



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:47 PM GMT

PDB ID : 4PUO
Title : Crystal structure of HIV-1 reverse transcriptase in complex with RNA/DNA and Nevirapine
Authors : Das, K.; Martinez, S.E.; Arnold, E.
Deposited on : 2014-03-13
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

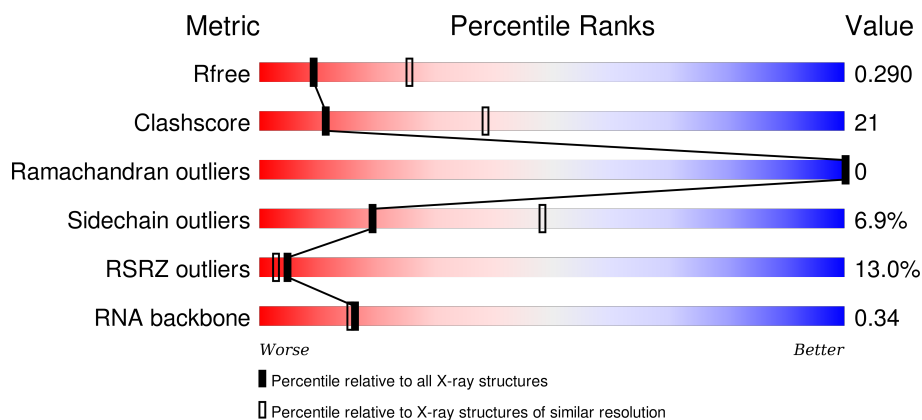
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>16%</div> <div>54%</div> <div>43%</div> <div>.</div> </div>
1	C	556	<div> <div>20%</div> <div>62%</div> <div>33%</div> <div>.</div> </div>
2	B	428	<div> <div>4%</div> <div>55%</div> <div>38%</div> <div>.</div> </div>
2	D	428	<div> <div>6%</div> <div>58%</div> <div>35%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	27	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>26%15%33%15%7%30%</div>
3	T	27	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>11%19%22%26%7%26%</div>
4	F	21	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>29%38%43%10%10%</div>
4	P	21	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>14%10%52%29%10%</div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17462 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

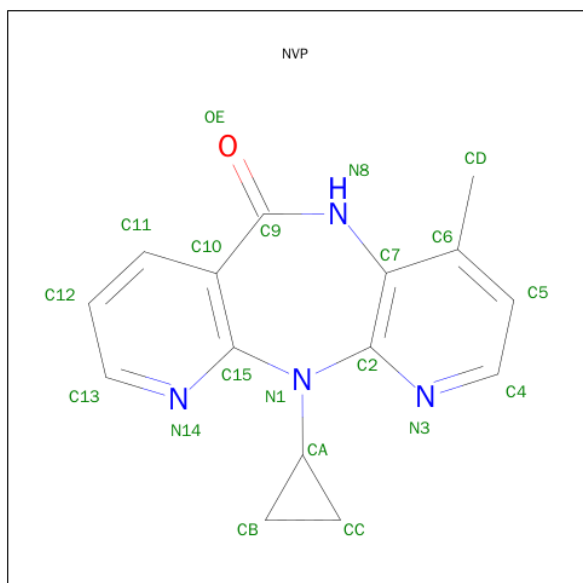
- Molecule 3 is a RNA chain called 5'-R(P*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	20	Total	C	N	O	P	0	0	0
			432	192	83	137	20			
3	E	19	Total	C	N	O	P	0	0	0
			408	182	77	130	19			

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

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

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

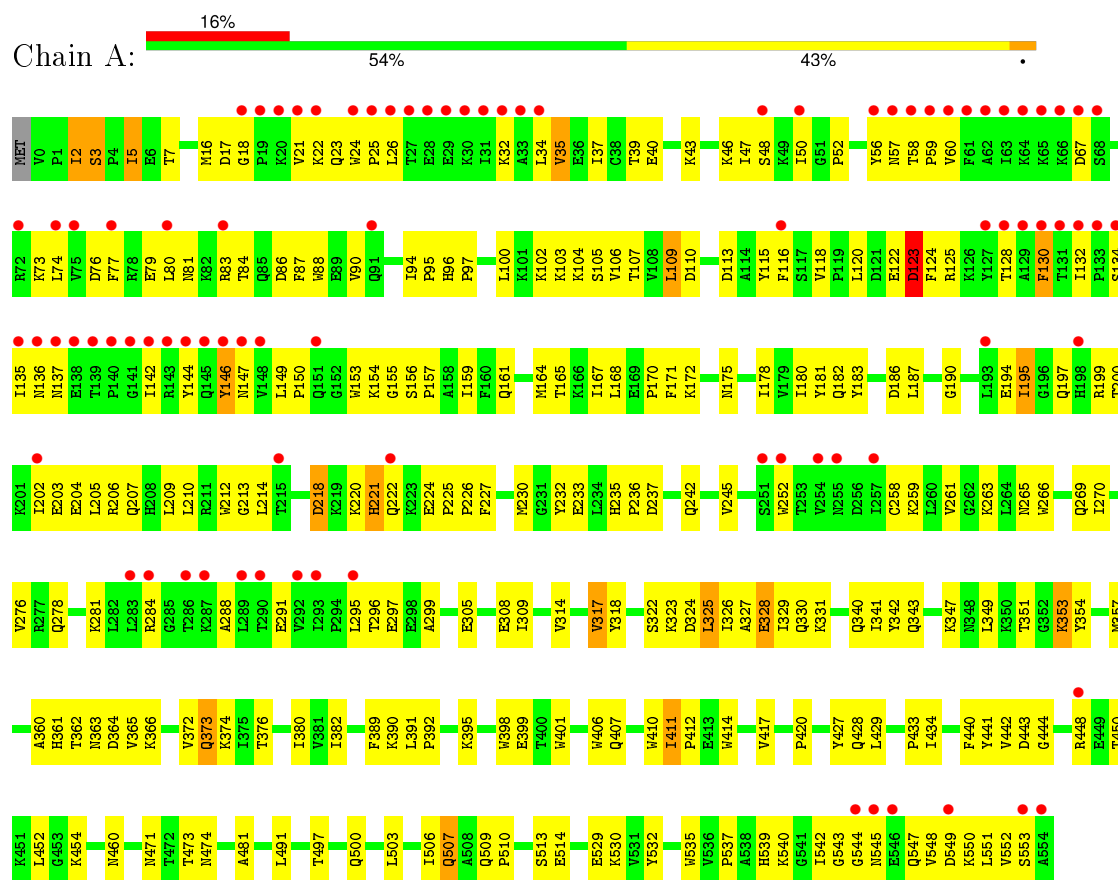


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	15	4	1		
5	C	1	Total	C	N	O	0	0
			20	15	4	1		

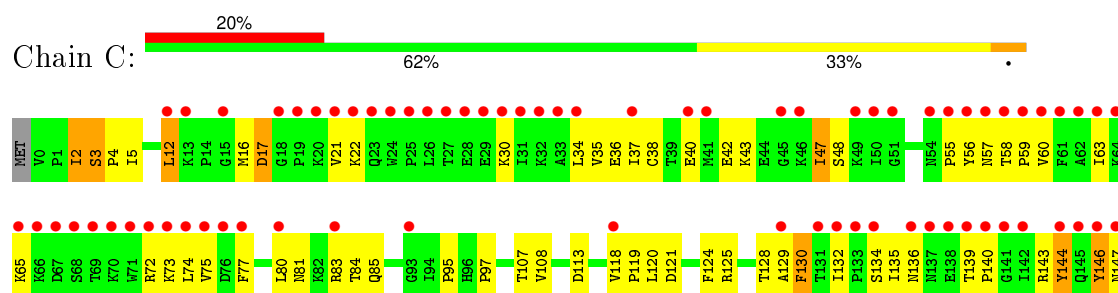
3 Residue-property plots

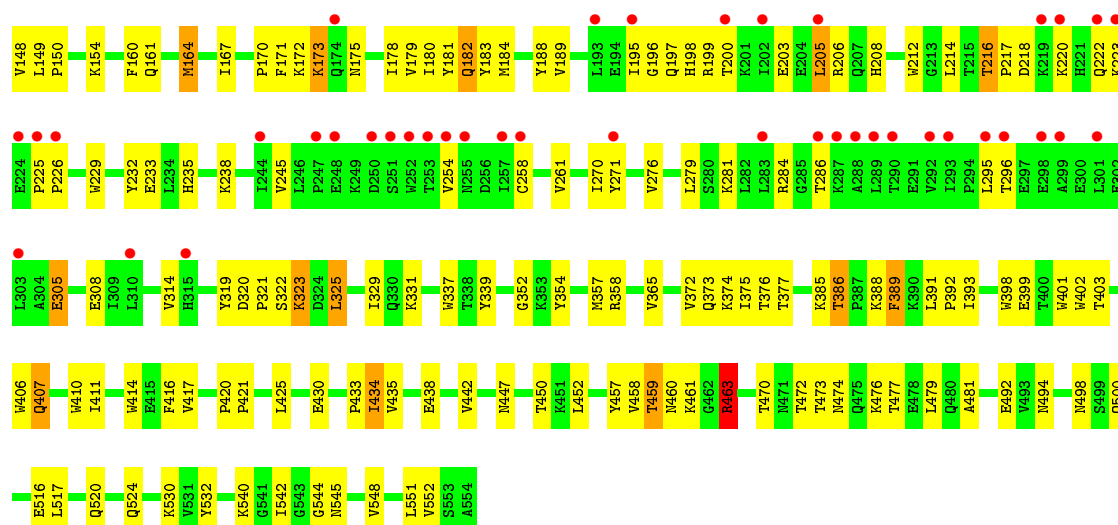
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: HIV-1 Reverse Transcriptase, p66 subunit

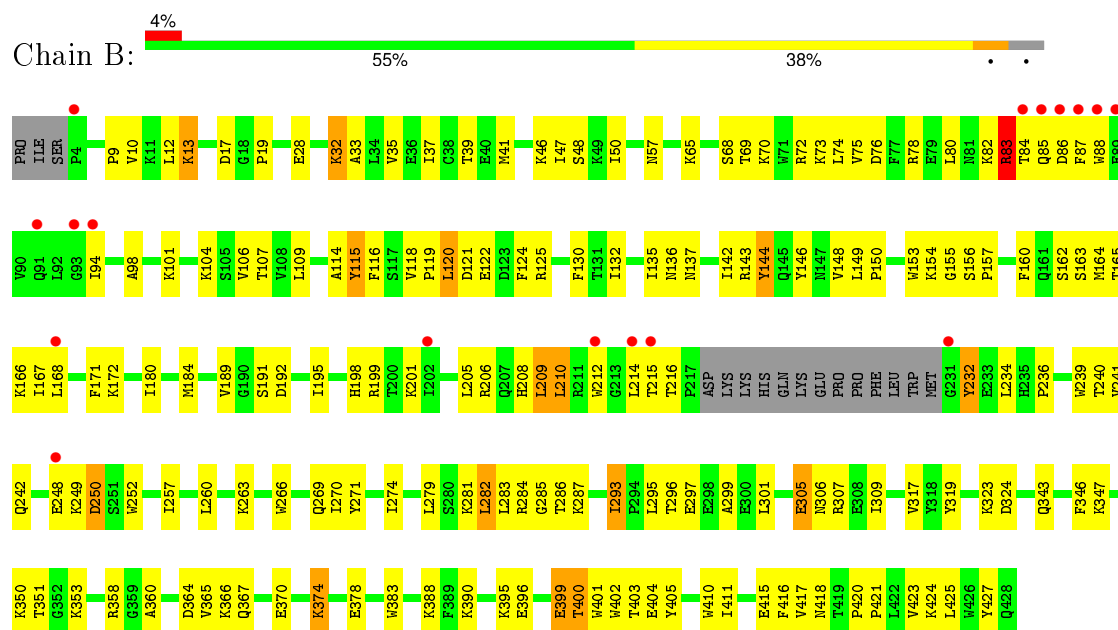


• Molecule 1: HIV-1 Reverse Transcriptase, p66 subunit

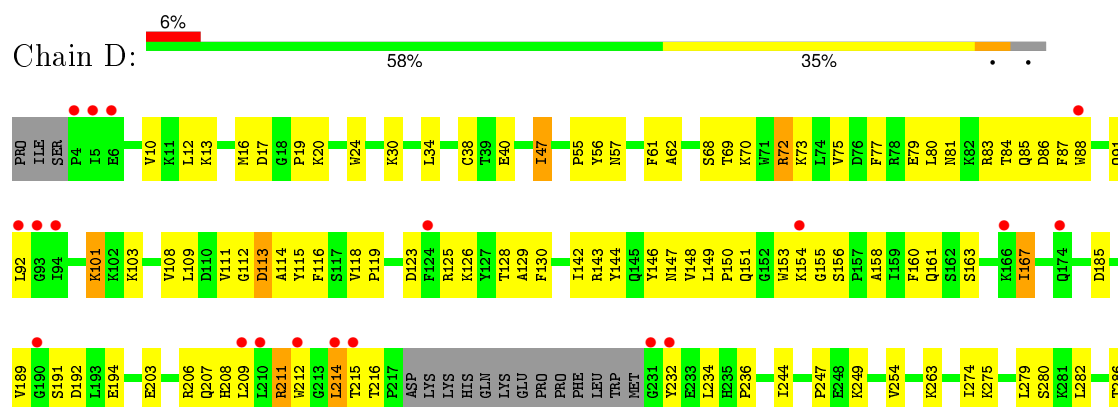


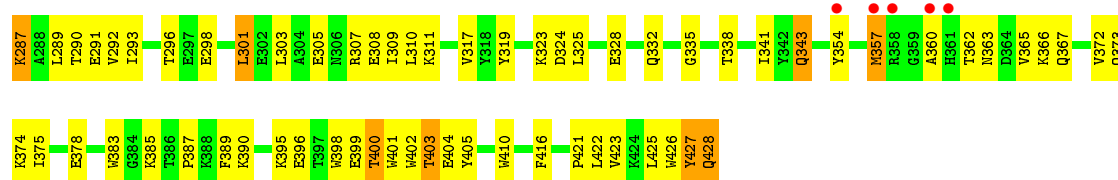


• Molecule 2: HIV-1 Reverse Transcriptase, p51 subunit



• Molecule 2: HIV-1 Reverse Transcriptase, p51 subunit





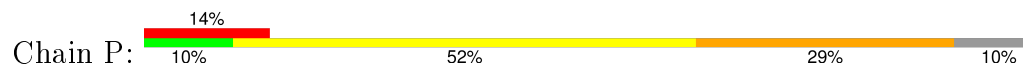
• Molecule 3: 5'-R(P*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'



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



• 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	89.74Å 132.13Å 141.96Å 90.00° 100.63° 90.00°	Depositor
Resolution (Å)	46.51 – 2.90 47.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.51-2.90) 98.4 (47.73-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.228 , 0.285 0.238 , 0.290	Depositor DCC
R_{free} test set	2136 reflections (3.11%)	DCC
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 70991 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17462	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.71	1/4630 (0.0%)	0.84	2/6290 (0.0%)
1	C	0.70	1/4624 (0.0%)	0.82	2/6283 (0.0%)
2	B	0.79	3/3497 (0.1%)	0.90	6/4751 (0.1%)
2	D	0.72	1/3497 (0.0%)	0.86	3/4751 (0.1%)
3	E	0.86	4/456 (0.9%)	1.54	6/709 (0.8%)
3	T	1.05	5/483 (1.0%)	1.55	9/752 (1.2%)
4	F	1.36	4/426 (0.9%)	1.14	5/655 (0.8%)
4	P	1.27	5/426 (1.2%)	1.24	4/655 (0.6%)
All	All	0.78	24/18039 (0.1%)	0.93	37/24846 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
2	B	0	2
All	All	0	5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	816	DG	C3'-C2'	-13.20	1.36	1.52
4	P	809	DC	O3'-P	-11.93	1.46	1.61
4	F	811	DG	C3'-C2'	-11.58	1.38	1.52
3	T	706	C	C4-N4	-10.87	1.24	1.33
4	F	815	DG	C3'-C2'	9.24	1.63	1.52
4	P	814	DC	C3'-C2'	-9.09	1.41	1.52
4	P	809	DC	C3'-C2'	-9.07	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	820	DC	C3'-C2'	8.03	1.61	1.52
3	T	706	C	C1'-N1	7.17	1.59	1.48
2	B	415	GLU	CG-CD	-6.67	1.42	1.51
3	T	717	C	C3'-C2'	-6.51	1.45	1.52
3	E	719	G	C3'-C2'	-6.46	1.45	1.52
3	T	711	C	C3'-C2'	-6.45	1.45	1.52
3	E	706	C	C1'-N1	6.40	1.58	1.48
3	E	706	C	N3-C4	5.77	1.38	1.33
3	T	706	C	N3-C4	5.69	1.38	1.33
2	B	400	THR	C-O	5.67	1.34	1.23
2	D	400	THR	C-O	5.61	1.34	1.23
1	A	328	GLU	CD-OE1	5.54	1.31	1.25
2	B	399	GLU	C-O	5.37	1.33	1.23
3	E	720	G	C3'-C2'	-5.37	1.46	1.52
1	C	389	PHE	CA-C	-5.36	1.39	1.52
4	P	818	DC	C3'-C2'	-5.09	1.46	1.52
4	P	811	DG	C3'-C2'	-5.08	1.46	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	706	C	N3-C4-C5	-19.31	114.17	121.90
3	T	706	C	N3-C4-C5	-19.22	114.21	121.90
3	E	706	C	C2-N3-C4	13.62	126.71	119.90
3	T	706	C	C2-N3-C4	13.56	126.68	119.90
4	P	812	DT	P-O3'-C3'	10.72	132.56	119.70
4	P	813	DT	P-O3'-C3'	8.29	129.64	119.70
2	D	301	LEU	CA-CB-CG	-7.82	97.31	115.30
3	T	711	C	C6-N1-C2	-7.55	117.28	120.30
2	B	364	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	C	463	ARG	NE-CZ-NH2	-7.40	116.60	120.30
4	F	815	DG	C4'-C3'-C2'	-7.29	96.54	103.10
3	E	706	C	C4-C5-C6	6.96	120.88	117.40
1	A	411	ILE	CG1-CB-CG2	-6.88	96.27	111.40
3	T	706	C	C4-C5-C6	6.80	120.80	117.40
3	T	706	C	C5-C4-N4	6.77	124.94	120.20
2	B	400	THR	C-N-CA	-6.76	104.81	121.70
4	F	820	DC	C4'-C3'-C2'	-6.65	97.12	103.10
1	C	4	PRO	N-CA-C	6.58	129.21	112.10
3	T	706	C	N1-C2-O2	6.43	122.76	118.90
3	E	706	C	N1-C2-O2	6.38	122.73	118.90
2	B	364	ASP	CB-CG-OD1	6.33	123.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	812	DT	OP1-P-O3'	6.25	118.96	105.20
3	T	719	G	P-O3'-C3'	6.22	127.16	119.70
2	D	214	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	325	LEU	CA-CB-CG	-5.93	101.67	115.30
4	P	820	DC	O4'-C4'-C3'	-5.81	102.17	104.50
3	E	706	C	N1-C2-N3	-5.74	115.18	119.20
3	T	706	C	N1-C2-N3	-5.67	115.23	119.20
4	F	815	DG	C3'-C2'-C1'	-5.43	95.98	102.50
2	B	420	PRO	C-N-CD	5.41	139.76	128.40
4	F	816	DG	C4'-C3'-C2'	5.41	107.97	103.10
3	E	723	C	C5'-C4'-O4'	5.38	115.55	109.10
2	D	400	THR	C-N-CA	-5.36	108.31	121.70
3	T	711	C	C5-C6-N1	5.33	123.67	121.00
4	F	816	DG	C3'-C2'-C1'	5.32	108.88	102.50
2	B	400	THR	O-C-N	-5.30	114.22	122.70
2	B	83	ARG	C-N-CA	-5.00	109.19	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ASP	Mainchain
1	A	35	VAL	Mainchain
2	B	400	THR	Mainchain
2	B	83	ARG	Mainchain
1	C	389	PHE	Mainchain

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	195	0
1	C	4506	0	4560	163	0
2	B	3400	0	3433	163	0
2	D	3400	0	3433	138	0
3	E	408	0	207	10	0
3	T	432	0	218	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	382	0	215	20	0
4	P	382	0	215	30	0
5	A	20	0	14	0	0
5	C	20	0	14	1	0
All	All	17462	0	16880	700	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 21.

All (700) 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:423:VAL:HG13	2:D:426:TRP:HD1	1.11	1.13
2:B:421:PRO:HB3	2:B:424:LYS:HB2	1.32	1.11
1:A:545:ASN:HA	1:A:548:VAL:HG12	1.31	1.05
4:P:812:DT:H2'	4:P:813:DT:H71	1.39	1.02
1:A:128:THR:HG21	1:A:146:TYR:HB2	1.41	1.01
1:C:498:ASN:HD22	1:C:545:ASN:HD21	1.13	0.96
2:B:115:TYR:HD2	2:B:156:SER:HB3	1.30	0.96
1:C:21:VAL:H	1:C:57:ASN:HB2	1.28	0.96
1:A:545:ASN:CA	1:A:548:VAL:HG12	1.97	0.93
2:D:423:VAL:HG13	2:D:426:TRP:CD1	2.04	0.92
2:B:191:SER:HG	2:B:198:HIS:HD1	1.08	0.91
1:A:434:ILE:HD13	1:A:530:LYS:HB3	1.52	0.91
1:C:474:ASN:HD21	3:E:723:C:H4'	1.37	0.90
1:A:545:ASN:HA	1:A:548:VAL:CG1	2.02	0.88
1:C:107:THR:HG1	1:C:198:HIS:HE2	1.14	0.88
4:F:815:DG:N3	4:F:816:DG:N7	2.21	0.88
2:B:282:LEU:HD22	2:B:293:ILE:HD11	1.55	0.88
2:B:28:GLU:HB2	2:B:135:ILE:HD11	1.54	0.87
2:B:13:LYS:HD3	2:B:83:ARG:HA	1.54	0.87
1:A:547:GLN:O	1:A:550:LYS:HG2	1.75	0.87
1:A:434:ILE:CD1	1:A:530:LYS:HB3	2.05	0.87
1:A:544:GLY:O	1:A:548:VAL:HB	1.75	0.86
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.57	0.86
1:C:500:GLN:HE22	2:D:422:LEU:HD23	1.40	0.86
2:D:209:LEU:HB3	2:D:214:LEU:HD23	1.59	0.85
1:C:452:LEU:HD11	1:C:470:THR:HG22	1.58	0.84
1:C:56:TYR:HB2	1:C:129:ALA:HB3	1.59	0.83
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.15	0.81
2:D:125:ARG:HE	2:D:147:ASN:HA	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:VAL:HG11	1:A:161:GLN:HB3	1.63	0.80
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.16	0.80
4:F:815:DG:C2	4:F:816:DG:C5	2.70	0.80
1:C:180:ILE:HG13	1:C:189:VAL:HG13	1.65	0.79
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.64	0.79
1:A:545:ASN:O	1:A:549:ASP:HB2	1.83	0.78
1:C:372:VAL:HG11	1:C:411:ILE:HG23	1.66	0.78
1:C:435:VAL:HG13	2:D:290:THR:HG21	1.66	0.77
2:B:421:PRO:CB	2:B:424:LYS:HB2	2.12	0.77
1:A:5:ILE:HG22	1:A:212:TRP:HD1	1.51	0.76
2:B:263:LYS:NZ	2:B:425:LEU:HB3	2.00	0.76
4:P:807:DC:H2'	4:P:808:DC:C6	2.20	0.76
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.22	0.75
1:C:498:ASN:ND2	1:C:545:ASN:HD21	1.84	0.75
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.18	0.75
1:C:5:ILE:HG22	1:C:212:TRP:HD1	1.52	0.75
2:D:423:VAL:CG1	2:D:426:TRP:HD1	1.96	0.75
1:C:57:ASN:HA	1:C:130:PHE:HA	1.68	0.74
2:D:421:PRO:HB2	2:D:423:VAL:H	1.50	0.73
1:C:458:VAL:HG23	1:C:548:VAL:HB	1.69	0.73
2:B:206:ARG:NH2	2:B:216:THR:O	2.22	0.73
4:P:812:DT:C6	4:P:813:DT:C7	2.71	0.72
2:B:425:LEU:HD12	2:B:425:LEU:N	2.04	0.72
1:C:261:VAL:HG13	1:C:276:VAL:HG21	1.71	0.71
2:D:86:ASP:OD1	2:D:87:PHE:N	2.24	0.71
1:A:32:LYS:NZ	1:A:134:SER:OG	2.20	0.71
4:F:807:DC:H2'	4:F:808:DC:C6	2.26	0.70
1:A:450:THR:O	1:A:452:LEU:HG	1.92	0.70
3:T:711:C:H2'	3:T:712:C:C6	2.26	0.69
1:A:79:GLU:OE1	1:A:83:ARG:NH1	2.25	0.69
2:B:195:ILE:HD11	2:B:199:ARG:HH21	1.58	0.69
2:B:250:ASP:N	2:B:250:ASP:OD1	2.14	0.69
1:A:175:ASN:HB3	1:A:178:ILE:HG12	1.75	0.68
2:D:317:VAL:HG23	2:D:317:VAL:O	1.92	0.68
4:P:808:DC:H2''	4:P:809:DC:C5'	2.23	0.68
1:A:324:ASP:O	1:A:343:GLN:HG2	1.93	0.68
1:C:65:LYS:HG2	1:C:72:ARG:HH22	1.59	0.68
2:B:47:ILE:HD12	2:B:144:TYR:CD2	2.29	0.68
3:E:711:C:H2'	3:E:712:C:C6	2.29	0.68
2:D:422:LEU:C	2:D:422:LEU:HD12	2.15	0.67
1:C:58:THR:HB	1:C:77:PHE:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ILE:HG22	2:B:144:TYR:HE1	1.58	0.67
1:A:261:VAL:HG13	1:A:276:VAL:HG21	1.77	0.67
1:A:60:VAL:HG21	1:A:132:ILE:HD12	1.75	0.67
4:P:812:DT:C6	4:P:813:DT:H71	2.30	0.66
1:A:544:GLY:O	1:A:548:VAL:CB	2.43	0.66
2:D:332:GLN:NE2	2:D:427:TYR:HB3	2.10	0.66
1:A:218:ASP:HA	1:A:220:LYS:HG2	1.77	0.66
1:A:305:GLU:O	1:A:309:ILE:HG13	1.95	0.66
1:A:245:VAL:O	1:A:263:LYS:NZ	2.20	0.66
1:C:434:ILE:CD1	1:C:530:LYS:HB3	2.26	0.66
1:C:305:GLU:HA	1:C:308:GLU:HB3	1.79	0.65
1:C:354:TYR:HD1	1:C:374:LYS:HD2	1.61	0.65
1:A:24:TRP:CD2	1:A:25:PRO:HD2	2.32	0.65
1:A:221:HIS:HB2	1:A:224:GLU:HB2	1.78	0.65
3:E:721:G:H2'	3:E:722:A:C8	2.31	0.65
1:A:167:ILE:O	1:A:170:PRO:HD2	1.97	0.65
4:F:809:DC:C5	4:F:810:DT:H73	2.31	0.65
2:D:80:LEU:HD23	2:D:153:TRP:CD1	2.32	0.65
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.78	0.65
1:A:123:ASP:N	1:A:123:ASP:OD1	2.29	0.64
2:B:28:GLU:HB2	2:B:135:ILE:CD1	2.27	0.64
1:A:26:LEU:HD22	1:A:60:VAL:HG11	1.79	0.64
2:D:423:VAL:O	2:D:426:TRP:HB2	1.96	0.64
2:D:101:LYS:O	2:D:236:PRO:HB2	1.97	0.64
3:E:709:C:H2'	3:E:710:G:H8	1.61	0.64
1:A:427:TYR:OH	1:A:510:PRO:HD2	1.98	0.64
1:A:118:VAL:HB	1:A:149:LEU:HG	1.78	0.64
3:T:710:G:C6	3:T:711:C:C4	2.85	0.64
2:B:107:THR:HG23	2:B:232:TYR:HB2	1.79	0.63
1:A:5:ILE:HG22	1:A:212:TRP:CD1	2.32	0.63
2:D:365:VAL:HG11	2:D:401:TRP:HB2	1.78	0.63
1:A:395:LYS:HD3	1:A:414:TRP:CH2	2.32	0.63
2:B:84:THR:HG21	2:B:153:TRP:CZ2	2.33	0.63
4:F:815:DG:C2	4:F:816:DG:N7	2.65	0.63
1:C:75:VAL:HG12	1:C:77:PHE:HD1	1.64	0.63
2:D:422:LEU:O	2:D:422:LEU:HD12	1.99	0.63
4:P:812:DT:C2'	4:P:813:DT:H71	2.22	0.63
4:P:810:DT:C2	4:P:811:DG:C8	2.87	0.63
2:B:180:ILE:HD13	2:B:189:VAL:HG22	1.81	0.62
1:A:135:ILE:HG23	1:A:136:ASN:H	1.63	0.62
2:D:279:LEU:O	2:D:282:LEU:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:HG11	1:A:401:TRP:CD1	2.35	0.62
1:C:35:VAL:HG23	1:C:134:SER:OG	1.99	0.62
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.35	0.62
1:C:60:VAL:HG23	1:C:132:ILE:HG21	1.80	0.62
2:B:142:ILE:CG2	2:B:144:TYR:HE1	2.13	0.61
1:C:48:SER:O	1:C:144:TYR:HB2	2.00	0.61
1:C:164:MET:HA	1:C:167:ILE:HD12	1.82	0.61
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.35	0.61
1:C:21:VAL:HG12	1:C:22:LYS:H	1.64	0.61
2:B:323:LYS:HB2	2:B:343:GLN:NE2	2.15	0.61
2:B:88:TRP:NE1	2:B:154:LYS:HB2	2.16	0.61
1:C:40:GLU:O	1:C:43:LYS:HB2	2.01	0.61
1:A:175:ASN:HB3	1:A:178:ILE:CG1	2.31	0.61
2:B:317:VAL:HG12	2:B:347:LYS:HG2	1.82	0.61
2:D:254:VAL:HG22	2:D:293:ILE:HD11	1.82	0.61
2:D:303:LEU:O	2:D:307:ARG:HG3	2.01	0.60
1:C:161:GLN:OE1	1:C:182:GLN:NE2	2.33	0.60
4:P:812:DT:C5	4:P:813:DT:H73	2.37	0.60
1:A:21:VAL:O	1:A:57:ASN:ND2	2.34	0.60
1:C:325:LEU:HB2	1:C:385:LYS:HE2	1.83	0.60
1:C:434:ILE:HD13	1:C:530:LYS:HB3	1.83	0.60
4:P:807:DC:H2'	4:P:808:DC:H6	1.64	0.60
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.83	0.60
1:A:120:LEU:HD23	1:A:125:ARG:HA	1.84	0.60
1:A:109:LEU:HD11	1:A:205:LEU:HD23	1.84	0.60
1:C:498:ASN:HD22	1:C:545:ASN:ND2	1.93	0.60
2:B:214:LEU:HD12	2:B:215:THR:H	1.65	0.60
1:C:329:ILE:O	1:C:392:PRO:HD3	2.01	0.60
1:A:296:THR:HG23	1:A:299:ALA:H	1.67	0.60
1:A:128:THR:O	1:A:128:THR:HG22	2.02	0.60
1:C:125:ARG:HE	1:C:147:ASN:HA	1.67	0.60
2:D:357:MET:O	2:D:360:ALA:HB2	2.01	0.60
2:B:118:VAL:HG12	2:B:119:PRO:O	2.01	0.59
2:B:403:THR:HG22	2:B:403:THR:O	2.02	0.59
2:B:252:TRP:NE1	2:B:295:LEU:HD11	2.17	0.59
1:A:199:ARG:NE	1:A:222:GLN:OE1	2.24	0.59
1:A:81:ASN:HD21	1:A:153:TRP:HA	1.67	0.59
2:B:353:LYS:HE3	2:B:427:TYR:CE1	2.37	0.59
2:B:84:THR:HG21	2:B:153:TRP:HZ2	1.68	0.59
1:A:543:GLY:HA2	2:B:283:LEU:O	2.02	0.59
2:B:120:LEU:HD23	2:B:125:ARG:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:808:DC:H2''	4:P:809:DC:H5''	1.84	0.58
1:C:457:TYR:HE1	1:C:463:ARG:HG2	1.67	0.58
2:D:399:GLU:HA	2:D:402:TRP:HD1	1.67	0.58
1:C:235:HIS:CD2	1:C:238:LYS:HE3	2.38	0.58
1:C:58:THR:H	1:C:130:PHE:HB2	1.68	0.58
2:B:209:LEU:HD22	2:B:214:LEU:HD23	1.85	0.58
4:F:807:DC:H2''	4:F:808:DC:C5'	2.33	0.58
1:A:362:THR:OG1	1:A:363:ASN:N	2.36	0.58
2:D:142:ILE:HG22	2:D:144:TYR:HE1	1.68	0.58
2:B:195:ILE:CG1	2:B:199:ARG:HE	2.16	0.58
3:E:721:G:H2'	3:E:722:A:H8	1.68	0.58
2:D:84:THR:HG21	2:D:153:TRP:HZ2	1.67	0.58
2:D:24:TRP:HZ2	2:D:61:PHE:CE2	2.22	0.58
1:C:206:ARG:HG2	1:C:216:THR:OG1	2.03	0.58
1:C:80:LEU:O	1:C:84:THR:OG1	2.20	0.58
2:D:111:VAL:HG23	2:D:115:TYR:HE2	1.66	0.58
2:D:354:TYR:CZ	2:D:374:LYS:HG2	2.39	0.58
1:A:225:PRO:HA	1:A:226:PRO:C	2.24	0.58
1:C:223:LYS:O	1:C:225:PRO:HD3	2.03	0.58
1:A:544:GLY:O	1:A:548:VAL:N	2.35	0.58
1:A:161:GLN:O	1:A:165:THR:OG1	2.21	0.58
1:A:46:LYS:HE3	1:A:116:PHE:HB3	1.85	0.58
4:P:809:DC:H1'	4:P:810:DT:H5'	1.85	0.58
4:P:812:DT:C2	4:P:813:DT:C6	2.91	0.58
2:D:398:TRP:O	2:D:402:TRP:HB3	2.04	0.58
2:B:88:TRP:CD1	2:B:154:LYS:HB2	2.38	0.57
2:D:125:ARG:NE	2:D:147:ASN:HA	2.15	0.57
1:C:494:ASN:HB3	2:D:289:LEU:HD12	1.86	0.57
1:A:103:LYS:O	1:A:236:PRO:HB3	2.04	0.57
2:D:274:ILE:O	2:D:275:LYS:HD3	2.04	0.57
2:B:13:LYS:HD2	2:B:86:ASP:HB3	1.87	0.57
1:A:210:LEU:O	1:A:213:GLY:N	2.29	0.57
1:A:204:GLU:O	1:A:207:GLN:HB2	2.05	0.57
2:B:366:LYS:HG3	2:B:405:TYR:CD1	2.40	0.57
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.28	0.57
1:C:181:TYR:CE2	1:C:183:TYR:HB2	2.40	0.56
1:A:149:LEU:HD13	1:A:156:SER:HA	1.87	0.56
2:D:387:PRO:HG2	2:D:389:PHE:CE1	2.41	0.56
1:C:376:THR:HG23	1:C:386:THR:HG23	1.87	0.56
2:B:205:LEU:O	2:B:209:LEU:HD12	2.04	0.56
4:F:815:DG:C4	4:F:816:DG:N7	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:ILE:HG22	2:B:144:TYR:CE1	2.39	0.56
2:D:73:LYS:NZ	2:D:146:TYR:OH	2.29	0.56
1:C:457:TYR:HA	1:C:548:VAL:HG21	1.86	0.56
2:D:85:GLN:HA	2:D:88:TRP:NE1	2.21	0.56
1:C:295:LEU:HG	1:C:296:THR:H	1.71	0.56
4:F:815:DG:C2	4:F:816:DG:C6	2.94	0.56
1:A:58:THR:OG1	1:A:130:PHE:HB2	2.05	0.56
4:F:807:DC:H2'	4:F:808:DC:H6	1.69	0.55
2:D:401:TRP:O	2:D:404:GLU:N	2.38	0.55
4:P:807:DC:H2''	4:P:808:DC:H5'	1.88	0.55
1:C:35:VAL:HB	1:C:134:SER:HB3	1.88	0.55
2:B:403:THR:O	2:B:403:THR:CG2	2.55	0.55
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.70	0.55
1:A:195:ILE:HG22	1:A:199:ARG:NH1	2.22	0.55
1:A:77:PHE:O	1:A:80:LEU:N	2.40	0.55
1:C:77:PHE:CD2	1:C:80:LEU:HB3	2.40	0.55
2:D:17:ASP:O	2:D:83:ARG:NH1	2.40	0.55
1:A:221:HIS:CG	1:A:224:GLU:HB2	2.41	0.55
2:B:120:LEU:HD12	2:B:149:LEU:HD23	1.87	0.55
1:A:503:LEU:O	1:A:507:GLN:HB2	2.07	0.55
1:A:373:GLN:HG3	2:B:401:TRP:CH2	2.42	0.55
1:A:86:ASP:OD1	1:A:154:LYS:NZ	2.39	0.55
2:D:263:LYS:HA	2:D:425:LEU:HD13	1.88	0.55
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.88	0.55
4:F:807:DC:H2''	4:F:808:DC:H5'	1.89	0.55
1:C:95:PRO:HG2	1:C:229:TRP:HH2	1.71	0.55
2:B:242:GLN:O	2:B:351:THR:OG1	2.25	0.55
2:D:282:LEU:HD21	2:D:296:THR:HG23	1.89	0.54
1:C:35:VAL:HG13	1:C:36:GLU:HG3	1.89	0.54
1:A:328:GLU:HB2	1:A:390:LYS:HB2	1.88	0.54
2:D:114:ALA:H	2:D:214:LEU:HD13	1.73	0.54
1:A:105:SER:O	1:A:190:GLY:HA2	2.07	0.54
1:C:38:CYS:O	1:C:42:GLU:OE1	2.25	0.54
3:T:711:C:O2'	3:T:712:C:OP1	2.25	0.54
1:A:322:SER:OG	1:A:323:LYS:HG2	2.07	0.54
1:A:59:PRO:O	1:A:76:ASP:HB3	2.07	0.54
2:D:395:LYS:HG3	2:D:416:PHE:CE2	2.41	0.54
2:B:69:THR:HG23	2:B:70:LYS:HE2	1.90	0.54
2:D:423:VAL:HG12	2:D:423:VAL:O	2.08	0.54
2:D:72:ARG:HD3	2:D:73:LYS:O	2.07	0.54
1:A:168:LEU:HD21	1:A:187:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:540:LYS:HB2	1:C:542:ILE:HG13	1.89	0.54
2:D:421:PRO:HB2	2:D:423:VAL:HB	1.90	0.54
3:T:714:G:C2	3:T:715:A:C4	2.96	0.54
1:A:317:VAL:HG23	1:A:318:TYR:N	2.23	0.54
1:C:452:LEU:CD1	1:C:470:THR:HG22	2.36	0.54
1:A:94:ILE:HD13	1:A:230:MET:CE	2.38	0.54
1:C:474:ASN:ND2	3:E:723:C:H4'	2.16	0.54
3:T:720:G:H2'	3:T:721:G:O4'	2.08	0.54
1:C:452:LEU:HD12	1:C:470:THR:HA	1.89	0.53
2:D:19:PRO:HD3	2:D:80:LEU:HD12	1.90	0.53
1:C:120:LEU:HD13	1:C:148:VAL:O	2.08	0.53
4:P:812:DT:C6	4:P:813:DT:H73	2.42	0.53
2:B:423:VAL:HG12	2:B:423:VAL:O	2.08	0.53
1:C:59:PRO:O	1:C:75:VAL:HG13	2.08	0.53
2:D:401:TRP:HB3	2:D:405:TYR:HE2	1.74	0.53
1:C:121:ASP:O	1:C:125:ARG:HG3	2.08	0.53
1:C:339:TYR:CZ	1:C:352:GLY:HA3	2.44	0.53
1:C:417:VAL:O	1:C:417:VAL:HG13	2.09	0.53
1:A:547:GLN:N	1:A:547:GLN:OE1	2.41	0.53
1:C:354:TYR:CD1	1:C:374:LYS:HD2	2.43	0.53
1:C:125:ARG:O	1:C:128:THR:OG1	2.25	0.53
2:D:115:TYR:HE1	2:D:156:SER:C	2.12	0.53
2:B:116:PHE:O	2:B:148:VAL:HG11	2.09	0.53
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.91	0.53
2:B:263:LYS:HZ2	2:B:425:LEU:HB3	1.70	0.52
2:B:82:LYS:O	2:B:85:GLN:HB3	2.09	0.52
2:B:76:ASP:OD1	2:B:78:ARG:NE	2.38	0.52
2:D:287:LYS:HG2	2:D:291:GLU:OE2	2.09	0.52
3:T:714:G:H2'	3:T:715:A:C8	2.45	0.52
1:C:438:GLU:HG3	1:C:461:LYS:HD3	1.92	0.52
2:D:85:GLN:HA	2:D:88:TRP:CE2	2.45	0.52
2:D:24:TRP:HZ2	2:D:61:PHE:HE2	1.57	0.52
1:A:18:GLY:HA3	1:A:56:TYR:CD1	2.43	0.52
2:B:162:SER:O	2:B:165:THR:HG22	2.10	0.52
4:P:809:DC:C5	4:P:810:DT:H73	2.44	0.52
1:C:406:TRP:CH2	1:C:407:GLN:HG3	2.44	0.52
2:B:115:TYR:O	2:B:149:LEU:HB2	2.09	0.52
1:C:97:PRO:HG2	1:C:232:TYR:CE1	2.44	0.52
1:C:197:GLN:O	1:C:200:THR:HB	2.10	0.52
2:B:263:LYS:HZ3	2:B:425:LEU:HB3	1.72	0.52
1:C:271:TYR:CZ	1:C:314:VAL:HG12	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:N	2:B:136:ASN:HD21	2.08	0.51
4:P:807:DC:H2''	4:P:808:DC:C5'	2.40	0.51
1:A:452:LEU:HD23	1:A:471:ASN:H	1.73	0.51
1:C:167:ILE:O	1:C:170:PRO:HD2	2.11	0.51
1:A:373:GLN:HG3	2:B:401:TRP:HH2	1.75	0.51
1:C:544:GLY:O	1:C:548:VAL:HG12	2.09	0.51
4:P:804:DA:H2''	4:P:805:DG:H8	1.75	0.51
2:B:401:TRP:O	2:B:404:GLU:N	2.42	0.51
2:D:88:TRP:CD1	2:D:154:LYS:HB3	2.45	0.51
3:T:714:G:H2'	3:T:715:A:H8	1.74	0.51
2:B:425:LEU:N	2:B:425:LEU:CD1	2.73	0.51
2:D:305:GLU:O	2:D:309:ILE:HG13	2.11	0.51
2:B:17:ASP:O	2:B:83:ARG:NH1	2.38	0.51
2:D:84:THR:HG21	2:D:153:TRP:CZ2	2.45	0.51
2:B:390:LYS:HB3	2:B:417:VAL:HG21	1.91	0.51
2:D:92:LEU:HD21	2:D:161:GLN:OE1	2.11	0.51
1:A:48:SER:O	1:A:144:TYR:HB2	2.11	0.51
1:A:233:GLU:HG3	1:A:242:GLN:HG2	1.92	0.51
1:C:220:LYS:HE2	1:C:222:GLN:HA	1.92	0.51
1:A:155:GLY:O	1:A:159:ILE:HB	2.11	0.51
2:D:109:LEU:HD22	2:D:216:THR:HG21	1.93	0.51
1:C:139:THR:HB	1:C:140:PRO:HD2	1.93	0.51
1:A:441:TYR:CD1	2:B:286:THR:HG23	2.46	0.51
1:C:199:ARG:NH2	1:C:223:LYS:HD3	2.26	0.51
1:A:317:VAL:HG23	1:A:318:TYR:O	2.11	0.51
4:P:808:DC:H2''	4:P:809:DC:H5'	1.92	0.51
2:B:130:PHE:CE2	2:B:144:TYR:HB2	2.46	0.51
2:D:118:VAL:HG12	2:D:119:PRO:O	2.11	0.51
1:C:2:ILE:HG22	1:C:3:SER:H	1.77	0.51
1:A:226:PRO:HB3	1:A:235:HIS:NE2	2.25	0.50
1:C:35:VAL:HG13	1:C:36:GLU:N	2.27	0.50
1:A:382:ILE:HA	2:B:136:ASN:OD1	2.11	0.50
2:D:68:SER:HB3	2:D:70:LYS:HE2	1.93	0.50
1:A:500:GLN:HG3	1:A:535:TRP:NE1	2.26	0.50
1:A:32:LYS:HZ2	1:A:35:VAL:HG21	1.76	0.50
1:A:34:LEU:HD21	1:A:132:ILE:HG21	1.92	0.50
3:E:720:G:H2'	3:E:721:G:C8	2.47	0.50
1:C:34:LEU:HD13	1:C:73:LYS:HE3	1.92	0.50
1:C:430:GLU:HG3	1:C:434:ILE:HD11	1.94	0.50
1:A:225:PRO:HD3	1:A:227:PHE:CE1	2.47	0.50
2:D:142:ILE:HG22	2:D:144:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:812:DT:C2	4:P:813:DT:C5	2.99	0.50
1:A:197:GLN:O	1:A:200:THR:HB	2.11	0.50
2:B:85:GLN:HG3	2:B:88:TRP:CH2	2.47	0.50
1:C:5:ILE:HG22	1:C:212:TRP:CD1	2.40	0.50
1:C:218:ASP:OD1	1:C:222:GLN:NE2	2.45	0.50
2:D:87:PHE:CE2	2:D:155:GLY:HA2	2.46	0.50
2:B:249:LYS:HG3	2:B:252:TRP:CH2	2.46	0.50
2:B:270:ILE:HG13	2:B:346:PHE:HD1	1.76	0.50
2:B:13:LYS:HD2	2:B:86:ASP:CB	2.42	0.49
1:A:106:VAL:HG12	1:A:227:PHE:HE2	1.77	0.49
2:B:252:TRP:CB	2:B:257:ILE:HD11	2.41	0.49
1:C:391:LEU:HD12	1:C:414:TRP:CE3	2.47	0.49
1:A:410:TRP:CZ2	1:A:412:PRO:HA	2.47	0.49
2:B:195:ILE:HG12	2:B:199:ARG:HE	1.77	0.49
2:B:47:ILE:HG22	2:B:146:TYR:HA	1.94	0.49
2:B:252:TRP:HB3	2:B:257:ILE:HD11	1.93	0.49
2:D:354:TYR:HE2	2:D:375:ILE:HG13	1.77	0.49
2:B:374:LYS:O	2:B:378:GLU:HG3	2.12	0.49
4:F:815:DG:N3	4:F:816:DG:C8	2.79	0.49
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.47	0.49
2:D:57:ASN:OD1	2:D:130:PHE:HA	2.13	0.49
2:B:74:LEU:HD12	2:B:75:VAL:N	2.27	0.49
2:D:56:TYR:O	2:D:143:ARG:NH2	2.45	0.49
1:A:5:ILE:CG2	1:A:212:TRP:HD1	2.23	0.49
2:D:400:THR:HB	2:D:401:TRP:CD1	2.47	0.49
2:D:47:ILE:HB	2:D:144:TYR:HD2	1.77	0.49
1:A:360:ALA:HA	1:A:514:GLU:OE2	2.12	0.49
1:A:327:ALA:O	1:A:389:PHE:HA	2.12	0.49
2:D:244:ILE:HB	2:D:310:LEU:HD22	1.94	0.49
2:B:206:ARG:HE	2:B:216:THR:HB	1.77	0.49
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.95	0.49
1:C:524:GLN:NE2	1:C:524:GLN:HA	2.27	0.49
2:D:155:GLY:O	2:D:158:ALA:N	2.46	0.49
1:A:164:MET:O	1:A:168:LEU:HD13	2.12	0.49
2:D:116:PHE:O	2:D:148:VAL:HG11	2.13	0.49
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.94	0.49
2:B:191:SER:OG	2:B:198:HIS:ND1	2.21	0.49
1:C:97:PRO:HG2	1:C:232:TYR:CD1	2.48	0.49
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.48	0.49
1:A:549:ASP:O	1:A:553:SER:HB2	2.13	0.49
2:D:13:LYS:HD3	2:D:86:ASP:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:GLY:H	2:B:287:LYS:HE2	1.78	0.49
2:B:136:ASN:O	2:B:137:ASN:HB2	2.12	0.49
2:B:266:TRP:O	2:B:269:GLN:N	2.41	0.49
4:F:815:DG:N2	4:F:816:DG:C5	2.81	0.48
1:C:172:LYS:HG2	1:C:180:ILE:HD13	1.94	0.48
2:D:427:TYR:CD1	2:D:427:TYR:C	2.86	0.48
1:C:35:VAL:O	1:C:38:CYS:HB3	2.12	0.48
2:D:214:LEU:HD12	2:D:215:THR:H	1.77	0.48
2:D:338:THR:HG21	2:D:427:TYR:HB2	1.95	0.48
2:D:366:LYS:HG3	2:D:405:TYR:CD1	2.48	0.48
1:C:391:LEU:O	1:C:393:ILE:N	2.39	0.48
1:C:500:GLN:NE2	2:D:422:LEU:HD23	2.18	0.48
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.47	0.48
2:D:354:TYR:OH	2:D:374:LYS:HG2	2.14	0.48
1:C:516:GLU:O	1:C:520:GLN:HG3	2.14	0.48
1:A:209:LEU:HD22	1:A:214:LEU:HD13	1.94	0.48
1:A:128:THR:O	1:A:128:THR:CG2	2.61	0.48
3:T:711:C:HO2'	3:T:712:C:P	2.35	0.48
1:A:24:TRP:CE3	1:A:25:PRO:HD2	2.49	0.48
1:A:281:LYS:HG2	1:A:284:ARG:NH2	2.29	0.48
1:C:358:ARG:NH2	2:D:396:GLU:OE1	2.46	0.48
1:C:447:ASN:OD1	1:C:450:THR:HG23	2.13	0.48
1:A:32:LYS:HD2	1:A:32:LYS:HA	1.62	0.48
3:E:709:C:H2'	3:E:710:G:C8	2.45	0.48
2:D:247:PRO:O	2:D:307:ARG:NH2	2.46	0.48
1:A:171:PHE:CZ	1:A:205:LEU:HB2	2.49	0.48
2:D:374:LYS:O	2:D:378:GLU:HG3	2.14	0.48
1:A:77:PHE:CE1	1:A:128:THR:HG23	2.48	0.48
1:C:548:VAL:O	1:C:552:VAL:HG13	2.14	0.48
1:C:473:THR:O	1:C:477:THR:HG23	2.13	0.48
1:C:65:LYS:HB3	1:C:72:ARG:HH12	1.79	0.47
1:A:365:VAL:HG11	1:A:401:TRP:CG	2.48	0.47
1:C:130:PHE:O	1:C:143:ARG:HB2	2.14	0.47
1:A:448:ARG:NH1	4:P:806:DT:O2	2.47	0.47
2:D:111:VAL:HG23	2:D:115:TYR:CE2	2.49	0.47
2:B:106:VAL:O	2:B:234:LEU:N	2.45	0.47
1:C:398:TRP:CZ2	1:C:411:ILE:HG13	2.50	0.47
1:A:252:TRP:CD1	1:A:295:LEU:HG	2.50	0.47
1:A:37:ILE:HA	1:A:40:GLU:CD	2.34	0.47
2:D:291:GLU:HG2	2:D:293:ILE:CD1	2.44	0.47
1:A:94:ILE:HD13	1:A:230:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:VAL:HG11	1:C:401:TRP:CD1	2.50	0.47
2:B:65:LYS:O	2:B:68:SER:HB3	2.15	0.47
1:A:50:ILE:HG22	1:A:52:PRO:HD2	1.95	0.47
2:D:30:LYS:HD3	2:D:62:ALA:O	2.15	0.47
1:C:37:ILE:HA	1:C:40:GLU:HB2	1.97	0.47
3:T:714:G:N2	3:T:715:A:C4	2.83	0.47
1:A:331:LYS:NZ	1:A:364:ASP:OD2	2.47	0.47
1:C:435:VAL:HG22	2:D:290:THR:HG21	1.97	0.47
1:C:161:GLN:NE2	1:C:184:MET:O	2.48	0.47
1:C:135:ILE:HG12	1:C:136:ASN:OD1	2.15	0.47
2:B:154:LYS:O	2:B:157:PRO:HD2	2.15	0.46
1:A:32:LYS:NZ	1:A:35:VAL:HG21	2.29	0.46
1:C:65:LYS:HG2	1:C:72:ARG:NH2	2.27	0.46
2:B:401:TRP:HB3	2:B:405:TYR:HE2	1.79	0.46
2:B:425:LEU:H	2:B:425:LEU:HD12	1.79	0.46
2:B:73:LYS:NZ	2:B:130:PHE:CZ	2.83	0.46
1:C:473:THR:OG1	1:C:476:LYS:HG3	2.15	0.46
1:A:376:THR:O	1:A:380:ILE:HG12	2.15	0.46
4:F:809:DC:C5	4:F:810:DT:C7	2.97	0.46
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.48	0.46
2:D:208:HIS:O	2:D:211:ARG:HG2	2.15	0.46
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.81	0.46
2:D:206:ARG:NH2	2:D:216:THR:O	2.49	0.46
1:A:2:ILE:HG22	1:A:3:SER:H	1.80	0.46
2:D:319:TYR:HD1	2:D:343:GLN:HE22	1.58	0.46
1:A:545:ASN:O	1:A:549:ASP:N	2.41	0.46
4:F:809:DC:C4	4:F:810:DT:H73	2.50	0.46
1:C:179:VAL:HG12	5:C:901:NVP:HCC2	1.97	0.46
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.98	0.46
2:B:101:LYS:O	2:B:236:PRO:HB2	2.15	0.46
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.79	0.46
1:C:120:LEU:HG	1:C:121:ASP:H	1.81	0.46
3:T:717:C:H2'	3:T:718:A:C8	2.51	0.46
2:B:297:GLU:O	2:B:301:LEU:HG	2.16	0.46
1:C:463:ARG:HB2	1:C:463:ARG:HE	1.23	0.46
4:F:809:DC:C6	4:F:810:DT:H71	2.51	0.46
1:C:2:ILE:HD12	1:C:2:ILE:H	1.80	0.46
1:C:17:ASP:O	1:C:83:ARG:HD3	2.15	0.46
1:C:281:LYS:O	1:C:284:ARG:HG3	2.15	0.46
1:A:326:ILE:O	1:A:341:ILE:HA	2.16	0.46
1:A:88:TRP:CD1	2:B:143:ARG:CZ	2.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:ALA:HA	2:B:367:GLN:OE1	2.15	0.46
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.98	0.46
1:C:58:THR:N	1:C:130:PHE:HB2	2.31	0.46
1:A:202:ILE:HG21	1:A:220:LYS:NZ	2.30	0.46
2:D:292:VAL:C	2:D:293:ILE:HD13	2.36	0.46
2:B:279:LEU:HD23	2:B:299:ALA:HB1	1.98	0.46
2:B:85:GLN:HA	2:B:88:TRP:CZ2	2.49	0.46
2:D:19:PRO:CD	2:D:80:LEU:HD12	2.46	0.46
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.98	0.46
2:D:108:VAL:HG12	2:D:232:TYR:O	2.15	0.46
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.30	0.45
1:C:173:LYS:HD2	1:C:173:LYS:HA	1.71	0.45
2:D:103:LYS:HD2	2:D:191:SER:HA	1.98	0.45
3:E:710:G:C6	3:E:711:C:C4	3.05	0.45
1:C:331:LYS:HB2	1:C:337:TRP:CZ3	2.51	0.45
1:A:391:LEU:HD12	1:A:414:TRP:CE3	2.51	0.45
1:A:34:LEU:HA	1:A:37:ILE:HB	1.97	0.45
2:D:282:LEU:HD21	2:D:296:THR:CG2	2.46	0.45
1:C:406:TRP:CZ3	1:C:407:GLN:HG3	2.52	0.45
1:A:102:LYS:HE2	1:A:237:ASP:HA	1.98	0.45
2:D:160:PHE:O	2:D:160:PHE:CD1	2.69	0.45
1:A:428:GLN:HA	1:A:509:GLN:OE1	2.17	0.45
2:B:10:VAL:HG13	2:B:87:PHE:CD1	2.50	0.45
2:D:341:ILE:HD11	2:D:375:ILE:HG23	1.98	0.45
2:B:50:ILE:HG12	2:B:143:ARG:HB2	1.98	0.45
1:A:347:LYS:HB2	1:A:347:LYS:HE3	1.77	0.45
2:B:78:ARG:O	2:B:82:LYS:HG3	2.15	0.45
1:A:221:HIS:CB	1:A:224:GLU:HB2	2.44	0.45
1:A:22:LYS:HE3	1:A:23:GLN:O	2.17	0.45
1:C:77:PHE:HD2	1:C:80:LEU:HB3	1.79	0.45
2:B:124:PHE:CE2	2:B:153:TRP:CZ2	3.04	0.45
1:A:398:TRP:CE2	1:A:411:ILE:HD12	2.52	0.45
1:C:226:PRO:HB3	1:C:235:HIS:CE1	2.52	0.45
2:D:115:TYR:O	2:D:149:LEU:HB2	2.17	0.45
1:C:195:ILE:HG12	1:C:199:ARG:HE	1.82	0.45
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.98	0.45
1:C:270:ILE:HG23	1:C:271:TYR:N	2.31	0.45
1:C:254:VAL:HG21	1:C:286:THR:HG21	1.97	0.45
1:A:270:ILE:HA	1:A:270:ILE:HD12	1.80	0.45
2:D:142:ILE:CG2	2:D:144:TYR:HE1	2.30	0.45
1:C:203:GLU:OE1	1:C:206:ARG:HD2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:TRP:O	2:B:402:TRP:C	2.55	0.45
2:B:358:ARG:NH2	2:B:405:TYR:O	2.50	0.45
2:D:79:GLU:O	2:D:83:ARG:HD2	2.17	0.45
1:A:172:LYS:HE3	1:A:180:ILE:HD12	1.98	0.45
2:B:274:ILE:HA	2:B:306:ASN:OD1	2.16	0.45
2:B:35:VAL:O	2:B:39:THR:HG23	2.16	0.45
2:D:373:GLN:HE21	2:D:373:GLN:HB3	1.59	0.45
1:C:149:LEU:HA	1:C:150:PRO:HD3	1.78	0.45
2:B:84:THR:O	2:B:87:PHE:N	2.49	0.45
1:A:34:LEU:HD22	1:A:73:LYS:HZ3	1.81	0.45
2:B:98:ALA:O	2:B:101:LYS:HE2	2.16	0.45
1:C:420:PRO:HA	1:C:421:PRO:C	2.36	0.45
1:C:107:THR:OG1	1:C:198:HIS:NE2	2.27	0.44
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.52	0.44
1:C:199:ARG:HH22	1:C:223:LYS:HD3	1.82	0.44
1:A:443:ASP:OD1	1:A:444:GLY:N	2.50	0.44
4:F:803:DC:H2'	4:F:804:DA:C8	2.52	0.44
2:B:115:TYR:CD1	2:B:115:TYR:N	2.85	0.44
2:B:154:LYS:C	2:B:157:PRO:HD2	2.37	0.44
2:D:427:TYR:CD1	2:D:428:GLN:O	2.70	0.44
1:C:128:THR:CB	1:C:146:TYR:HB2	2.47	0.44
2:B:279:LEU:HD23	2:B:279:LEU:HA	1.71	0.44
3:E:718:A:C6	3:E:719:G:C5	3.05	0.44
1:C:63:ILE:H	1:C:74:LEU:HD12	1.82	0.44
2:D:401:TRP:O	2:D:402:TRP:C	2.53	0.44
1:A:366:LYS:HE3	1:A:401:TRP:HH2	1.82	0.44
1:C:30:LYS:N	1:C:30:LYS:HD2	2.31	0.44
1:A:265:ASN:OD1	1:A:353:LYS:HD3	2.18	0.44
2:D:167:ILE:HG12	2:D:167:ILE:O	2.17	0.44
2:B:166:LYS:HB2	2:B:166:LYS:HE3	1.66	0.44
4:P:809:DC:C5	4:P:810:DT:C7	3.00	0.44
2:D:12:LEU:HD23	2:D:16:MET:O	2.18	0.44
1:C:388:LYS:H	1:C:388:LYS:HG3	1.65	0.44
1:A:142:ILE:HD12	1:A:142:ILE:HA	1.88	0.44
1:A:329:ILE:O	1:A:392:PRO:HD3	2.18	0.44
1:C:430:GLU:HB2	1:C:532:TYR:HB2	1.98	0.44
1:C:410:TRP:CE2	2:D:363:ASN:ND2	2.86	0.44
1:A:440:PHE:CD1	1:A:440:PHE:N	2.86	0.44
2:B:78:ARG:HD3	2:B:411:ILE:O	2.18	0.44
1:A:125:ARG:HD3	1:A:147:ASN:HD22	1.83	0.44
2:D:396:GLU:OE2	2:D:396:GLU:N	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:THR:HG21	1:A:146:TYR:CD2	2.52	0.44
2:D:112:GLY:HA3	2:D:151:GLN:OE1	2.18	0.44
2:D:149:LEU:HD13	2:D:156:SER:HA	2.00	0.44
1:A:186:ASP:C	1:A:187:LEU:HD23	2.38	0.44
2:B:206:ARG:NE	2:B:216:THR:HB	2.32	0.44
1:C:473:THR:HG21	4:F:809:DC:P	2.57	0.44
1:A:203:GLU:HA	1:A:206:ARG:HD3	2.00	0.44
2:D:323:LYS:O	2:D:385:LYS:NZ	2.51	0.43
2:B:210:LEU:HA	2:B:214:LEU:O	2.18	0.43
1:C:416:PHE:CD1	1:C:417:VAL:N	2.86	0.43
1:A:325:LEU:HA	1:A:325:LEU:HD23	1.66	0.43
2:D:301:LEU:HA	2:D:301:LEU:HD23	1.45	0.43
2:B:28:GLU:HG3	2:B:32:LYS:HD3	1.99	0.43
2:B:214:LEU:HD12	2:B:215:THR:N	2.33	0.43
2:B:281:LYS:O	2:B:284:ARG:HG2	2.18	0.43
1:A:545:ASN:C	1:A:548:VAL:HG12	2.36	0.43
1:C:206:ARG:HH22	1:C:218:ASP:HB2	1.83	0.43
2:D:372:VAL:HG13	2:D:389:PHE:CE2	2.53	0.43
2:B:305:GLU:O	2:B:309:ILE:HG13	2.18	0.43
2:D:20:LYS:HD3	2:D:55:PRO:O	2.18	0.43
1:A:278:GLN:HB2	1:A:299:ALA:HA	2.01	0.43
1:C:226:PRO:HB2	1:C:233:GLU:HG2	2.00	0.43
1:C:320:ASP:OD1	1:C:322:SER:OG	2.27	0.43
1:A:361:HIS:ND1	1:A:513:SER:OG	2.38	0.43
1:C:21:VAL:HG23	1:C:57:ASN:O	2.19	0.43
2:D:113:ASP:HB2	2:D:214:LEU:HD12	2.00	0.43
2:B:82:LYS:HA	2:B:85:GLN:HB2	2.01	0.43
1:C:457:TYR:C	1:C:457:TYR:CD1	2.91	0.43
2:D:47:ILE:HD12	2:D:144:TYR:CD2	2.53	0.43
1:C:160:PHE:CD1	1:C:160:PHE:C	2.91	0.43
4:P:817:DG:C6	4:P:818:DC:C4	3.07	0.43
2:D:114:ALA:N	2:D:214:LEU:HD13	2.33	0.43
4:P:806:DT:H2'	4:P:807:DC:C6	2.53	0.43
1:A:218:ASP:C	1:A:220:LYS:N	2.72	0.43
2:D:81:ASN:HB3	2:D:154:LYS:HD3	2.00	0.43
2:B:350:LYS:NZ	2:B:378:GLU:OE2	2.42	0.43
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.54	0.43
1:A:544:GLY:HA2	1:A:547:GLN:HB2	2.01	0.43
2:B:115:TYR:H	2:B:115:TYR:HD1	1.65	0.43
2:D:75:VAL:HB	2:D:77:PHE:CE2	2.54	0.43
2:D:335:GLY:HA2	2:D:367:GLN:HE22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LEU:O	1:C:205:LEU:HG	2.17	0.43
1:A:542:ILE:HG12	2:B:283:LEU:CD1	2.49	0.43
1:C:171:PHE:CZ	1:C:205:LEU:HB2	2.54	0.43
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.01	0.43
1:A:497:THR:O	1:A:535:TRP:HA	2.19	0.43
1:A:22:LYS:HG2	1:A:23:GLN:N	2.34	0.43
1:A:104:LYS:HE2	1:A:104:LYS:HB2	1.79	0.43
2:B:120:LEU:HD13	2:B:150:PRO:HD3	2.01	0.42
1:A:224:GLU:N	1:A:225:PRO:HD2	2.34	0.42
1:C:524:GLN:HE21	1:C:524:GLN:HA	1.84	0.42
1:A:259:LYS:HG3	4:P:819:DG:OP1	2.18	0.42
1:A:128:THR:HG21	1:A:146:TYR:HD2	1.83	0.42
2:B:41:MET:HG2	2:B:46:LYS:HD3	2.01	0.42
4:P:815:DG:N3	4:P:816:DG:C8	2.87	0.42
1:A:34:LEU:HD22	1:A:73:LYS:NZ	2.33	0.42
2:D:111:VAL:HG22	2:D:185:ASP:O	2.19	0.42
2:B:239:TRP:CZ3	2:B:378:GLU:HB3	2.54	0.42
1:A:88:TRP:CZ2	2:B:57:ASN:HB2	2.54	0.42
2:B:172:LYS:HE2	2:B:180:ILE:HB	2.01	0.42
1:C:35:VAL:HG23	1:C:134:SER:CB	2.49	0.42
1:A:94:ILE:CD1	1:A:230:MET:CE	2.97	0.42
2:D:325:LEU:HB2	2:D:387:PRO:HA	2.01	0.42
1:A:87:PHE:HE2	1:A:154:LYS:HB2	1.85	0.42
1:A:95:PRO:HA	2:B:136:ASN:O	2.20	0.42
1:C:175:ASN:HB3	1:C:178:ILE:HD13	2.00	0.42
2:D:149:LEU:HA	2:D:150:PRO:HD3	1.80	0.42
1:A:433:PRO:HD3	1:A:532:TYR:CZ	2.55	0.42
1:C:479:LEU:HB2	1:C:517:LEU:HD21	2.00	0.42
2:D:34:LEU:HA	2:D:34:LEU:HD23	1.78	0.42
1:A:43:LYS:HD3	1:A:43:LYS:HA	1.63	0.42
1:A:406:TRP:HH2	2:B:418:ASN:CB	2.33	0.42
2:B:319:TYR:CD2	2:B:383:TRP:HD1	2.38	0.42
1:C:323:LYS:HE2	1:C:323:LYS:HB3	1.51	0.42
1:C:279:LEU:HD23	1:C:279:LEU:HA	1.72	0.42
1:A:550:LYS:CG	1:A:551:LEU:N	2.82	0.42
2:D:328:GLU:HG3	2:D:390:LYS:HG3	2.02	0.42
2:B:160:PHE:CD1	2:B:160:PHE:O	2.73	0.42
2:B:370:GLU:HG3	2:B:374:LYS:HD2	2.02	0.42
1:A:429:LEU:HD11	1:A:506:ILE:HG22	2.02	0.42
1:A:276:VAL:HG12	1:A:353:LYS:NZ	2.35	0.42
2:B:257:ILE:H	2:B:257:ILE:HG12	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:PRO:HG3	2:B:80:LEU:HB2	2.02	0.42
1:A:454:LYS:HG3	1:A:552:VAL:HG13	2.02	0.42
2:B:33:ALA:O	2:B:37:ILE:HD12	2.20	0.42
2:B:248:GLU:HG2	2:B:307:ARG:HH12	1.85	0.42
4:F:807:DC:H2"	4:F:808:DC:O5'	2.19	0.41
2:B:132:ILE:HB	2:B:142:ILE:HB	2.02	0.41
1:C:433:PRO:HD3	1:C:532:TYR:CZ	2.55	0.41
2:D:303:LEU:HG	2:D:307:ARG:NH1	2.35	0.41
1:C:206:ARG:HH21	1:C:217:PRO:C	2.23	0.41
2:D:128:THR:OG1	2:D:146:TYR:HB2	2.20	0.41
1:C:63:ILE:H	1:C:74:LEU:CD1	2.33	0.41
1:C:399:GLU:O	1:C:403:THR:HG23	2.20	0.41
1:C:551:LEU:HD23	1:C:551:LEU:HA	1.70	0.41
2:B:153:TRP:CZ2	2:B:155:GLY:HA3	2.55	0.41
1:A:448:ARG:HE	1:A:448:ARG:HB2	1.52	0.41
2:D:10:VAL:HG13	2:D:87:PHE:CD1	2.56	0.41
3:T:720:G:C4	3:T:721:G:C8	3.08	0.41
1:A:194:GLU:CD	1:A:197:GLN:H	2.24	0.41
2:D:203:GLU:O	2:D:207:GLN:HG2	2.20	0.41
1:A:288:ALA:HB3	1:A:291:GLU:HG3	2.02	0.41
2:B:154:LYS:HG2	2:B:184:MET:SD	2.61	0.41
2:B:206:ARG:NH1	2:B:232:TYR:OH	2.53	0.41
1:A:60:VAL:HA	1:A:76:ASP:HB3	2.01	0.41
1:C:434:ILE:HG13	1:C:494:ASN:OD1	2.20	0.41
2:B:171:PHE:CE2	2:B:205:LEU:HB2	2.55	0.41
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.54	0.41
2:D:395:LYS:NZ	4:F:813:DT:OP1	2.32	0.41
1:C:399:GLU:HA	1:C:402:TRP:CD1	2.56	0.41
2:B:12:LEU:HD12	2:B:124:PHE:HE1	1.84	0.41
4:P:809:DC:C6	4:P:810:DT:C7	3.04	0.41
4:P:810:DT:C2	4:P:811:DG:N7	2.89	0.41
2:B:209:LEU:O	2:B:214:LEU:N	2.53	0.41
2:D:280:SER:C	2:D:282:LEU:N	2.72	0.41
1:C:167:ILE:HG22	1:C:208:HIS:HE1	1.85	0.41
4:P:814:DC:H2"	4:P:815:DG:H8	1.85	0.41
2:B:167:ILE:HG23	2:B:212:TRP:CG	2.56	0.41
1:A:128:THR:HG21	1:A:146:TYR:CB	2.29	0.41
2:D:209:LEU:HB3	2:D:214:LEU:CD2	2.39	0.41
4:P:809:DC:C6	4:P:810:DT:H71	2.55	0.41
2:D:308:GLU:O	2:D:311:LYS:HB2	2.19	0.41
1:A:84:THR:HG23	1:A:124:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:396:GLU:N	2:B:396:GLU:OE2	2.50	0.41
2:D:402:TRP:CG	2:D:403:THR:N	2.88	0.41
1:C:319:TYR:CZ	1:C:321:PRO:HA	2.56	0.41
2:B:421:PRO:HB3	2:B:424:LYS:CB	2.24	0.41
2:B:249:LYS:HB2	2:B:252:TRP:CZ2	2.54	0.41
2:D:112:GLY:O	2:D:115:TYR:HB2	2.21	0.41
2:D:319:TYR:CD2	2:D:383:TRP:HD1	2.38	0.41
1:C:12:LEU:HG	1:C:124:PHE:HE2	1.85	0.41
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.70	0.41
1:C:108:VAL:HG22	1:C:188:TYR:CD2	2.56	0.41
1:C:118:VAL:HA	1:C:119:PRO:HD2	1.63	0.41
2:D:317:VAL:CG2	2:D:317:VAL:O	2.63	0.41
2:B:252:TRP:HB3	2:B:257:ILE:CD1	2.50	0.41
1:C:460:ASN:HA	2:D:286:THR:HG22	2.01	0.41
1:A:434:ILE:HD11	1:A:530:LYS:HB3	1.97	0.41
1:C:417:VAL:CG1	1:C:417:VAL:O	2.69	0.41
1:A:460:ASN:HA	2:B:286:THR:O	2.21	0.41
2:D:56:TYR:HD2	2:D:126:LYS:O	2.04	0.41
2:D:324:ASP:O	2:D:343:GLN:HG3	2.20	0.41
2:B:164:MET:HE2	2:B:168:LEU:HD11	2.02	0.41
2:B:189:VAL:HG21	2:B:205:LEU:HD23	2.03	0.41
1:C:139:THR:HB	1:C:140:PRO:CD	2.50	0.41
1:A:194:GLU:OE2	1:A:197:GLN:HB2	2.21	0.41
2:D:163:SER:O	2:D:167:ILE:HG22	2.21	0.41
2:B:104:LYS:HB2	2:B:192:ASP:HA	2.03	0.41
2:B:109:LEU:HD22	2:B:206:ARG:NH1	2.36	0.40
4:F:809:DC:C6	4:F:810:DT:C7	3.04	0.40
1:C:196:GLY:HA2	1:C:199:ARG:HD2	2.02	0.40
1:A:100:LEU:O	1:A:318:TYR:HB3	2.22	0.40
1:A:96:HIS:H	2:B:136:ASN:HD21	1.68	0.40
1:A:326:ILE:HB	1:A:342:TYR:CE1	2.55	0.40
2:D:103:LYS:HD3	2:D:192:ASP:OD1	2.21	0.40
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.87	0.40
2:B:84:THR:O	2:B:85:GLN:C	2.58	0.40
1:A:537:PRO:O	1:A:542:ILE:HD12	2.21	0.40
2:B:423:VAL:O	2:B:423:VAL:CG1	2.69	0.40
2:D:69:THR:H	2:D:70:LYS:HZ3	1.68	0.40
2:B:270:ILE:HG13	2:B:346:PHE:CD1	2.56	0.40
1:A:266:TRP:O	1:A:269:GLN:HG2	2.22	0.40
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.56	0.40
2:B:9:PRO:HA	2:B:121:ASP:CG	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:PRO:CB	2:B:424:LYS:CB	2.92	0.40
1:A:545:ASN:O	1:A:548:VAL:HG12	2.21	0.40
2:B:282:LEU:HD23	2:B:282:LEU:HA	1.74	0.40
1:C:47:ILE:HG21	1:C:144:TYR:CE2	2.56	0.40
1:A:46:LYS:O	1:A:47:ILE:HG13	2.22	0.40
1:C:459:THR:CG2	1:C:461:LYS:H	2.34	0.40
4:P:814:DC:H2"	4:P:815:DG:C8	2.57	0.40
1:C:81:ASN:HB3	1:C:154:LYS:HG3	2.02	0.40
1:C:214:LEU:HD23	1:C:214:LEU:HA	1.51	0.40
2:D:423:VAL:CG1	2:D:423:VAL:O	2.70	0.40
1:C:55:PRO:HA	1:C:143:ARG:NH2	2.36	0.40
2:D:87:PHE:O	2:D:91:GLN:HB3	2.21	0.40
1:A:543:GLY:HA2	2:B:285:GLY:O	2.21	0.40
2:D:57:ASN:HA	2:D:129:ALA:O	2.21	0.40
1:A:325:LEU:HD21	1:A:349:LEU:HD13	2.03	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%)	523 (95%)	30 (5%)	0	100	100
1	C	553/556 (100%)	522 (94%)	31 (6%)	0	100	100
2	B	408/428 (95%)	396 (97%)	12 (3%)	0	100	100
2	D	408/428 (95%)	398 (98%)	10 (2%)	0	100	100
All	All	1922/1968 (98%)	1839 (96%)	83 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	457 (92%)	38 (8%)	16	42
1	C	494/497 (99%)	462 (94%)	32 (6%)	21	52
2	B	374/390 (96%)	347 (93%)	27 (7%)	18	46
2	D	374/390 (96%)	351 (94%)	23 (6%)	23	56
All	All	1737/1774 (98%)	1617 (93%)	120 (7%)	19	48

All (120) 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	7	THR
1	A	16	MET
1	A	17	ASP
1	A	39	THR
1	A	67	ASP
1	A	74	LEU
1	A	107	THR
1	A	109	LEU
1	A	110	ASP
1	A	113	ASP
1	A	122	GLU
1	A	123	ASP
1	A	130	PHE
1	A	137	ASN
1	A	146	TYR
1	A	182	GLN
1	A	195	ILE
1	A	218	ASP
1	A	221	HIS
1	A	258	CYS
1	A	297	GLU

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Mol	Chain	Res	Type
1	A	308	GLU
1	A	314	VAL
1	A	317	VAL
1	A	353	LYS
1	A	357	MET
1	A	373	GLN
1	A	399	GLU
1	A	417	VAL
1	A	420	PRO
1	A	473	THR
1	A	474	ASN
1	A	507	GLN
1	A	529	GLU
1	A	539	HIS
2	B	13	LYS
2	B	32	LYS
2	B	48	SER
2	B	72	ARG
2	B	94	ILE
2	B	115	TYR
2	B	120	LEU
2	B	144	TYR
2	B	163	SER
2	B	201	LYS
2	B	208	HIS
2	B	209	LEU
2	B	210	LEU
2	B	232	TYR
2	B	240	THR
2	B	241	VAL
2	B	250	ASP
2	B	271	TYR
2	B	282	LEU
2	B	293	ILE
2	B	296	THR
2	B	305	GLU
2	B	324	ASP
2	B	374	LYS
2	B	388	LYS
2	B	399	GLU
2	B	410	TRP
1	C	2	ILE

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Mol	Chain	Res	Type
1	C	3	SER
1	C	12	LEU
1	C	16	MET
1	C	17	ASP
1	C	47	ILE
1	C	85	GLN
1	C	113	ASP
1	C	130	PHE
1	C	144	TYR
1	C	146	TYR
1	C	164	MET
1	C	173	LYS
1	C	182	GLN
1	C	205	LEU
1	C	216	THR
1	C	245	VAL
1	C	258	CYS
1	C	305	GLU
1	C	323	LYS
1	C	325	LEU
1	C	357	MET
1	C	373	GLN
1	C	375	ILE
1	C	377	THR
1	C	386	THR
1	C	407	GLN
1	C	425	LEU
1	C	434	ILE
1	C	459	THR
1	C	463	ARG
1	C	472	THR
2	D	38	CYS
2	D	40	GLU
2	D	47	ILE
2	D	72	ARG
2	D	101	LYS
2	D	113	ASP
2	D	123	ASP
2	D	167	ILE
2	D	189	VAL
2	D	194	GLU
2	D	211	ARG

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Mol	Chain	Res	Type
2	D	212	TRP
2	D	234	LEU
2	D	249	LYS
2	D	287	LYS
2	D	298	GLU
2	D	343	GLN
2	D	357	MET
2	D	362	THR
2	D	403	THR
2	D	410	TRP
2	D	427	TYR
2	D	428	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
2	B	161	GLN
1	C	222	GLN
1	C	474	ASN
1	C	500	GLN
1	C	545	ASN
2	D	367	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	18/27 (66%)	8 (44%)	3 (16%)
3	T	19/27 (70%)	10 (52%)	4 (21%)
All	All	37/54 (68%)	18 (48%)	7 (18%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	708	G
3	T	712	C
3	T	715	A
3	T	716	A
3	T	717	C
3	T	718	A

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Mol	Chain	Res	Type
3	T	720	G
3	T	721	G
3	T	724	U
3	T	725	G
3	E	712	C
3	E	714	G
3	E	715	A
3	E	717	C
3	E	720	G
3	E	721	G
3	E	723	C
3	E	724	U

All (7) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	T	711	C
3	T	714	G
3	T	719	G
3	T	720	G
3	E	711	C
3	E	714	G
3	E	720	G

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NVP	A	901	-	18,23,23	1.90	5 (27%)	18,34,34	2.66	6 (33%)
5	NVP	C	901	-	18,23,23	1.94	6 (33%)	18,34,34	1.77	6 (33%)

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	-	-	0/0/6/6	0/2/4/4
5	NVP	C	901	-	-	0/0/6/6	0/2/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	NVP	C10-C15	-2.68	1.37	1.40
5	C	901	NVP	C10-C15	-2.04	1.38	1.40
5	C	901	NVP	CB-CA	2.03	1.52	1.48
5	A	901	NVP	C15-N14	2.58	1.39	1.35
5	C	901	NVP	C2-N3	2.83	1.39	1.35
5	C	901	NVP	C15-N14	3.33	1.40	1.35
5	A	901	NVP	C2-N3	3.38	1.40	1.35
5	A	901	NVP	C4-N3	3.62	1.39	1.32
5	A	901	NVP	C13-N14	3.69	1.39	1.32
5	C	901	NVP	C4-N3	3.75	1.40	1.32
5	C	901	NVP	C13-N14	3.85	1.40	1.32

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	NVP	CC-CA-N1	-4.46	113.65	118.25
5	C	901	NVP	CC-CA-N1	-3.62	114.52	118.25
5	A	901	NVP	C7-C2-N3	-3.57	118.98	122.90
5	A	901	NVP	C10-C15-N14	-2.75	120.26	123.53
5	C	901	NVP	C12-C13-N14	-2.70	119.71	123.94
5	A	901	NVP	C12-C13-N14	-2.49	120.04	123.94
5	C	901	NVP	C5-C4-N3	-2.42	120.75	124.56
5	C	901	NVP	C10-C15-N14	-2.25	120.86	123.53
5	C	901	NVP	CD-C6-C7	2.30	122.34	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	901	NVP	C11-C10-C15	3.33	120.11	117.00
5	A	901	NVP	C11-C10-C15	5.65	122.28	117.00
5	A	901	NVP	CD-C6-C7	5.81	126.14	119.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	901	NVP	1	0

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%)	0.97	88 (15%) 3 1	17, 82, 185, 221	0
1	C	555/556 (99%)	1.13	113 (20%) 1 1	13, 89, 191, 219	0
2	B	412/428 (96%)	0.20	17 (4%) 41 34	18, 58, 108, 135	0
2	D	412/428 (96%)	0.33	24 (5%) 26 20	20, 67, 119, 144	0
3	E	19/27 (70%)	1.82	7 (36%) 0 0	130, 171, 195, 201	0
3	T	20/27 (74%)	0.97	3 (15%) 3 2	123, 141, 184, 191	0
4	F	19/21 (90%)	1.77	6 (31%) 1 0	91, 157, 195, 202	0
4	P	19/21 (90%)	0.87	3 (15%) 3 1	85, 134, 175, 177	0
All	All	2011/2064 (97%)	0.74	261 (12%) 5 3	13, 73, 179, 221	0

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	27.9
1	A	132	ILE	23.0
1	A	60	VAL	22.4
1	A	62	ALA	18.3
1	A	26	LEU	14.7
1	C	31	ILE	14.2
1	C	133	PRO	14.0
1	C	62	ALA	13.9
1	A	61	PHE	10.8
1	C	33	ALA	10.7
1	C	26	LEU	10.0
1	C	72	ARG	10.0
1	A	27	THR	9.7
1	A	25	PRO	9.6
1	C	132	ILE	9.5
1	A	75	VAL	9.2

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Mol	Chain	Res	Type	RSRZ
1	C	59	PRO	9.0
1	C	136	ASN	8.9
2	B	215	THR	8.8
1	C	68	SER	8.6
1	A	136	ASN	8.6
1	C	247	PRO	8.5
1	A	134	SER	8.5
1	A	59	PRO	8.4
1	C	32	LYS	8.3
2	D	214	LEU	8.2
1	A	31	ILE	8.2
2	B	214	LEU	8.0
1	C	71	TRP	7.9
1	A	142	ILE	7.8
1	C	61	PHE	7.7
1	A	138	GLU	7.7
2	D	215	THR	7.5
1	A	67	ASP	7.5
1	A	131	THR	7.5
1	C	30	LYS	7.3
1	A	34	LEU	7.2
1	C	34	LEU	7.1
1	A	139	THR	6.9
1	A	553	SER	6.8
1	C	144	TYR	6.8
1	A	68	SER	6.7
1	C	69	THR	6.6
1	C	25	PRO	6.5
2	D	93	GLY	6.5
1	C	27	THR	6.4
1	C	142	ILE	6.3
1	A	33	ALA	6.3
1	C	252	TRP	6.3
1	C	140	PRO	6.2
1	C	24	TRP	6.1
1	C	21	VAL	6.1
1	C	255	ASN	6.1
1	A	22	LYS	6.1
1	C	63	ILE	6.0
1	A	137	ASN	6.0
1	C	54	ASN	5.8
1	C	257	ILE	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	74	LEU	5.7
1	A	144	TYR	5.7
1	C	223	LYS	5.7
1	A	130	PHE	5.6
1	C	310	LEU	5.4
1	A	21	VAL	5.3
1	A	287	LYS	5.3
1	C	18	GLY	5.3
4	F	805	DG	5.2
1	C	51	GLY	5.1
1	C	37	ILE	5.0
1	C	55	PRO	5.0
1	C	19	PRO	5.0
3	T	725	G	4.9
1	A	24	TRP	4.9
2	D	209	LEU	4.8
2	B	88	TRP	4.8
1	C	131	THR	4.7
1	C	290	THR	4.7
2	D	5	ILE	4.7
1	A	66	LYS	4.7
2	B	231	GLY	4.7
2	D	94	ILE	4.7
1	A	128	THR	4.6
1	C	74	LEU	4.6
1	C	139	THR	4.6
1	A	193	LEU	4.6
4	F	815	DG	4.6
1	A	56	TYR	4.6
1	C	70	LYS	4.5
1	A	28	GLU	4.5
1	A	283	LEU	4.4
1	C	64	LYS	4.4
1	C	141	GLY	4.4
1	C	58	THR	4.4
1	C	134	SER	4.4
4	F	816	DG	4.4
3	E	723	C	4.4
2	D	6	GLU	4.3
1	A	146	TYR	4.2
2	D	360	ALA	4.2
1	C	73	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	554	ALA	4.2
1	C	145	GLN	4.0
1	C	253	THR	4.0
1	A	148	VAL	3.9
1	A	151	GLN	3.8
1	C	283	LEU	3.8
1	C	254	VAL	3.8
1	C	292	VAL	3.8
1	A	19	PRO	3.8
1	C	20	LYS	3.8
1	A	135	ILE	3.7
1	C	66	LYS	3.7
1	C	289	LEU	3.7
1	A	544	GLY	3.7
1	C	174	GLN	3.6
4	P	803	DC	3.6
1	C	76	ASP	3.6
1	C	195	ILE	3.5
1	C	224	GLU	3.5
2	D	231	GLY	3.5
1	C	222	GLN	3.5
1	A	129	ALA	3.5
1	A	63	ILE	3.4
1	C	138	GLU	3.4
1	C	65	LYS	3.4
1	C	23	GLN	3.4
1	A	202	ILE	3.4
1	C	293	ILE	3.4
2	B	86	ASP	3.3
1	A	257	ILE	3.3
1	C	296	THR	3.3
2	D	166	LYS	3.3
4	F	813	DT	3.3
1	A	57	ASN	3.3
1	A	143	ARG	3.3
1	A	289	LEU	3.3
1	C	60	VAL	3.2
1	A	80	LEU	3.2
2	D	212	TRP	3.2
1	C	28	GLU	3.2
1	C	295	LEU	3.2
3	E	716	A	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	4	PRO	3.1
3	E	724	U	3.1
1	A	140	PRO	3.1
1	A	65	LYS	3.1
2	D	354	TYR	3.1
1	A	127	TYR	3.1
3	E	713	C	3.1
1	A	58	THR	3.1
2	B	94	ILE	3.1
1	C	57	ASN	3.0
1	A	18	GLY	3.0
1	C	67	ASP	3.0
1	A	198	HIS	3.0
2	D	210	LEU	3.0
1	C	50	ILE	3.0
3	E	714	G	3.0
1	C	93	GLY	3.0
1	A	77	PHE	3.0
1	C	202	ILE	2.9
1	A	251	SER	2.9
2	B	93	GLY	2.9
1	C	193	LEU	2.9
1	C	137	ASN	2.9
2	B	85	GLN	2.9
1	A	254	VAL	2.9
1	A	72	ARG	2.9
1	C	15	GLY	2.8
1	A	50	ILE	2.8
1	C	251	SER	2.8
2	B	212	TRP	2.8
4	P	804	DA	2.8
1	A	141	GLY	2.8
3	E	715	A	2.8
1	C	40	GLU	2.7
4	F	804	DA	2.7
1	C	286	THR	2.7
1	C	80	LEU	2.7
2	D	190	GLY	2.7
1	A	222	GLN	2.7
1	C	22	LYS	2.6
2	B	87	PHE	2.6
1	C	12	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	284	ARG	2.6
2	D	124	PHE	2.6
1	C	301	LEU	2.6
1	C	200	THR	2.6
2	B	202	ILE	2.6
1	C	226	PRO	2.6
3	T	706	C	2.6
1	A	30	LYS	2.6
1	C	49	LYS	2.6
4	F	817	DG	2.6
1	C	315	HIS	2.5
1	A	32	LYS	2.5
1	C	248	GLU	2.5
1	A	292	VAL	2.5
1	C	29	GLU	2.5
1	C	147	ASN	2.5
1	A	293	ILE	2.5
2	D	92	LEU	2.5
1	C	288	ALA	2.5
1	A	549	ASP	2.5
1	C	287	LYS	2.5
1	C	146	TYR	2.5
1	C	299	ALA	2.5
1	A	295	LEU	2.4
2	D	358	ARG	2.4
1	A	64	LYS	2.4
1	C	46	LYS	2.4
3	E	721	G	2.4
2	B	248	GLU	2.4
2	D	174	GLN	2.4
1	C	219	LYS	2.4
1	C	220	LYS	2.4
4	P	816	DG	2.4
2	D	361	HIS	2.4
1	A	29	GLU	2.3
1	A	546	GLU	2.3
2	B	91	GLN	2.3
2	D	232	TYR	2.3
1	C	41	MET	2.3
2	D	357	MET	2.3
2	D	154	LYS	2.3
1	C	77	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	258	CYS	2.3
1	A	286	THR	2.2
1	C	45	GLY	2.2
2	B	168	LEU	2.2
1	A	91	GLN	2.2
1	A	83	ARG	2.2
1	C	205	LEU	2.2
2	B	89	GLU	2.2
2	D	4	PRO	2.2
1	A	116	PHE	2.2
1	A	20	LYS	2.2
1	C	129	ALA	2.2
2	B	84	THR	2.2
1	A	252	TRP	2.2
1	C	56	TYR	2.2
1	C	118	VAL	2.2
1	A	48	SER	2.2
1	C	298	GLU	2.2
1	C	244	ILE	2.1
2	D	88	TRP	2.1
1	A	215	THR	2.1
1	A	545	ASN	2.1
1	C	225	PRO	2.1
1	A	290	THR	2.1
1	A	145	GLN	2.1
1	C	75	VAL	2.1
1	C	250	ASP	2.1
1	A	147	ASN	2.1
1	C	271	TYR	2.1
3	T	724	U	2.1
1	C	303	LEU	2.1
1	C	83	ARG	2.1
1	C	13	LYS	2.0
1	A	448	ARG	2.0
1	A	255	ASN	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
5	NVP	A	901	20/20	0.94	0.23	-0.16	49,56,65,67	0
5	NVP	C	901	20/20	0.96	0.25	-0.23	58,68,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.