



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:57 PM UTC

PDB ID : 4PWD / pdb_00004pwd
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:

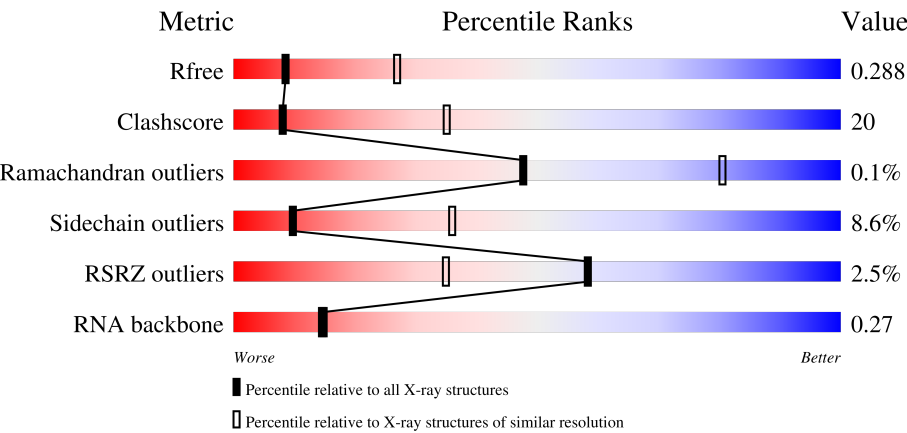
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	3% 52% 42% 6% .
1	C	556	3% 60% 34% 5%
2	B	428	% 51% 40% 5% .
2	D	428	2% 51% 40% 5% .

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Mol	Chain	Length	Quality of chain
3	E	27	
3	T	27	
4	F	21	
4	P	21	

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

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

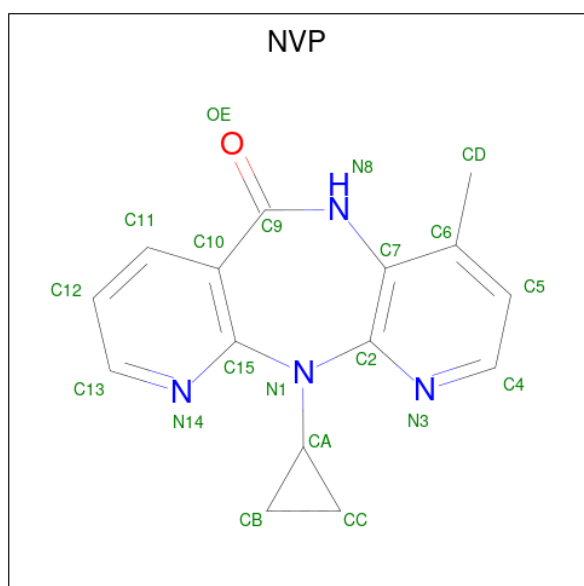
- Molecule 3 is a RNA chain called 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*GP*AP*AP*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*U)-3'.

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'.

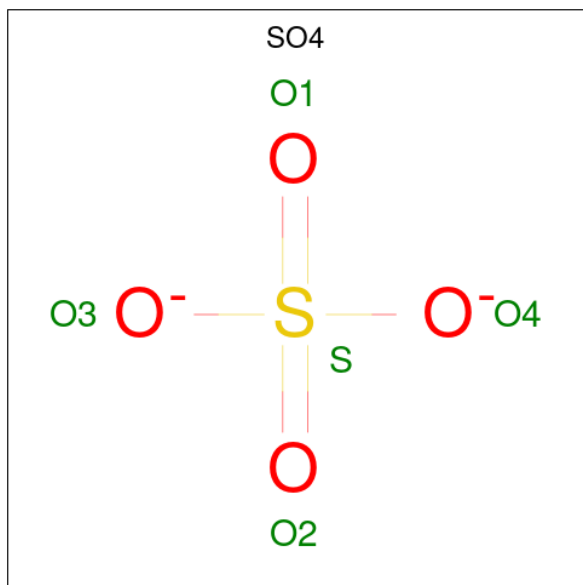
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	19	Total	C	N	O	P	0	0	0
			382	182	67	115	18			
4	F	19	Total	C	N	O	P	0	0	0
			382	182	67	115	18			

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

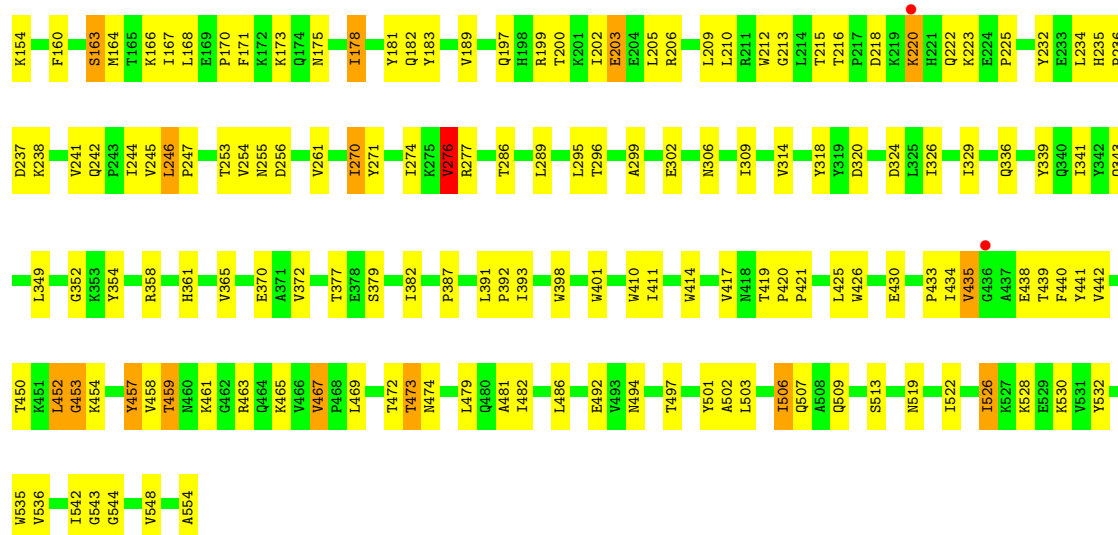


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		
6	C	1	Total	Ca	0	0
			1	1		

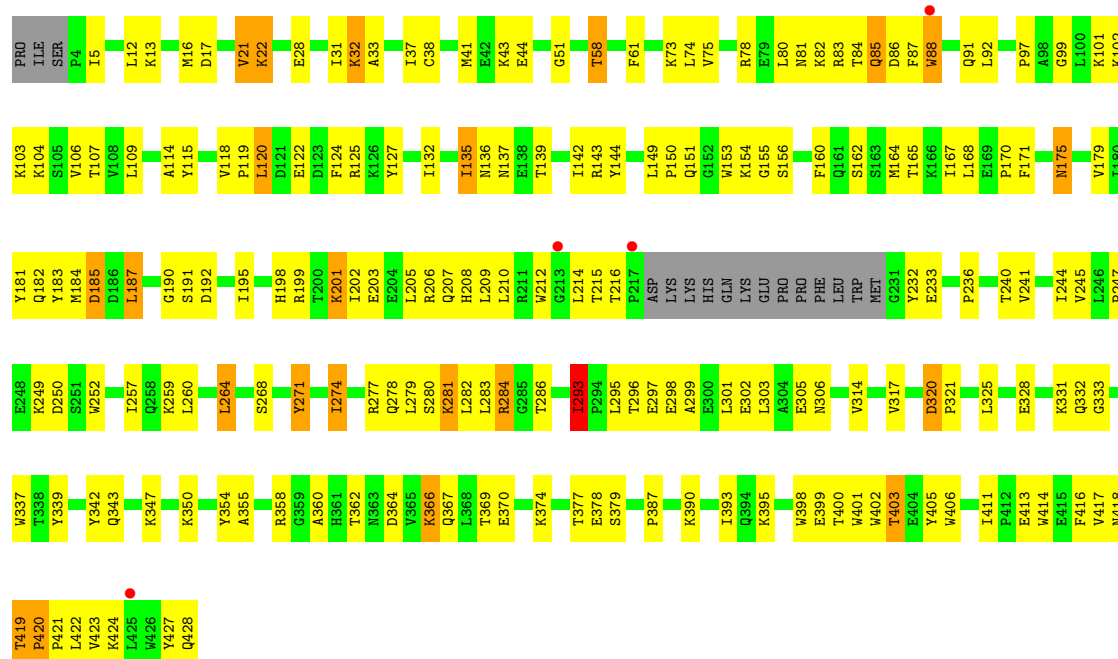
- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



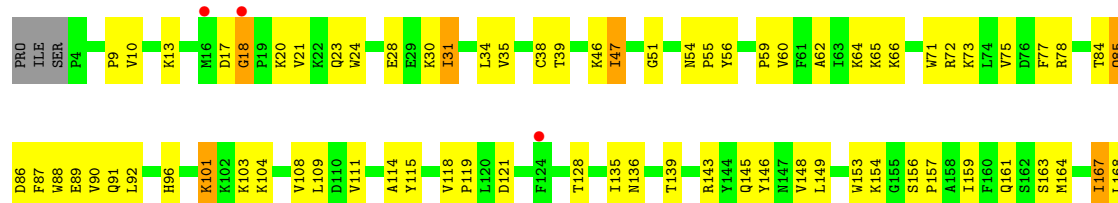
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		

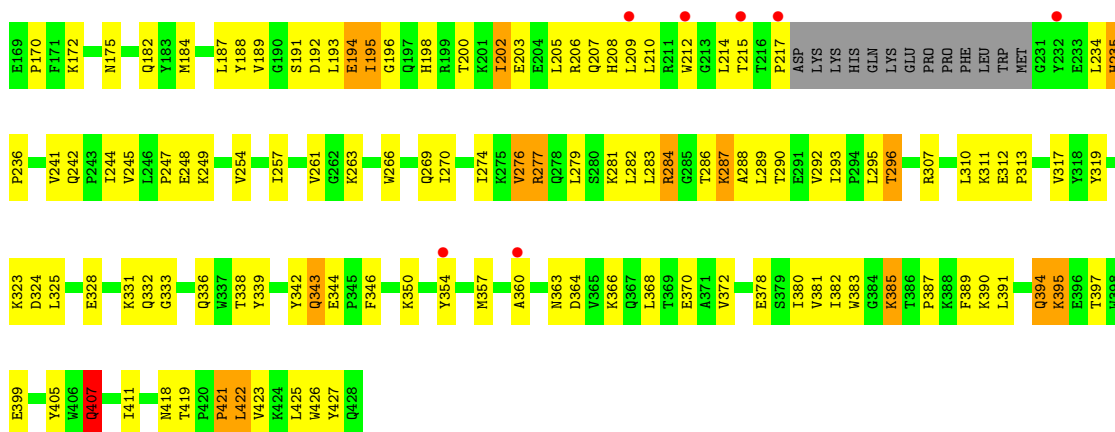


• Molecule 2: HIV-1 Reverse Transcriptase, P51 subunit



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





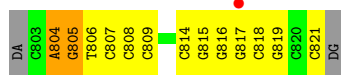
• Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*GP*AP*AP*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*U)-3'



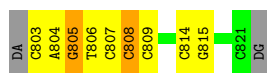
• Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*GP*AP*AP*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*U)-3'



• 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

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 44.68 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (44.68-3.00) 96.1 (44.68-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 0.288	Depositor DCC
R_{free} test set	1841 reflections (2.86%)	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)	0.33 , 83.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

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: 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	0.95	6/4624 (0.1%)	1.25	47/6283 (0.7%)
1	C	0.89	4/4624 (0.1%)	1.20	32/6283 (0.5%)
2	B	0.93	3/3497 (0.1%)	1.23	30/4751 (0.6%)
2	D	0.90	1/3497 (0.0%)	1.25	33/4751 (0.7%)
3	E	0.52	0/482	0.88	1/750 (0.1%)
3	T	0.61	0/508	1.02	2/791 (0.3%)
4	F	0.58	0/426	0.77	2/655 (0.3%)
4	P	0.67	0/426	0.88	2/655 (0.3%)
All	All	0.89	14/18084 (0.1%)	1.20	149/24919 (0.6%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	SER	CA-C	6.73	1.59	1.52
2	B	419	THR	C-N	6.61	1.39	1.33
1	A	466	VAL	C-O	-6.40	1.17	1.24
1	C	457	TYR	CA-C	-6.03	1.45	1.52
1	C	467	VAL	CA-CB	-6.01	1.47	1.54
1	A	429	LEU	C-O	-5.63	1.17	1.23
1	C	440	PHE	CA-C	-5.62	1.46	1.52
2	D	288	ALA	CA-CB	-5.56	1.44	1.53
1	A	495	ILE	CA-CB	-5.55	1.47	1.54
2	B	401	TRP	C-O	-5.42	1.17	1.24
1	A	495	ILE	C-O	-5.17	1.18	1.24
1	A	365	VAL	CA-CB	-5.15	1.48	1.54
2	B	355	ALA	CA-CB	-5.15	1.44	1.53
1	C	522	ILE	CA-CB	-5.03	1.48	1.54

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	139	THR	CA-C-N	-14.45	101.78	119.84
2	D	139	THR	C-N-CA	-14.45	101.78	119.84
2	B	139	THR	CA-C-N	-11.65	108.51	120.98
2	B	139	THR	C-N-CA	-11.65	108.51	120.98
4	P	804	DA	C2'-C3'-O3'	11.38	128.57	111.50
1	C	118	VAL	CA-C-N	9.72	130.33	119.83
1	C	118	VAL	C-N-CA	9.72	130.33	119.83
1	C	24	TRP	CA-C-N	9.71	131.97	119.84
1	C	24	TRP	C-N-CA	9.71	131.97	119.84
1	A	149	LEU	CA-C-N	9.08	128.84	119.76
1	A	149	LEU	C-N-CA	9.08	128.84	119.76
2	B	51	GLY	CA-C-N	8.70	128.92	119.87
2	B	51	GLY	C-N-CA	8.70	128.92	119.87
2	D	54	ASN	CA-C-N	8.57	128.78	119.87
2	D	54	ASN	C-N-CA	8.57	128.78	119.87
2	B	284	ARG	N-CA-C	8.20	120.95	111.11
1	A	29	GLU	N-CA-C	8.02	119.80	111.14
1	A	18	GLY	CA-C-N	7.98	128.13	120.31
1	A	18	GLY	C-N-CA	7.98	128.13	120.31
1	A	141	GLY	N-CA-C	7.92	121.63	110.38
2	B	21	VAL	N-CA-C	7.80	119.64	109.58
2	D	195	ILE	N-CA-C	7.80	118.55	110.36
2	B	419	THR	CA-C-N	-7.79	113.97	119.66
2	B	419	THR	C-N-CA	-7.79	113.97	119.66
1	C	134	SER	N-CA-C	7.76	119.43	110.97
3	T	713	C	C3'-C2'-O2'	-7.40	99.60	110.70
1	C	4	PRO	N-CA-C	7.34	127.60	112.47
2	D	96	HIS	N-CA-C	7.27	120.19	109.50
2	D	284	ARG	N-CA-C	7.26	120.06	111.71
4	F	808	DC	C2'-C3'-O3'	-7.25	100.63	111.50
1	C	453	GLY	N-CA-C	7.20	121.41	110.18
2	B	293	ILE	CA-C-N	7.15	127.72	120.14
2	B	293	ILE	C-N-CA	7.15	127.72	120.14
2	B	271	TYR	CA-C-N	7.11	126.81	119.56
2	B	271	TYR	C-N-CA	7.11	126.81	119.56
2	D	235	HIS	CA-C-N	7.11	128.72	119.84
2	D	235	HIS	C-N-CA	7.11	128.72	119.84
1	C	62	ALA	N-CA-C	7.05	119.65	109.14
4	F	805	DG	C2'-C3'-O3'	7.03	122.04	111.50
1	A	93	GLY	N-CA-C	-6.97	102.78	111.70
1	A	391	LEU	N-CA-C	6.93	121.61	109.48
1	C	78	ARG	N-CA-C	-6.88	104.92	113.38
3	T	712	C	C3'-C2'-O2'	-6.87	100.40	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	GLY	CA-C-N	6.85	128.41	119.84
1	C	18	GLY	C-N-CA	6.85	128.41	119.84
1	A	195	ILE	N-CA-C	6.84	118.42	110.62
1	A	382	ILE	N-CA-C	6.84	116.96	110.74
1	A	552	VAL	N-CA-C	6.82	121.97	112.35
1	A	184	MET	CB-CA-C	-6.67	108.90	116.63
2	D	324	ASP	N-CA-C	6.67	119.90	110.50
2	D	51	GLY	CA-C-N	6.65	126.33	119.82
2	D	51	GLY	C-N-CA	6.65	126.33	119.82
1	A	65	LYS	N-CA-C	6.65	120.23	109.40
1	A	435	VAL	N-CA-C	6.56	117.89	109.30
2	D	270	ILE	N-CA-C	-6.55	105.32	111.48
2	B	85	GLN	N-CA-C	6.51	118.92	111.11
1	A	92	LEU	N-CA-C	-6.45	105.28	113.02
1	C	220	LYS	N-CA-C	6.38	118.10	110.19
1	A	25	PRO	N-CA-C	6.37	121.21	111.15
1	C	324	ASP	N-CA-C	6.36	119.90	110.48
1	A	21	VAL	N-CA-C	6.24	118.92	108.81
1	A	62	ALA	N-CA-C	6.24	118.89	109.41
1	C	276	VAL	N-CA-C	6.20	118.97	112.83
2	D	346	PHE	CA-C-N	-6.15	114.03	123.14
2	D	346	PHE	C-N-CA	-6.15	114.03	123.14
1	A	74	LEU	N-CA-C	6.11	118.59	108.99
2	D	287	LYS	N-CA-C	6.09	119.59	110.14
1	C	118	VAL	N-CA-C	6.08	117.32	107.71
1	A	410	TRP	N-CA-C	6.07	118.35	108.76
2	B	43	LYS	N-CA-C	-5.99	104.08	111.33
2	D	385	LYS	N-CA-C	-5.94	100.05	109.07
1	A	31	ILE	N-CA-C	5.91	120.68	113.00
2	D	391	LEU	N-CA-C	5.91	117.46	109.24
2	B	320	ASP	CA-C-N	5.88	126.29	119.47
2	B	320	ASP	C-N-CA	5.88	126.29	119.47
2	B	420	PRO	CA-C-N	-5.87	113.17	120.79
2	B	420	PRO	C-N-CA	-5.87	113.17	120.79
1	A	293	ILE	CA-C-N	5.86	126.35	120.14
1	A	293	ILE	C-N-CA	5.86	126.35	120.14
1	C	8	VAL	CA-C-N	5.86	125.87	119.90
1	C	8	VAL	C-N-CA	5.86	125.87	119.90
1	A	453	GLY	N-CA-C	5.84	120.12	110.55
3	E	714	G	C2'-C3'-O3'	5.83	122.45	113.70
1	A	432	GLU	CA-C-N	5.82	127.12	119.84
1	A	432	GLU	C-N-CA	5.82	127.12	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	805	DG	C2'-C3'-O3'	5.82	120.23	111.50
2	B	259	LYS	N-CA-C	-5.82	104.94	111.28
1	A	51	GLY	N-CA-C	5.79	124.15	112.34
1	A	198	HIS	N-CA-C	-5.76	104.92	111.14
1	A	242	GLN	CA-C-N	5.75	126.08	119.93
1	A	242	GLN	C-N-CA	5.75	126.08	119.93
1	A	3	SER	N-CA-C	5.74	122.00	108.40
1	A	276	VAL	N-CA-C	5.73	118.40	112.90
2	D	193	LEU	N-CA-C	5.72	118.08	110.53
1	C	382	ILE	N-CA-C	5.71	116.36	110.82
1	C	320	ASP	CA-C-N	5.69	126.95	119.84
1	C	320	ASP	C-N-CA	5.69	126.95	119.84
1	A	312	GLU	CA-C-N	-5.64	114.94	120.98
1	A	312	GLU	C-N-CA	-5.64	114.94	120.98
1	A	388	LYS	N-CA-C	-5.63	100.11	109.46
2	B	88	TRP	CA-CB-CG	5.59	124.22	113.60
2	B	333	GLY	N-CA-C	5.58	119.91	112.65
1	A	106	VAL	N-CA-C	5.57	116.08	107.78
1	C	4	PRO	CB-CA-C	-5.56	102.39	111.56
1	C	473	THR	N-CA-C	5.56	118.75	110.52
2	D	419	THR	CA-C-N	-5.53	114.69	120.38
2	D	419	THR	C-N-CA	-5.53	114.69	120.38
2	D	175	ASN	CA-C-N	5.50	125.12	119.56
2	D	175	ASN	C-N-CA	5.50	125.12	119.56
2	D	96	HIS	CA-C-N	5.48	126.69	119.84
2	D	96	HIS	C-N-CA	5.48	126.69	119.84
1	A	94	ILE	CA-C-N	5.46	125.40	119.78
1	A	94	ILE	C-N-CA	5.46	125.40	119.78
2	D	381	VAL	CA-C-N	-5.46	117.62	122.97
2	D	381	VAL	C-N-CA	-5.46	117.62	122.97
1	A	320	ASP	CA-C-N	5.46	126.66	119.84
1	A	320	ASP	C-N-CA	5.46	126.66	119.84
2	D	184	MET	CB-CA-C	-5.46	110.27	116.54
2	B	420	PRO	O-C-N	5.43	123.81	121.31
2	B	403	THR	N-CA-C	5.42	119.39	112.34
2	D	407	GLN	N-CA-C	5.38	120.71	113.72
1	C	246	LEU	CA-C-N	5.37	125.13	119.76
1	C	246	LEU	C-N-CA	5.37	125.13	119.76
1	A	190	GLY	N-CA-C	5.35	119.11	110.87
1	C	149	LEU	CA-C-N	5.34	126.52	119.84
1	C	149	LEU	C-N-CA	5.34	126.52	119.84
1	A	219	LYS	N-CA-C	-5.33	106.47	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	168	LEU	N-CA-C	5.33	118.95	112.23
1	C	467	VAL	N-CA-C	5.32	113.80	107.73
1	C	129	ALA	N-CA-C	5.31	117.98	110.50
2	D	85	GLN	N-CA-C	5.28	117.72	111.33
2	B	175	ASN	CA-C-N	5.28	124.78	119.19
2	B	175	ASN	C-N-CA	5.28	124.78	119.19
2	B	233	GLU	N-CA-C	5.24	117.83	110.23
2	D	421	PRO	CA-N-CD	-5.21	104.70	112.00
1	C	17	ASP	N-CA-C	5.18	116.86	109.14
1	C	242	GLN	CA-C-N	5.15	125.15	119.90
1	C	242	GLN	C-N-CA	5.15	125.15	119.90
1	A	505	ILE	N-CA-C	5.15	115.37	110.53
1	A	277	ARG	N-CA-C	5.13	117.26	111.11
1	A	493	VAL	N-CA-C	5.12	114.62	108.06
2	B	401	TRP	N-CA-C	5.12	120.38	113.72
1	A	118	VAL	N-CA-C	5.10	113.54	107.73
2	D	18	GLY	CA-C-N	-5.08	114.68	119.76
2	D	18	GLY	C-N-CA	-5.08	114.68	119.76
1	A	143	ARG	N-CA-C	5.05	115.72	108.74
2	B	414	TRP	N-CA-C	5.05	116.92	108.99
2	B	296	THR	N-CA-C	-5.03	103.85	110.43
1	C	28	GLU	N-CA-C	5.02	119.04	113.01

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	179	0
1	C	4506	0	4560	158	0
2	B	3400	0	3433	148	0
2	D	3400	0	3433	127	0
3	E	431	0	220	20	0
3	T	454	0	231	20	0
4	F	382	0	215	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	661	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 20.

All (661) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:160:PHE:HE1	1:A:164:MET:HE2	1.50	0.75
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: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
2:B:191:SER:HG	2:B:198:HIS:HD1	1.34	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
1:A:206:ARG:HH11	1:A:220:LYS:HZ3	1.35	0.72
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
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
2:D:422:LEU:C	2:D:422:LEU:HD23	2.16	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:A:225:PRO:HA	1:A:226:PRO:C	2.20	0.67
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
2:D:164:MET:HE1	2:D:209:LEU:HD21	1.78	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: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
2:D:164:MET:HE3	2:D:168:LEU:HG	1.80	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
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
1:A:160:PHE:CE1	1:A:164:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LYS:O	1:A:343:GLN:NE2	2.33	0.62
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
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
1:C:122:GLU:H	1:C:122:GLU:CD	2.11	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
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
1:A:420:PRO:HA	1:A:421:PRO:C	2.29	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
2:D:194:GLU:CD	2:D:195:ILE:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:395:LYS:NZ	1:A:414:TRP:O	2.32	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:C:30:LYS:HZ1	1:C:64:LYS:HD2	1.71	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:A:77:PHE:O	1:A:80:LEU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:457:TYR:C	1:C:457:TYR:CD1	2.85	0.53
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:160:PHE:CD1	1:A:160:PHE:C	2.85	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
2:B:175:ASN:OD1	2:B:201:LYS:NZ	2.36	0.52
1:A:282:LEU:HB3	1:A:293:ILE:HG21	1.91	0.52
2:D:72:ARG:HD3	2:D:73:LYS:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:420:PRO:HA	1:C:421:PRO:C	2.34	0.52
1:C:474:ASN:ND2	3:E:722:A:O2'	2.43	0.51
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:160:PHE:C	1:A:160:PHE:HD1	2.20	0.49
1:A:398:TRP:NE1	1:A:402:TRP:CD1	2.79	0.49
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
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
2:D:66:LYS:HG3	2:D:407:GLN:CD	2.38	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:164:MET:HE1	2:B:209:LEU:HD21	1.96	0.48
1:C:85:GLN:C	1:C:154:LYS:HZ1	2.20	0.48
1:A:47:ILE:HG23	1:A:144:TYR:HD2	1.79	0.48
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: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: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:160:PHE:C	1:C:160:PHE:CD1	2.90	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
2:B:331:LYS:NZ	2:B:364:ASP:OD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:245:VAL:O	1:A:263:LYS:NZ	2.46	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:342:TYR:CD1	1:A:342:TYR:C	2.95	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
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:B:13:LYS:HG3	2:B:16:MET:HE1	1.99	0.45
2:B:82:LYS:NZ	2:B:413:GLU:OE2	2.46	0.45
2:D:28:GLU:HA	2:D:135:ILE:HD11	1.99	0.45
1:C:361:HIS:HD1	1:C:513:SER:HG	1.61	0.44
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
2:D:191:SER:OG	2:D:198:HIS:ND1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:218:ASP:C	1:A:220:LYS:N	2.76	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
2:D:331:LYS:NZ	2:D:364:ASP:OD2	2.46	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:A:277:ARG:HB2	1:A:336:GLN:CD	2.43	0.43
1:C:41:MET:HE3	1:C:41:MET:HB2	1.68	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:398:TRP:O	1:A:399:GLU:C	2.60	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
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
2:D:23:GLN:HG3	2:D:24:TRP:O	2.19	0.42
1:C:37:ILE:HA	1:C:40:GLU:CD	2.44	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:B:328:GLU:OE1	2:B:342:TYR:OH	2.33	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:292:VAL:C	2:D:293:ILE:HD13	2.45	0.42
2:D:339:TYR:CE1	2:D:354:TYR:CE2	3.08	0.42
2:D:357:MET:HE3	2:D:357:MET:HB2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:218:ASP:C	1:C:220:LYS:H	2.28	0.42
1:C:246:LEU:HA	1:C:247:PRO:HD3	1.84	0.42
1:C:277:ARG:HB2	1:C:336:GLN:CD	2.45	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
2:D:153:TRP:CD1	2:D:154:LYS:H	2.38	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
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
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
2:B:16:MET:HB2	2:B:16:MET:HE3	1.82	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
2:D:115:TYR:HE1	2:D:156:SER:C	2.28	0.41
3:T:719:G:H2'	3:T:720:G:H8	1.84	0.41
1:A:199:ARG:HE	1:A:222:GLN:CD	2.27	0.41
2:B:320:ASP:OD1	2:B:320:ASP:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:THR:HG22	1:C:256:ASP:CG	2.45	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:103:LYS:HA	2:B:103:LYS:HD3	1.92	0.41
1:C:479:LEU:HD11	1:C:501:TYR:CE2	2.56	0.41
2:D:104:LYS:HD2	2:D:192:ASP:HB3	2.03	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:77:PHE:O	2:D:78:ARG:C	2.63	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:360:ALA:HA	2:B:367:GLN:CD	2.46	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

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%)	525 (95%)	27 (5%)	1 (0%)	43	76
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%)	48	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	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	494/497 (99%)	450 (91%)	44 (9%)	9	34
1	C	494/497 (99%)	459 (93%)	35 (7%)	13	43
2	B	374/390 (96%)	338 (90%)	36 (10%)	8	31
2	D	374/390 (96%)	340 (91%)	34 (9%)	9	33
All	All	1736/1774 (98%)	1587 (91%)	149 (9%)	10	36

All (149) 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	21	VAL
1	A	74	LEU
1	A	84	THR
1	A	109	LEU
1	A	123	ASP
1	A	130	PHE
1	A	131	THR
1	A	132	ILE
1	A	135	ILE
1	A	137	ASN
1	A	142	ILE
1	A	146	TYR
1	A	182	GLN
1	A	189	VAL
1	A	221	HIS
1	A	228	LEU

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Mol	Chain	Res	Type
1	A	230	MET
1	A	258	CYS
1	A	292	VAL
1	A	297	GLU
1	A	301	LEU
1	A	308	GLU
1	A	317	VAL
1	A	338	THR
1	A	357	MET
1	A	373	GLN
1	A	399	GLU
1	A	420	PRO
1	A	428	GLN
1	A	435	VAL
1	A	442	VAL
1	A	463	ARG
1	A	469	LEU
1	A	472	THR
1	A	473	THR
1	A	493	VAL
1	A	507	GLN
1	A	529	GLU
1	A	530	LYS
1	A	533	LEU
1	A	547	GLN
2	B	12	LEU
2	B	21	VAL
2	B	22	LYS
2	B	31	ILE
2	B	32	LYS
2	B	58	THR
2	B	73	LYS
2	B	120	LEU
2	B	135	ILE
2	B	143	ARG
2	B	151	GLN
2	B	185	ASP
2	B	187	LEU
2	B	201	LYS
2	B	206	ARG
2	B	240	THR
2	B	241	VAL

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Mol	Chain	Res	Type
2	B	245	VAL
2	B	250	ASP
2	B	257	ILE
2	B	264	LEU
2	B	268	SER
2	B	274	ILE
2	B	277	ARG
2	B	280	SER
2	B	281	LYS
2	B	293	ILE
2	B	302	GLU
2	B	305	GLU
2	B	321	PRO
2	B	362	THR
2	B	366	LYS
2	B	369	THR
2	B	377	THR
2	B	400	THR
2	B	403	THR
1	C	2	ILE
1	C	3	SER
1	C	21	VAL
1	C	35	VAL
1	C	47	ILE
1	C	50	ILE
1	C	128	THR
1	C	130	PHE
1	C	138	GLU
1	C	140	PRO
1	C	142	ILE
1	C	144	TYR
1	C	146	TYR
1	C	163	SER
1	C	168	LEU
1	C	173	LYS
1	C	178	ILE
1	C	182	GLN
1	C	189	VAL
1	C	203	GLU
1	C	209	LEU
1	C	215	THR
1	C	234	LEU

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Mol	Chain	Res	Type
1	C	270	ILE
1	C	276	VAL
1	C	314	VAL
1	C	358	ARG
1	C	377	THR
1	C	435	VAL
1	C	452	LEU
1	C	459	THR
1	C	472	THR
1	C	497	THR
1	C	506	ILE
1	C	526	ILE
2	D	31	ILE
2	D	35	VAL
2	D	39	THR
2	D	47	ILE
2	D	90	VAL
2	D	101	LYS
2	D	108	VAL
2	D	109	LEU
2	D	167	ILE
2	D	189	VAL
2	D	194	GLU
2	D	202	ILE
2	D	212	TRP
2	D	234	LEU
2	D	245	VAL
2	D	248	GLU
2	D	249	LYS
2	D	254	VAL
2	D	274	ILE
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	343	GLN
2	D	344	GLU
2	D	385	LYS
2	D	390	LYS
2	D	394	GLN

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Mol	Chain	Res	Type
2	D	395	LYS
2	D	397	THR
2	D	407	GLN
2	D	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	367	GLN
1	A	373	GLN
1	A	394	GLN
1	A	428	GLN
2	B	151	GLN
2	B	242	GLN
2	B	255	ASN
2	B	269	GLN
2	B	332	GLN
2	B	428	GLN
1	C	54	ASN
1	C	85	GLN
1	C	147	ASN
1	C	151	GLN
1	C	161	GLN
1	C	175	ASN
1	C	182	GLN
1	C	474	ASN
1	C	487	GLN
1	C	507	GLN
2	D	147	ASN
2	D	174	GLN
2	D	258	GLN
2	D	278	GLN
2	D	373	GLN

5.3.3 RNA ⓘ

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%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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
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 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	$\# Z > 2$
5	NVP	A	901	-	23,23,23	1.67	5 (21%)	34,34,34	3.61	16 (47%)
7	SO4	B	501	-	4,4,4	0.45	0	6,6,6	0.68	0
5	NVP	C	901	-	23,23,23	1.50	5 (21%)	34,34,34	4.50	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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	NVP	C2-N3	4.00	1.41	1.34
5	C	901	NVP	C15-N14	3.20	1.40	1.34
5	A	901	NVP	C15-N14	3.06	1.40	1.34
5	A	901	NVP	C4-N3	2.98	1.40	1.34
5	C	901	NVP	C2-N3	2.79	1.39	1.34
5	A	901	NVP	C10-C15	-2.60	1.37	1.40
5	A	901	NVP	C13-N14	2.55	1.39	1.34
5	C	901	NVP	C4-N3	2.52	1.39	1.34
5	C	901	NVP	C13-N14	2.28	1.39	1.34
5	C	901	NVP	C10-C15	-2.21	1.37	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	901	NVP	C7-C2-N1	18.04	127.07	120.14
5	A	901	NVP	C7-C2-N1	13.65	125.38	120.14
5	A	901	NVP	C7-N8-C9	-9.07	120.80	128.29
5	C	901	NVP	N3-C2-N1	-6.84	111.50	116.67
5	C	901	NVP	C7-N8-C9	-6.63	122.82	128.29
5	C	901	NVP	OE-C9-N8	-6.43	114.11	120.38
5	C	901	NVP	C6-C7-N8	-6.36	113.55	119.18
5	C	901	NVP	C10-C9-N8	5.75	125.83	120.22
5	C	901	NVP	CC-CA-N1	-5.16	113.04	116.09
5	C	901	NVP	C2-C7-N8	4.69	125.88	121.46
5	A	901	NVP	OE-C9-N8	-4.33	116.16	120.38
5	A	901	NVP	C10-C9-N8	4.23	124.35	120.22
5	C	901	NVP	N14-C15-N1	-4.22	113.48	116.67
5	A	901	NVP	N14-C15-N1	-3.83	113.77	116.67
5	C	901	NVP	C15-C10-C9	3.71	127.64	124.01
5	A	901	NVP	C15-N1-CA	3.56	119.15	116.34
5	C	901	NVP	C10-C15-N1	3.55	125.38	120.95
5	A	901	NVP	C2-N1-CA	3.37	119.00	116.34
5	A	901	NVP	C11-C10-C15	3.29	120.47	117.23
5	A	901	NVP	C10-C15-N1	3.15	124.88	120.95
5	C	901	NVP	C15-N1-CA	3.12	118.80	116.34
5	C	901	NVP	C15-N1-C2	3.10	118.71	115.29
5	A	901	NVP	C15-C10-C9	3.08	127.02	124.01
5	A	901	NVP	C6-C7-C2	2.98	121.35	119.03
5	A	901	NVP	C6-C7-N8	-2.95	116.57	119.18
5	A	901	NVP	N3-C2-N1	-2.91	114.47	116.67
5	C	901	NVP	C11-C10-C15	2.76	119.95	117.23
5	A	901	NVP	C12-C13-N14	-2.71	119.12	123.42
5	C	901	NVP	C12-C13-N14	-2.69	119.16	123.42
5	A	901	NVP	CD-C6-C7	2.64	124.64	121.42
5	C	901	NVP	C11-C10-C9	-2.61	112.40	116.76
5	A	901	NVP	C11-C10-C9	-2.54	112.52	116.76
5	C	901	NVP	C5-C4-N3	-2.32	121.13	123.97

There are no chirality outliers.

All (1) torsion outliers are listed below:

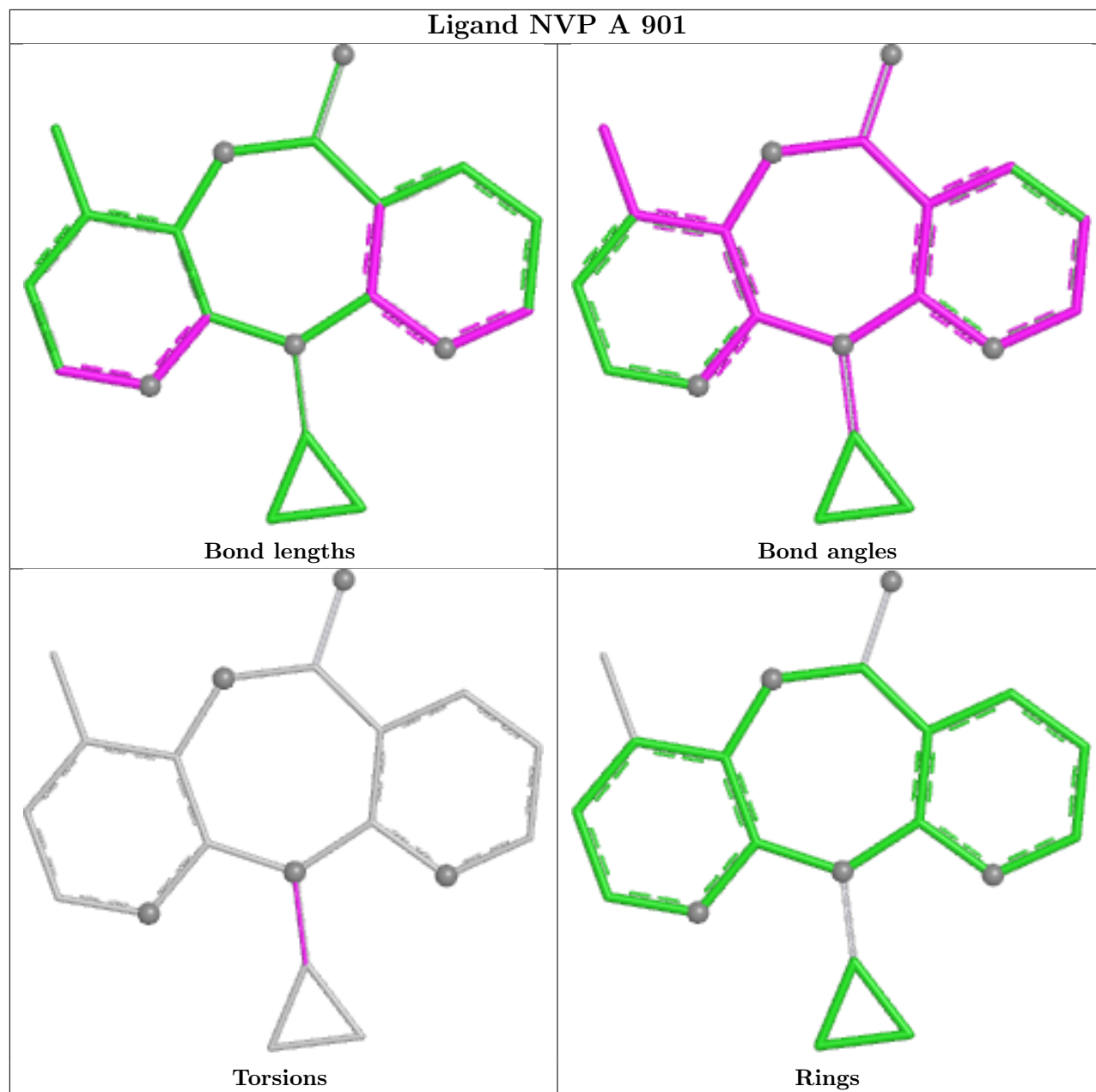
Mol	Chain	Res	Type	Atoms
5	A	901	NVP	CC-CA-N1-C15

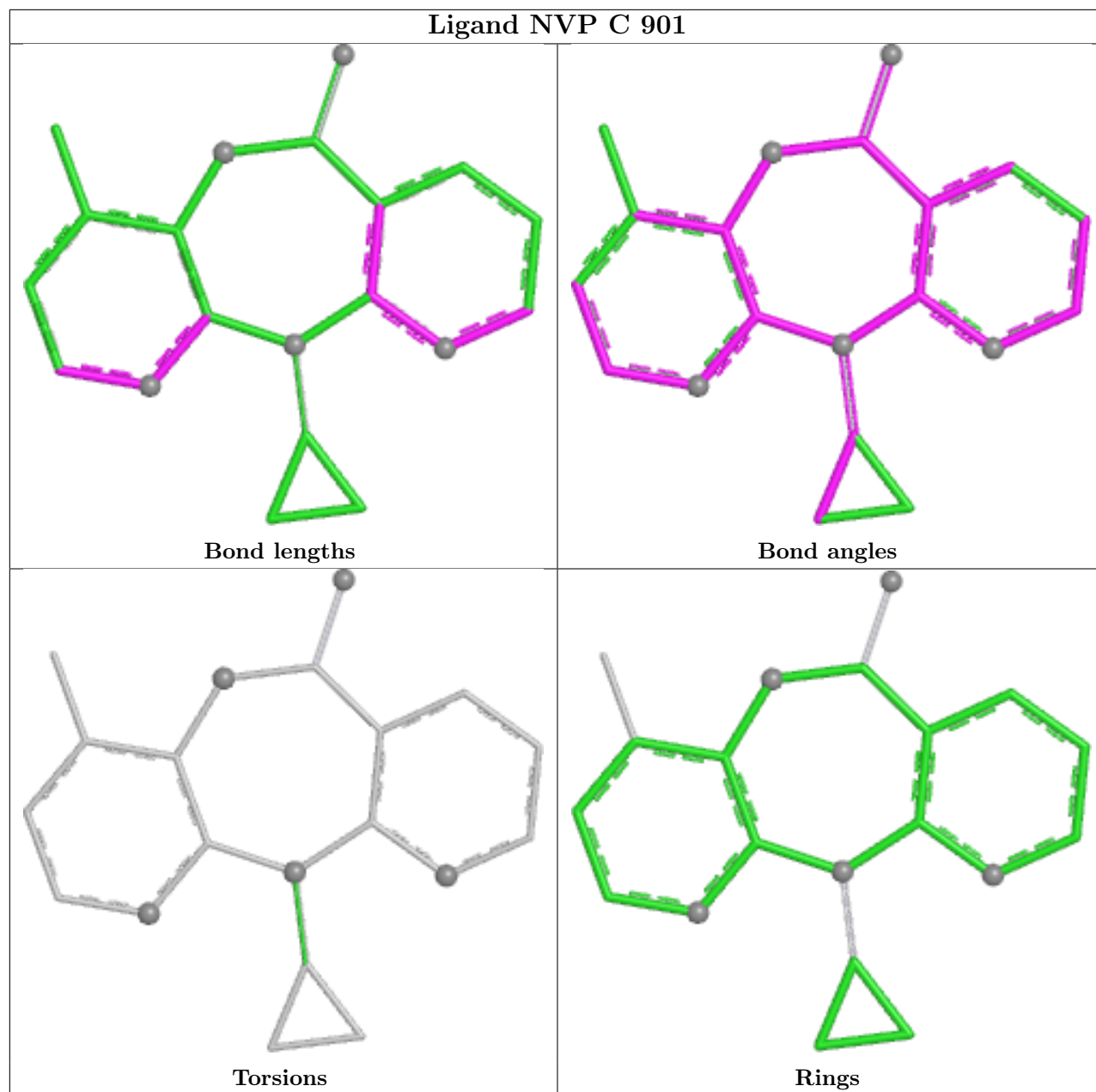
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	901	NVP	1	0
7	B	501	SO4	2	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%)	0.08	15 (2%) 56 33	17, 78, 180, 206	0
1	C	555/556 (99%)	0.14	19 (3%) 48 27	14, 83, 188, 209	0
2	B	412/428 (96%)	-0.21	4 (0%) 79 59	22, 60, 106, 131	0
2	D	412/428 (96%)	-0.08	10 (2%) 59 36	21, 64, 116, 141	0
3	E	20/27 (74%)	0.78	1 (5%) 34 18	126, 143, 174, 194	0
3	T	21/27 (77%)	0.19	0 100 100	81, 105, 147, 174	0
4	F	19/21 (90%)	0.48	0 100 100	83, 126, 184, 188	0
4	P	19/21 (90%)	0.35	1 (5%) 32 16	60, 105, 147, 159	0
All	All	2013/2064 (97%)	0.02	50 (2%) 58 35	14, 71, 167, 209	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	ILE	7.1
1	A	133	PRO	6.1
1	C	33	ALA	4.3
1	C	91	GLN	3.8
2	B	217	PRO	3.5
1	A	60	VAL	3.5
1	C	146	TYR	3.4
1	C	140	PRO	2.9
1	A	62	ALA	2.9
1	A	34	LEU	2.8
2	D	360	ALA	2.8
2	D	215	THR	2.8
1	C	59	PRO	2.7
1	C	63	ILE	2.7
2	D	124	PHE	2.7
1	C	31	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	723	C	2.6
1	C	84	THR	2.6
1	A	135	ILE	2.6
1	A	19	PRO	2.6
2	D	16	MET	2.5
1	C	128	THR	2.5
1	A	174	GLN	2.5
2	B	425	LEU	2.4
1	C	436	GLY	2.4
1	C	124	PHE	2.4
2	D	217	PRO	2.4
2	D	232	TYR	2.4
1	C	46	LYS	2.4
1	C	52	PRO	2.3
1	C	69	THR	2.3
2	D	354	TYR	2.3
1	C	54	ASN	2.3
1	A	134	SER	2.3
1	A	198	HIS	2.2
1	A	223	LYS	2.2
4	P	817	DG	2.2
1	A	146	TYR	2.2
2	D	18	GLY	2.2
1	C	32	LYS	2.1
1	A	31	ILE	2.1
1	C	55	PRO	2.1
2	B	213	GLY	2.1
1	C	135	ILE	2.1
1	A	50	ILE	2.1
2	D	212	TRP	2.1
1	C	220	LYS	2.0
2	D	209	LEU	2.0
2	B	88	TRP	2.0
1	A	26	LEU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

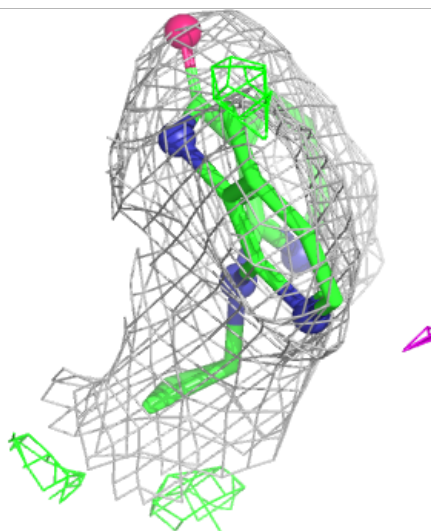
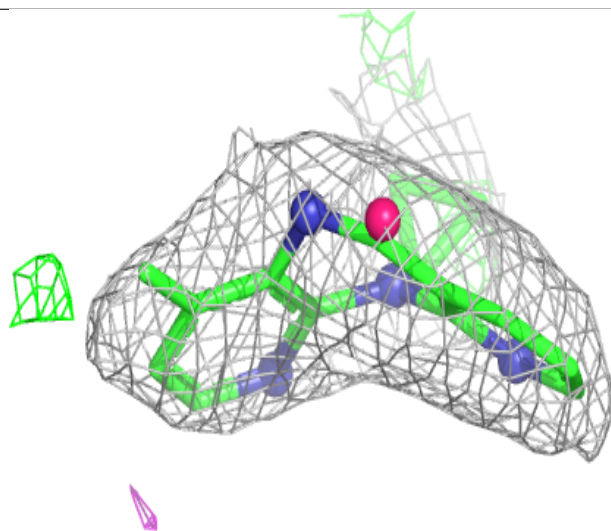
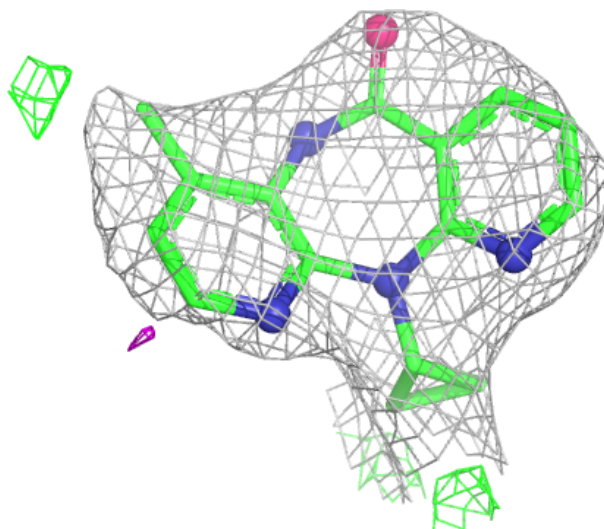
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NVP	A	901	20/20	0.90	0.15	59,68,72,79	0
6	CA	C	902	1/1	0.95	0.05	73,73,73,73	0
5	NVP	C	901	20/20	0.96	0.09	61,66,74,76	0
7	SO4	B	501	5/5	0.96	0.15	42,48,54,71	0
6	CA	A	902	1/1	0.97	0.05	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.

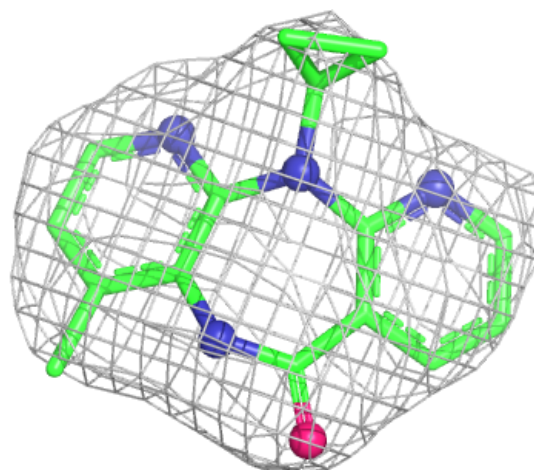
Electron density around NVP A 901:

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

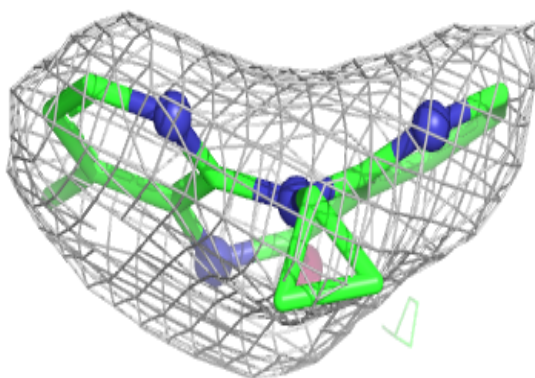


Electron density around NVP C 901:

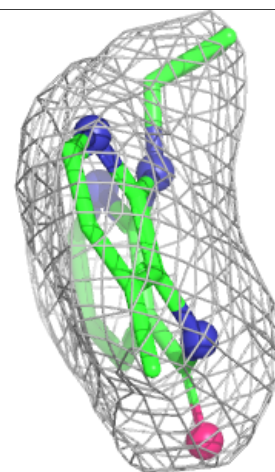
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



P



D



A

6.5 Other polymers [i](#)

There are no such residues in this entry.