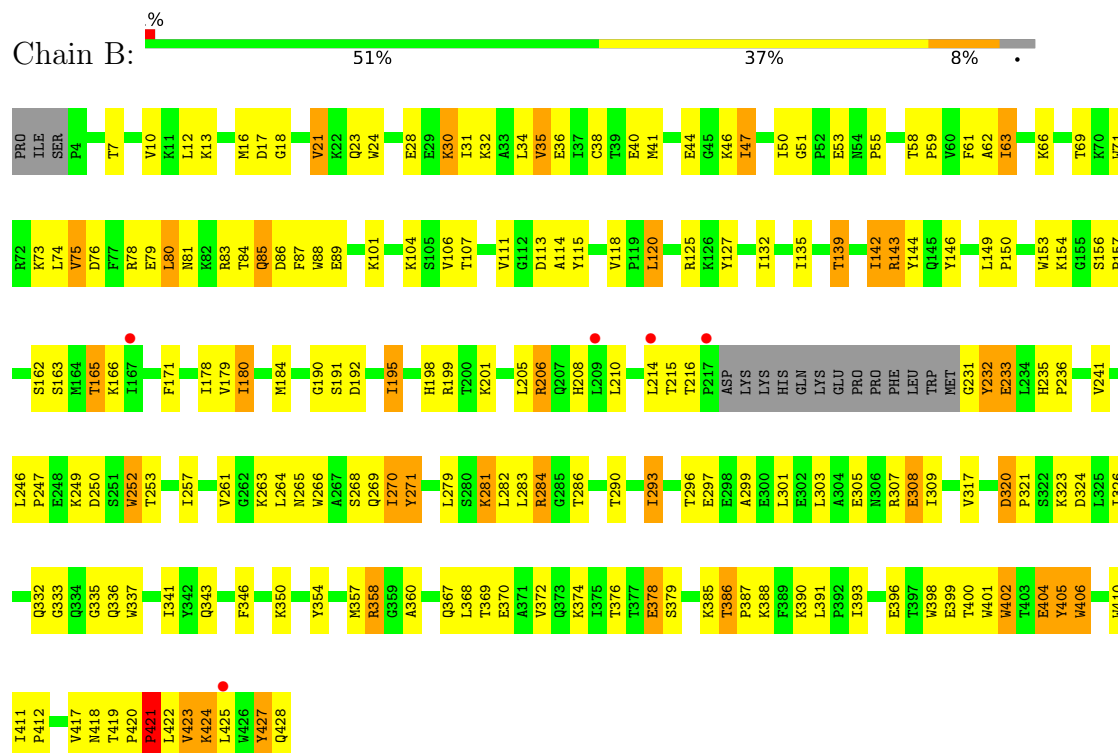


- Molecule 1: HIV-1 reverse transcriptase, p66 subunit

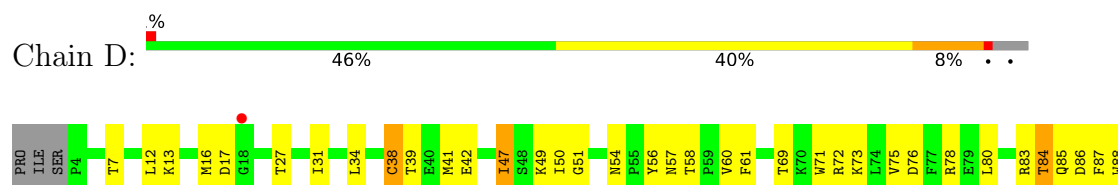


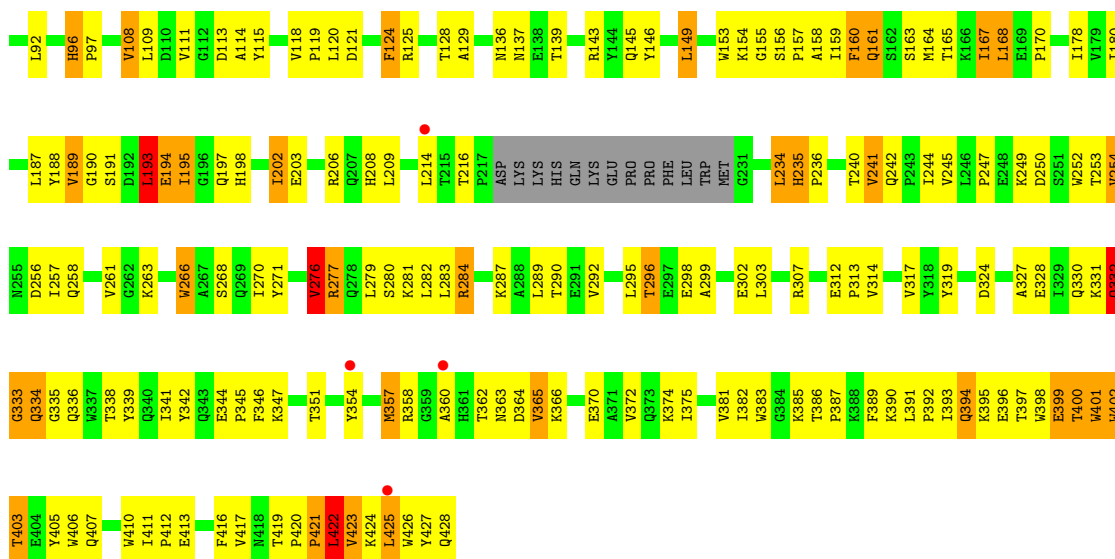


• Molecule 2: HIV-1 reverse transcriptase, p51 subunit



• Molecule 2: HIV-1 reverse transcriptase, p51 subunit





• Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*G)-3'

Chain T: 7% 29% 29% 36%



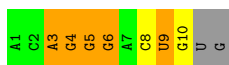
• Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*G)-3'

Chain E: 21% 14% 29% 36%



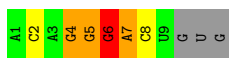
• Molecule 4: 5'-R(P*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'

Chain t: 25% 17% 42% 17%



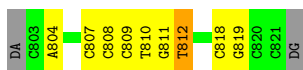
• Molecule 4: 5'-R(P*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'

Chain e: 25% 17% 25% 8% 25%



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

Chain P: 48% 38% 5% 10%



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

Chain F:  38% 43% 10% 10%

DA	C803	A804	G805	T806	C807	C808	C809	T810	G811	T812	T813	C814	C821	DG
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.72Å 131.05Å 141.63Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	46.39 – 3.30 46.39 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.39-3.30) 98.4 (46.39-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.235 , 0.317 0.236 , 0.311	Depositor DCC
R_{free} test set	1420 reflections (2.89%)	wwPDB-VP
Wilson B-factor (Å ²)	77.7	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17428	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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

5.1 Standard geometry

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

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	0.81	2/4630 (0.0%)	1.29	49/6290 (0.8%)
1	C	0.83	2/4624 (0.0%)	1.31	57/6283 (0.9%)
2	B	0.82	1/3497 (0.0%)	1.29	38/4751 (0.8%)
2	D	0.86	2/3497 (0.1%)	1.37	51/4751 (1.1%)
3	E	0.24	0/213	0.55	0/330
3	T	0.24	0/213	0.51	0/330
4	e	0.40	0/219	0.98	3/338 (0.9%)
4	t	0.29	0/245	0.66	0/379
5	F	0.50	0/426	0.68	2/655 (0.3%)
5	P	0.45	0/426	0.61	1/655 (0.2%)
All	All	0.80	7/17990 (0.0%)	1.26	201/24762 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	1
2	B	0	1
2	D	0	2
All	All	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	389	PHE	CA-C	-8.63	1.42	1.52
1	A	389	PHE	CA-C	-7.50	1.43	1.52
2	D	270	ILE	CA-CB	-7.23	1.48	1.55
1	C	440	PHE	CA-C	-6.90	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	THR	C-O	5.72	1.30	1.24
1	A	156	SER	N-CA	-5.67	1.42	1.46
2	D	400	THR	C-O	5.35	1.30	1.24

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	THR	CA-C-N	-14.94	101.16	119.84
2	D	139	THR	C-N-CA	-14.94	101.16	119.84
2	B	402	TRP	N-CA-C	-14.50	95.56	111.36
1	C	386	THR	CA-C-N	14.47	134.35	120.03
1	C	386	THR	C-N-CA	14.47	134.35	120.03
1	A	386	THR	CA-C-N	13.70	133.59	120.03
1	A	386	THR	C-N-CA	13.70	133.59	120.03
1	C	0	VAL	CA-C-N	12.84	133.23	120.52
1	C	0	VAL	C-N-CA	12.84	133.23	120.52
1	C	128	THR	N-CA-C	11.20	127.28	113.17
1	C	125	ARG	N-CA-C	-11.00	99.29	111.28
1	A	156	SER	N-CA-C	-10.81	97.47	112.17
2	D	402	TRP	N-CA-C	-10.59	99.74	111.07
1	A	149	LEU	CA-C-N	10.05	129.81	119.76
1	A	149	LEU	C-N-CA	10.05	129.81	119.76
2	B	139	THR	CA-C-N	-9.54	110.77	120.98
2	B	139	THR	C-N-CA	-9.54	110.77	120.98
1	C	34	LEU	N-CA-C	9.42	123.28	111.69
2	B	386	THR	CA-C-N	9.42	129.85	120.52
2	B	386	THR	C-N-CA	9.42	129.85	120.52
2	D	335	GLY	CA-C-N	-9.41	108.63	122.65
2	D	335	GLY	C-N-CA	-9.41	108.63	122.65
1	C	124	PHE	N-CA-C	-9.19	101.83	113.23
1	C	388	LYS	CA-C-N	-9.06	109.80	122.93
1	C	388	LYS	C-N-CA	-9.06	109.80	122.93
2	D	235	HIS	CA-C-N	8.89	130.96	119.84
2	D	235	HIS	C-N-CA	8.89	130.96	119.84
2	D	51	GLY	CA-C-N	8.63	128.28	119.82
2	D	51	GLY	C-N-CA	8.63	128.28	119.82
1	A	29	GLU	N-CA-C	8.59	120.56	111.03
2	B	400	THR	CA-C-N	-8.57	107.44	122.26
2	B	400	THR	C-N-CA	-8.57	107.44	122.26
2	D	54	ASN	CA-C-N	8.54	128.76	119.87
2	D	54	ASN	C-N-CA	8.54	128.76	119.87
2	B	284	ARG	N-CA-C	8.49	121.30	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	334	GLN	N-CA-C	-8.46	99.68	111.52
1	A	453	GLY	N-CA-C	8.43	124.37	110.55
1	C	118	VAL	CA-C-N	8.36	128.86	119.83
1	C	118	VAL	C-N-CA	8.36	128.86	119.83
1	A	141	GLY	N-CA-C	8.33	122.21	110.38
2	D	422	LEU	N-CA-C	-8.26	102.77	113.17
1	C	129	ALA	N-CA-C	8.04	121.29	110.35
1	C	40	GLU	N-CA-C	-7.85	101.83	111.40
1	A	8	VAL	CA-C-N	7.77	128.25	119.93
1	A	8	VAL	C-N-CA	7.77	128.25	119.93
1	C	43	LYS	N-CA-C	7.74	120.46	111.02
1	C	24	TRP	CA-C-N	7.55	129.28	119.84
1	C	24	TRP	C-N-CA	7.55	129.28	119.84
5	F	809	DC	C5'-C4'-O4'	7.51	120.67	109.40
2	D	332	GLN	O-C-N	-7.48	112.99	122.34
1	A	320	ASP	CA-C-N	7.43	129.13	119.84
1	A	320	ASP	C-N-CA	7.43	129.13	119.84
2	B	24	TRP	CA-C-N	7.43	127.48	119.90
2	B	24	TRP	C-N-CA	7.43	127.48	119.90
1	A	0	VAL	CA-C-N	7.36	129.04	119.84
1	A	0	VAL	C-N-CA	7.36	129.04	119.84
1	A	389	PHE	CA-C-N	-7.30	112.74	123.11
1	A	389	PHE	C-N-CA	-7.30	112.74	123.11
1	C	224	GLU	CA-C-N	7.23	127.82	120.38
1	C	224	GLU	C-N-CA	7.23	127.82	120.38
2	B	423	VAL	N-CA-C	-7.21	105.69	112.83
2	D	400	THR	CA-C-N	-7.20	108.98	121.66
2	D	400	THR	C-N-CA	-7.20	108.98	121.66
2	D	160	PHE	N-CA-C	-7.18	104.26	113.16
1	C	389	PHE	N-CA-C	-7.18	98.04	109.59
2	D	161	GLN	N-CA-C	-7.18	103.54	111.36
2	D	276	VAL	N-CA-C	7.17	119.78	112.90
2	D	159	ILE	CA-C-N	-7.17	109.40	122.38
2	D	159	ILE	C-N-CA	-7.17	109.40	122.38
1	C	18	GLY	CA-C-N	7.15	128.77	119.84
1	C	18	GLY	C-N-CA	7.15	128.77	119.84
2	D	386	THR	CA-C-N	7.12	127.29	120.31
2	D	386	THR	C-N-CA	7.12	127.29	120.31
1	A	432	GLU	CA-C-N	7.08	127.11	119.89
1	A	432	GLU	C-N-CA	7.08	127.11	119.89
5	P	812	DT	C5'-C4'-O4'	-7.06	98.81	109.40
2	B	418	ASN	N-CA-C	7.01	120.29	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	206	ARG	N-CA-C	-6.98	103.67	111.28
1	C	320	ASP	CA-C-N	6.97	127.55	119.47
1	C	320	ASP	C-N-CA	6.97	127.55	119.47
2	B	404	GLU	N-CA-C	6.97	121.01	112.23
1	A	125	ARG	N-CA-C	-6.88	103.01	111.33
2	B	271	TYR	CA-C-N	6.87	126.57	119.56
2	B	271	TYR	C-N-CA	6.87	126.57	119.56
1	C	51	GLY	CA-C-N	6.79	126.93	119.87
1	C	51	GLY	C-N-CA	6.79	126.93	119.87
1	A	434	ILE	N-CA-C	6.74	117.56	107.51
1	C	467	VAL	N-CA-C	6.68	115.35	107.73
1	C	35	VAL	N-CA-C	6.68	117.37	110.36
2	B	406	TRP	N-CA-C	6.62	119.38	109.25
2	D	96	HIS	N-CA-C	6.61	119.21	109.50
1	C	389	PHE	CA-C-O	-6.60	113.71	120.71
1	A	457	TYR	N-CA-C	6.58	118.21	108.60
1	C	382	ILE	N-CA-C	6.58	117.20	110.82
2	D	381	VAL	CA-C-N	-6.56	116.54	122.97
2	D	381	VAL	C-N-CA	-6.56	116.54	122.97
1	C	46	LYS	N-CA-C	-6.56	105.27	113.20
1	C	277	ARG	N-CA-C	6.55	118.08	111.07
1	C	62	ALA	N-CA-C	6.55	118.89	109.14
2	D	69	THR	N-CA-C	-6.54	105.05	113.16
1	A	363	ASN	N-CA-C	6.50	117.71	108.74
1	C	123	ASP	CA-C-N	-6.46	110.29	121.66
1	C	123	ASP	C-N-CA	-6.46	110.29	121.66
1	A	40	GLU	N-CA-C	-6.44	104.18	111.07
2	B	85	GLN	N-CA-C	6.40	118.79	111.11
2	B	320	ASP	CA-C-N	6.39	126.88	119.47
2	B	320	ASP	C-N-CA	6.39	126.88	119.47
1	C	38	CYS	CA-C-N	-6.38	110.84	122.38
1	C	38	CYS	C-N-CA	-6.38	110.84	122.38
2	D	168	LEU	N-CA-C	6.36	119.16	111.40
1	A	382	ILE	N-CA-C	6.31	116.49	110.74
2	D	190	GLY	N-CA-C	6.31	121.58	110.80
1	A	198	HIS	N-CA-C	-6.27	104.37	111.14
1	C	149	LEU	CA-C-N	6.23	127.63	119.84
1	C	149	LEU	C-N-CA	6.23	127.63	119.84
2	B	12	LEU	N-CA-C	-6.21	100.46	109.59
1	C	92	LEU	N-CA-C	-6.14	105.43	113.17
2	D	96	HIS	CA-C-N	6.13	127.51	119.84
2	D	96	HIS	C-N-CA	6.13	127.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	LYS	N-CA-C	-6.13	105.51	112.87
1	A	124	PHE	N-CA-C	-6.12	105.81	113.28
1	A	28	GLU	N-CA-C	6.11	118.91	111.82
1	A	221	HIS	N-CA-C	6.09	118.33	108.34
2	B	51	GLY	CA-C-N	6.09	126.20	119.87
2	B	51	GLY	C-N-CA	6.09	126.20	119.87
1	A	456	GLY	N-CA-C	6.08	120.00	111.19
2	B	400	THR	N-CA-C	6.07	117.56	111.07
1	C	531	VAL	N-CA-C	6.06	116.60	107.75
2	D	284	ARG	N-CA-C	6.05	118.67	111.71
2	B	270	ILE	N-CA-C	6.04	116.67	110.82
1	A	388	LYS	CA-C-N	-6.03	113.67	122.65
1	A	388	LYS	C-N-CA	-6.03	113.67	122.65
1	A	367	GLN	N-CA-C	6.00	117.83	111.28
1	A	32	LYS	N-CA-C	-5.96	105.50	112.89
2	B	252	TRP	N-CA-C	5.89	118.12	108.52
2	D	327	ALA	N-CA-C	-5.87	100.14	109.59
1	C	276	VAL	N-CA-C	5.86	118.63	112.83
1	C	118	VAL	N-CA-C	5.84	116.94	107.71
2	D	324	ASP	N-CA-C	5.78	118.65	110.50
1	C	389	PHE	CB-CA-C	5.77	119.77	109.38
1	C	31	ILE	N-CA-C	5.75	120.95	113.07
1	C	333	GLY	N-CA-C	5.73	119.41	112.48
1	C	134	SER	N-CA-C	5.70	117.18	110.97
1	C	399	GLU	N-CA-C	5.68	117.15	111.07
1	A	229	TRP	N-CA-C	5.64	117.57	107.80
2	B	293	ILE	CA-C-N	5.64	126.12	120.14
2	B	293	ILE	C-N-CA	5.64	126.12	120.14
1	A	389	PHE	CB-CA-C	5.64	118.95	109.48
1	C	453	GLY	N-CA-C	5.62	118.95	110.18
2	D	240	THR	N-CA-C	5.59	118.02	108.90
4	e	4	G	OP2-P-O3'	-5.57	91.28	108.00
1	A	224	GLU	N-CA-C	5.53	122.03	109.81
1	A	128	THR	N-CA-C	5.51	119.72	112.89
2	D	193	LEU	N-CA-C	5.51	117.81	110.53
2	D	401	TRP	N-CA-C	-5.50	106.42	113.23
1	A	92	LEU	N-CA-C	-5.49	106.43	113.02
2	D	364	ASP	N-CA-C	5.49	116.94	111.07
1	C	389	PHE	CA-C-N	-5.48	115.38	123.05
1	C	389	PHE	C-N-CA	-5.48	115.38	123.05
1	A	195	ILE	N-CA-C	5.48	116.86	110.62
2	D	250	ASP	N-CA-C	5.47	118.41	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e	4	G	OP1-P-O3'	5.45	124.34	108.00
2	B	71	TRP	N-CA-C	5.44	117.58	109.25
2	D	149	LEU	CA-C-N	5.41	125.84	119.99
2	D	149	LEU	C-N-CA	5.41	125.84	119.99
1	A	106	VAL	N-CA-C	5.41	115.84	107.78
1	A	31	ILE	N-CA-C	5.38	120.00	113.00
2	D	270	ILE	N-CA-C	-5.38	106.42	111.48
2	D	195	ILE	N-CA-C	5.37	116.00	110.36
2	D	407	GLN	N-CA-C	5.37	120.70	113.72
2	B	400	THR	CA-C-O	5.34	126.43	120.82
2	D	333	GLY	N-CA-C	5.33	119.58	112.65
2	D	266	TRP	N-CA-C	-5.31	105.16	111.69
2	B	410	TRP	N-CA-C	5.30	118.30	110.46
2	B	165	THR	N-CA-C	-5.29	105.62	111.71
2	B	333	GLY	N-CA-C	5.28	119.33	112.68
1	A	357	MET	N-CA-C	-5.28	100.57	108.96
2	D	406	TRP	N-CA-C	5.28	117.35	108.96
2	D	124	PHE	N-CA-C	5.28	118.88	112.23
1	C	509	GLN	CB-CA-C	-5.26	107.46	111.20
4	e	6	G	OP1-P-O3'	5.24	123.72	108.00
1	C	293	ILE	CA-C-N	5.22	125.22	120.21
1	C	293	ILE	C-N-CA	5.22	125.22	120.21
1	C	373	GLN	N-CA-C	5.22	117.05	111.36
2	D	58	THR	N-CA-C	-5.20	102.29	110.14
1	A	143	ARG	N-CA-C	5.19	115.90	108.74
1	C	130	PHE	N-CA-C	5.18	115.37	108.38
1	A	487	GLN	N-CA-C	5.14	116.89	111.28
5	F	812	DT	C5'-C4'-O4'	5.13	117.10	109.40
1	A	93	GLY	N-CA-C	-5.11	105.16	111.70
1	A	504	GLY	CA-C-N	-5.11	114.02	120.56
1	A	504	GLY	C-N-CA	-5.11	114.02	120.56
2	B	235	HIS	CA-C-N	5.10	125.39	119.47
2	B	235	HIS	C-N-CA	5.10	125.39	119.47
1	A	254	VAL	N-CA-C	5.08	118.18	111.17
2	B	405	TYR	N-CA-C	5.08	119.17	112.92
1	C	101	LYS	N-CA-C	-5.07	103.83	110.53
2	B	421	PRO	CA-C-N	-5.07	114.20	122.26
2	B	421	PRO	C-N-CA	-5.07	114.20	122.26
2	D	71	TRP	N-CA-C	5.05	117.62	110.50
2	D	397	THR	N-CA-C	-5.05	105.78	111.28

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ASP	Mainchain
1	A	35	VAL	Mainchain
1	A	389	PHE	Mainchain
2	B	421	PRO	Peptide
1	C	389	PHE	Mainchain
2	D	332	GLN	Mainchain
2	D	421	PRO	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	4512	0	4571	219	0
1	C	4506	0	4560	182	0
2	B	3400	0	3433	146	0
2	D	3400	0	3433	161	0
3	E	192	0	100	9	0
3	T	192	0	100	8	0
4	e	196	0	99	7	0
4	t	219	0	110	7	0
5	F	382	0	215	13	0
5	P	382	0	215	13	0
6	A	20	0	14	1	0
6	C	20	0	14	1	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	e	5	0	0	0	0
All	All	17428	0	16864	738	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 22.

All (738) 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)
1:C:416:PHE:HD1	1:C:417:VAL:N	1.53	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:VAL:H	1:C:57:ASN:HB2	1.23	1.01
1:C:416:PHE:CD1	1:C:417:VAL:N	2.30	0.98
1:A:416:PHE:CD1	1:A:417:VAL:N	2.38	0.92
1:A:416:PHE:HD1	1:A:417:VAL:N	1.69	0.91
1:A:328:GLU:HB2	1:A:390:LYS:HB2	1.53	0.91
2:B:115:TYR:HD2	2:B:156:SER:HB3	1.41	0.84
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.40	0.84
1:C:416:PHE:HD1	1:C:417:VAL:H	1.25	0.82
1:C:416:PHE:HE1	1:C:417:VAL:O	1.64	0.81
1:A:255:ASN:HD22	1:A:289:LEU:HD11	1.45	0.80
1:C:354:TYR:HD1	1:C:374:LYS:HD2	1.46	0.80
1:C:372:VAL:HG11	1:C:411:ILE:HG23	1.64	0.79
3:E:13:C:H2'	3:E:14:G:H8	1.46	0.79
1:C:469:LEU:HD11	1:C:480:GLN:HG2	1.64	0.77
2:D:357:MET:O	2:D:360:ALA:HB2	1.85	0.77
2:D:421:PRO:HB2	2:D:423:VAL:H	1.49	0.76
1:A:288:ALA:HB3	1:A:291:GLU:HG3	1.68	0.76
1:C:395:LYS:HD3	1:C:414:TRP:CZ2	2.20	0.76
1:A:416:PHE:HE1	1:A:417:VAL:O	1.69	0.76
1:C:175:ASN:HB3	1:C:178:ILE:HD13	1.68	0.76
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.68	0.76
1:A:434:ILE:HD12	1:A:494:ASN:OD1	1.86	0.75
2:D:282:LEU:HD21	2:D:296:THR:H	1.50	0.75
1:A:281:LYS:HG2	1:A:284:ARG:HH21	1.51	0.74
3:E:12:C:H2'	3:E:13:C:H6	1.52	0.74
1:A:416:PHE:CE1	1:A:417:VAL:O	2.40	0.74
2:D:396:GLU:OE2	2:D:396:GLU:N	2.20	0.74
1:C:195:ILE:HD11	1:C:199:ARG:HH21	1.52	0.74
1:C:416:PHE:CE1	1:C:417:VAL:O	2.40	0.74
2:B:358:ARG:NE	2:B:370:GLU:OE1	2.20	0.73
1:A:416:PHE:CE1	1:A:417:VAL:C	2.67	0.73
1:C:416:PHE:CE1	1:C:417:VAL:C	2.68	0.72
1:A:261:VAL:HG13	1:A:276:VAL:HG21	1.72	0.72
2:D:86:ASP:OD1	2:D:87:PHE:N	2.23	0.72
2:B:76:ASP:OD2	2:B:78:ARG:NH2	2.21	0.72
1:A:416:PHE:HD1	1:A:417:VAL:H	1.38	0.72
1:C:218:ASP:OD2	1:C:222:GLN:NE2	2.23	0.71
1:C:317:VAL:HG23	1:C:349:LEU:HD23	1.72	0.71
1:A:175:ASN:OD1	1:A:201:LYS:NZ	2.21	0.71
1:A:416:PHE:CD1	1:A:416:PHE:C	2.68	0.71
1:A:419:THR:O	1:A:422:LEU:CD2	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:5:G:H2'	4:t:6:G:C8	2.26	0.70
2:B:118:VAL:HB	2:B:149:LEU:HG	1.74	0.70
1:A:417:VAL:O	1:A:417:VAL:HG13	1.90	0.70
3:E:12:C:H2'	3:E:13:C:C6	2.27	0.69
1:C:494:ASN:HB3	2:D:289:LEU:HD12	1.75	0.69
1:C:59:PRO:HG2	1:C:76:ASP:HB3	1.74	0.69
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.73	0.69
1:C:502:ALA:O	1:C:506:ILE:HG12	1.93	0.69
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.08	0.68
1:C:416:PHE:CD1	1:C:416:PHE:C	2.64	0.68
1:C:458:VAL:HG23	1:C:548:VAL:HB	1.75	0.68
4:e:7:A:H2'	4:e:8:C:O4'	1.93	0.68
1:A:221:HIS:HB2	1:A:224:GLU:HB2	1.75	0.68
2:B:171:PHE:HD2	2:B:205:LEU:HD13	1.60	0.67
1:A:260:LEU:HD21	1:A:279:LEU:HD13	1.75	0.66
1:C:305:GLU:HA	1:C:308:GLU:HB3	1.77	0.66
1:C:395:LYS:HZ3	1:C:414:TRP:NE1	1.94	0.65
1:A:103:LYS:O	1:A:236:PRO:HB3	1.96	0.65
2:D:421:PRO:HB2	2:D:423:VAL:N	2.11	0.65
2:B:191:SER:OG	2:B:198:HIS:ND1	2.25	0.65
2:B:357:MET:HE3	2:B:367:GLN:HG2	1.78	0.65
1:C:389:PHE:HB3	1:C:391:LEU:HD21	1.77	0.65
5:F:804:DA:H2''	5:F:805:DG:H5'	1.79	0.65
1:A:218:ASP:HA	1:A:220:LYS:HG2	1.77	0.65
2:B:84:THR:O	2:B:87:PHE:HB3	1.97	0.65
2:D:393:ILE:HD13	2:D:398:TRP:HB2	1.78	0.65
1:A:400:THR:O	1:A:404:GLU:HG2	1.97	0.64
1:A:56:TYR:HB2	1:A:129:ALA:HB3	1.79	0.64
1:C:58:THR:HB	1:C:77:PHE:HB3	1.79	0.64
1:C:223:LYS:O	1:C:225:PRO:HD3	1.98	0.64
1:A:26:LEU:HD22	1:A:60:VAL:HG11	1.78	0.64
1:C:418:ASN:O	1:C:418:ASN:ND2	2.30	0.64
2:D:257:ILE:O	2:D:261:VAL:HG23	1.97	0.64
1:A:454:LYS:HA	1:A:469:LEU:HD12	1.80	0.64
1:A:21:VAL:O	1:A:57:ASN:ND2	2.31	0.63
2:B:214:LEU:HD12	2:B:215:THR:H	1.62	0.63
1:C:390:LYS:HA	1:C:415:GLU:O	1.98	0.63
2:D:209:LEU:HB3	2:D:214:LEU:HD23	1.80	0.63
1:C:77:PHE:CD2	1:C:80:LEU:HB3	2.34	0.63
1:A:209:LEU:HD22	1:A:214:LEU:HD13	1.81	0.63
1:C:343:GLN:HG3	1:C:349:LEU:HD11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:t:5:G:H2'	4:t:6:G:H8	1.61	0.63
2:B:142:ILE:HG22	2:B:144:TYR:HE1	1.61	0.63
1:A:123:ASP:OD1	1:A:123:ASP:N	2.31	0.62
1:A:483:TYR:HA	1:A:486:LEU:HD12	1.80	0.62
1:C:129:ALA:HB1	1:C:143:ARG:HD2	1.82	0.62
1:C:394:GLN:OE1	1:C:416:PHE:CE2	2.53	0.62
1:C:75:VAL:HG12	1:C:77:PHE:HD1	1.65	0.62
1:C:95:PRO:HD3	2:D:137:ASN:HB2	1.81	0.62
1:C:161:GLN:HE21	1:C:161:GLN:HA	1.62	0.62
3:T:7:G:H2'	3:T:8:G:C8	2.35	0.61
5:P:811:DG:H2''	5:P:812:DT:H72	1.82	0.61
1:A:106:VAL:HG12	1:A:227:PHE:HE2	1.64	0.61
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.13	0.61
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.28	0.61
1:C:163:SER:HA	1:C:166:LYS:HE3	1.80	0.61
2:D:332:GLN:HG3	2:D:338:THR:HG23	1.83	0.61
1:C:261:VAL:HG13	1:C:276:VAL:HG21	1.82	0.61
1:C:123:ASP:O	1:C:126:LYS:HG2	2.00	0.61
2:D:84:THR:HG21	2:D:153:TRP:HZ2	1.65	0.61
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.81	0.61
2:B:376:THR:HG23	2:B:386:THR:HG22	1.83	0.61
1:C:21:VAL:HG12	1:C:22:LYS:H	1.65	0.61
1:A:458:VAL:HG12	2:B:286:THR:HG21	1.83	0.61
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.82	0.61
1:A:195:ILE:HG22	1:A:199:ARG:HH12	1.65	0.60
1:A:419:THR:O	1:A:422:LEU:HD23	2.00	0.60
2:B:350:LYS:NZ	2:B:378:GLU:OE2	2.28	0.60
2:D:111:VAL:HG23	2:D:115:TYR:HE1	1.65	0.60
1:A:118:VAL:HB	1:A:149:LEU:HG	1.84	0.60
1:A:24:TRP:CD2	1:A:25:PRO:HD2	2.37	0.60
1:C:254:VAL:HG21	1:C:286:THR:HG21	1.84	0.60
5:P:809:DC:C5	5:P:810:DT:H73	2.36	0.60
5:F:806:DT:C2	5:F:807:DC:C5	2.90	0.60
5:F:807:DC:H2'	5:F:808:DC:H6	1.66	0.60
1:C:97:PRO:HG2	1:C:232:TYR:CE2	2.36	0.60
1:C:390:LYS:HG2	1:C:415:GLU:HG2	1.84	0.60
1:A:236:PRO:HA	6:A:901:NVP:H12	1.83	0.60
1:A:204:GLU:O	1:A:207:GLN:HB2	2.01	0.59
2:B:80:LEU:HD23	2:B:153:TRP:CD1	2.37	0.59
1:C:188:TYR:HH	1:C:229:TRP:CD1	2.20	0.59
2:D:280:SER:O	2:D:283:LEU:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:282:LEU:HD21	2:D:296:THR:HG22	1.84	0.59
2:B:28:GLU:HG3	2:B:32:LYS:HE2	1.84	0.59
5:F:811:DG:N2	4:e:2:C:O2	2.30	0.59
1:A:279:LEU:HD23	1:A:299:ALA:HB1	1.84	0.59
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.71	0.59
1:A:2:ILE:HG22	1:A:3:SER:H	1.68	0.59
1:A:79:GLU:OE1	1:A:83:ARG:NH1	2.35	0.59
1:C:417:VAL:O	1:C:417:VAL:HG13	2.01	0.59
2:D:399:GLU:HA	2:D:402:TRP:HD1	1.68	0.59
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.85	0.59
3:E:7:G:H2'	3:E:8:G:C8	2.38	0.59
1:A:362:THR:OG1	1:A:363:ASN:N	2.34	0.59
1:C:387:PRO:HG2	1:C:389:PHE:CZ	2.38	0.59
2:D:423:VAL:HG13	2:D:426:TRP:CD1	2.37	0.59
2:B:115:TYR:O	2:B:149:LEU:HB2	2.03	0.59
2:D:277:ARG:HH11	2:D:277:ARG:H	1.49	0.58
2:D:399:GLU:HA	2:D:402:TRP:CD1	2.38	0.58
1:A:225:PRO:HA	1:A:226:PRO:C	2.28	0.58
2:B:171:PHE:HE2	2:B:205:LEU:HB2	1.66	0.58
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.39	0.58
1:A:416:PHE:CE1	1:A:418:ASN:HA	2.38	0.58
2:B:279:LEU:HD23	2:B:299:ALA:HB1	1.86	0.58
1:C:90:VAL:HG11	1:C:161:GLN:HB2	1.85	0.58
2:D:88:TRP:CG	2:D:154:LYS:HG2	2.39	0.58
2:D:354:TYR:HE2	2:D:375:ILE:HG13	1.69	0.58
3:E:11:C:H2'	3:E:12:C:C6	2.39	0.58
1:A:132:ILE:HG12	1:A:133:PRO:HD2	1.85	0.58
1:A:420:PRO:HA	1:A:421:PRO:C	2.27	0.58
5:P:807:DC:H2'	5:P:808:DC:C6	2.39	0.58
1:A:548:VAL:O	1:A:552:VAL:HG22	2.02	0.58
1:C:100:LEU:O	1:C:318:TYR:HB3	2.04	0.58
1:C:124:PHE:HA	1:C:127:TYR:HD2	1.68	0.58
2:D:50:ILE:HD13	2:D:145:GLN:HB3	1.84	0.58
2:D:366:LYS:HG3	2:D:405:TYR:CD1	2.38	0.58
4:e:5:G:H2'	4:e:6:G:C8	2.39	0.58
2:B:50:ILE:HD11	2:B:143:ARG:CZ	2.33	0.58
2:B:246:LEU:HD12	2:B:307:ARG:HG2	1.86	0.58
1:C:80:LEU:O	1:C:84:THR:OG1	2.21	0.58
2:D:422:LEU:HG	2:D:422:LEU:O	1.99	0.58
1:A:134:SER:OG	1:A:135:ILE:N	2.34	0.57
2:D:92:LEU:HD21	2:D:161:GLN:OE1	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:807:DC:H2'	5:F:808:DC:C6	2.40	0.57
1:A:337:TRP:CZ3	1:A:368:LEU:HD13	2.40	0.57
1:A:483:TYR:O	1:A:487:GLN:HG3	2.05	0.57
2:B:270:ILE:HG13	2:B:346:PHE:HD1	1.69	0.57
2:D:279:LEU:HG	2:D:302:GLU:OE1	2.04	0.57
1:C:399:GLU:O	1:C:403:THR:HG23	2.03	0.57
1:A:135:ILE:HG23	1:A:136:ASN:H	1.69	0.57
1:A:326:ILE:HD13	1:A:388:LYS:HB3	1.86	0.57
1:A:537:PRO:HD2	1:A:542:ILE:CD1	2.34	0.57
3:T:8:G:H2'	3:T:9:C:H6	1.69	0.57
1:A:473:THR:HG23	1:A:476:LYS:HG3	1.85	0.57
1:C:253:THR:HG23	1:C:256:ASP:H	1.70	0.57
1:C:435:VAL:HG13	2:D:290:THR:HG21	1.86	0.57
2:D:277:ARG:HH11	2:D:277:ARG:N	2.02	0.57
1:A:5:ILE:HG22	1:A:212:TRP:CD1	2.39	0.57
1:A:543:GLY:HA2	2:B:283:LEU:O	2.05	0.57
5:P:807:DC:H2''	5:P:808:DC:O5'	2.05	0.57
1:A:77:PHE:O	1:A:80:LEU:N	2.38	0.57
2:B:18:GLY:HA3	2:B:127:TYR:HD1	1.70	0.57
1:A:21:VAL:H	1:A:57:ASN:HB3	1.70	0.57
2:D:47:ILE:HG22	2:D:146:TYR:HA	1.85	0.56
2:D:118:VAL:HG12	2:D:119:PRO:O	2.05	0.56
1:A:115:TYR:HD2	1:A:151:GLN:HE22	1.53	0.56
1:A:419:THR:C	1:A:422:LEU:HD21	2.30	0.56
1:A:419:THR:O	1:A:422:LEU:HD21	2.05	0.56
2:B:421:PRO:HB3	2:B:424:LYS:HB2	1.88	0.56
1:C:394:GLN:OE1	1:C:416:PHE:HE2	1.88	0.56
1:C:459:THR:HG23	1:C:461:LYS:H	1.69	0.56
1:A:130:PHE:CZ	1:A:132:ILE:HB	2.40	0.56
1:A:486:LEU:O	1:A:528:LYS:HE3	2.05	0.56
2:B:281:LYS:O	2:B:284:ARG:HG2	2.06	0.56
5:F:809:DC:C5	5:F:810:DT:H73	2.41	0.56
3:T:11:C:O2'	3:T:12:C:OP1	2.24	0.56
1:C:234:LEU:HD12	6:C:901:NVP:HCD2	1.86	0.56
2:D:170:PRO:HB2	2:D:208:HIS:HE1	1.71	0.56
1:A:80:LEU:O	1:A:84:THR:OG1	2.24	0.55
1:C:364:ASP:HB3	1:C:423:VAL:HG13	1.88	0.55
1:C:365:VAL:HG11	1:C:401:TRP:CD1	2.41	0.55
1:C:479:LEU:HD23	1:C:521:ILE:HD12	1.87	0.55
1:C:57:ASN:HA	1:C:130:PHE:HA	1.88	0.55
1:C:459:THR:CG2	1:C:461:LYS:H	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:SER:HB3	1:A:385:LYS:O	2.07	0.55
2:D:88:TRP:CD2	2:D:154:LYS:HG2	2.42	0.55
2:B:171:PHE:CD2	2:B:205:LEU:HD13	2.39	0.55
1:C:491:LEU:HB3	1:C:529:GLU:HB2	1.87	0.55
1:C:115:TYR:HE1	1:C:160:PHE:HD2	1.55	0.55
1:C:497:THR:HG1	1:C:499:SER:H	1.55	0.55
3:T:9:C:H2'	3:T:10:G:H8	1.72	0.55
2:B:266:TRP:O	2:B:269:GLN:N	2.33	0.55
2:B:401:TRP:HB3	2:B:405:TYR:HE2	1.71	0.55
1:A:123:ASP:O	1:A:126:LYS:HG2	2.07	0.55
1:A:266:TRP:O	1:A:269:GLN:HG2	2.06	0.55
2:B:297:GLU:O	2:B:301:LEU:HG	2.07	0.55
2:D:194:GLU:CD	2:D:195:ILE:H	2.14	0.55
1:A:154:LYS:O	1:A:157:PRO:HD2	2.07	0.54
2:D:276:VAL:H	2:D:277:ARG:HH12	1.55	0.54
3:T:8:G:H2'	3:T:9:C:C6	2.42	0.54
2:B:142:ILE:HG22	2:B:144:TYR:CE1	2.41	0.54
1:C:463:ARG:C	1:C:464:GLN:HG2	2.31	0.54
2:D:332:GLN:NE2	2:D:427:TYR:HB3	2.22	0.54
1:A:417:VAL:O	1:A:417:VAL:CG1	2.54	0.54
1:A:305:GLU:O	1:A:309:ILE:HG13	2.07	0.54
1:C:339:TYR:CE2	1:C:341:ILE:HD11	2.43	0.54
2:D:96:HIS:ND1	2:D:97:PRO:HD2	2.22	0.54
2:B:374:LYS:O	2:B:378:GLU:HG2	2.08	0.54
2:B:390:LYS:HB3	2:B:417:VAL:HG21	1.90	0.54
1:C:97:PRO:HG2	1:C:232:TYR:CD2	2.42	0.54
2:D:247:PRO:O	2:D:307:ARG:NH2	2.41	0.54
1:A:167:ILE:O	1:A:170:PRO:HD2	2.07	0.54
2:B:41:MET:HG2	2:B:46:LYS:HD2	1.88	0.54
2:D:85:GLN:HA	2:D:88:TRP:NE1	2.22	0.54
1:A:60:VAL:HG21	1:A:132:ILE:HD12	1.89	0.54
2:B:423:VAL:C	2:B:425:LEU:H	2.16	0.54
2:D:13:LYS:NZ	2:D:85:GLN:OE1	2.37	0.54
2:D:235:HIS:N	2:D:236:PRO:HD3	2.23	0.54
2:D:261:VAL:HG13	2:D:276:VAL:HG11	1.90	0.54
2:D:401:TRP:O	2:D:402:TRP:C	2.50	0.54
1:A:394:GLN:OE1	1:A:416:PHE:CE2	2.61	0.53
1:A:331:LYS:HE2	1:A:333:GLY:HA2	1.89	0.53
1:A:437:ALA:HB1	1:A:493:VAL:HA	1.90	0.53
2:B:34:LEU:HD21	2:B:62:ALA:HB2	1.90	0.53
2:B:398:TRP:O	2:B:402:TRP:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ASP:OD1	2:D:78:ARG:NE	2.41	0.53
1:A:339:TYR:CG	1:A:375:ILE:HD11	2.43	0.53
1:A:525:LEU:HD23	1:A:531:VAL:HG21	1.90	0.53
1:C:78:ARG:HB3	1:C:82:LYS:NZ	2.23	0.53
2:D:241:VAL:HG12	2:D:351:THR:H	1.72	0.53
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.43	0.53
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.42	0.53
4:e:7:A:C6	4:e:8:C:C5	2.97	0.53
1:C:325:LEU:HD11	1:C:383:TRP:CD2	2.44	0.53
1:A:232:TYR:O	1:A:242:GLN:NE2	2.36	0.53
2:B:104:LYS:HB2	2:B:192:ASP:HA	1.90	0.53
2:D:423:VAL:HG13	2:D:426:TRP:HD1	1.74	0.53
1:C:277:ARG:NH1	1:C:334:GLN:O	2.42	0.53
2:B:17:ASP:O	2:B:83:ARG:HD3	2.09	0.53
4:t:3:A:N1	5:P:810:DT:N3	2.57	0.53
1:A:525:LEU:CD2	1:A:531:VAL:HG21	2.38	0.53
1:C:107:THR:HG23	1:C:222:GLN:O	2.09	0.53
1:C:334:GLN:HB2	1:C:336:GLN:HE21	1.73	0.53
2:D:261:VAL:HG13	2:D:276:VAL:CG1	2.39	0.53
3:E:14:G:O6	5:F:814:DC:N4	2.42	0.52
1:A:259:LYS:HA	5:P:818:DC:H2''	1.92	0.52
2:B:360:ALA:HA	2:B:367:GLN:OE1	2.09	0.52
5:P:818:DC:H2'	5:P:819:DG:H8	1.74	0.52
1:A:24:TRP:CG	1:A:25:PRO:HD2	2.44	0.52
2:B:206:ARG:HE	2:B:216:THR:HB	1.74	0.52
1:C:220:LYS:HG3	1:C:222:GLN:HG2	1.92	0.52
1:C:357:MET:HE2	1:C:362:THR:HG22	1.91	0.52
1:C:77:PHE:CE2	1:C:80:LEU:HB3	2.45	0.52
1:C:354:TYR:CD1	1:C:374:LYS:HD2	2.37	0.52
5:F:803:DC:H2'	5:F:804:DA:C8	2.43	0.52
1:A:255:ASN:ND2	1:A:289:LEU:HD21	2.25	0.52
1:C:47:ILE:HG22	1:C:48:SER:N	2.25	0.52
2:D:34:LEU:O	2:D:38:CYS:HB2	2.09	0.52
1:C:206:ARG:HG2	1:C:216:THR:OG1	2.10	0.52
1:A:277:ARG:HB2	1:A:336:GLN:CD	2.34	0.52
1:C:18:GLY:HA3	1:C:56:TYR:CD1	2.44	0.52
2:D:401:TRP:HB3	2:D:405:TYR:HE2	1.75	0.52
5:P:818:DC:C2	5:P:819:DG:C8	2.98	0.52
3:E:13:C:H2'	3:E:14:G:C8	2.36	0.52
2:B:85:GLN:NE2	2:B:89:GLU:OE2	2.43	0.52
2:B:101:LYS:O	2:B:236:PRO:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:TRP:HZ3	2:B:406:TRP:CD2	2.27	0.52
1:C:450:THR:OG1	1:C:452:LEU:HB2	2.10	0.52
1:A:19:PRO:O	1:A:56:TYR:HA	2.10	0.52
1:A:503:LEU:O	1:A:507:GLN:HB2	2.10	0.52
1:A:105:SER:O	1:A:190:GLY:HA2	2.10	0.52
1:A:391:LEU:O	1:A:393:ILE:N	2.42	0.51
2:D:393:ILE:HG12	2:D:394:GLN:N	2.25	0.51
1:C:35:VAL:O	1:C:38:CYS:HB3	2.09	0.51
1:C:395:LYS:NZ	1:C:414:TRP:NE1	2.57	0.51
1:C:430:GLU:HB2	1:C:532:TYR:HB2	1.92	0.51
1:C:270:ILE:HG23	1:C:271:TYR:H	1.75	0.51
1:A:516:GLU:O	1:A:520:GLN:HG3	2.10	0.51
2:D:72:ARG:HD3	2:D:73:LYS:O	2.10	0.51
2:D:191:SER:OG	2:D:198:HIS:ND1	2.33	0.51
1:A:503:LEU:HD12	1:A:533:LEU:HG	1.92	0.51
2:B:50:ILE:HG12	2:B:143:ARG:HB2	1.92	0.51
2:B:146:TYR:CG	2:B:150:PRO:HB3	2.46	0.51
2:D:61:PHE:HZ	2:D:402:TRP:HH2	1.59	0.51
2:D:402:TRP:CE2	2:D:403:THR:HG22	2.45	0.51
4:e:6:G:H2'	4:e:7:A:C8	2.46	0.51
1:A:416:PHE:CD1	1:A:417:VAL:C	2.89	0.51
1:C:279:LEU:HG	1:C:302:GLU:OE1	2.11	0.51
1:A:48:SER:O	1:A:144:TYR:HB2	2.11	0.51
1:A:198:HIS:O	1:A:202:ILE:HG12	2.11	0.51
2:B:47:ILE:HB	2:B:144:TYR:HD2	1.75	0.51
1:C:390:LYS:HG2	1:C:415:GLU:CG	2.41	0.51
1:A:149:LEU:HD13	1:A:156:SER:HA	1.92	0.51
1:A:325:LEU:HD11	1:A:383:TRP:CD2	2.46	0.50
2:D:87:PHE:HE2	2:D:155:GLY:HA2	1.75	0.50
2:D:341:ILE:HD11	2:D:375:ILE:HG23	1.92	0.50
1:A:171:PHE:CD2	1:A:205:LEU:HD12	2.45	0.50
2:B:30:LYS:HD3	2:B:62:ALA:O	2.11	0.50
2:B:379:SER:OG	2:B:385:LYS:O	2.29	0.50
1:A:329:ILE:O	1:A:392:PRO:HD3	2.11	0.50
2:B:142:ILE:CG2	2:B:144:TYR:HE1	2.24	0.50
1:C:153:TRP:HB3	1:C:156:SER:OG	2.12	0.50
1:A:160:PHE:CD1	1:A:160:PHE:C	2.89	0.50
1:A:366:LYS:HG3	1:A:401:TRP:CZ2	2.46	0.50
1:A:418:ASN:OD1	1:A:418:ASN:O	2.30	0.50
2:B:282:LEU:HD21	2:B:296:THR:HG23	1.94	0.50
1:C:270:ILE:HG23	1:C:271:TYR:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLU:O	2:B:308:GLU:HB3	2.12	0.50
1:A:342:TYR:CD1	1:A:342:TYR:C	2.89	0.50
1:C:389:PHE:CE2	1:C:412:PRO:HG2	2.46	0.50
1:A:211:ARG:HD3	1:A:212:TRP:HZ3	1.76	0.50
1:A:493:VAL:HG22	1:A:494:ASN:N	2.26	0.50
2:B:58:THR:HG22	2:B:75:VAL:HG12	1.94	0.50
1:C:226:PRO:HB3	1:C:235:HIS:CE1	2.45	0.50
1:C:429:LEU:N	1:C:429:LEU:HD23	2.27	0.50
2:D:13:LYS:HG2	2:D:83:ARG:O	2.10	0.50
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.45	0.50
4:t:3:A:H2'	4:t:4:G:C8	2.47	0.50
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.93	0.50
2:B:81:ASN:HB3	2:B:154:LYS:HG3	1.93	0.50
2:D:84:THR:HG21	2:D:153:TRP:CZ2	2.46	0.50
3:T:7:G:H2'	3:T:8:G:H8	1.75	0.50
1:A:114:ALA:HB1	1:A:160:PHE:CE2	2.47	0.49
2:B:393:ILE:HG21	2:B:398:TRP:HB2	1.95	0.49
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.47	0.49
1:A:97:PRO:HG2	1:A:232:TYR:CE1	2.46	0.49
1:A:438:GLU:HG2	1:A:461:LYS:HG3	1.92	0.49
1:A:498:ASN:OD1	1:A:498:ASN:O	2.30	0.49
2:D:155:GLY:O	2:D:158:ALA:N	2.45	0.49
2:D:281:LYS:HA	2:D:284:ARG:HG3	1.94	0.49
2:D:358:ARG:HG2	2:D:366:LYS:HD3	1.93	0.49
4:t:4:G:O2'	4:t:5:G:OP1	2.28	0.49
1:A:66:LYS:HD3	1:A:67:ASP:H	1.77	0.49
1:A:327:ALA:HB2	1:A:341:ILE:HG23	1.95	0.49
2:B:13:LYS:HB3	2:B:86:ASP:HB3	1.94	0.49
2:B:370:GLU:O	2:B:374:LYS:HG3	2.13	0.49
2:D:78:ARG:HD3	2:D:411:ILE:HG22	1.93	0.49
1:A:171:PHE:O	1:A:175:ASN:ND2	2.40	0.49
1:C:58:THR:H	1:C:130:PHE:HB2	1.78	0.49
3:E:14:G:C6	5:F:814:DC:N4	2.81	0.49
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.94	0.49
2:B:40:GLU:HG3	2:B:44:GLU:OE2	2.12	0.49
1:C:171:PHE:CG	1:C:205:LEU:HD12	2.46	0.49
2:B:107:THR:HG23	2:B:232:TYR:HB2	1.95	0.49
2:D:333:GLY:O	2:D:336:GLN:N	2.43	0.49
2:B:336:GLN:C	2:B:337:TRP:CD1	2.91	0.49
1:C:241:VAL:HG21	1:C:244:ILE:HD11	1.95	0.49
2:B:305:GLU:O	2:B:309:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TRP:CD1	1:A:295:LEU:HG	2.48	0.48
1:C:60:VAL:HG21	1:C:132:ILE:HD13	1.93	0.48
2:D:249:LYS:HD2	2:D:252:TRP:CD2	2.48	0.48
1:A:224:GLU:N	1:A:225:PRO:HD2	2.28	0.48
2:B:66:LYS:HE2	2:B:66:LYS:HB2	1.61	0.48
1:C:473:THR:HG21	5:F:809:DC:P	2.54	0.48
2:D:276:VAL:H	2:D:277:ARG:NH1	2.12	0.48
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.48	0.48
2:D:282:LEU:CD2	2:D:296:THR:HG22	2.43	0.48
1:A:78:ARG:HA	1:A:81:ASN:HD22	1.78	0.48
1:A:202:ILE:O	1:A:206:ARG:HG3	2.14	0.48
2:B:78:ARG:HD3	2:B:411:ILE:O	2.13	0.48
1:A:60:VAL:HG22	1:A:75:VAL:HA	1.94	0.48
1:A:90:VAL:HG11	1:A:161:GLN:HB3	1.96	0.48
1:A:336:GLN:C	1:A:337:TRP:CD1	2.92	0.48
1:A:402:TRP:HB2	1:A:409:THR:HG23	1.96	0.48
1:C:30:LYS:HD2	1:C:30:LYS:N	2.29	0.48
2:D:398:TRP:CD1	2:D:416:PHE:CZ	3.01	0.48
1:A:5:ILE:HG22	1:A:212:TRP:HD1	1.78	0.48
1:C:416:PHE:CD1	1:C:417:VAL:C	2.92	0.48
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.49	0.48
2:B:253:THR:O	2:B:257:ILE:HG12	2.13	0.48
1:C:44:GLU:N	1:C:44:GLU:OE2	2.47	0.48
2:D:319:TYR:OH	2:D:385:LYS:NZ	2.25	0.48
1:A:180:ILE:HG12	1:A:189:VAL:HG13	1.96	0.47
1:C:49:LYS:O	1:C:50:ILE:HD12	2.14	0.47
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.29	0.47
1:C:55:PRO:HA	1:C:143:ARG:NH2	2.29	0.47
2:D:13:LYS:NZ	2:D:85:GLN:HB3	2.29	0.47
1:A:5:ILE:CG2	1:A:212:TRP:HD1	2.27	0.47
1:C:122:GLU:O	1:C:125:ARG:N	2.46	0.47
2:D:398:TRP:HD1	2:D:416:PHE:HZ	1.63	0.47
3:T:9:C:H2'	3:T:10:G:C8	2.50	0.47
2:B:120:LEU:HD23	2:B:125:ARG:HG3	1.96	0.47
1:C:58:THR:N	1:C:130:PHE:HB2	2.29	0.47
5:F:807:DC:H2''	5:F:808:DC:C5'	2.44	0.47
1:A:55:PRO:HD2	1:A:56:TYR:CE2	2.49	0.47
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.96	0.47
1:A:465:LYS:HG3	1:A:466:VAL:N	2.28	0.47
1:C:139:THR:HB	1:C:140:PRO:HD2	1.96	0.47
5:P:818:DC:C2	5:P:819:DG:N7	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:TRP:CZ2	1:A:411:ILE:HG13	2.49	0.47
1:C:95:PRO:HB3	2:D:136:ASN:O	2.15	0.47
1:C:524:GLN:OE1	1:C:524:GLN:HA	2.14	0.47
1:A:58:THR:OG1	1:A:130:PHE:HB2	2.15	0.47
1:A:233:GLU:HG3	1:A:242:GLN:HG2	1.97	0.47
1:A:524:GLN:O	1:A:528:LYS:HG2	2.14	0.47
2:B:53:GLU:O	2:B:55:PRO:HD3	2.14	0.47
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.80	0.47
1:C:398:TRP:CZ2	1:C:411:ILE:HG13	2.50	0.47
2:D:61:PHE:CZ	2:D:402:TRP:CH2	3.03	0.47
2:D:279:LEU:O	2:D:282:LEU:HB2	2.13	0.47
3:T:12:C:H2'	3:T:13:C:C6	2.49	0.47
1:A:31:ILE:O	1:A:34:LEU:HG	2.15	0.47
1:A:218:ASP:C	1:A:220:LYS:N	2.72	0.47
1:A:408:ALA:O	2:B:393:ILE:HG13	2.15	0.47
1:C:486:LEU:O	1:C:528:LYS:NZ	2.41	0.47
1:A:480:GLN:O	1:A:483:TYR:HB3	2.15	0.47
2:B:337:TRP:CZ3	2:B:368:LEU:HD13	2.50	0.47
2:B:421:PRO:O	2:B:422:LEU:HD23	2.14	0.47
2:D:394:GLN:OE1	2:D:394:GLN:HA	2.14	0.47
1:A:171:PHE:HB2	1:A:208:HIS:CD2	2.50	0.46
1:A:389:PHE:HB2	1:A:414:TRP:HB2	1.96	0.46
1:C:44:GLU:HB2	1:C:46:LYS:HD2	1.97	0.46
2:D:252:TRP:HE3	2:D:256:ASP:HB3	1.80	0.46
1:A:473:THR:O	1:A:477:THR:HG23	2.16	0.46
2:B:282:LEU:HD23	2:B:282:LEU:HA	1.60	0.46
2:D:354:TYR:CE2	2:D:375:ILE:HG13	2.49	0.46
1:A:389:PHE:HB2	1:A:414:TRP:CB	2.45	0.46
4:t:3:A:H2'	4:t:4:G:H8	1.81	0.46
1:A:501:TYR:CE1	1:A:505:ILE:HD11	2.50	0.46
1:A:536:VAL:HB	1:A:542:ILE:CD1	2.46	0.46
1:A:328:GLU:CG	1:A:330:GLN:HE21	2.29	0.46
1:A:495:ILE:O	1:A:532:TYR:O	2.34	0.46
2:B:379:SER:OG	2:B:387:PRO:HD3	2.16	0.46
1:C:144:TYR:CD1	1:C:144:TYR:C	2.92	0.46
1:C:395:LYS:HZ3	1:C:414:TRP:CD1	2.34	0.46
1:C:395:LYS:NZ	1:C:414:TRP:CE2	2.83	0.46
1:C:424:LYS:HE2	1:C:426:TRP:CD2	2.51	0.46
2:B:354:TYR:OH	2:B:378:GLU:OE1	2.23	0.46
2:B:391:LEU:O	2:B:393:ILE:N	2.48	0.46
2:B:401:TRP:O	2:B:402:TRP:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:TYR:HB2	1:C:129:ALA:HB3	1.96	0.46
1:C:167:ILE:O	1:C:170:PRO:HD2	2.16	0.46
2:D:266:TRP:CD1	2:D:422:LEU:HD11	2.51	0.46
4:e:4:G:H2'	4:e:5:G:C8	2.51	0.46
1:A:328:GLU:HG2	1:A:330:GLN:HE21	1.80	0.46
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.98	0.46
2:B:106:VAL:HG22	2:B:190:GLY:HA3	1.97	0.46
1:C:56:TYR:HD2	1:C:129:ALA:HB3	1.80	0.46
1:C:197:GLN:O	1:C:200:THR:HB	2.15	0.46
2:D:57:ASN:HA	2:D:129:ALA:O	2.16	0.46
5:P:818:DC:O2	5:P:819:DG:C8	2.69	0.46
1:A:167:ILE:HD13	1:A:214:LEU:HD11	1.96	0.46
2:B:13:LYS:HE3	2:B:16:MET:HE1	1.98	0.46
2:D:61:PHE:HZ	2:D:402:TRP:CH2	2.33	0.46
2:D:115:TYR:O	2:D:149:LEU:HB2	2.16	0.46
1:A:395:LYS:O	1:A:399:GLU:HB2	2.15	0.45
1:A:438:GLU:HB3	1:A:440:PHE:CE1	2.51	0.45
1:A:186:ASP:N	1:A:186:ASP:OD1	2.49	0.45
2:B:249:LYS:HB2	2:B:252:TRP:CZ2	2.51	0.45
1:C:103:LYS:HE3	1:C:179:VAL:HG21	1.98	0.45
1:C:438:GLU:OE1	1:C:461:LYS:HD2	2.15	0.45
2:D:357:MET:HB3	2:D:370:GLU:OE1	2.16	0.45
2:B:13:LYS:NZ	2:B:85:GLN:HB3	2.31	0.45
1:C:391:LEU:HD12	1:C:414:TRP:CE3	2.51	0.45
2:D:382:ILE:HG22	2:D:383:TRP:CD2	2.52	0.45
2:B:214:LEU:HD12	2:B:215:THR:N	2.31	0.45
2:B:396:GLU:OE2	2:B:396:GLU:N	2.47	0.45
2:D:87:PHE:CE2	2:D:155:GLY:HA2	2.51	0.45
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.99	0.45
2:D:115:TYR:CD2	2:D:156:SER:HB3	2.51	0.45
2:D:118:VAL:HB	2:D:149:LEU:HD12	1.97	0.45
2:D:333:GLY:O	2:D:334:GLN:C	2.59	0.45
2:B:162:SER:O	2:B:165:THR:HG22	2.16	0.45
1:C:0:VAL:HA	1:C:1:PRO:HD2	1.78	0.45
2:B:18:GLY:HA3	2:B:127:TYR:CD1	2.49	0.45
2:B:73:LYS:HG2	2:B:74:LEU:N	2.31	0.45
2:B:195:ILE:O	2:B:199:ARG:HG3	2.16	0.45
1:C:65:LYS:HD3	1:C:72:ARG:HH22	1.80	0.45
1:C:115:TYR:O	1:C:149:LEU:HB2	2.17	0.45
1:C:115:TYR:CE1	1:C:160:PHE:HD2	2.35	0.45
2:D:203:GLU:HA	2:D:206:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:811:DG:N2	5:F:812:DT:C2	2.85	0.45
2:B:58:THR:HG23	2:B:76:ASP:O	2.17	0.45
2:B:154:LYS:HD3	2:B:184:MET:SD	2.56	0.45
1:A:221:HIS:CB	1:A:224:GLU:HB2	2.44	0.45
2:D:296:THR:HG23	2:D:299:ALA:H	1.81	0.45
1:A:395:LYS:HE2	1:A:414:TRP:CE2	2.52	0.45
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.52	0.45
2:B:257:ILE:HB	2:B:283:LEU:HD21	1.99	0.45
2:B:419:THR:O	2:B:420:PRO:C	2.59	0.45
1:C:125:ARG:O	1:C:128:THR:OG1	2.35	0.45
1:C:195:ILE:O	1:C:199:ARG:HG3	2.17	0.45
2:D:114:ALA:HB1	2:D:160:PHE:CZ	2.52	0.45
2:D:399:GLU:O	2:D:403:THR:HG23	2.17	0.45
1:A:365:VAL:HG21	1:A:425:LEU:HD21	1.99	0.44
1:C:417:VAL:O	1:C:417:VAL:CG1	2.65	0.44
1:A:78:ARG:HG2	1:A:82:LYS:HE3	1.99	0.44
1:A:390:LYS:HZ2	1:A:390:LYS:HG2	1.52	0.44
1:C:164:MET:HE2	1:C:187:LEU:HD21	1.99	0.44
1:C:410:TRP:CE2	2:D:363:ASN:ND2	2.85	0.44
2:D:164:MET:HE3	2:D:168:LEU:HG	1.99	0.44
1:A:101:LYS:HE2	1:A:101:LYS:HB2	1.66	0.44
1:A:406:TRP:HB3	2:B:421:PRO:HG3	2.00	0.44
1:C:365:VAL:HG11	1:C:401:TRP:CG	2.52	0.44
4:e:6:G:O2'	4:e:7:A:OP1	2.35	0.44
2:B:369:THR:CG2	2:B:406:TRP:HE3	2.30	0.44
1:C:457:TYR:C	1:C:457:TYR:CD1	2.96	0.44
2:B:74:LEU:HD12	2:B:75:VAL:N	2.33	0.44
1:C:122:GLU:O	1:C:125:ARG:HB2	2.17	0.44
1:C:319:TYR:CZ	1:C:321:PRO:HA	2.53	0.44
1:C:441:TYR:CG	1:C:544:GLY:HA3	2.53	0.44
2:D:163:SER:O	2:D:167:ILE:HG22	2.18	0.44
1:A:77:PHE:HB3	1:A:80:LEU:HB3	2.00	0.44
1:C:410:TRP:HZ3	2:D:401:TRP:CZ3	2.36	0.44
2:D:283:LEU:HD23	2:D:283:LEU:HA	1.74	0.44
2:D:421:PRO:CB	2:D:423:VAL:H	2.25	0.44
1:C:425:LEU:HD22	1:C:509:GLN:OE1	2.17	0.44
1:A:376:THR:O	1:A:380:ILE:HG13	2.18	0.44
1:A:425:LEU:HD23	1:A:425:LEU:HA	1.72	0.44
2:B:423:VAL:C	2:B:425:LEU:N	2.76	0.44
2:D:12:LEU:HD12	2:D:124:PHE:HE1	1.82	0.44
2:D:280:SER:C	2:D:282:LEU:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:HD21	1:A:264:LEU:HD21	2.00	0.43
1:A:339:TYR:CD1	1:A:375:ILE:HD11	2.53	0.43
1:A:323:LYS:O	1:A:343:GLN:NE2	2.50	0.43
1:A:326:ILE:HB	1:A:342:TYR:CE1	2.53	0.43
1:A:473:THR:HG23	1:A:476:LYS:HE3	2.01	0.43
1:C:339:TYR:HE2	1:C:341:ILE:HD11	1.83	0.43
2:D:328:GLU:OE1	2:D:342:TYR:OH	2.22	0.43
4:t:9:U:N3	5:P:804:DA:N1	2.50	0.43
1:A:65:LYS:HD3	1:A:72:ARG:NE	2.34	0.43
2:B:153:TRP:O	2:B:157:PRO:HD2	2.18	0.43
1:C:124:PHE:O	1:C:125:ARG:C	2.60	0.43
2:D:157:PRO:O	2:D:161:GLN:HB2	2.18	0.43
2:D:234:LEU:C	2:D:236:PRO:HD3	2.43	0.43
1:A:129:ALA:HA	1:A:144:TYR:O	2.18	0.43
1:A:238:LYS:HE3	1:A:315:HIS:CG	2.53	0.43
1:A:325:LEU:HD22	1:A:341:ILE:HG22	2.01	0.43
1:C:65:LYS:HB3	1:C:72:ARG:NH2	2.33	0.43
1:C:390:LYS:HB3	1:C:417:VAL:HB	1.99	0.43
2:D:41:MET:HE2	2:D:47:ILE:HD13	1.99	0.43
2:D:242:GLN:O	2:D:242:GLN:HG3	2.19	0.43
1:A:306:ASN:HA	1:A:309:ILE:HD12	1.99	0.43
1:A:373:GLN:HG3	2:B:401:TRP:CH2	2.54	0.43
1:C:41:MET:HE3	1:C:41:MET:HB2	1.95	0.43
1:C:122:GLU:HA	1:C:125:ARG:HD2	2.01	0.43
1:C:441:TYR:CD2	1:C:544:GLY:HA3	2.53	0.43
1:A:61:PHE:H	1:A:76:ASP:HB2	1.83	0.43
2:B:28:GLU:HA	2:B:135:ILE:HD11	2.01	0.43
1:C:377:THR:O	1:C:381:VAL:HG23	2.19	0.43
2:D:56:TYR:O	2:D:143:ARG:NH2	2.51	0.43
1:A:124:PHE:O	1:A:125:ARG:C	2.61	0.43
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.82	0.43
1:C:90:VAL:HG23	1:C:91:GLN:HG2	2.01	0.43
1:C:237:ASP:OD1	1:C:238:LYS:N	2.52	0.43
1:A:255:ASN:HD22	1:A:289:LEU:CD1	2.25	0.43
1:A:440:PHE:HA	1:A:459:THR:HG22	2.01	0.43
1:A:536:VAL:O	1:A:536:VAL:HG23	2.18	0.43
2:B:247:PRO:O	2:B:307:ARG:NH2	2.47	0.43
1:A:160:PHE:C	1:A:160:PHE:HD1	2.26	0.43
1:C:12:LEU:HD23	1:C:84:THR:HA	2.00	0.43
1:C:518:VAL:O	1:C:522:ILE:HG13	2.18	0.43
2:D:80:LEU:O	2:D:83:ARG:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:263:LYS:HA	2:D:425:LEU:HD23	2.00	0.43
2:D:372:VAL:HG13	2:D:389:PHE:CZ	2.54	0.43
2:B:41:MET:HE2	2:B:47:ILE:CD1	2.49	0.43
2:B:368:LEU:O	2:B:372:VAL:HG23	2.18	0.43
2:D:42:GLU:OE2	2:D:49:LYS:HG3	2.18	0.43
2:D:330:GLN:OE1	2:D:338:THR:OG1	2.33	0.43
2:D:357:MET:HE3	2:D:357:MET:HB2	1.90	0.43
2:D:398:TRP:HD1	2:D:416:PHE:CZ	2.37	0.43
1:A:171:PHE:CD1	1:A:171:PHE:C	2.96	0.42
1:A:454:LYS:HE2	1:A:454:LYS:HB3	1.67	0.42
1:C:10:VAL:HG13	1:C:87:PHE:HZ	1.84	0.42
1:C:18:GLY:HA3	1:C:56:TYR:CE1	2.54	0.42
1:C:220:LYS:HE2	1:C:222:GLN:HA	2.01	0.42
2:B:31:ILE:HD12	2:B:135:ILE:HG13	2.01	0.42
1:C:452:LEU:HD23	1:C:469:LEU:O	2.19	0.42
2:D:419:THR:HA	2:D:420:PRO:HD3	1.86	0.42
1:C:160:PHE:C	1:C:160:PHE:CD1	2.95	0.42
1:A:259:LYS:HG3	5:P:819:DG:P	2.58	0.42
2:B:265:ASN:O	2:B:268:SER:OG	2.33	0.42
1:C:123:ASP:HA	1:C:126:LYS:NZ	2.34	0.42
1:C:366:LYS:HE2	1:C:405:TYR:OH	2.19	0.42
2:B:84:THR:HG21	2:B:153:TRP:HZ2	1.85	0.42
2:D:312:GLU:HB3	2:D:313:PRO:HD2	2.00	0.42
2:D:338:THR:HG21	2:D:427:TYR:HB2	2.01	0.42
2:D:339:TYR:CD2	2:D:375:ILE:HG12	2.55	0.42
2:B:61:PHE:CE2	2:B:63:ILE:HG22	2.55	0.42
2:B:231:GLY:C	2:B:233:GLU:H	2.28	0.42
2:B:320:ASP:OD1	2:B:320:ASP:C	2.62	0.42
1:C:480:GLN:O	1:C:483:TYR:HB3	2.19	0.42
2:D:187:LEU:HD12	2:D:187:LEU:HA	1.80	0.42
2:D:398:TRP:CD1	2:D:416:PHE:CE1	3.07	0.42
1:A:537:PRO:HD2	1:A:542:ILE:HD11	2.01	0.42
2:B:35:VAL:HG12	2:B:36:GLU:N	2.34	0.42
2:D:85:GLN:HA	2:D:88:TRP:CD1	2.54	0.42
2:D:108:VAL:HB	2:D:188:TYR:HD1	1.85	0.42
1:A:172:LYS:HE2	1:A:180:ILE:HB	2.02	0.42
1:A:225:PRO:HD3	1:A:227:PHE:CE1	2.55	0.42
1:A:255:ASN:HB2	1:A:289:LEU:HG	2.00	0.42
1:C:296:THR:O	1:C:300:GLU:HB2	2.20	0.42
2:D:193:LEU:HD23	2:D:197:GLN:HB3	2.02	0.42
2:D:331:LYS:O	2:D:424:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:TRP:HB3	2:D:405:TYR:CE2	2.53	0.42
1:A:191:SER:HB2	1:A:193:LEU:HG	2.02	0.42
1:A:249:LYS:HB3	1:A:249:LYS:HE3	1.77	0.42
1:A:407:GLN:HG2	2:B:393:ILE:HA	2.02	0.42
1:A:410:TRP:CZ2	1:A:412:PRO:HA	2.54	0.42
1:A:433:PRO:HB2	2:B:290:THR:CG2	2.49	0.42
2:B:157:PRO:HG3	2:B:184:MET:HA	2.01	0.42
2:B:261:VAL:HA	2:B:264:LEU:HD12	2.02	0.42
1:C:362:THR:OG1	1:C:363:ASN:N	2.53	0.42
1:C:491:LEU:HD13	1:C:529:GLU:OE1	2.18	0.42
1:C:494:ASN:HB3	2:D:289:LEU:CD1	2.47	0.42
2:D:354:TYR:CZ	2:D:374:LYS:HG2	2.55	0.42
3:E:7:G:H2'	3:E:8:G:H8	1.84	0.42
1:C:427:TYR:CE2	1:C:525:LEU:HD13	2.55	0.41
2:D:249:LYS:HD2	2:D:252:TRP:CE3	2.55	0.41
2:D:254:VAL:O	2:D:258:GLN:HG3	2.19	0.41
1:A:32:LYS:HD3	1:A:134:SER:O	2.20	0.41
1:A:171:PHE:CE2	1:A:205:LEU:HD12	2.55	0.41
2:B:206:ARG:O	2:B:210:LEU:HB2	2.20	0.41
2:B:249:LYS:HG3	2:B:252:TRP:CZ3	2.54	0.41
2:B:401:TRP:C	2:B:404:GLU:H	2.28	0.41
2:B:411:ILE:HG22	2:B:412:PRO:O	2.19	0.41
1:A:108:VAL:HG12	1:A:227:PHE:CE1	2.55	0.41
1:C:5:ILE:HG13	1:C:119:PRO:HG3	2.02	0.41
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.73	0.41
2:D:115:TYR:HE2	2:D:156:SER:C	2.28	0.41
2:D:280:SER:O	2:D:282:LEU:N	2.53	0.41
1:A:257:ILE:HD11	1:A:295:LEU:HD21	2.03	0.41
2:B:179:VAL:C	2:B:180:ILE:HG12	2.45	0.41
1:C:122:GLU:CD	1:C:122:GLU:H	2.28	0.41
1:C:296:THR:HB	1:C:299:ALA:HB3	2.02	0.41
2:D:252:TRP:CE3	2:D:256:ASP:HB3	2.55	0.41
2:B:263:LYS:HE3	2:B:425:LEU:O	2.19	0.41
1:C:95:PRO:HA	2:D:136:ASN:OD1	2.19	0.41
1:C:435:VAL:HG22	2:D:290:THR:HG21	2.01	0.41
2:D:128:THR:OG1	2:D:146:TYR:HB2	2.21	0.41
2:D:155:GLY:O	2:D:156:SER:C	2.64	0.41
2:D:398:TRP:CD1	2:D:416:PHE:HZ	2.39	0.41
1:A:160:PHE:HE1	1:A:164:MET:HE2	1.84	0.41
1:A:206:ARG:HB3	1:A:216:THR:OG1	2.20	0.41
2:B:332:GLN:CD	2:B:427:TYR:CD1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:GLU:OE1	2:D:195:ILE:N	2.53	0.41
2:D:253:THR:O	2:D:257:ILE:HG12	2.21	0.41
2:D:280:SER:O	2:D:281:LYS:C	2.60	0.41
1:A:257:ILE:O	1:A:260:LEU:HB3	2.21	0.41
1:A:259:LYS:HG3	5:P:819:DG:OP1	2.21	0.41
1:A:434:ILE:CD1	1:A:494:ASN:OD1	2.64	0.41
2:B:419:THR:O	2:B:419:THR:HG22	2.20	0.41
1:C:386:THR:HA	1:C:387:PRO:HD2	1.62	0.41
2:D:391:LEU:HA	2:D:392:PRO:HD3	1.92	0.41
1:A:247:PRO:O	1:A:307:ARG:NH2	2.45	0.41
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.29	0.41
1:A:389:PHE:HB3	1:A:391:LEU:HG	2.02	0.41
1:A:497:THR:O	1:A:535:TRP:HA	2.21	0.41
2:B:115:TYR:N	2:B:115:TYR:CD1	2.89	0.41
1:C:13:LYS:HG3	1:C:84:THR:O	2.21	0.41
1:C:124:PHE:C	1:C:126:LYS:N	2.75	0.41
2:D:7:THR:HB	2:D:121:ASP:HA	2.02	0.41
2:D:17:ASP:O	2:D:83:ARG:HD3	2.20	0.41
1:A:259:LYS:HE3	1:A:263:LYS:HE3	2.02	0.41
1:A:398:TRP:CH2	1:A:411:ILE:HG13	2.56	0.41
1:A:457:TYR:HA	1:A:548:VAL:HG21	2.03	0.41
2:B:10:VAL:HG13	2:B:87:PHE:CE2	2.56	0.41
2:B:270:ILE:HG22	2:B:271:TYR:CD1	2.56	0.41
2:B:335:GLY:HA2	2:B:367:GLN:OE1	2.21	0.41
2:B:425:LEU:HD13	2:B:425:LEU:HA	1.67	0.41
1:C:135:ILE:HG12	1:C:136:ASN:OD1	2.21	0.41
1:C:221:HIS:ND1	1:C:224:GLU:HB2	2.35	0.41
1:C:228:LEU:HA	1:C:232:TYR:O	2.21	0.41
2:D:12:LEU:HD23	2:D:16:MET:O	2.21	0.41
2:D:60:VAL:HG21	2:D:73:LYS:HD2	2.02	0.41
2:D:78:ARG:HD3	2:D:411:ILE:O	2.21	0.41
2:D:113:ASP:HB2	2:D:214:LEU:HD12	2.03	0.41
2:D:387:PRO:HG2	2:D:389:PHE:CE1	2.56	0.41
1:A:54:ASN:ND2	1:A:143:ARG:HE	2.19	0.41
1:A:88:TRP:HD1	2:B:143:ARG:HD2	1.84	0.41
1:A:210:LEU:HD12	1:A:210:LEU:HA	1.74	0.41
1:A:354:TYR:CZ	1:A:370:GLU:HB3	2.56	0.41
1:A:363:ASN:HB2	1:A:511:ASP:OD2	2.21	0.41
2:B:257:ILE:HG12	2:B:257:ILE:H	1.63	0.41
2:B:401:TRP:O	2:B:404:GLU:N	2.54	0.41
2:D:115:TYR:HD2	2:D:156:SER:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:LEU:O	2:D:307:ARG:HG3	2.20	0.41
1:A:78:ARG:O	1:A:82:LYS:HG3	2.21	0.40
1:A:206:ARG:NH2	1:A:216:THR:O	2.53	0.40
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.56	0.40
2:B:166:LYS:HB2	2:B:166:LYS:HE3	1.72	0.40
2:B:367:GLN:HE21	2:B:367:GLN:HB2	1.72	0.40
1:C:120:LEU:HD23	1:C:125:ARG:HA	2.02	0.40
1:C:479:LEU:HD23	1:C:521:ILE:CD1	2.50	0.40
2:D:333:GLY:C	2:D:336:GLN:H	2.27	0.40
1:A:278:GLN:HB2	1:A:299:ALA:HA	2.03	0.40
1:A:540:LYS:HD3	1:A:540:LYS:HA	1.30	0.40
2:B:257:ILE:O	2:B:261:VAL:HG23	2.21	0.40
1:C:58:THR:O	1:C:130:PHE:HD2	2.04	0.40
2:D:180:ILE:HD13	2:D:189:VAL:HB	2.03	0.40
1:A:271:TYR:O	1:A:274:ILE:HD13	2.21	0.40
2:B:53:GLU:OE1	2:B:53:GLU:N	2.39	0.40
1:C:70:LYS:HB2	1:C:70:LYS:HE3	1.82	0.40
1:C:354:TYR:OH	1:C:370:GLU:HB3	2.21	0.40
2:D:345:PRO:O	2:D:346:PHE:HB2	2.20	0.40
2:D:358:ARG:HG2	2:D:366:LYS:CD	2.51	0.40
1:A:73:LYS:HG2	1:A:74:LEU:N	2.36	0.40
2:B:21:VAL:HG13	2:B:59:PRO:HD3	2.04	0.40
2:B:38:CYS:HB3	2:B:144:TYR:CE2	2.57	0.40
1:C:48:SER:O	1:C:144:TYR:HB2	2.22	0.40
2:D:202:ILE:HD13	2:D:202:ILE:HA	1.74	0.40
2:D:268:SER:HA	2:D:271:TYR:O	2.21	0.40
2:D:303:LEU:HD12	2:D:303:LEU:HA	1.72	0.40
2:D:372:VAL:HG13	2:D:389:PHE:CE2	2.56	0.40
2:D:423:VAL:C	2:D:425:LEU:H	2.29	0.40
5:F:809:DC:C6	5:F:810:DT:C7	3.05	0.40
1:A:239:TRP:HB3	1:A:318:TYR:OH	2.21	0.40
1:A:326:ILE:O	1:A:341:ILE:HA	2.21	0.40
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.22	0.40
2:B:357:MET:HE3	2:B:357:MET:HB2	1.61	0.40
1:C:104:LYS:HB2	1:C:104:LYS:HE3	1.84	0.40
1:C:225:PRO:HB2	1:C:226:PRO:HA	2.03	0.40
1:C:330:GLN:NE2	1:C:340:GLN:OE1	2.50	0.40
1:C:339:TYR:CE1	1:C:352:GLY:HA3	2.57	0.40
2:D:206:ARG:NH2	2:D:216:THR:O	2.43	0.40
2:D:411:ILE:HA	2:D:412:PRO:HD2	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/556 (100%)	526 (95%)	26 (5%)	1 (0%)	43	71
1	C	553/556 (100%)	522 (94%)	30 (5%)	1 (0%)	43	71
2	B	408/428 (95%)	395 (97%)	13 (3%)	0	100	100
2	D	408/428 (95%)	397 (97%)	11 (3%)	0	100	100
All	All	1922/1968 (98%)	1840 (96%)	80 (4%)	2 (0%)	48	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	C	4	PRO

5.3.2 Protein sidechains

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	495/497 (100%)	425 (86%)	70 (14%)	3	14
1	C	494/497 (99%)	432 (87%)	62 (13%)	4	18
2	B	374/390 (96%)	332 (89%)	42 (11%)	6	22
2	D	374/390 (96%)	326 (87%)	48 (13%)	4	18
All	All	1737/1774 (98%)	1515 (87%)	222 (13%)	4	18

All (222) 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	8	VAL
1	A	36	GLU
1	A	37	ILE
1	A	63	ILE
1	A	74	LEU
1	A	90	VAL
1	A	105	SER
1	A	107	THR
1	A	109	LEU
1	A	113	ASP
1	A	115	TYR
1	A	118	VAL
1	A	123	ASP
1	A	131	THR
1	A	132	ILE
1	A	137	ASN
1	A	142	ILE
1	A	146	TYR
1	A	156	SER
1	A	161	GLN
1	A	184	MET
1	A	188	TYR
1	A	193	LEU
1	A	205	LEU
1	A	210	LEU
1	A	221	HIS
1	A	222	GLN
1	A	228	LEU
1	A	244	ILE
1	A	245	VAL
1	A	254	VAL
1	A	258	CYS
1	A	292	VAL
1	A	296	THR
1	A	308	GLU
1	A	310	LEU
1	A	317	VAL
1	A	324	ASP
1	A	325	LEU
1	A	326	ILE

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Mol	Chain	Res	Type
1	A	328	GLU
1	A	341	ILE
1	A	365	VAL
1	A	372	VAL
1	A	373	GLN
1	A	375	ILE
1	A	379	SER
1	A	387	PRO
1	A	397	THR
1	A	399	GLU
1	A	442	VAL
1	A	448	ARG
1	A	452	LEU
1	A	463	ARG
1	A	470	THR
1	A	472	THR
1	A	473	THR
1	A	474	ASN
1	A	482	ILE
1	A	498	ASN
1	A	507	GLN
1	A	516	GLU
1	A	529	GLU
1	A	530	LYS
1	A	533	LEU
1	A	540	LYS
1	A	551	LEU
2	B	7	THR
2	B	21	VAL
2	B	30	LYS
2	B	35	VAL
2	B	47	ILE
2	B	63	ILE
2	B	69	THR
2	B	75	VAL
2	B	80	LEU
2	B	111	VAL
2	B	113	ASP
2	B	120	LEU
2	B	132	ILE
2	B	139	THR
2	B	142	ILE

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Mol	Chain	Res	Type
2	B	143	ARG
2	B	163	SER
2	B	178	ILE
2	B	180	ILE
2	B	195	ILE
2	B	201	LYS
2	B	208	HIS
2	B	232	TYR
2	B	233	GLU
2	B	241	VAL
2	B	250	ASP
2	B	281	LYS
2	B	293	ILE
2	B	303	LEU
2	B	308	GLU
2	B	317	VAL
2	B	321	PRO
2	B	324	ASP
2	B	326	ILE
2	B	341	ILE
2	B	358	ARG
2	B	378	GLU
2	B	388	LYS
2	B	399	GLU
2	B	424	LYS
2	B	427	TYR
2	B	428	GLN
1	C	2	ILE
1	C	3	SER
1	C	8	VAL
1	C	16	MET
1	C	21	VAL
1	C	34	LEU
1	C	35	VAL
1	C	38	CYS
1	C	42	GLU
1	C	50	ILE
1	C	63	ILE
1	C	86	ASP
1	C	94	ILE
1	C	113	ASP
1	C	122	GLU

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Mol	Chain	Res	Type
1	C	126	LYS
1	C	128	THR
1	C	130	PHE
1	C	140	PRO
1	C	142	ILE
1	C	144	TYR
1	C	163	SER
1	C	168	LEU
1	C	173	LYS
1	C	182	GLN
1	C	184	MET
1	C	195	ILE
1	C	205	LEU
1	C	209	LEU
1	C	210	LEU
1	C	216	THR
1	C	244	ILE
1	C	246	LEU
1	C	255	ASN
1	C	276	VAL
1	C	314	VAL
1	C	324	ASP
1	C	325	LEU
1	C	334	GLN
1	C	361	HIS
1	C	365	VAL
1	C	372	VAL
1	C	373	GLN
1	C	377	THR
1	C	393	ILE
1	C	434	ILE
1	C	435	VAL
1	C	442	VAL
1	C	452	LEU
1	C	454	LYS
1	C	459	THR
1	C	464	GLN
1	C	472	THR
1	C	479	LEU
1	C	482	ILE
1	C	493	VAL
1	C	497	THR

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Mol	Chain	Res	Type
1	C	505	ILE
1	C	507	GLN
1	C	540	LYS
1	C	542	ILE
1	C	552	VAL
2	D	27	THR
2	D	31	ILE
2	D	38	CYS
2	D	39	THR
2	D	47	ILE
2	D	75	VAL
2	D	84	THR
2	D	108	VAL
2	D	109	LEU
2	D	165	THR
2	D	167	ILE
2	D	178	ILE
2	D	189	VAL
2	D	193	LEU
2	D	194	GLU
2	D	202	ILE
2	D	234	LEU
2	D	241	VAL
2	D	244	ILE
2	D	245	VAL
2	D	254	VAL
2	D	276	VAL
2	D	277	ARG
2	D	287	LYS
2	D	292	VAL
2	D	295	LEU
2	D	296	THR
2	D	298	GLU
2	D	314	VAL
2	D	317	VAL
2	D	344	GLU
2	D	347	LYS
2	D	357	MET
2	D	362	THR
2	D	365	VAL
2	D	390	LYS
2	D	394	GLN

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Mol	Chain	Res	Type
2	D	395	LYS
2	D	399	GLU
2	D	400	THR
2	D	403	THR
2	D	410	TRP
2	D	413	GLU
2	D	417	VAL
2	D	422	LEU
2	D	423	VAL
2	D	425	LEU
2	D	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	151	GLN
1	A	161	GLN
1	A	182	GLN
1	A	255	ASN
1	A	418	ASN
1	A	447	ASN
1	A	475	GLN
1	A	507	GLN
1	A	545	ASN
2	B	85	GLN
2	B	151	GLN
2	B	242	GLN
2	B	315	HIS
1	C	161	GLN
1	C	255	ASN
1	C	269	GLN
1	C	418	ASN
1	C	507	GLN
2	D	137	ASN
2	D	208	HIS
2	D	255	ASN
2	D	258	GLN
2	D	269	GLN
2	D	278	GLN
2	D	336	GLN
2	D	418	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	8/14 (57%)	3 (37%)	2 (25%)
3	T	8/14 (57%)	5 (62%)	1 (12%)
4	e	8/12 (66%)	3 (37%)	0
4	t	9/12 (75%)	7 (77%)	0
All	All	33/52 (63%)	18 (54%)	3 (9%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	9	C
3	T	11	C
3	T	12	C
3	T	13	C
3	T	14	G
4	t	3	A
4	t	4	G
4	t	5	G
4	t	6	G
4	t	8	C
4	t	9	U
4	t	10	G
3	E	12	C
3	E	13	C
3	E	14	G
4	e	5	G
4	e	6	G
4	e	7	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	T	11	C
3	E	11	C
3	E	13	C

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
6	NVP	C	901	-	23,23,23	1.51	5 (21%)	34,34,34	4.81	19 (55%)
6	NVP	A	901	-	23,23,23	1.45	4 (17%)	34,34,34	3.73	15 (44%)
8	SO4	e	801	-	4,4,4	0.26	0	6,6,6	0.15	0

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

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

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	901	NVP	C2-N3	3.44	1.40	1.34
6	C	901	NVP	C15-N14	3.11	1.40	1.34
6	C	901	NVP	C2-N3	3.06	1.40	1.34
6	A	901	NVP	C15-N14	2.83	1.39	1.34
6	C	901	NVP	C4-N3	2.78	1.40	1.34
6	A	901	NVP	C4-N3	2.71	1.40	1.34
6	A	901	NVP	C13-N14	2.56	1.40	1.34
6	C	901	NVP	C13-N14	2.44	1.39	1.34
6	C	901	NVP	C9-N8	-2.05	1.33	1.35

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	901	NVP	C7-C2-N1	19.22	127.52	120.14
6	A	901	NVP	C7-C2-N1	13.58	125.36	120.14
6	A	901	NVP	C7-N8-C9	-10.68	119.48	128.29
6	C	901	NVP	C7-N8-C9	-7.92	121.76	128.29
6	C	901	NVP	C6-C7-N8	-7.35	112.67	119.18
6	C	901	NVP	OE-C9-N8	-6.12	114.41	120.38
6	C	901	NVP	N3-C2-N1	-5.79	112.29	116.67
6	C	901	NVP	N14-C15-N1	-5.12	112.80	116.67
6	C	901	NVP	C10-C15-N1	4.83	126.97	120.95
6	C	901	NVP	C2-C7-N8	4.81	125.99	121.46
6	C	901	NVP	CC-CA-N1	-4.77	113.27	116.09
6	C	901	NVP	C10-C9-N8	4.71	124.81	120.22
6	C	901	NVP	C15-N1-C2	4.66	120.42	115.29
6	A	901	NVP	C11-C10-C15	4.52	121.67	117.23
6	A	901	NVP	C10-C15-N1	4.48	126.53	120.95
6	A	901	NVP	N14-C15-N1	-4.47	113.29	116.67
6	C	901	NVP	C15-C10-C9	3.94	127.86	124.01
6	A	901	NVP	C6-C7-N8	-3.90	115.73	119.18
6	A	901	NVP	C10-C9-N8	3.57	123.70	120.22
6	A	901	NVP	OE-C9-N8	-3.51	116.96	120.38
6	C	901	NVP	C5-C4-N3	-3.47	119.72	123.97
6	A	901	NVP	C11-C10-C9	-3.31	111.23	116.76
6	C	901	NVP	C11-C10-C15	3.21	120.39	117.23
6	A	901	NVP	N3-C2-N1	-3.16	114.28	116.67
6	A	901	NVP	C15-C10-C9	3.16	127.09	124.01
6	C	901	NVP	C11-C10-C9	-3.00	111.75	116.76
6	C	901	NVP	C6-C7-C2	2.97	121.34	119.03
6	A	901	NVP	C6-C7-C2	2.84	121.24	119.03
6	C	901	NVP	CB-CA-N1	2.45	117.54	116.09
6	C	901	NVP	C12-C13-N14	-2.36	119.69	123.42
6	C	901	NVP	C4-N3-C2	2.23	120.10	115.05
6	A	901	NVP	C5-C4-N3	-2.11	121.39	123.97
6	A	901	NVP	C15-N1-CA	2.07	117.98	116.34
6	A	901	NVP	C12-C13-N14	-2.06	120.16	123.42

There are no chirality outliers.

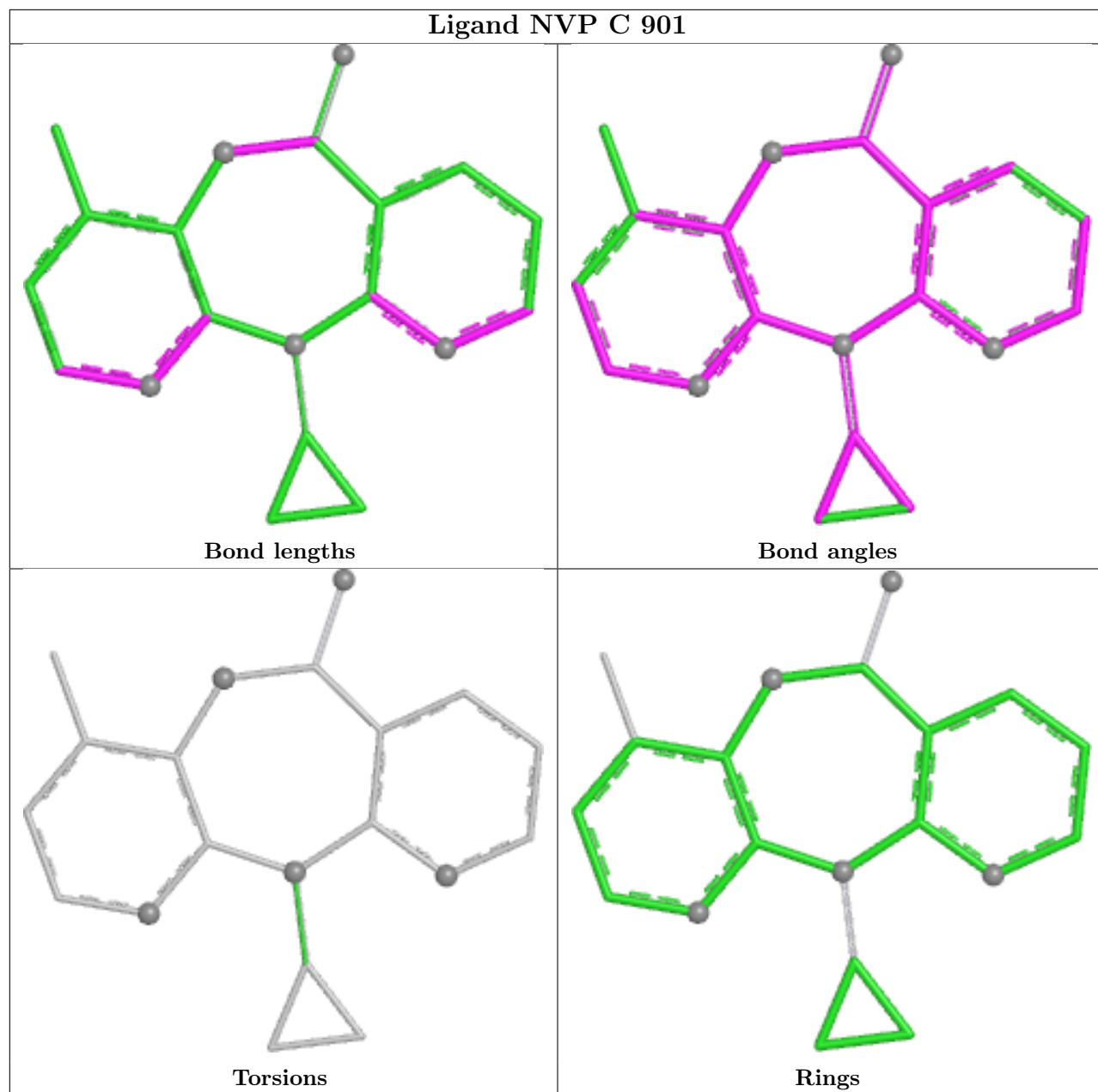
There are no torsion outliers.

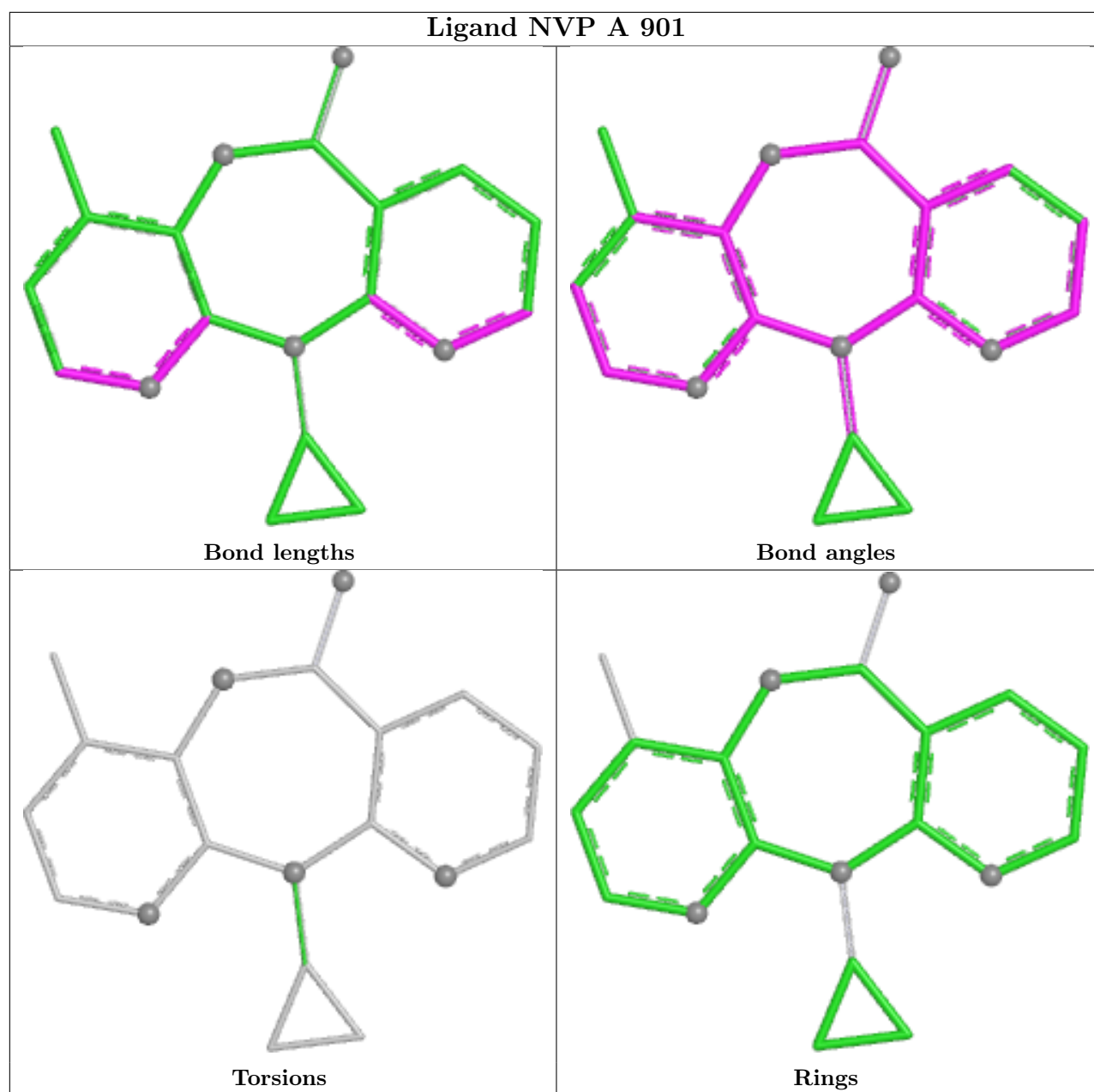
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	901	NVP	1	0
6	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 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	555/556 (99%)	-0.09	13 (2%) 61 42	21, 82, 195, 225	0
1	C	555/556 (99%)	-0.04	15 (2%) 56 37	16, 93, 206, 228	0
2	B	412/428 (96%)	-0.32	5 (1%) 76 58	23, 64, 113, 140	0
2	D	412/428 (96%)	-0.19	5 (1%) 76 58	22, 68, 120, 150	0
3	E	9/14 (64%)	-0.17	0 100 100	149, 156, 179, 197	0
3	T	9/14 (64%)	-0.10	0 100 100	139, 144, 168, 201	0
4	e	9/12 (75%)	0.29	0 100 100	127, 136, 165, 175	0
4	t	10/12 (83%)	-0.03	0 100 100	103, 124, 159, 172	0
5	F	19/21 (90%)	0.08	0 100 100	96, 140, 198, 200	0
5	P	19/21 (90%)	0.02	0 100 100	78, 125, 174, 176	0
All	All	2009/2062 (97%)	-0.14	38 (1%) 66 48	16, 76, 185, 228	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	ILE	5.2
1	A	133	PRO	4.7
1	C	135	ILE	3.3
2	D	214	LEU	3.1
2	B	214	LEU	3.1
1	C	241	VAL	3.0
1	C	140	PRO	2.9
1	C	33	ALA	2.9
1	A	35	VAL	2.7
2	B	167	ILE	2.7
1	C	31	ILE	2.6
1	C	183	TYR	2.6
1	C	54	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	217	PRO	2.5
1	C	34	LEU	2.5
1	C	214	LEU	2.5
1	C	37	ILE	2.4
1	C	71	TRP	2.3
1	C	276	VAL	2.3
1	A	26	LEU	2.3
2	B	209	LEU	2.3
1	A	34	LEU	2.2
2	D	425	LEU	2.2
2	B	425	LEU	2.2
1	A	214	LEU	2.2
2	D	354	TYR	2.1
1	A	151	GLN	2.1
1	A	89	GLU	2.1
1	A	546	GLU	2.1
1	C	60	VAL	2.1
1	C	30	LYS	2.1
1	A	31	ILE	2.1
2	D	18	GLY	2.1
1	A	60	VAL	2.0
1	A	73	LYS	2.0
1	A	37	ILE	2.0
2	D	360	ALA	2.0
1	C	188	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

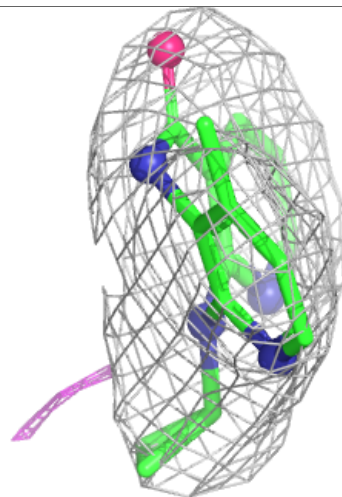
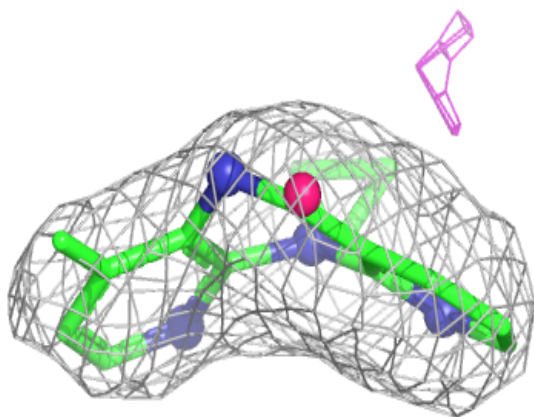
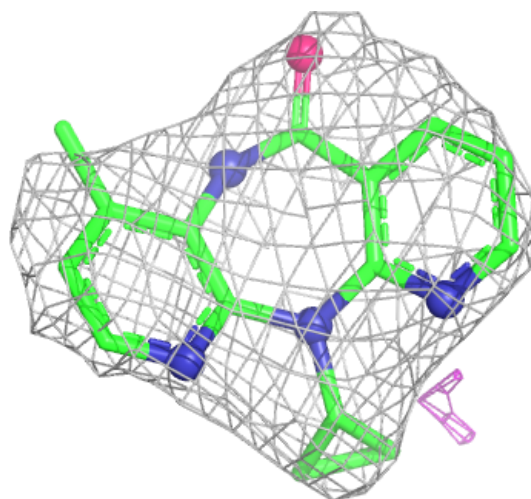
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	SO4	e	801	5/5	0.44	0.09	173,175,182,185	0
6	NVP	A	901	20/20	0.89	0.12	64,72,79,79	0
7	MN	A	902	1/1	0.95	0.09	73,73,73,73	0
6	NVP	C	901	20/20	0.95	0.11	79,85,91,93	0
7	MN	C	902	1/1	0.98	0.03	63,63,63,63	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.

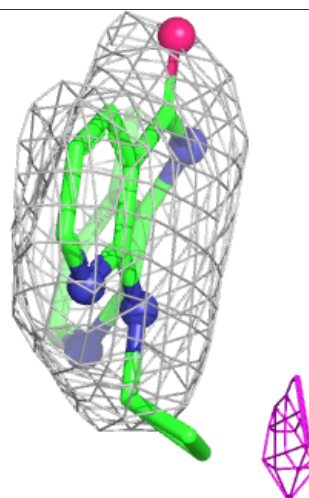
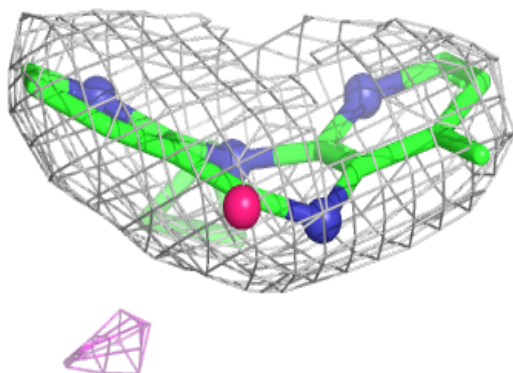
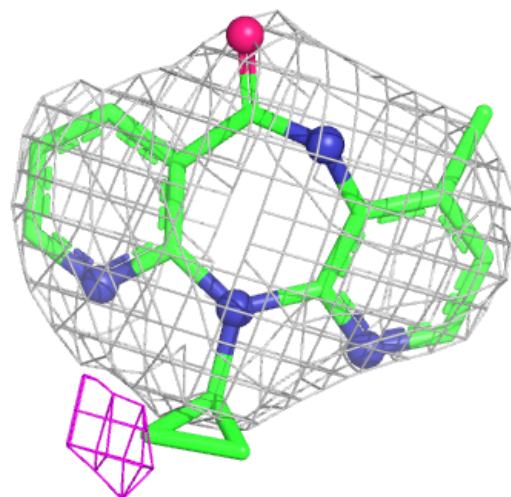
Electron density around NVP A 901:

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 [i](#)

There are no such residues in this entry.