



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:48 PM UTC

PDB ID : 1T05 / pdb_00001t05
Title : HIV-1 reverse transcriptase crosslinked to template-primer with tenofovir-diphosphate bound as the incoming nucleotide substrate
Authors : Tuske, S.; Sarafianos, S.G.; Ding, J.; Arnold, E.
Deposited on : 2004-04-07
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

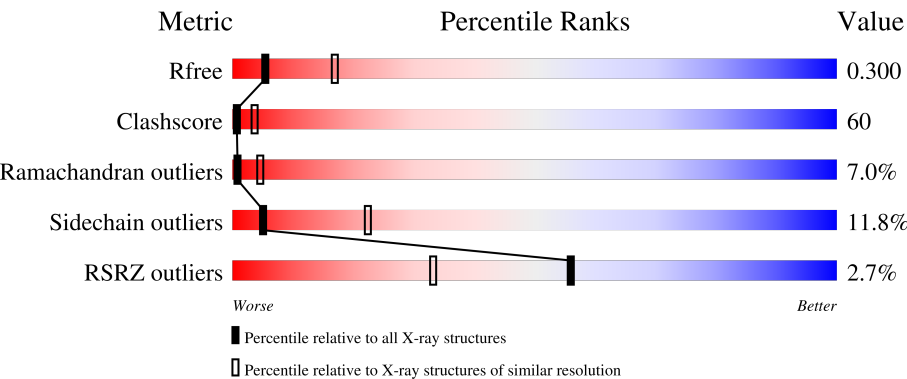
1 Overall quality at a glance i

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)

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	T	27	
2	P	21	
3	A	558	
4	B	437	

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	GOL	A	824	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8898 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 DNA chain called oligonucleotide template.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	24	Total	C	N	O	P	0	0	0
			494	233	97	141	23			

- Molecule 2 is a DNA chain called oligonucleotide primer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	20	Total	C	N	O	P	0	0	0
			403	192	72	120	19			

- Molecule 3 is a protein called POL polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	554	Total	C	N	O	S	0	0	0
			4506	2917	749	832	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 4 is a protein called POL polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	414	Total	C	N	O	S	0	0	0
			3415	2221	567	621	6			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P04585
B	430	GLY	-	cloning artifact	UNP P04585

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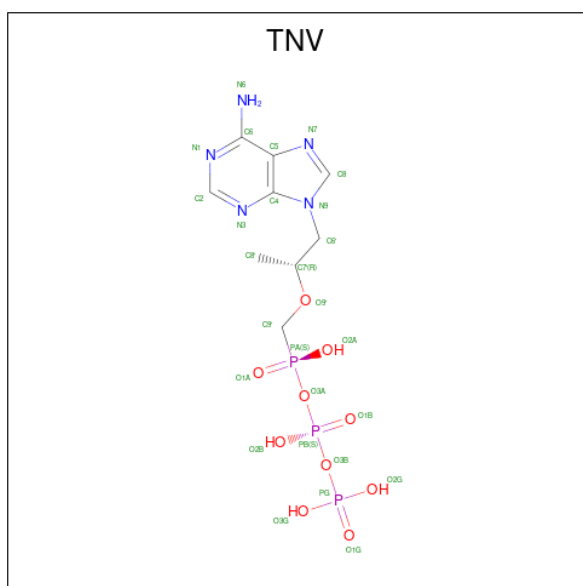
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Chain	Residue	Modelled	Actual	Comment	Reference
B	431	GLY	-	cloning artifact	UNP P04585
B	432	HIS	-	expression tag	UNP P04585
B	433	HIS	-	expression tag	UNP P04585
B	434	HIS	-	expression tag	UNP P04585
B	435	HIS	-	expression tag	UNP P04585
B	436	HIS	-	expression tag	UNP P04585
B	437	HIS	-	expression tag	UNP P04585

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is [2-(6-AMINO-9H-PURIN-9-YL)-1-METHYLETHOXY]METHYL-TRIPHOSPHATE (CCD ID: TNV) (formula: C₉H₁₆N₅O₁₀P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	9	5	10	3		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	T	2	Total	O	0	0
			2	2		
8	P	3	Total	O	0	0
			3	3		
8	A	10	Total	O	0	0
			10	10		
8	B	6	Total	O	0	0
			6	6		

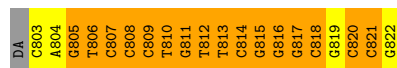
3 Residue-property plots

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

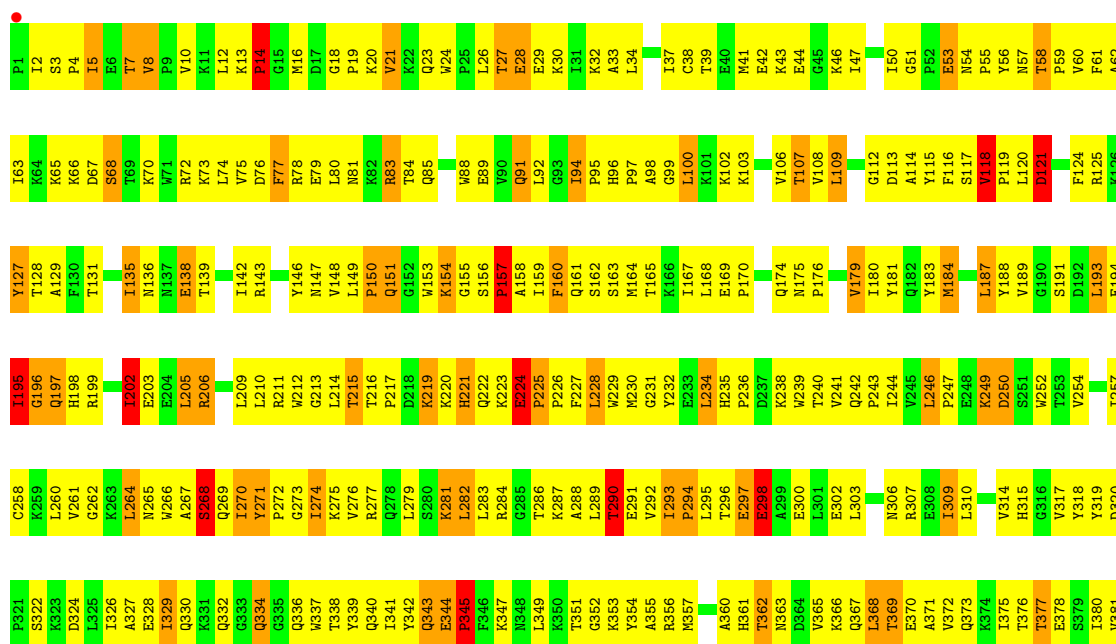
- Molecule 1: oligonucleotide template

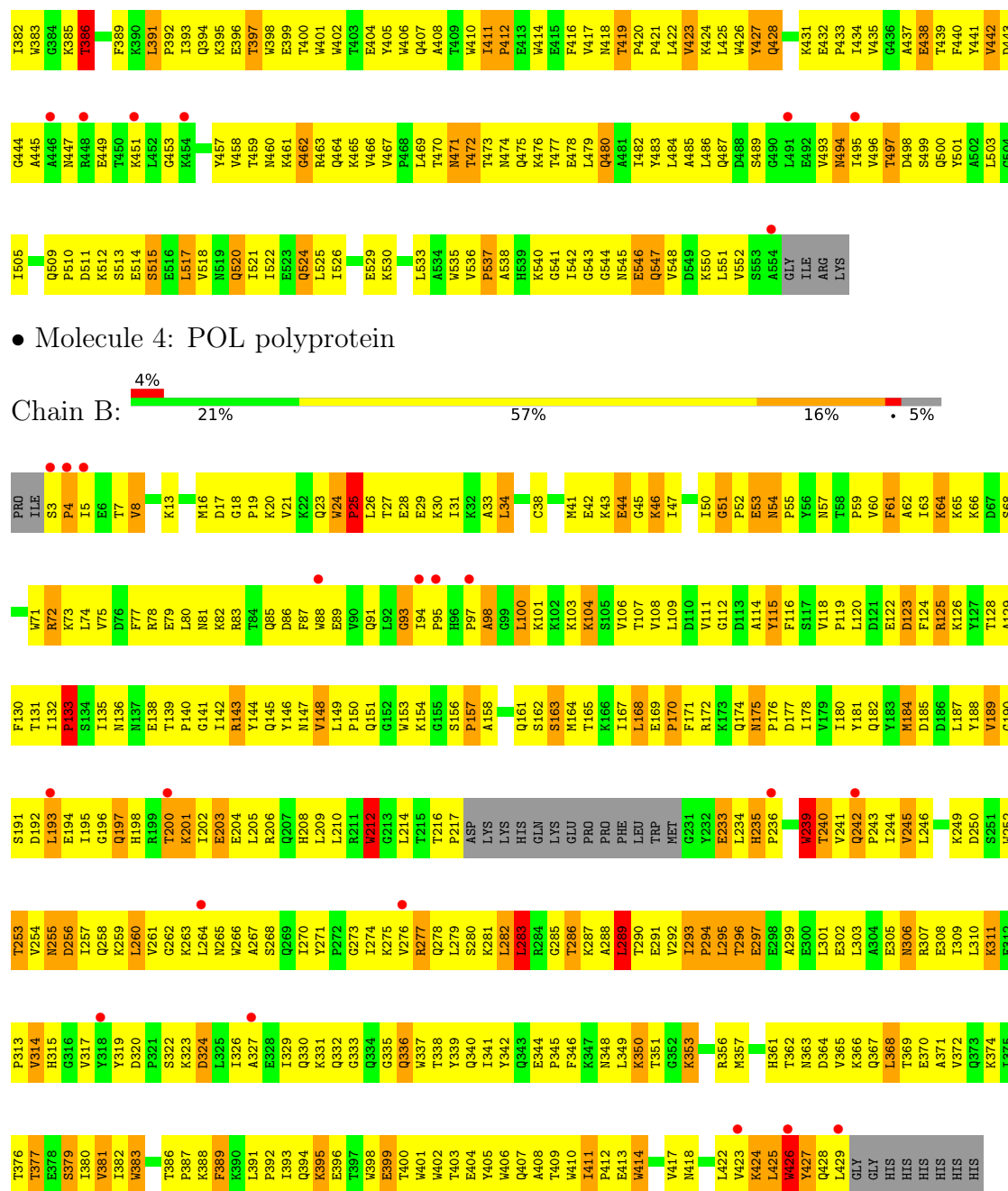


- Molecule 2: oligonucleotide primer



- Molecule 3: POL polyprotein





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	171.57Å 171.57Å 156.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	81.8 (20.00-3.00) 91.0 (20.00-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.253 , 0.292 0.268 , 0.300	Depositor DCC
R_{free} test set	1926 reflections (4.01%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.063 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8898	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MRG, MG, TNV, DDG

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	T	0.39	0/555	1.39	21/856 (2.5%)
2	P	0.39	0/400	1.52	22/612 (3.6%)
3	A	0.67	1/4624 (0.0%)	1.22	51/6282 (0.8%)
4	B	0.55	0/3512	1.20	35/4774 (0.7%)
All	All	0.60	1/9091 (0.0%)	1.24	129/12524 (1.0%)

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
3	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	ILE	CA-CB	-6.93	1.47	1.54

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3	SER	CA-C-N	19.15	143.77	119.84
4	B	3	SER	C-N-CA	19.15	143.77	119.84
4	B	295	LEU	N-CA-C	12.48	129.27	112.30
4	B	3	SER	C-N-CD	-11.84	76.44	125.00
4	B	5	ILE	N-CA-C	9.69	120.46	111.45
3	A	174	GLN	OE1-CD-NE2	-9.22	113.38	122.60
3	A	225	PRO	N-CA-C	-8.68	100.11	110.70
3	A	92	LEU	N-CA-C	8.51	120.56	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8	VAL	N-CA-C	8.40	116.25	107.76
3	A	391	LEU	CA-C-N	7.98	129.82	119.84
3	A	391	LEU	C-N-CA	7.98	129.82	119.84
3	A	118	VAL	CA-C-N	7.94	128.00	119.90
3	A	118	VAL	C-N-CA	7.94	128.00	119.90
2	P	814	DC	C2'-C3'-O3'	-7.70	99.95	111.50
3	A	474	ASN	N-CA-C	-7.64	103.84	113.01
3	A	8	VAL	CA-C-N	7.62	129.37	119.84
3	A	8	VAL	C-N-CA	7.62	129.37	119.84
1	T	711	DC	C2'-C3'-O3'	-7.62	100.07	111.50
3	A	281	LYS	N-CA-C	-7.47	103.63	112.89
3	A	147	ASN	N-CA-C	-7.45	104.70	114.31
1	T	718	DA	N9-C1'-C2'	7.44	124.66	113.50
3	A	411	ILE	CA-C-N	7.44	129.13	119.84
3	A	411	ILE	C-N-CA	7.44	129.13	119.84
4	B	51	GLY	CA-C-N	7.43	128.37	120.12
4	B	51	GLY	C-N-CA	7.43	128.37	120.12
2	P	815	DG	C2'-C3'-O3'	-7.38	100.42	111.50
2	P	807	DC	C2'-C3'-O3'	-7.38	100.43	111.50
4	B	311	LYS	N-CA-C	-7.30	104.90	113.88
1	T	712	DC	C2'-C3'-O3'	-7.30	100.56	111.50
1	T	706	DC	C2'-C3'-O3'	-7.21	100.69	111.50
1	T	714	DG	C2'-C3'-O3'	-7.21	100.69	111.50
2	P	813	DT	C2'-C3'-O3'	-7.19	100.71	111.50
2	P	815	DG	N9-C1'-C2'	7.19	124.28	113.50
4	B	212	TRP	N-CA-C	-7.12	104.22	114.12
4	B	4	PRO	N-CA-C	7.09	127.07	112.47
1	T	720	DG	C2'-C3'-O3'	-7.07	100.90	111.50
3	A	219	LYS	N-CA-C	-7.07	95.75	110.80
2	P	809	DC	C2'-C3'-O3'	-7.06	100.91	111.50
1	T	715	DA	C2'-C3'-O3'	-7.00	101.00	111.50
3	A	344	GLU	CA-C-N	6.97	128.56	119.84
3	A	344	GLU	C-N-CA	6.97	128.56	119.84
3	A	224	GLU	CA-C-N	-6.96	113.22	120.38
3	A	224	GLU	C-N-CA	-6.96	113.22	120.38
3	A	8	VAL	N-CA-C	6.89	115.58	107.73
3	A	51	GLY	CA-C-N	6.87	126.47	119.19
3	A	51	GLY	C-N-CA	6.87	126.47	119.19
2	P	812	DT	C2'-C3'-O3'	-6.80	101.30	111.50
3	A	189	VAL	N-CA-C	6.80	116.50	106.85
3	A	174	GLN	CG-CD-NE2	6.73	126.49	116.40
1	T	716	DA	C2'-C3'-O3'	-6.71	101.44	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	721	DG	C2'-C3'-O3'	-6.66	101.51	111.50
3	A	28	GLU	N-CA-C	-6.64	105.15	113.18
3	A	234	LEU	N-CA-C	6.61	120.41	107.98
3	A	271	TYR	CA-C-N	6.58	126.60	119.89
3	A	271	TYR	C-N-CA	6.58	126.60	119.89
1	T	717	DC	C2'-C3'-O3'	-6.56	101.66	111.50
1	T	724	DT	C2'-C3'-O3'	-6.54	101.69	111.50
2	P	804	DA	C2'-C3'-O3'	-6.50	101.75	111.50
1	T	722	DA	C2'-C3'-O3'	-6.47	101.79	111.50
1	T	719	DG	N9-C1'-C2'	6.45	123.18	113.50
4	B	250	ASP	N-CA-C	-6.43	105.36	113.72
2	P	818	DC	C2'-C3'-O3'	-6.42	101.87	111.50
1	T	718	DA	C2'-C3'-O3'	-6.39	101.92	111.50
2	P	816	DG	C2'-C3'-O3'	-6.38	101.94	111.50
4	B	391	LEU	CA-C-N	6.36	127.79	119.84
4	B	391	LEU	C-N-CA	6.36	127.79	119.84
1	T	719	DG	C2'-C3'-O3'	-6.36	101.96	111.50
2	P	806	DT	C2'-C3'-O3'	-6.26	102.11	111.50
3	A	467	VAL	CA-C-N	6.25	126.22	120.03
3	A	467	VAL	C-N-CA	6.25	126.22	120.03
3	A	397	THR	N-CA-C	-6.25	103.77	111.33
4	B	147	ASN	N-CA-C	-6.23	106.22	113.88
3	A	297	GLU	N-CA-C	-6.20	103.45	111.02
4	B	54	ASN	CA-C-N	6.19	127.58	119.84
4	B	54	ASN	C-N-CA	6.19	127.58	119.84
2	P	810	DT	C2'-C3'-O3'	-6.17	102.24	111.50
4	B	64	LYS	N-CA-C	-6.07	100.86	109.96
3	A	442	VAL	N-CA-C	6.06	118.50	109.17
2	P	813	DT	N1-C1'-C2'	6.05	122.57	113.50
2	P	805	DG	C2'-C3'-O3'	-6.03	102.46	111.50
3	A	343	GLN	N-CA-C	-6.01	107.18	114.75
2	P	803	DC	C2'-C3'-O3'	-6.00	102.50	111.50
1	T	713	DC	C2'-C3'-O3'	-5.99	102.51	111.50
2	P	820	DC	C2'-C3'-O3'	-5.98	102.53	111.50
3	A	213	GLY	CA-C-N	-5.97	114.76	123.00
3	A	213	GLY	C-N-CA	-5.97	114.76	123.00
2	P	811	DG	C2'-C3'-O3'	-5.96	102.56	111.50
2	P	814	DC	N1-C1'-C2'	5.91	122.37	113.50
4	B	411	ILE	CA-C-N	5.81	125.78	120.03
4	B	411	ILE	C-N-CA	5.81	125.78	120.03
4	B	24	TRP	CA-C-N	5.72	126.99	119.84
4	B	24	TRP	C-N-CA	5.72	126.99	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	405	TYR	N-CA-C	5.72	120.42	113.38
1	T	705	DT	N1-C1'-C2'	-5.72	104.92	113.50
3	A	187	LEU	N-CA-C	5.72	117.73	108.41
3	A	290	THR	N-CA-C	-5.70	106.67	113.97
3	A	386	THR	CA-C-N	5.67	125.42	119.76
3	A	386	THR	C-N-CA	5.67	125.42	119.76
4	B	324	ASP	N-CA-C	5.66	118.75	109.76
4	B	296	THR	N-CA-C	5.64	117.42	108.79
1	T	723	DC	C2'-C3'-O3'	-5.63	103.06	111.50
1	T	715	DA	N9-C1'-C2'	5.61	121.92	113.50
4	B	377	THR	N-CA-C	-5.59	104.19	111.02
3	A	179	VAL	CB-CA-C	-5.58	103.58	111.38
3	A	215	THR	N-CA-C	5.56	118.69	109.46
4	B	306	ASN	N-CA-C	-5.55	105.12	112.34
2	P	821	DC	C2'-C3'-O3'	-5.50	103.24	111.50
4	B	168	LEU	N-CA-C	5.49	119.98	113.28
3	A	274	ILE	N-CA-C	-5.47	101.85	109.45
2	P	808	DC	C2'-C3'-O3'	-5.45	103.32	111.50
4	B	294	PRO	N-CA-C	-5.43	101.29	112.47
3	A	249	LYS	N-CA-C	5.41	122.33	110.80
3	A	360	ALA	N-CA-C	-5.38	107.37	114.31
3	A	369	THR	N-CA-C	-5.38	105.53	112.68
1	T	710	DG	C2'-C3'-O3'	-5.37	103.45	111.50
4	B	131	THR	N-CA-C	5.37	117.73	107.75
3	A	127	TYR	N-CA-C	5.35	117.81	111.33
1	T	720	DG	N9-C1'-C2'	5.32	121.48	113.50
4	B	5	ILE	CB-CA-C	-5.29	104.99	111.92
2	P	809	DC	N1-C1'-C2'	5.27	121.41	113.50
3	A	292	VAL	N-CA-C	5.26	115.17	108.12
3	A	497	THR	N-CA-C	5.21	117.30	109.23
2	P	807	DC	N1-C1'-C2'	5.20	121.30	113.50
4	B	301	LEU	N-CA-C	-5.10	105.42	111.69
4	B	44	GLU	N-CA-C	-5.09	104.40	110.41
4	B	143	ARG	N-CA-C	5.09	117.37	110.35
3	A	391	LEU	N-CA-C	5.03	117.48	109.64
3	A	514	GLU	N-CA-C	-5.03	107.10	113.18
4	B	426	TRP	N-CA-C	-5.01	105.83	112.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	160	PHE	Sidechain

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	T	494	0	269	24	0
2	P	403	0	224	30	0
3	A	4506	0	4567	548	0
4	B	3415	0	3448	473	0
5	A	2	0	0	0	0
6	A	27	0	12	7	0
7	A	18	0	21	5	0
7	B	12	0	14	1	0
8	A	10	0	0	1	0
8	B	6	0	0	1	0
8	P	3	0	0	0	0
8	T	2	0	0	0	0
All	All	8898	0	8555	1042	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 60.

All (1042) 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)
3:A:498:ASP:HB2	3:A:538:ALA:HB2	1.31	1.08
3:A:103:LYS:H	7:A:824:GOL:H32	1.13	1.08
3:A:205:LEU:HD22	3:A:209:LEU:HD11	1.35	1.07
3:A:408:ALA:HB1	4:B:364:ASP:HB3	1.37	1.07
3:A:72:ARG:HH12	6:A:823:TNV:H8'3	1.12	1.07
4:B:140:PRO:HA	8:B:441:HOH:O	1.54	1.06
4:B:278:GLN:HB3	4:B:299:ALA:HA	1.40	1.03
3:A:517:LEU:HD22	3:A:521:ILE:HD11	1.43	1.00
4:B:194:GLU:H	4:B:197:GLN:HE22	1.07	0.98
4:B:44:GLU:O	4:B:46:LYS:HD2	1.65	0.94
4:B:332:GLN:HB2	4:B:336:GLN:HB3	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:122:GLU:HA	4:B:125:ARG:HD2	1.50	0.93
4:B:167:ILE:HG23	4:B:212:TRP:CE3	2.04	0.93
3:A:484:LEU:HA	3:A:487:GLN:HE21	1.30	0.93
3:A:324:ASP:O	3:A:343:GLN:HG2	1.69	0.93
4:B:104:LYS:HB2	4:B:192:ASP:HA	1.51	0.92
3:A:254:VAL:HG13	3:A:283:LEU:HD22	1.51	0.92
3:A:419:THR:H	3:A:422:LEU:HD21	1.33	0.92
3:A:493:VAL:HG12	3:A:494:ASN:H	1.34	0.92
3:A:222:GLN:N	3:A:224:GLU:HG3	1.84	0.91
3:A:317:VAL:HG22	3:A:318:TYR:H	1.32	0.91
3:A:221:HIS:HE1	3:A:228:LEU:HB2	1.36	0.91
4:B:369:THR:HG22	4:B:398:TRP:CH2	2.05	0.91
3:A:484:LEU:HD23	3:A:487:GLN:NE2	1.86	0.90
3:A:439:THR:HG21	4:B:289:LEU:HD13	1.50	0.90
3:A:47:ILE:HG22	3:A:146:TYR:HA	1.54	0.90
3:A:293:ILE:HG13	3:A:294:PRO:HD2	1.53	0.88
4:B:326:ILE:HG22	4:B:327:ALA:H	1.36	0.88
1:T:705:DT:H3	6:A:823:TNV:HN61	1.22	0.87
3:A:135:ILE:H	3:A:135:ILE:HD12	1.39	0.87
3:A:199:ARG:HH21	3:A:223:LYS:HB2	1.40	0.87
4:B:246:LEU:HD22	4:B:260:LEU:HD11	1.58	0.85
3:A:72:ARG:HH12	6:A:823:TNV:C8'	1.87	0.85
3:A:156:SER:HB2	3:A:157:PRO:HD3	1.59	0.85
3:A:103:LYS:H	7:A:824:GOL:C3	1.89	0.85
4:B:326:ILE:HG22	4:B:327:ALA:N	1.88	0.84
3:A:222:GLN:H	3:A:224:GLU:HG3	1.38	0.83
4:B:194:GLU:HG3	4:B:196:GLY:H	1.43	0.83
3:A:72:ARG:NH1	6:A:823:TNV:H8'3	1.94	0.83
3:A:500:GLN:HG2	4:B:422:LEU:HD22	1.59	0.83
4:B:252:TRP:HB3	4:B:257:ILE:HD11	1.59	0.82
3:A:205:LEU:HD22	3:A:209:LEU:CD1	2.08	0.82
4:B:296:THR:HB	4:B:299:ALA:HB3	1.60	0.82
4:B:194:GLU:H	4:B:197:GLN:NE2	1.78	0.82
3:A:59:PRO:HG2	3:A:76:ASP:HB3	1.59	0.81
4:B:118:VAL:HB	4:B:149:LEU:HD12	1.62	0.81
4:B:175:ASN:HD21	4:B:201:LYS:HE2	1.47	0.80
4:B:389:PHE:HD1	4:B:389:PHE:H	1.30	0.80
3:A:95:PRO:HA	4:B:136:ASN:O	1.80	0.79
3:A:417:VAL:O	3:A:417:VAL:HG13	1.81	0.79
4:B:365:VAL:O	4:B:369:THR:HG23	1.81	0.79
3:A:72:ARG:HG2	3:A:74:LEU:HD21	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:326:ILE:CG2	4:B:327:ALA:H	1.96	0.79
3:A:397:THR:HG21	3:A:424:LYS:HA	1.63	0.79
3:A:498:ASP:CB	3:A:538:ALA:HB2	2.12	0.79
4:B:276:VAL:HG22	4:B:280:SER:HB3	1.63	0.79
3:A:362:THR:HG22	3:A:366:LYS:HD3	1.64	0.79
4:B:62:ALA:HB1	4:B:71:TRP:HE3	1.48	0.79
3:A:157:PRO:O	3:A:161:GLN:HG3	1.83	0.78
4:B:401:TRP:O	4:B:404:GLU:HB2	1.83	0.78
3:A:441:TYR:HB2	3:A:458:VAL:HG12	1.66	0.78
3:A:246:LEU:HD21	3:A:264:LEU:HD11	1.65	0.78
3:A:199:ARG:NH2	3:A:223:LYS:HB2	1.99	0.78
4:B:266:TRP:HB3	4:B:426:TRP:CZ2	2.19	0.77
4:B:79:GLU:O	4:B:83:ARG:HG3	1.84	0.77
3:A:116:PHE:C	3:A:148:VAL:HG21	2.09	0.77
4:B:335:GLY:HA3	4:B:356:ARG:HB2	1.66	0.77
1:T:714:DG:H4'	3:A:286:THR:HG21	1.66	0.76
3:A:67:ASP:O	3:A:68:SER:HB2	1.85	0.76
4:B:372:VAL:HG13	4:B:389:PHE:CE2	2.21	0.76
4:B:61:PHE:HE2	4:B:63:ILE:HD11	1.50	0.76
3:A:205:LEU:CD2	3:A:209:LEU:HD11	2.15	0.76
3:A:16:MET:HE2	3:A:83:ARG:HD2	1.68	0.76
3:A:50:ILE:HD12	3:A:54:ASN:HB3	1.67	0.76
3:A:220:LYS:O	3:A:220:LYS:HG3	1.86	0.76
4:B:287:LYS:HE2	4:B:287:LYS:HA	1.68	0.76
4:B:314:VAL:HG22	4:B:315:HIS:H	1.50	0.76
4:B:114:ALA:CB	4:B:214:LEU:HD22	2.16	0.75
3:A:478:GLU:HG2	3:A:499:SER:HB3	1.68	0.75
4:B:120:LEU:HD12	4:B:149:LEU:HD23	1.67	0.75
4:B:278:GLN:HB3	4:B:299:ALA:CA	2.16	0.75
4:B:240:THR:HG22	4:B:241:VAL:H	1.51	0.75
3:A:408:ALA:HA	4:B:364:ASP:OD1	1.85	0.75
2:P:818:DC:H2''	2:P:819:DG:H5'	1.69	0.74
4:B:239:TRP:HA	4:B:239:TRP:CE3	2.22	0.74
3:A:149:LEU:CD2	3:A:156:SER:HA	2.17	0.74
4:B:115:TYR:CD1	4:B:156:SER:HB3	2.22	0.74
3:A:484:LEU:HA	3:A:487:GLN:NE2	2.01	0.74
4:B:171:PHE:HA	4:B:174:GLN:HG3	1.70	0.74
4:B:180:ILE:HD11	4:B:205:LEU:HD11	1.67	0.74
3:A:537:PRO:HG2	4:B:262:GLY:HA2	1.68	0.74
4:B:406:TRP:O	4:B:407:GLN:HG3	1.87	0.74
3:A:544:GLY:O	3:A:548:VAL:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3:SER:OG	3:A:5:ILE:HG22	1.86	0.73
3:A:118:VAL:HB	3:A:149:LEU:CD1	2.18	0.73
4:B:262:GLY:O	4:B:265:ASN:HB3	1.88	0.73
3:A:221:HIS:CE1	3:A:228:LEU:HB2	2.23	0.73
4:B:406:TRP:CH2	4:B:412:PRO:HD2	2.23	0.73
4:B:266:TRP:HB3	4:B:426:TRP:HZ2	1.50	0.73
4:B:329:ILE:HG22	4:B:330:GLN:N	2.04	0.73
3:A:103:LYS:N	7:A:824:GOL:H32	1.97	0.73
4:B:115:TYR:HD1	4:B:156:SER:HB3	1.54	0.72
4:B:388:LYS:HD2	4:B:388:LYS:O	1.88	0.72
3:A:509:GLN:N	3:A:510:PRO:HD3	2.04	0.72
3:A:478:GLU:O	3:A:482:ILE:HG13	1.88	0.72
3:A:470:THR:HG22	3:A:471:ASN:OD1	1.89	0.72
3:A:76:ASP:O	3:A:78:ARG:N	2.21	0.72
3:A:221:HIS:HB3	3:A:224:GLU:HB2	1.72	0.72
3:A:337:TRP:CZ3	3:A:368:LEU:HD23	2.24	0.72
3:A:441:TYR:HB3	3:A:548:VAL:HG21	1.72	0.71
3:A:206:ARG:HG2	3:A:216:THR:OG1	1.89	0.71
3:A:317:VAL:HG22	3:A:318:TYR:N	2.04	0.71
3:A:529:GLU:O	3:A:530:LYS:HG3	1.91	0.71
3:A:89:GLU:OE1	3:A:89:GLU:HA	1.90	0.71
3:A:242:GLN:HB3	3:A:243:PRO:HD2	1.72	0.71
3:A:293:ILE:HG13	3:A:294:PRO:CD	2.21	0.70
4:B:120:LEU:HB2	4:B:148:VAL:O	1.91	0.70
4:B:255:ASN:ND2	4:B:259:LYS:HE2	2.06	0.70
4:B:65:LYS:HB2	4:B:68:SER:HB3	1.73	0.70
3:A:3:SER:HB2	3:A:212:TRP:O	1.91	0.70
3:A:257:ILE:O	3:A:261:VAL:HG23	1.92	0.70
4:B:115:TYR:OH	4:B:157:PRO:HB3	1.90	0.70
4:B:44:GLU:HB2	4:B:46:LYS:HE3	1.73	0.70
4:B:233:GLU:CD	4:B:233:GLU:H	1.97	0.70
3:A:221:HIS:CE1	3:A:228:LEU:H	2.09	0.70
4:B:329:ILE:HG22	4:B:330:GLN:H	1.57	0.70
3:A:391:LEU:C	3:A:417:VAL:HG12	2.16	0.70
4:B:60:VAL:HG12	4:B:75:VAL:HG22	1.73	0.70
3:A:97:PRO:HA	3:A:100:LEU:CD2	2.21	0.70
4:B:98:ALA:HA	4:B:101:LYS:HD3	1.72	0.70
3:A:406:TRP:CD1	3:A:407:GLN:HG3	2.26	0.70
4:B:406:TRP:HH2	4:B:412:PRO:HD2	1.55	0.70
3:A:451:LYS:HB3	3:A:471:ASN:HA	1.74	0.69
4:B:326:ILE:CG2	4:B:327:ALA:N	2.54	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:482:ILE:O	3:A:486:LEU:HG	1.92	0.69
4:B:372:VAL:HA	4:B:389:PHE:HE2	1.56	0.69
3:A:135:ILE:HD12	3:A:135:ILE:N	2.06	0.69
4:B:175:ASN:N	4:B:176:PRO:HD3	2.08	0.69
3:A:84:THR:HG22	3:A:85:GLN:N	2.08	0.69
3:A:59:PRO:HG2	3:A:76:ASP:CB	2.23	0.69
3:A:391:LEU:HB2	3:A:414:TRP:CE3	2.28	0.69
3:A:498:ASP:HB2	3:A:538:ALA:CB	2.17	0.69
4:B:24:TRP:HH2	4:B:61:PHE:CD1	2.10	0.69
4:B:379:SER:OG	4:B:387:PRO:HD3	1.93	0.69
3:A:2:ILE:HD11	3:A:46:LYS:HD2	1.75	0.69
4:B:61:PHE:CE2	4:B:63:ILE:HD11	2.27	0.68
3:A:91:GLN:CG	3:A:161:GLN:HE22	2.07	0.68
4:B:168:LEU:HD12	4:B:172:ARG:NH2	2.08	0.68
4:B:242:GLN:HE21	4:B:353:LYS:HE3	1.58	0.68
3:A:410:TRP:CH2	3:A:412:PRO:HA	2.29	0.68
4:B:167:ILE:HA	4:B:212:TRP:CZ3	2.29	0.68
3:A:417:VAL:HG22	3:A:419:THR:CG2	2.24	0.68
3:A:518:VAL:HA	3:A:521:ILE:HD12	1.75	0.68
4:B:255:ASN:HB3	4:B:289:LEU:HG	1.76	0.68
3:A:402:TRP:HH2	4:B:362:THR:HB	1.59	0.67
3:A:420:PRO:HA	3:A:421:PRO:C	2.18	0.67
4:B:25:PRO:O	4:B:26:LEU:HD23	1.95	0.67
4:B:260:LEU:O	4:B:264:LEU:HD12	1.95	0.67
4:B:170:PRO:HB2	4:B:208:HIS:CE1	2.29	0.67
3:A:518:VAL:O	3:A:522:ILE:HG13	1.95	0.67
4:B:314:VAL:HG22	4:B:315:HIS:N	2.08	0.67
4:B:368:LEU:HD23	4:B:368:LEU:O	1.94	0.67
3:A:394:GLN:HB2	3:A:397:THR:OG1	1.95	0.67
4:B:103:LYS:HG3	4:B:191:SER:O	1.95	0.67
3:A:453:GLY:O	3:A:469:LEU:N	2.27	0.67
3:A:91:GLN:HG3	3:A:161:GLN:HE22	1.60	0.67
4:B:114:ALA:HB1	4:B:214:LEU:HD22	1.77	0.67
4:B:254:VAL:HB	4:B:289:LEU:HA	1.77	0.67
3:A:58:THR:HG22	3:A:59:PRO:HD2	1.77	0.66
3:A:164:MET:HG3	3:A:168:LEU:HD12	1.76	0.66
3:A:109:LEU:HD23	3:A:109:LEU:N	2.09	0.66
3:A:242:GLN:HB3	3:A:243:PRO:CD	2.25	0.66
4:B:78:ARG:O	4:B:82:LYS:HG3	1.95	0.66
4:B:254:VAL:O	4:B:258:GLN:HG3	1.96	0.66
4:B:277:ARG:HA	4:B:280:SER:OG	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:369:THR:HG22	4:B:398:TRP:CZ3	2.30	0.66
4:B:406:TRP:CD1	4:B:408:ALA:H	2.13	0.66
4:B:239:TRP:HA	4:B:239:TRP:HE3	1.61	0.66
3:A:13:LYS:HG2	3:A:84:THR:O	1.96	0.66
4:B:100:LEU:HD23	4:B:101:LYS:N	2.10	0.66
4:B:194:GLU:N	4:B:197:GLN:HE22	1.88	0.66
3:A:336:GLN:C	3:A:337:TRP:CD1	2.74	0.65
3:A:392:PRO:O	3:A:423:VAL:HG23	1.96	0.65
3:A:439:THR:CG2	4:B:289:LEU:HD13	2.24	0.65
3:A:517:LEU:O	3:A:520:GLN:HG2	1.96	0.65
4:B:50:ILE:HG21	4:B:145:GLN:HB2	1.76	0.65
3:A:149:LEU:HD23	3:A:156:SER:HA	1.78	0.65
4:B:120:LEU:HD21	4:B:124:PHE:HD2	1.60	0.65
3:A:97:PRO:HA	3:A:100:LEU:HD22	1.77	0.65
4:B:233:GLU:C	4:B:234:LEU:HD12	2.20	0.65
3:A:369:THR:O	3:A:373:GLN:HG3	1.96	0.65
4:B:85:GLN:HA	4:B:88:TRP:CE2	2.32	0.65
3:A:402:TRP:CH2	4:B:362:THR:HB	2.32	0.65
3:A:223:LYS:C	3:A:225:PRO:HD2	2.22	0.65
4:B:368:LEU:HD23	4:B:368:LEU:C	2.21	0.65
3:A:457:TYR:CE2	3:A:465:LYS:HB3	2.31	0.65
3:A:221:HIS:H	3:A:221:HIS:CD2	2.14	0.64
3:A:376:THR:HG23	3:A:386:THR:HG22	1.79	0.64
3:A:339:TYR:CZ	3:A:352:GLY:HA3	2.31	0.64
4:B:93:GLY:C	4:B:94:ILE:HD12	2.22	0.64
4:B:151:GLN:HB3	4:B:185:ASP:OD2	1.97	0.64
3:A:273:GLY:H	3:A:338:THR:HG21	1.62	0.64
3:A:427:TYR:HE1	3:A:522:ILE:HG23	1.63	0.64
4:B:126:LYS:HA	4:B:145:GLN:OE1	1.96	0.64
3:A:53:GLU:H	3:A:53:GLU:CD	2.06	0.64
4:B:308:GLU:HA	4:B:311:LYS:HE2	1.78	0.64
4:B:243:PRO:O	4:B:244:ILE:HD13	1.98	0.64
3:A:344:GLU:HB2	3:A:347:LYS:HB2	1.79	0.64
4:B:72:ARG:HG3	4:B:72:ARG:HH11	1.62	0.64
4:B:244:ILE:HG23	4:B:426:TRP:HB3	1.80	0.64
4:B:278:GLN:HB2	4:B:302:GLU:CD	2.23	0.64
3:A:347:LYS:HE2	3:A:347:LYS:HA	1.80	0.64
3:A:547:GLN:O	3:A:551:LEU:HG	1.96	0.64
4:B:85:GLN:HG3	4:B:86:ASP:N	2.12	0.64
4:B:320:ASP:OD2	4:B:323:LYS:HE2	1.97	0.64
3:A:376:THR:HG23	3:A:386:THR:CG2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:114:ALA:HB2	4:B:214:LEU:HD22	1.80	0.63
3:A:135:ILE:H	3:A:135:ILE:CD1	2.10	0.63
3:A:303:LEU:HD21	3:A:307:ARG:NH2	2.14	0.63
4:B:109:LEU:HD11	4:B:206:ARG:NH2	2.14	0.63
3:A:202:ILE:HG22	3:A:203:GLU:N	2.13	0.63
3:A:434:ILE:H	3:A:494:ASN:HD21	1.47	0.63
3:A:497:THR:O	3:A:535:TRP:HA	1.97	0.63
4:B:170:PRO:HB2	4:B:208:HIS:HE1	1.63	0.63
4:B:341:ILE:HD12	4:B:350:LYS:HB3	1.80	0.63
3:A:238:LYS:HD2	3:A:315:HIS:CD2	2.34	0.62
3:A:337:TRP:CH2	3:A:368:LEU:HB2	2.34	0.62
4:B:59:PRO:O	4:B:75:VAL:HG13	1.98	0.62
4:B:369:THR:HG22	4:B:398:TRP:HH2	1.61	0.62
3:A:23:GLN:OE1	3:A:59:PRO:HA	2.00	0.62
3:A:417:VAL:HG22	3:A:419:THR:HG22	1.81	0.62
3:A:441:TYR:HB2	3:A:458:VAL:CG1	2.28	0.62
4:B:330:GLN:O	4:B:337:TRP:HA	1.99	0.62
3:A:370:GLU:HA	3:A:373:GLN:HG3	1.82	0.62
3:A:222:GLN:C	3:A:224:GLU:H	2.07	0.62
4:B:241:VAL:HG12	4:B:242:GLN:H	1.64	0.62
3:A:247:PRO:HG2	3:A:260:LEU:CD1	2.30	0.62
4:B:54:ASN:O	4:B:143:ARG:NH2	2.32	0.62
4:B:249:LYS:HE2	4:B:256:ASP:OD1	2.00	0.62
3:A:540:LYS:O	3:A:542:ILE:HG13	1.99	0.62
4:B:62:ALA:HB1	4:B:71:TRP:CE3	2.31	0.62
3:A:540:LYS:HD3	3:A:540:LYS:C	2.24	0.62
4:B:100:LEU:HD23	4:B:101:LYS:H	1.64	0.62
4:B:106:VAL:HG12	4:B:107:THR:N	2.15	0.62
4:B:291:GLU:O	4:B:293:ILE:HG23	1.99	0.62
3:A:127:TYR:C	3:A:129:ALA:H	2.08	0.62
3:A:222:GLN:O	3:A:227:PHE:CE2	2.53	0.62
3:A:458:VAL:HG22	3:A:459:THR:H	1.65	0.62
3:A:473:THR:O	3:A:477:THR:HG23	1.99	0.62
4:B:34:LEU:H	4:B:34:LEU:HD23	1.64	0.61
3:A:438:GLU:OE1	3:A:461:LYS:HD2	1.99	0.61
4:B:380:ILE:C	4:B:382:ILE:H	2.08	0.61
1:T:707:DG:H2''	1:T:708:DG:H5'	1.82	0.61
3:A:368:LEU:HD11	3:A:391:LEU:HD22	1.81	0.61
4:B:252:TRP:HB3	4:B:257:ILE:CD1	2.31	0.61
4:B:274:ILE:HG23	4:B:306:ASN:CG	2.25	0.61
4:B:296:THR:HG22	4:B:297:GLU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:275:LYS:HD3	3:A:332:GLN:CD	2.25	0.61
4:B:33:ALA:O	4:B:34:LEU:C	2.42	0.61
3:A:164:MET:HA	3:A:167:ILE:HD12	1.83	0.61
4:B:148:VAL:HG23	4:B:149:LEU:N	2.15	0.61
4:B:372:VAL:HA	4:B:389:PHE:CE2	2.36	0.60
2:P:822:DDG:H2'	6:A:823:TNV:H6'1	1.82	0.60
3:A:221:HIS:HA	3:A:224:GLU:OE1	2.00	0.60
4:B:193:LEU:HD12	4:B:198:HIS:N	2.16	0.60
4:B:376:THR:HG1	4:B:389:PHE:HZ	1.49	0.60
3:A:75:VAL:HB	3:A:77:PHE:CE2	2.37	0.60
4:B:27:THR:HB	4:B:29:GLU:HG2	1.82	0.60
3:A:270:ILE:O	3:A:272:PRO:HD3	2.01	0.60
4:B:208:HIS:O	4:B:212:TRP:HB2	2.01	0.60
2:P:815:DG:H2'	2:P:816:DG:H8	1.67	0.60
3:A:183:TYR:O	3:A:184:MET:HB3	2.01	0.60
4:B:30:LYS:O	4:B:33:ALA:HB3	2.01	0.60
3:A:521:ILE:O	3:A:525:LEU:HG	2.02	0.60
3:A:102:LYS:HE3	8:A:827:HOH:O	2.00	0.60
4:B:241:VAL:HA	4:B:351:THR:O	2.02	0.60
3:A:63:ILE:CD1	3:A:74:LEU:HD11	2.31	0.60
4:B:241:VAL:HG12	4:B:242:GLN:N	2.17	0.59
3:A:76:ASP:C	3:A:78:ARG:H	2.10	0.59
3:A:427:TYR:CE1	3:A:522:ILE:HG23	2.36	0.59
3:A:478:GLU:HG2	3:A:499:SER:CB	2.31	0.59
3:A:547:GLN:H	3:A:547:GLN:NE2	2.00	0.59
4:B:406:TRP:CD1	4:B:407:GLN:N	2.70	0.59
1:T:706:DC:H2'	1:T:707:DG:C8	2.37	0.59
3:A:416:PHE:HZ	3:A:422:LEU:CD1	2.15	0.59
3:A:546:GLU:HB3	3:A:547:GLN:NE2	2.18	0.59
3:A:68:SER:C	3:A:70:LYS:H	2.09	0.59
3:A:332:GLN:HG3	3:A:338:THR:OG1	2.02	0.59
4:B:428:GLN:HG2	4:B:429:LEU:HD13	1.84	0.59
3:A:63:ILE:HD13	3:A:74:LEU:HD11	1.83	0.59
3:A:109:LEU:N	3:A:109:LEU:CD2	2.65	0.59
3:A:377:THR:HG22	3:A:378:GLU:N	2.17	0.59
4:B:111:VAL:HG12	4:B:216:THR:OG1	2.03	0.59
3:A:39:THR:HG22	3:A:43:LYS:HE3	1.85	0.59
3:A:118:VAL:HB	3:A:149:LEU:HD12	1.84	0.59
3:A:391:LEU:HB2	3:A:414:TRP:HE3	1.68	0.59
4:B:255:ASN:OD1	4:B:256:ASP:N	2.36	0.59
3:A:232:TYR:HB3	3:A:240:THR:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:484:LEU:HD23	3:A:487:GLN:HE22	1.65	0.59
4:B:278:GLN:CB	4:B:299:ALA:HA	2.26	0.59
3:A:72:ARG:CG	3:A:74:LEU:HD21	2.32	0.58
4:B:296:THR:HB	4:B:299:ALA:CB	2.31	0.58
4:B:394:GLN:O	4:B:395:LYS:C	2.45	0.58
4:B:47:ILE:HG22	4:B:145:GLN:O	2.03	0.58
4:B:241:VAL:HG22	4:B:350:LYS:HD2	1.84	0.58
4:B:356:ARG:HG3	4:B:367:GLN:NE2	2.17	0.58
3:A:4:PRO:O	3:A:5:ILE:C	2.44	0.58
3:A:75:VAL:HB	3:A:77:PHE:CD2	2.39	0.58
3:A:417:VAL:O	3:A:417:VAL:CG1	2.50	0.58
4:B:169:GLU:C	4:B:171:PHE:H	2.10	0.58
4:B:193:LEU:HB2	4:B:197:GLN:HE21	1.68	0.58
1:T:720:DG:H2'	1:T:721:DG:C8	2.39	0.58
3:A:10:VAL:HG23	3:A:124:PHE:CD1	2.38	0.58
3:A:405:TYR:CE2	3:A:407:GLN:HB2	2.39	0.58
4:B:306:ASN:HA	4:B:309:ILE:HD12	1.85	0.58
3:A:181:TYR:HB2	3:A:188:TYR:HB3	1.85	0.58
3:A:479:LEU:O	3:A:482:ILE:N	2.37	0.58
3:A:288:ALA:C	3:A:290:THR:H	2.12	0.58
4:B:115:TYR:H	4:B:115:TYR:HD2	1.52	0.58
4:B:389:PHE:CD1	4:B:389:PHE:N	2.72	0.58
3:A:24:TRP:CD1	3:A:26:LEU:HD23	2.39	0.57
4:B:85:GLN:HA	4:B:88:TRP:CZ2	2.39	0.57
4:B:194:GLU:N	4:B:197:GLN:NE2	2.50	0.57
3:A:30:LYS:O	3:A:33:ALA:N	2.35	0.57
4:B:271:TYR:CD2	4:B:309:ILE:HG22	2.39	0.57
4:B:19:PRO:HG3	4:B:80:LEU:HD13	1.87	0.57
3:A:221:HIS:CD2	3:A:221:HIS:N	2.73	0.57
4:B:23:GLN:NE2	4:B:26:LEU:HD21	2.19	0.57
4:B:288:ALA:O	4:B:291:GLU:HG3	2.04	0.57
3:A:72:ARG:HG2	3:A:74:LEU:CD2	2.34	0.57
3:A:77:PHE:O	3:A:81:ASN:ND2	2.37	0.57
3:A:281:LYS:O	3:A:284:ARG:HG3	2.04	0.57
4:B:108:VAL:HG13	4:B:188:TYR:CE2	2.40	0.57
4:B:417:VAL:HG22	4:B:418:ASN:N	2.19	0.57
1:T:720:DG:O6	2:P:807:DC:N4	2.37	0.57
2:P:816:DG:H2'	2:P:817:MRG:H8	1.86	0.57
3:A:281:LYS:HG3	3:A:284:ARG:CZ	2.35	0.57
3:A:432:GLU:OE2	3:A:433:PRO:HD2	2.04	0.57
3:A:84:THR:CG2	3:A:85:GLN:N	2.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:416:PHE:CZ	3:A:422:LEU:HD13	2.40	0.56
3:A:548:VAL:O	3:A:552:VAL:HG22	2.05	0.56
4:B:205:LEU:HD23	4:B:205:LEU:O	2.05	0.56
3:A:96:HIS:O	3:A:99:GLY:N	2.35	0.56
4:B:161:GLN:O	4:B:165:THR:HG23	2.04	0.56
4:B:181:TYR:HD2	4:B:188:TYR:HD1	1.53	0.56
4:B:255:ASN:C	4:B:257:ILE:N	2.62	0.56
4:B:273:GLY:O	4:B:309:ILE:HD13	2.05	0.56
2:P:820:DC:H2''	2:P:821:DC:H5'	1.87	0.56
3:A:180:ILE:CG2	3:A:187:LEU:HD22	2.36	0.56
4:B:13:LYS:HD3	4:B:86:ASP:H	1.70	0.56
4:B:78:ARG:HD3	4:B:411:ILE:HG22	1.87	0.56
4:B:80:LEU:O	4:B:83:ARG:N	2.35	0.56
4:B:330:GLN:HB2	4:B:338:THR:OG1	2.05	0.56
3:A:88:TRP:O	3:A:89:GLU:C	2.49	0.56
3:A:470:THR:C	3:A:472:THR:H	2.13	0.56
4:B:271:TYR:HD2	4:B:309:ILE:HG22	1.70	0.56
4:B:274:ILE:HG12	4:B:309:ILE:HD12	1.86	0.56
3:A:53:GLU:CD	3:A:53:GLU:N	2.64	0.56
4:B:143:ARG:O	4:B:144:TYR:CG	2.59	0.56
3:A:193:LEU:HD13	3:A:198:HIS:HA	1.86	0.56
3:A:275:LYS:CG	3:A:332:GLN:NE2	2.69	0.56
4:B:20:LYS:HG2	4:B:55:PRO:O	2.06	0.56
4:B:288:ALA:HB3	4:B:291:GLU:HG3	1.88	0.56
4:B:395:LYS:CG	4:B:399:GLU:OE2	2.54	0.56
3:A:493:VAL:HG12	3:A:494:ASN:N	2.15	0.56
3:A:274:ILE:HG22	3:A:275:LYS:N	2.19	0.56
4:B:78:ARG:HD3	4:B:411:ILE:O	2.06	0.56
4:B:100:LEU:HA	4:B:103:LYS:HB2	1.87	0.56
4:B:206:ARG:HH12	4:B:216:THR:HB	1.71	0.56
4:B:376:THR:HG23	4:B:386:THR:HG22	1.88	0.56
3:A:267:ALA:O	3:A:269:GLN:N	2.38	0.56
3:A:441:TYR:HA	3:A:496:VAL:HG12	1.87	0.56
4:B:104:LYS:HD2	4:B:192:ASP:C	2.31	0.56
3:A:28:GLU:O	3:A:32:LYS:HB2	2.06	0.55
3:A:220:LYS:O	3:A:220:LYS:CG	2.53	0.55
3:A:362:THR:HG22	3:A:366:LYS:CD	2.34	0.55
4:B:194:GLU:HB3	4:B:197:GLN:OE1	2.05	0.55
3:A:19:PRO:O	3:A:20:LYS:HG3	2.07	0.55
3:A:372:VAL:HG13	3:A:389:PHE:CE1	2.42	0.55
4:B:274:ILE:HD11	4:B:310:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:815:DG:H2'	2:P:816:DG:C8	2.41	0.55
3:A:97:PRO:HD3	3:A:232:TYR:CE2	2.41	0.55
3:A:121:ASP:O	3:A:125:ARG:HG3	2.06	0.55
4:B:366:LYS:O	4:B:370:GLU:HG3	2.05	0.55
1:T:714:DG:H4'	3:A:286:THR:CG2	2.37	0.55
3:A:529:GLU:O	3:A:529:GLU:HG2	2.06	0.55
4:B:278:GLN:HB2	4:B:302:GLU:OE2	2.06	0.55
3:A:81:ASN:HB3	3:A:154:LYS:HB2	1.87	0.55
3:A:136:ASN:HB2	3:A:138:GLU:HG3	1.88	0.55
3:A:23:GLN:HE21	3:A:26:LEU:HD21	1.71	0.55
3:A:306:ASN:HA	3:A:309:ILE:HG13	1.88	0.55
4:B:206:ARG:HH22	4:B:216:THR:HG22	1.72	0.55
4:B:275:LYS:O	4:B:306:ASN:ND2	2.39	0.55
3:A:188:TYR:HE2	3:A:234:LEU:CD1	2.19	0.55
3:A:354:TYR:CD2	3:A:371:ALA:HA	2.42	0.55
3:A:406:TRP:NE1	3:A:407:GLN:HG3	2.22	0.55
4:B:62:ALA:O	4:B:63:ILE:HD13	2.07	0.55
3:A:464:GLN:HG2	3:A:465:LYS:N	2.22	0.55
3:A:509:GLN:N	3:A:510:PRO:CD	2.70	0.55
4:B:255:ASN:C	4:B:257:ILE:H	2.14	0.55
4:B:395:LYS:HG3	4:B:399:GLU:OE2	2.07	0.55
3:A:63:ILE:HD11	3:A:72:ARG:HD2	1.89	0.54
3:A:274:ILE:HA	3:A:306:ASN:OD1	2.07	0.54
3:A:529:GLU:O	3:A:530:LYS:CG	2.55	0.54
4:B:292:VAL:HG12	4:B:294:PRO:HD3	1.90	0.54
3:A:138:GLU:OE1	3:A:139:THR:HG23	2.07	0.54
3:A:265:ASN:OD1	3:A:353:LYS:NZ	2.40	0.54
3:A:401:TRP:O	3:A:405:TYR:HB2	2.06	0.54
3:A:416:PHE:HZ	3:A:422:LEU:HD13	1.71	0.54
4:B:54:ASN:HB3	4:B:143:ARG:HH21	1.71	0.54
4:B:180:ILE:CD1	4:B:205:LEU:HD11	2.37	0.54
3:A:249:LYS:HG3	3:A:252:TRP:CE2	2.43	0.54
3:A:472:THR:OG1	3:A:476:LYS:HB2	2.08	0.54
3:A:493:VAL:O	3:A:494:ASN:ND2	2.41	0.54
3:A:522:ILE:HA	3:A:525:LEU:HD12	1.90	0.54
4:B:181:TYR:HB3	4:B:188:TYR:HB2	1.90	0.54
3:A:254:VAL:HG13	3:A:283:LEU:CD2	2.32	0.54
3:A:275:LYS:HD3	3:A:332:GLN:OE1	2.08	0.54
3:A:396:GLU:O	3:A:397:THR:C	2.51	0.54
3:A:484:LEU:CA	3:A:487:GLN:HE21	2.10	0.54
4:B:122:GLU:HA	4:B:125:ARG:CD	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:270:ILE:HG22	4:B:271:TYR:CD1	2.42	0.54
2:P:819:DG:H2'	2:P:820:DC:C6	2.43	0.54
3:A:109:LEU:HD23	3:A:187:LEU:O	2.08	0.54
4:B:109:LEU:HG	4:B:216:THR:HG21	1.90	0.54
4:B:193:LEU:HB2	4:B:197:GLN:NE2	2.23	0.54
1:T:711:DC:H2'	1:T:712:DC:C6	2.43	0.53
3:A:395:LYS:O	3:A:395:LYS:HD3	2.07	0.53
3:A:457:TYR:CZ	3:A:465:LYS:HB3	2.43	0.53
4:B:382:ILE:O	4:B:383:TRP:CG	2.61	0.53
2:P:819:DG:H2''	2:P:820:DC:H5'	1.90	0.53
3:A:276:VAL:HA	3:A:302:GLU:CD	2.33	0.53
3:A:371:ALA:O	3:A:372:VAL:C	2.51	0.53
4:B:303:LEU:HD11	4:B:307:ARG:NH2	2.23	0.53
3:A:34:LEU:HD11	3:A:62:ALA:HB2	1.91	0.53
4:B:382:ILE:HG22	4:B:383:TRP:CD2	2.43	0.53
4:B:60:VAL:O	4:B:61:PHE:HB3	2.09	0.53
4:B:282:LEU:O	4:B:283:LEU:HB3	2.08	0.53
4:B:329:ILE:CG2	4:B:330:GLN:H	2.21	0.53
4:B:406:TRP:CD1	4:B:407:GLN:H	2.25	0.53
4:B:408:ALA:C	4:B:410:TRP:H	2.17	0.53
3:A:470:THR:O	3:A:472:THR:N	2.41	0.53
3:A:498:ASP:HA	3:A:536:VAL:O	2.09	0.53
4:B:81:ASN:HB3	4:B:154:LYS:HD2	1.90	0.53
4:B:396:GLU:CD	4:B:396:GLU:H	2.17	0.53
4:B:382:ILE:O	4:B:382:ILE:CG2	2.57	0.53
4:B:395:LYS:CE	4:B:399:GLU:OE2	2.57	0.53
4:B:77:PHE:O	4:B:78:ARG:C	2.51	0.53
4:B:100:LEU:HG	4:B:381:VAL:HG12	1.90	0.53
3:A:5:ILE:HG23	3:A:5:ILE:O	2.09	0.53
3:A:339:TYR:CE1	3:A:352:GLY:C	2.87	0.52
3:A:74:LEU:CD2	3:A:151:GLN:HG2	2.39	0.52
4:B:369:THR:OG1	4:B:370:GLU:N	2.41	0.52
4:B:413:GLU:O	4:B:414:TRP:HB3	2.10	0.52
1:T:709:DC:H2'	1:T:710:DG:C8	2.44	0.52
3:A:229:TRP:CD2	3:A:230:MET:HG2	2.44	0.52
4:B:330:GLN:OE1	4:B:340:GLN:NE2	2.37	0.52
1:T:709:DC:H2'	1:T:710:DG:H8	1.74	0.52
3:A:39:THR:CG2	3:A:43:LYS:HE3	2.39	0.52
3:A:545:ASN:O	3:A:546:GLU:C	2.52	0.52
4:B:244:ILE:CG2	4:B:426:TRP:HB3	2.39	0.52
4:B:255:ASN:O	4:B:257:ILE:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:376:THR:OG1	4:B:389:PHE:CZ	2.62	0.52
3:A:155:GLY:O	3:A:156:SER:C	2.53	0.52
3:A:239:TRP:CE3	3:A:240:THR:N	2.77	0.52
4:B:77:PHE:O	4:B:80:LEU:N	2.39	0.52
3:A:121:ASP:OD2	3:A:124:PHE:HB2	2.09	0.52
3:A:244:ILE:CD1	3:A:267:ALA:HB2	2.39	0.52
3:A:420:PRO:HA	3:A:422:LEU:N	2.25	0.52
4:B:425:LEU:C	4:B:427:TYR:N	2.65	0.52
3:A:72:ARG:NH1	6:A:823:TNV:C8'	2.62	0.52
3:A:354:TYR:C	3:A:354:TYR:CD1	2.86	0.52
3:A:500:GLN:HG2	4:B:422:LEU:CD2	2.36	0.52
1:T:704:DG:H5''	1:T:704:DG:N3	2.24	0.52
4:B:382:ILE:O	4:B:382:ILE:HG22	2.09	0.52
3:A:153:TRP:O	3:A:155:GLY:N	2.43	0.52
3:A:461:LYS:C	3:A:463:ARG:H	2.17	0.52
4:B:64:LYS:NZ	4:B:71:TRP:HE1	2.08	0.52
4:B:163:SER:O	4:B:167:ILE:HG13	2.09	0.52
4:B:332:GLN:HE22	4:B:425:LEU:CD1	2.23	0.52
4:B:376:THR:OG1	4:B:389:PHE:HZ	1.93	0.52
2:P:819:DG:H2'	2:P:820:DC:H6	1.75	0.52
3:A:334:GLN:OE1	3:A:334:GLN:HA	2.10	0.52
3:A:354:TYR:HE1	3:A:356:ARG:CB	2.22	0.52
3:A:442:VAL:O	3:A:443:ASP:HB2	2.09	0.52
4:B:103:LYS:HG3	4:B:191:SER:C	2.35	0.52
4:B:194:GLU:HB3	4:B:197:GLN:CD	2.35	0.52
3:A:13:LYS:O	3:A:14:PRO:C	2.53	0.51
3:A:156:SER:HB2	3:A:157:PRO:CD	2.38	0.51
4:B:153:TRP:HB3	4:B:156:SER:OG	2.10	0.51
3:A:41:MET:O	3:A:42:GLU:C	2.54	0.51
3:A:441:TYR:CD2	3:A:544:GLY:HA3	2.45	0.51
3:A:191:SER:OG	3:A:193:LEU:HD12	2.11	0.51
4:B:120:LEU:HD13	4:B:150:PRO:HD3	1.91	0.51
4:B:281:LYS:C	4:B:283:LEU:H	2.19	0.51
3:A:247:PRO:HD2	3:A:260:LEU:HD12	1.93	0.51
3:A:426:TRP:O	3:A:427:TYR:HB3	2.10	0.51
4:B:78:ARG:CD	4:B:411:ILE:HG22	2.41	0.51
2:P:818:DC:H2'	2:P:819:DG:H8	1.75	0.51
4:B:235:HIS:N	4:B:236:PRO:HD3	2.24	0.51
3:A:222:GLN:C	3:A:224:GLU:N	2.67	0.51
3:A:254:VAL:HB	3:A:289:LEU:HA	1.92	0.51
4:B:106:VAL:CG1	4:B:107:THR:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:189:VAL:HG21	4:B:202:ILE:HD12	1.91	0.51
3:A:440:PHE:O	3:A:496:VAL:HG12	2.11	0.51
4:B:365:VAL:HG23	4:B:366:LYS:H	1.75	0.51
3:A:2:ILE:CD1	3:A:46:LYS:HD2	2.40	0.51
3:A:55:PRO:HG2	3:A:56:TYR:CE2	2.46	0.51
3:A:94:ILE:HG23	3:A:95:PRO:CD	2.40	0.51
4:B:157:PRO:HG2	4:B:158:ALA:H	1.75	0.51
3:A:10:VAL:HG23	3:A:10:VAL:O	2.11	0.50
3:A:28:GLU:HG2	3:A:32:LYS:HD3	1.92	0.50
3:A:235:HIS:HB2	3:A:238:LYS:O	2.10	0.50
1:T:723:DC:H2'	1:T:724:DT:C6	2.47	0.50
3:A:77:PHE:HE2	3:A:150:PRO:HB2	1.75	0.50
3:A:127:TYR:C	3:A:129:ALA:N	2.70	0.50
1:T:704:DG:N3	1:T:704:DG:H2'	2.26	0.50
3:A:486:LEU:HD13	3:A:524:GLN:HB3	1.94	0.50
3:A:501:TYR:CE1	3:A:505:ILE:HD11	2.47	0.50
2:P:814:DC:H2'	2:P:815:DG:C8	2.46	0.50
3:A:513:SER:OG	3:A:515:SER:HB3	2.11	0.50
3:A:77:PHE:O	3:A:81:ASN:CG	2.55	0.50
3:A:293:ILE:CG1	3:A:294:PRO:HD2	2.34	0.50
3:A:546:GLU:HG3	3:A:547:GLN:N	2.24	0.50
4:B:290:THR:HG22	4:B:290:THR:O	2.12	0.50
4:B:329:ILE:CG2	4:B:330:GLN:N	2.71	0.50
3:A:91:GLN:HG2	3:A:161:GLN:NE2	2.26	0.50
3:A:136:ASN:HB2	3:A:138:GLU:OE2	2.12	0.50
4:B:365:VAL:HG23	4:B:366:LYS:N	2.27	0.50
3:A:435:VAL:HG22	4:B:290:THR:HG21	1.93	0.50
4:B:24:TRP:CH2	4:B:61:PHE:CD1	2.96	0.50
4:B:233:GLU:O	4:B:234:LEU:HD12	2.12	0.50
4:B:367:GLN:O	4:B:368:LEU:C	2.55	0.50
3:A:317:VAL:CG2	3:A:318:TYR:H	2.15	0.50
3:A:319:TYR:CD1	3:A:383:TRP:CD1	3.00	0.50
4:B:154:LYS:O	4:B:157:PRO:HD2	2.11	0.50
4:B:305:GLU:C	4:B:307:ARG:N	2.68	0.50
3:A:33:ALA:O	3:A:37:ILE:HG12	2.10	0.49
3:A:163:SER:O	3:A:167:ILE:HG13	2.11	0.49
3:A:406:TRP:O	4:B:331:LYS:HD3	2.12	0.49
4:B:42:GLU:C	4:B:44:GLU:H	2.20	0.49
4:B:242:GLN:HB2	4:B:353:LYS:NZ	2.27	0.49
3:A:8:VAL:O	3:A:10:VAL:HG13	2.12	0.49
3:A:41:MET:O	3:A:44:GLU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:51:GLY:C	4:B:53:GLU:OE2	2.55	0.49
4:B:122:GLU:C	4:B:124:PHE:H	2.20	0.49
4:B:154:LYS:C	4:B:157:PRO:HD2	2.37	0.49
3:A:131:THR:OG1	3:A:143:ARG:HG2	2.12	0.49
3:A:297:GLU:HA	3:A:300:GLU:HB2	1.95	0.49
3:A:501:TYR:O	3:A:505:ILE:HG13	2.12	0.49
3:A:246:LEU:HD22	3:A:310:LEU:HD12	1.93	0.49
3:A:447:ASN:ND2	3:A:449:GLU:H	2.10	0.49
4:B:342:TYR:CD1	4:B:342:TYR:C	2.89	0.49
3:A:276:VAL:O	3:A:277:ARG:C	2.53	0.49
3:A:434:ILE:HB	3:A:494:ASN:ND2	2.26	0.49
3:A:460:ASN:HA	4:B:286:THR:O	2.12	0.49
3:A:484:LEU:O	3:A:486:LEU:N	2.46	0.49
2:P:811:DG:H2'	2:P:812:DT:C6	2.47	0.49
3:A:375:ILE:O	3:A:376:THR:C	2.55	0.49
3:A:437:ALA:O	3:A:439:THR:N	2.45	0.49
4:B:348:ASN:C	4:B:350:LYS:H	2.21	0.49
1:T:724:DT:H2'	1:T:725:DG:C8	2.48	0.49
3:A:160:PHE:CE2	3:A:164:MET:HE2	2.48	0.49
3:A:154:LYS:O	3:A:154:LYS:HG2	2.12	0.49
3:A:239:TRP:HE3	3:A:240:THR:N	2.11	0.49
3:A:372:VAL:HG13	3:A:389:PHE:CZ	2.48	0.49
3:A:477:THR:O	3:A:478:GLU:C	2.56	0.49
3:A:543:GLY:C	3:A:545:ASN:H	2.21	0.49
4:B:78:ARG:NE	4:B:411:ILE:HG22	2.27	0.49
4:B:210:LEU:C	4:B:212:TRP:H	2.21	0.49
4:B:406:TRP:CD1	4:B:408:ALA:N	2.79	0.49
3:A:16:MET:HE2	3:A:83:ARG:CD	2.41	0.49
4:B:249:LYS:HB2	4:B:252:TRP:CE2	2.48	0.49
4:B:372:VAL:O	4:B:389:PHE:CZ	2.66	0.49
2:P:807:DC:H2'	2:P:808:DC:C6	2.48	0.49
2:P:818:DC:H2''	2:P:819:DG:C5'	2.40	0.49
3:A:46:LYS:O	3:A:47:ILE:HG23	2.12	0.49
3:A:106:VAL:HG12	3:A:107:THR:N	2.27	0.49
3:A:149:LEU:HD22	3:A:156:SER:HA	1.93	0.49
3:A:329:ILE:HG22	3:A:330:GLN:N	2.28	0.49
4:B:43:LYS:HG2	4:B:43:LYS:O	2.13	0.49
4:B:314:VAL:CG2	4:B:315:HIS:H	2.21	0.49
1:T:706:DC:H2'	1:T:707:DG:H8	1.77	0.48
3:A:269:GLN:HA	3:A:351:THR:O	2.13	0.48
3:A:277:ARG:NH1	3:A:355:ALA:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:537:PRO:CG	4:B:262:GLY:HA2	2.42	0.48
4:B:242:GLN:CB	4:B:353:LYS:NZ	2.76	0.48
3:A:37:ILE:HD13	3:A:37:ILE:N	2.28	0.48
3:A:222:GLN:H	3:A:224:GLU:CG	2.18	0.48
3:A:420:PRO:HB3	3:A:421:PRO:HA	1.95	0.48
3:A:458:VAL:HG22	3:A:459:THR:N	2.28	0.48
3:A:18:GLY:H	3:A:56:TYR:HE1	1.62	0.48
4:B:273:GLY:O	4:B:309:ILE:CD1	2.61	0.48
3:A:354:TYR:HE1	3:A:356:ARG:HB2	1.79	0.48
3:A:391:LEU:HD12	3:A:414:TRP:CB	2.43	0.48
3:A:451:LYS:O	3:A:471:ASN:N	2.46	0.48
3:A:462:GLY:O	3:A:463:ARG:C	2.56	0.48
4:B:112:GLY:HA2	4:B:115:TYR:CD2	2.48	0.48
4:B:175:ASN:N	4:B:176:PRO:CD	2.76	0.48
4:B:181:TYR:O	4:B:187:LEU:HD12	2.13	0.48
2:P:810:DT:OP1	3:A:361:HIS:NE2	2.42	0.48
3:A:91:GLN:CG	3:A:161:GLN:NE2	2.75	0.48
3:A:115:TYR:OH	3:A:157:PRO:HG3	2.13	0.48
4:B:13:LYS:HD2	4:B:86:ASP:HB2	1.96	0.48
4:B:197:GLN:O	4:B:200:THR:N	2.45	0.48
4:B:285:GLY:O	4:B:287:LYS:N	2.42	0.48
3:A:247:PRO:HG2	3:A:260:LEU:HD13	1.95	0.48
4:B:195:ILE:C	4:B:197:GLN:N	2.71	0.48
3:A:164:MET:HG3	3:A:168:LEU:CD1	2.41	0.48
3:A:391:LEU:HD12	3:A:414:TRP:CE3	2.48	0.48
4:B:241:VAL:HG13	4:B:351:THR:OG1	2.13	0.48
4:B:245:VAL:O	4:B:263:LYS:NZ	2.47	0.48
4:B:253:THR:HG23	4:B:256:ASP:HB2	1.96	0.48
4:B:369:THR:O	4:B:370:GLU:C	2.56	0.48
4:B:249:LYS:HD2	4:B:256:ASP:OD2	2.14	0.48
3:A:320:ASP:OD1	3:A:322:SER:HB3	2.13	0.48
3:A:376:THR:O	3:A:380:ILE:HG13	2.14	0.48
4:B:175:ASN:H	4:B:176:PRO:HD3	1.77	0.48
3:A:78:ARG:HA	3:A:81:ASN:ND2	2.28	0.47
3:A:225:PRO:HB3	3:A:227:PHE:CE1	2.49	0.47
3:A:326:ILE:HD12	3:A:342:TYR:CE2	2.49	0.47
3:A:391:LEU:HD12	3:A:414:TRP:HB2	1.96	0.47
4:B:260:LEU:HG	4:B:264:LEU:HD12	1.95	0.47
4:B:320:ASP:CG	4:B:322:SER:HG	2.22	0.47
4:B:376:THR:O	4:B:377:THR:C	2.56	0.47
3:A:38:CYS:O	3:A:39:THR:C	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:94:ILE:HG23	3:A:95:PRO:HD2	1.96	0.47
3:A:398:TRP:O	3:A:399:GLU:C	2.57	0.47
4:B:401:TRP:O	4:B:404:GLU:N	2.45	0.47
3:A:23:GLN:NE2	3:A:26:LEU:HD21	2.28	0.47
3:A:146:TYR:CE2	3:A:150:PRO:HA	2.49	0.47
3:A:484:LEU:C	3:A:486:LEU:H	2.23	0.47
4:B:333:GLY:O	4:B:336:GLN:HB2	2.14	0.47
3:A:406:TRP:O	4:B:331:LYS:HB3	2.14	0.47
3:A:427:TYR:C	3:A:428:GLN:OE1	2.57	0.47
4:B:79:GLU:OE2	4:B:83:ARG:NH1	2.47	0.47
4:B:368:LEU:HD23	4:B:372:VAL:HG23	1.94	0.47
3:A:96:HIS:O	3:A:97:PRO:C	2.55	0.47
3:A:209:LEU:HB3	3:A:214:LEU:HB2	1.96	0.47
4:B:115:TYR:CE1	4:B:156:SER:C	2.92	0.47
4:B:235:HIS:N	4:B:235:HIS:ND1	2.63	0.47
4:B:287:LYS:HD3	4:B:291:GLU:OE1	2.14	0.47
4:B:380:ILE:C	4:B:382:ILE:N	2.70	0.47
4:B:414:TRP:HD1	4:B:414:TRP:O	1.98	0.47
3:A:115:TYR:O	3:A:148:VAL:HG22	2.14	0.47
3:A:221:HIS:HA	3:A:224:GLU:CD	2.39	0.47
3:A:484:LEU:HA	3:A:487:GLN:HG2	1.96	0.47
4:B:243:PRO:C	4:B:244:ILE:HD13	2.39	0.47
3:A:489:SER:HB2	3:A:493:VAL:HG22	1.95	0.47
3:A:493:VAL:CG1	3:A:494:ASN:H	2.14	0.47
3:A:546:GLU:HB3	3:A:547:GLN:HE21	1.80	0.47
4:B:124:PHE:O	4:B:126:LYS:N	2.48	0.47
4:B:175:ASN:ND2	4:B:201:LYS:HE2	2.23	0.47
4:B:242:GLN:HB2	4:B:243:PRO:HD2	1.97	0.47
4:B:257:ILE:O	4:B:261:VAL:HG23	2.15	0.47
3:A:158:ALA:HB1	4:B:52:PRO:HB2	1.97	0.47
3:A:247:PRO:CG	3:A:260:LEU:CD1	2.93	0.47
4:B:202:ILE:O	4:B:206:ARG:HG3	2.14	0.47
4:B:372:VAL:HG13	4:B:389:PHE:CZ	2.49	0.47
4:B:428:GLN:CG	4:B:429:LEU:HD13	2.44	0.47
2:P:820:DC:H4'	3:A:266:TRP:CE2	2.50	0.47
3:A:96:HIS:ND1	3:A:98:ALA:HB3	2.29	0.47
3:A:288:ALA:C	3:A:290:THR:N	2.72	0.47
4:B:276:VAL:HG13	4:B:277:ARG:N	2.30	0.47
4:B:299:ALA:O	4:B:302:GLU:HB3	2.15	0.47
3:A:498:ASP:O	3:A:535:TRP:NE1	2.48	0.47
4:B:97:PRO:O	4:B:100:LEU:HD22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:234:LEU:HB3	4:B:236:PRO:HD3	1.97	0.47
4:B:402:TRP:CG	4:B:403:THR:N	2.83	0.47
3:A:363:ASN:HA	3:A:511:ASP:OD1	2.15	0.46
4:B:263:LYS:C	4:B:265:ASN:H	2.23	0.46
4:B:305:GLU:O	4:B:308:GLU:N	2.40	0.46
3:A:279:LEU:N	3:A:302:GLU:OE2	2.34	0.46
3:A:427:TYR:HD1	3:A:526:ILE:HG12	1.80	0.46
4:B:164:MET:O	4:B:165:THR:C	2.58	0.46
1:T:715:DA:C6	1:T:716:DA:C6	3.04	0.46
3:A:274:ILE:C	3:A:275:LYS:HG3	2.39	0.46
3:A:434:ILE:CB	3:A:494:ASN:HD21	2.28	0.46
4:B:295:LEU:O	4:B:296:THR:OG1	2.31	0.46
2:P:812:DT:H2''	2:P:813:DT:H5'	1.97	0.46
2:P:817:MRG:H4'	3:A:289:LEU:HD21	1.97	0.46
3:A:3:SER:CB	3:A:212:TRP:O	2.62	0.46
4:B:135:ILE:HD12	4:B:135:ILE:O	2.15	0.46
4:B:141:GLY:C	4:B:142:ILE:HD13	2.41	0.46
4:B:276:VAL:HG13	4:B:277:ARG:H	1.79	0.46
4:B:314:VAL:CG2	4:B:315:HIS:N	2.77	0.46
4:B:401:TRP:O	4:B:402:TRP:C	2.59	0.46
4:B:393:ILE:HG12	4:B:394:GLN:N	2.30	0.46
3:A:367:GLN:C	3:A:369:THR:N	2.73	0.46
3:A:432:GLU:CD	3:A:433:PRO:HD2	2.40	0.46
3:A:438:GLU:O	3:A:440:PHE:CD1	2.69	0.46
3:A:503:LEU:HD23	4:B:422:LEU:HD23	1.98	0.46
4:B:106:VAL:HA	4:B:190:GLY:HA2	1.97	0.46
4:B:296:THR:CG2	4:B:297:GLU:N	2.79	0.46
4:B:345:PRO:O	4:B:346:PHE:HB2	2.16	0.46
2:P:812:DT:H2'	2:P:813:DT:H6	1.81	0.46
3:A:61:PHE:CD1	3:A:61:PHE:N	2.84	0.46
3:A:103:LYS:O	7:A:824:GOL:H31	2.15	0.46
3:A:160:PHE:HE2	3:A:164:MET:HE2	1.79	0.46
3:A:195:ILE:HG22	3:A:199:ARG:HD2	1.96	0.46
3:A:339:TYR:CD1	3:A:352:GLY:O	2.69	0.46
3:A:405:TYR:HE2	3:A:407:GLN:HB2	1.81	0.46
3:A:442:VAL:HG13	3:A:495:ILE:HG23	1.97	0.46
4:B:142:ILE:HD13	4:B:142:ILE:N	2.31	0.46
4:B:281:LYS:O	4:B:283:LEU:N	2.49	0.46
4:B:400:THR:HG22	4:B:401:TRP:CD2	2.51	0.46
2:P:822:DDG:H2'	3:A:184:MET:HG2	1.97	0.46
3:A:47:ILE:O	3:A:47:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:78:ARG:HA	3:A:81:ASN:HD22	1.80	0.46
4:B:276:VAL:CG2	4:B:280:SER:HB3	2.40	0.46
3:A:224:GLU:O	3:A:225:PRO:C	2.57	0.46
3:A:244:ILE:HD13	3:A:267:ALA:HB2	1.98	0.46
3:A:547:GLN:H	3:A:547:GLN:HE21	1.62	0.46
4:B:27:THR:HG22	4:B:28:GLU:N	2.31	0.46
4:B:162:SER:O	4:B:164:MET:N	2.49	0.46
4:B:164:MET:HG2	4:B:182:GLN:OE1	2.16	0.46
4:B:408:ALA:O	4:B:410:TRP:N	2.48	0.46
3:A:303:LEU:HD21	3:A:307:ARG:CZ	2.46	0.46
3:A:460:ASN:HD22	4:B:288:ALA:HB2	1.80	0.46
3:A:473:THR:H	3:A:476:LYS:HB2	1.81	0.46
3:A:484:LEU:O	3:A:487:GLN:HG2	2.15	0.46
4:B:195:ILE:C	4:B:197:GLN:H	2.23	0.46
4:B:200:THR:O	4:B:204:GLU:HG3	2.16	0.46
4:B:408:ALA:C	4:B:410:TRP:N	2.74	0.46
2:P:812:DT:H2'	2:P:813:DT:C6	2.51	0.45
3:A:377:THR:O	3:A:381:VAL:HG23	2.16	0.45
3:A:484:LEU:C	3:A:486:LEU:N	2.72	0.45
4:B:27:THR:HG22	4:B:28:GLU:H	1.82	0.45
4:B:44:GLU:HB2	4:B:46:LYS:CE	2.45	0.45
1:T:707:DG:O3'	3:A:89:GLU:HG3	2.17	0.45
3:A:270:ILE:HD12	3:A:270:ILE:HA	1.68	0.45
4:B:41:MET:HB3	4:B:47:ILE:HG12	1.98	0.45
4:B:425:LEU:C	4:B:427:TYR:H	2.22	0.45
3:A:240:THR:OG1	3:A:241:VAL:N	2.50	0.45
3:A:398:TRP:C	3:A:400:THR:N	2.73	0.45
3:A:517:LEU:HD22	3:A:521:ILE:CD1	2.30	0.45
4:B:361:HIS:CD2	4:B:363:ASN:HB2	2.51	0.45
2:P:809:DC:H2''	2:P:810:DT:C5'	2.47	0.45
3:A:194:GLU:C	3:A:196:GLY:N	2.74	0.45
3:A:458:VAL:HG12	3:A:548:VAL:HG22	1.98	0.45
3:A:459:THR:C	3:A:461:LYS:H	2.24	0.45
4:B:114:ALA:O	4:B:116:PHE:N	2.50	0.45
4:B:169:GLU:C	4:B:171:PHE:N	2.75	0.45
3:A:194:GLU:O	3:A:195:ILE:C	2.58	0.45
3:A:281:LYS:C	3:A:283:LEU:H	2.23	0.45
3:A:341:ILE:HG22	3:A:342:TYR:N	2.32	0.45
3:A:427:TYR:CD2	3:A:427:TYR:O	2.69	0.45
4:B:252:TRP:CB	4:B:257:ILE:HD11	2.39	0.45
4:B:317:VAL:HG23	4:B:317:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:73:LYS:O	3:A:74:LEU:HD23	2.16	0.45
3:A:473:THR:C	3:A:475:GLN:N	2.75	0.45
3:A:483:TYR:CE1	3:A:520:GLN:HG3	2.51	0.45
4:B:87:PHE:HA	4:B:91:GLN:NE2	2.31	0.45
4:B:128:THR:CB	4:B:146:TYR:HB2	2.47	0.45
3:A:7:THR:HG22	3:A:119:PRO:HB2	1.99	0.45
4:B:41:MET:HE1	4:B:146:TYR:CE2	2.52	0.45
4:B:47:ILE:HA	4:B:145:GLN:O	2.17	0.45
4:B:62:ALA:CB	4:B:71:TRP:CE3	2.98	0.45
4:B:78:ARG:NE	4:B:411:ILE:CG2	2.80	0.45
4:B:395:LYS:HE3	4:B:399:GLU:OE2	2.16	0.45
2:P:809:DC:H2''	2:P:810:DT:H5'	1.98	0.45
3:A:158:ALA:HB1	4:B:52:PRO:CB	2.46	0.45
3:A:198:HIS:CD2	3:A:198:HIS:C	2.95	0.45
3:A:367:GLN:HA	3:A:370:GLU:CG	2.47	0.45
3:A:461:LYS:O	3:A:463:ARG:N	2.49	0.45
3:A:498:ASP:OD2	3:A:538:ALA:HB2	2.16	0.45
4:B:162:SER:C	4:B:164:MET:N	2.74	0.45
4:B:169:GLU:OE1	4:B:169:GLU:HA	2.14	0.45
4:B:426:TRP:H	4:B:426:TRP:HE3	1.63	0.45
3:A:296:THR:O	3:A:300:GLU:N	2.33	0.45
3:A:328:GLU:HG2	3:A:330:GLN:NE2	2.31	0.45
4:B:81:ASN:O	4:B:88:TRP:HZ2	1.99	0.45
4:B:293:ILE:HB	4:B:295:LEU:HD13	1.99	0.45
4:B:302:GLU:O	4:B:305:GLU:HB3	2.17	0.45
4:B:332:GLN:HE22	4:B:425:LEU:HD12	1.80	0.45
3:A:223:LYS:C	3:A:225:PRO:CD	2.90	0.45
3:A:252:TRP:CZ3	3:A:260:LEU:HD22	2.52	0.45
3:A:264:LEU:HD23	3:A:274:ILE:CG2	2.46	0.45
3:A:264:LEU:HD23	3:A:274:ILE:HG23	1.99	0.45
3:A:391:LEU:C	3:A:393:ILE:H	2.25	0.45
3:A:418:ASN:C	3:A:419:THR:HG22	2.41	0.45
4:B:242:GLN:HG2	4:B:353:LYS:HG2	1.99	0.45
3:A:12:LEU:HD23	3:A:84:THR:HA	1.97	0.44
3:A:114:ALA:HB1	3:A:160:PHE:CE1	2.52	0.44
3:A:118:VAL:O	3:A:148:VAL:HG23	2.16	0.44
4:B:109:LEU:CD1	4:B:216:THR:HG21	2.47	0.44
4:B:120:LEU:CD1	4:B:150:PRO:HD3	2.46	0.44
4:B:266:TRP:C	4:B:268:SER:H	2.26	0.44
1:T:714:DG:H5'	3:A:286:THR:HG23	2.00	0.44
3:A:21:VAL:HG13	3:A:59:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:326:ILE:HG22	3:A:327:ALA:N	2.31	0.44
2:P:816:DG:H2'	2:P:817:MRG:C8	2.46	0.44
3:A:117:SER:N	3:A:148:VAL:HG21	2.33	0.44
3:A:194:GLU:O	3:A:196:GLY:N	2.50	0.44
3:A:252:TRP:CE3	3:A:257:ILE:HD13	2.51	0.44
3:A:420:PRO:CB	3:A:421:PRO:HA	2.47	0.44
4:B:23:GLN:HE22	4:B:26:LEU:HD21	1.83	0.44
4:B:149:LEU:HA	4:B:150:PRO:HD3	1.82	0.44
4:B:209:LEU:HD22	4:B:214:LEU:HD12	2.00	0.44
3:A:159:ILE:O	3:A:163:SER:OG	2.33	0.44
3:A:169:GLU:HB3	3:A:170:PRO:HD3	1.98	0.44
4:B:115:TYR:HE1	4:B:156:SER:C	2.24	0.44
4:B:180:ILE:HA	4:B:188:TYR:O	2.17	0.44
3:A:57:ASN:HB2	3:A:143:ARG:NH2	2.32	0.44
3:A:88:TRP:CD1	4:B:143:ARG:HD3	2.53	0.44
3:A:349:LEU:HA	3:A:349:LEU:HD23	1.75	0.44
3:A:365:VAL:HG22	3:A:393:ILE:CD1	2.48	0.44
4:B:94:ILE:HD12	4:B:94:ILE:N	2.32	0.44
4:B:122:GLU:C	4:B:124:PHE:N	2.75	0.44
4:B:259:LYS:C	4:B:261:VAL:N	2.75	0.44
4:B:393:ILE:HG12	4:B:394:GLN:H	1.82	0.44
3:A:13:LYS:O	3:A:16:MET:HG3	2.16	0.44
3:A:149:LEU:HD21	3:A:159:ILE:HB	1.98	0.44
3:A:221:HIS:HE1	3:A:228:LEU:CB	2.20	0.44
4:B:184:MET:HB3	4:B:185:ASP:H	1.55	0.44
4:B:206:ARG:NH1	4:B:216:THR:HB	2.32	0.44
2:P:813:DT:H2'	2:P:814:DC:C6	2.53	0.44
3:A:79:GLU:O	3:A:80:LEU:C	2.60	0.44
3:A:96:HIS:N	4:B:136:ASN:OD1	2.44	0.44
4:B:424:LYS:O	4:B:425:LEU:O	2.36	0.44
3:A:224:GLU:N	3:A:225:PRO:CD	2.81	0.44
3:A:416:PHE:CZ	3:A:418:ASN:HA	2.53	0.44
3:A:480:GLN:HG2	3:A:517:LEU:HD11	2.00	0.44
4:B:17:ASP:CG	4:B:18:GLY:N	2.76	0.44
3:A:296:THR:O	3:A:297:GLU:C	2.60	0.43
3:A:367:GLN:C	3:A:369:THR:H	2.26	0.43
3:A:408:ALA:O	4:B:393:ILE:HG13	2.18	0.43
3:A:453:GLY:C	3:A:469:LEU:HB2	2.43	0.43
4:B:65:LYS:HE3	4:B:72:ARG:HB2	2.00	0.43
4:B:233:GLU:CD	4:B:233:GLU:N	2.72	0.43
4:B:255:ASN:HA	4:B:258:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:357:MET:HE2	4:B:374:LYS:NZ	2.33	0.43
4:B:368:LEU:C	4:B:368:LEU:CD2	2.89	0.43
2:P:818:DC:H2'	2:P:819:DG:C8	2.51	0.43
3:A:118:VAL:HA	3:A:119:PRO:HD3	1.69	0.43
3:A:136:ASN:HB2	3:A:138:GLU:CG	2.47	0.43
3:A:287:LYS:HD2	3:A:291:GLU:OE2	2.18	0.43
4:B:174:GLN:NE2	4:B:175:ASN:OD1	2.52	0.43
1:T:724:DT:H2'	1:T:725:DG:H8	1.82	0.43
3:A:394:GLN:C	3:A:396:GLU:N	2.75	0.43
3:A:423:VAL:O	3:A:424:LYS:HB3	2.19	0.43
3:A:470:THR:C	3:A:472:THR:N	2.76	0.43
4:B:31:ILE:C	4:B:33:ALA:N	2.75	0.43
4:B:257:ILE:C	4:B:259:LYS:N	2.75	0.43
3:A:24:TRP:CD1	3:A:24:TRP:O	2.72	0.43
3:A:286:THR:O	3:A:287:LYS:HG2	2.18	0.43
3:A:391:LEU:HA	3:A:392:PRO:HD3	1.58	0.43
4:B:85:GLN:O	4:B:89:GLU:N	2.51	0.43
4:B:177:ASP:CG	4:B:178:ILE:H	2.26	0.43
3:A:242:GLN:O	3:A:243:PRO:C	2.61	0.43
3:A:367:GLN:HA	3:A:370:GLU:HG2	1.99	0.43
3:A:465:LYS:O	3:A:466:VAL:HG13	2.17	0.43
4:B:21:VAL:HB	4:B:59:PRO:HD3	1.99	0.43
4:B:254:VAL:HG12	4:B:258:GLN:OE1	2.18	0.43
4:B:260:LEU:HG	4:B:264:LEU:CD1	2.49	0.43
3:A:68:SER:C	3:A:70:LYS:N	2.76	0.43
3:A:279:LEU:HB2	3:A:302:GLU:OE1	2.17	0.43
3:A:365:VAL:HG22	3:A:393:ILE:HD12	2.01	0.43
3:A:427:TYR:HE1	3:A:522:ILE:CG2	2.30	0.43
4:B:253:THR:O	4:B:257:ILE:HG12	2.19	0.43
1:T:716:DA:H2'	1:T:717:DC:O4'	2.18	0.43
3:A:54:ASN:O	3:A:143:ARG:NH1	2.51	0.43
3:A:60:VAL:HG12	3:A:75:VAL:HG22	2.00	0.43
3:A:76:ASP:C	3:A:78:ARG:N	2.74	0.43
3:A:88:TRP:HD1	4:B:143:ARG:HD3	1.83	0.43
3:A:288:ALA:HB3	3:A:291:GLU:HB2	2.01	0.43
3:A:345:PRO:O	7:A:825:GOL:H31	2.19	0.43
3:A:511:ASP:HA	3:A:522:ILE:HG21	1.99	0.43
3:A:27:THR:OG1	3:A:29:GLU:HB3	2.19	0.43
3:A:275:LYS:HG3	3:A:332:GLN:NE2	2.34	0.43
3:A:297:GLU:O	3:A:300:GLU:N	2.52	0.43
4:B:259:LYS:O	4:B:261:VAL:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:318:TYR:O	3:A:349:LEU:HD21	2.19	0.43
3:A:354:TYR:CE2	3:A:371:ALA:HA	2.54	0.43
4:B:100:LEU:HG	4:B:381:VAL:CG1	2.48	0.43
4:B:253:THR:HG23	4:B:256:ASP:CB	2.49	0.43
3:A:150:PRO:HG2	3:A:153:TRP:HB2	2.01	0.43
3:A:163:SER:O	3:A:164:MET:C	2.62	0.43
3:A:244:ILE:O	3:A:244:ILE:HG12	2.18	0.43
3:A:297:GLU:O	3:A:298:GLU:C	2.62	0.43
3:A:445:ALA:C	3:A:477:THR:HG21	2.44	0.43
3:A:540:LYS:HD2	3:A:542:ILE:HD11	2.01	0.43
4:B:296:THR:HG22	4:B:297:GLU:H	1.83	0.43
4:B:363:ASN:O	4:B:367:GLN:HG3	2.19	0.43
4:B:402:TRP:CD2	4:B:403:THR:N	2.87	0.43
4:B:65:LYS:CB	4:B:68:SER:HB3	2.47	0.42
4:B:93:GLY:O	4:B:94:ILE:HG13	2.18	0.42
4:B:118:VAL:HB	4:B:149:LEU:CD1	2.40	0.42
4:B:167:ILE:HG23	4:B:212:TRP:CD2	2.51	0.42
4:B:180:ILE:HD11	4:B:205:LEU:CD1	2.45	0.42
4:B:382:ILE:HG22	4:B:383:TRP:CE3	2.52	0.42
7:B:438:GOL:H32	7:B:439:GOL:O1	2.18	0.42
3:A:270:ILE:HG23	3:A:271:TYR:CD2	2.54	0.42
3:A:500:GLN:CG	4:B:422:LEU:HD22	2.41	0.42
4:B:34:LEU:N	4:B:34:LEU:CD2	2.82	0.42
4:B:168:LEU:HD12	4:B:172:ARG:CZ	2.49	0.42
3:A:112:GLY:O	3:A:113:ASP:C	2.61	0.42
3:A:441:TYR:HB3	3:A:548:VAL:CG2	2.47	0.42
4:B:38:CYS:SG	4:B:130:PHE:HE2	2.42	0.42
4:B:339:TYR:HE2	4:B:341:ILE:HD11	1.83	0.42
4:B:380:ILE:O	4:B:382:ILE:N	2.52	0.42
3:A:50:ILE:HD12	3:A:54:ASN:CB	2.43	0.42
3:A:95:PRO:HG2	3:A:230:MET:HE2	2.01	0.42
3:A:293:ILE:HG13	3:A:294:PRO:N	2.34	0.42
4:B:242:GLN:HB2	4:B:353:LYS:HZ1	1.83	0.42
3:A:197:GLN:CD	3:A:197:GLN:H	2.26	0.42
3:A:221:HIS:H	3:A:221:HIS:HD2	1.61	0.42
3:A:267:ALA:C	3:A:269:GLN:H	2.27	0.42
3:A:473:THR:C	3:A:475:GLN:H	2.27	0.42
4:B:77:PHE:O	4:B:79:GLU:N	2.52	0.42
4:B:198:HIS:O	4:B:202:ILE:HG12	2.20	0.42
4:B:263:LYS:C	4:B:265:ASN:N	2.77	0.42
3:A:27:THR:HG1	3:A:29:GLU:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:77:PHE:CE2	3:A:150:PRO:HB2	2.54	0.42
3:A:215:THR:O	3:A:217:PRO:HD3	2.19	0.42
3:A:239:TRP:CE3	3:A:240:THR:CA	3.02	0.42
3:A:392:PRO:N	3:A:417:VAL:HG12	2.34	0.42
3:A:434:ILE:HB	3:A:494:ASN:HD21	1.85	0.42
4:B:24:TRP:HH2	4:B:61:PHE:CE1	2.37	0.42
4:B:38:CYS:O	4:B:47:ILE:HD11	2.20	0.42
4:B:72:ARG:HH11	4:B:72:ARG:CG	2.27	0.42
4:B:174:GLN:O	4:B:175:ASN:OD1	2.37	0.42
4:B:342:TYR:CB	4:B:348:ASN:HA	2.49	0.42
3:A:80:LEU:HD12	3:A:80:LEU:O	2.20	0.42
3:A:231:GLY:C	3:A:242:GLN:NE2	2.78	0.42
3:A:294:PRO:O	3:A:294:PRO:HG2	2.20	0.42
4:B:140:PRO:O	4:B:142:ILE:HD13	2.19	0.42
4:B:203:GLU:OE2	4:B:206:ARG:HD2	2.20	0.42
4:B:266:TRP:C	4:B:268:SER:N	2.78	0.42
1:T:713:DC:H2'	1:T:714:DG:C8	2.55	0.42
4:B:41:MET:HE1	4:B:146:TYR:OH	2.19	0.42
4:B:77:PHE:C	4:B:79:GLU:N	2.77	0.42
4:B:115:TYR:CE1	4:B:156:SER:HB3	2.55	0.42
4:B:143:ARG:O	4:B:144:TYR:CD2	2.73	0.42
4:B:197:GLN:O	4:B:198:HIS:C	2.63	0.42
1:T:705:DT:H2''	1:T:706:DC:C5'	2.50	0.42
3:A:382:ILE:HG22	3:A:383:TRP:CE2	2.55	0.42
3:A:402:TRP:C	3:A:404:GLU:N	2.77	0.42
4:B:41:MET:HE1	4:B:146:TYR:HE2	1.85	0.42
4:B:66:LYS:C	4:B:68:SER:H	2.28	0.42
4:B:332:GLN:NE2	4:B:425:LEU:CD1	2.83	0.42
3:A:475:GLN:C	3:A:477:THR:N	2.76	0.42
3:A:511:ASP:C	3:A:512:LYS:HG2	2.45	0.42
4:B:13:LYS:HE3	4:B:85:GLN:HG2	2.02	0.42
4:B:73:LYS:O	4:B:74:LEU:HB2	2.20	0.42
4:B:279:LEU:HD11	4:B:303:LEU:HA	2.02	0.42
3:A:228:LEU:HD22	3:A:228:LEU:HA	1.83	0.41
3:A:391:LEU:HD12	3:A:414:TRP:CD2	2.55	0.41
3:A:417:VAL:HG22	3:A:419:THR:HG21	2.00	0.41
3:A:500:GLN:O	3:A:501:TYR:C	2.63	0.41
4:B:16:MET:HB3	4:B:17:ASP:H	1.63	0.41
4:B:281:LYS:C	4:B:283:LEU:N	2.78	0.41
4:B:356:ARG:HG3	4:B:367:GLN:HE21	1.85	0.41
3:A:287:LYS:HG3	3:A:291:GLU:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:31:ILE:C	4:B:33:ALA:H	2.28	0.41
4:B:242:GLN:HB3	4:B:353:LYS:HZ2	1.86	0.41
4:B:368:LEU:O	4:B:371:ALA:HB3	2.20	0.41
3:A:161:GLN:O	3:A:162:SER:C	2.61	0.41
3:A:231:GLY:O	3:A:242:GLN:HG3	2.19	0.41
3:A:249:LYS:HG3	3:A:252:TRP:NE1	2.35	0.41
3:A:265:ASN:O	3:A:268:SER:OG	2.27	0.41
3:A:279:LEU:O	3:A:282:LEU:CB	2.69	0.41
3:A:363:ASN:O	3:A:367:GLN:HG3	2.20	0.41
4:B:273:GLY:C	4:B:309:ILE:HD13	2.45	0.41
4:B:344:GLU:OE1	4:B:344:GLU:HA	2.20	0.41
2:P:805:DG:H2'	2:P:806:DT:O5'	2.21	0.41
3:A:46:LYS:C	3:A:47:ILE:HG23	2.46	0.41
3:A:72:ARG:CD	3:A:74:LEU:HD21	2.51	0.41
3:A:441:TYR:O	3:A:457:TYR:HA	2.19	0.41
4:B:54:ASN:HB3	4:B:143:ARG:NH2	2.35	0.41
4:B:66:LYS:C	4:B:68:SER:N	2.78	0.41
4:B:341:ILE:H	4:B:341:ILE:HG13	1.70	0.41
3:A:246:LEU:HD11	3:A:264:LEU:HD12	2.03	0.41
3:A:279:LEU:O	3:A:282:LEU:HB2	2.20	0.41
3:A:398:TRP:O	3:A:400:THR:N	2.54	0.41
3:A:522:ILE:O	3:A:525:LEU:N	2.54	0.41
3:A:546:GLU:OE2	3:A:550:LYS:HB2	2.20	0.41
4:B:21:VAL:HG12	4:B:59:PRO:CG	2.51	0.41
4:B:66:LYS:HB2	4:B:407:GLN:HE21	1.84	0.41
4:B:128:THR:OG1	4:B:146:TYR:HB2	2.19	0.41
4:B:348:ASN:C	4:B:350:LYS:N	2.77	0.41
3:A:106:VAL:CG1	3:A:107:THR:N	2.84	0.41
4:B:63:ILE:HG21	4:B:407:GLN:HA	2.02	0.41
4:B:194:GLU:HB3	4:B:197:GLN:NE2	2.35	0.41
4:B:313:PRO:O	4:B:314:VAL:O	2.39	0.41
4:B:417:VAL:CG2	4:B:418:ASN:N	2.83	0.41
3:A:391:LEU:HD12	3:A:414:TRP:CG	2.56	0.41
4:B:115:TYR:HE1	4:B:157:PRO:N	2.19	0.41
4:B:189:VAL:HB	4:B:202:ILE:HD11	2.01	0.41
4:B:241:VAL:CG1	4:B:242:GLN:H	2.33	0.41
3:A:210:LEU:HA	3:A:214:LEU:O	2.21	0.41
3:A:339:TYR:CG	3:A:375:ILE:HD11	2.55	0.41
3:A:341:ILE:CG2	3:A:342:TYR:N	2.83	0.41
4:B:132:ILE:HG22	4:B:133:PRO:N	2.34	0.41
4:B:267:ALA:N	4:B:426:TRP:HE1	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:65:LYS:HE2	3:A:72:ARG:HB2	2.03	0.41
3:A:107:THR:HA	3:A:227:PHE:CE2	2.55	0.41
3:A:175:ASN:N	3:A:176:PRO:HD3	2.35	0.41
3:A:249:LYS:HB2	3:A:250:ASP:H	1.74	0.41
3:A:306:ASN:HA	3:A:309:ILE:CD1	2.51	0.41
4:B:50:ILE:CG2	4:B:145:GLN:HB2	2.49	0.41
4:B:162:SER:C	4:B:164:MET:H	2.29	0.41
4:B:189:VAL:HG11	4:B:202:ILE:HD13	2.03	0.41
4:B:194:GLU:O	4:B:198:HIS:N	2.49	0.41
4:B:216:THR:HA	4:B:217:PRO:HD3	1.96	0.41
3:A:94:ILE:HG22	3:A:95:PRO:O	2.20	0.40
3:A:95:PRO:HB2	3:A:229:TRP:HH2	1.86	0.40
3:A:341:ILE:O	3:A:342:TYR:HB3	2.21	0.40
6:A:823:TNV:H6'1	6:A:823:TNV:H9'1	1.51	0.40
4:B:279:LEU:HD11	4:B:303:LEU:CA	2.52	0.40
4:B:368:LEU:HD11	4:B:392:PRO:HD2	2.02	0.40
2:P:805:DG:H2'	2:P:806:DT:O4'	2.20	0.40
3:A:181:TYR:CD2	4:B:138:GLU:HA	2.56	0.40
3:A:226:PRO:HG2	3:A:226:PRO:O	2.21	0.40
3:A:262:GLY:O	3:A:265:ASN:HB2	2.22	0.40
3:A:367:GLN:O	3:A:369:THR:N	2.55	0.40
3:A:416:PHE:HZ	3:A:422:LEU:HD11	1.86	0.40
4:B:7:THR:HG22	4:B:119:PRO:HG2	2.03	0.40
4:B:8:VAL:O	4:B:8:VAL:HG23	2.22	0.40
4:B:57:ASN:HA	4:B:129:ALA:O	2.22	0.40
4:B:112:GLY:HA2	4:B:115:TYR:CE2	2.57	0.40
4:B:365:VAL:O	4:B:366:LYS:C	2.64	0.40
4:B:410:TRP:O	4:B:411:ILE:HG13	2.21	0.40
4:B:423:VAL:HG21	4:B:426:TRP:CH2	2.56	0.40
1:T:705:DT:H2''	1:T:706:DC:H5'	2.04	0.40
1:T:714:DG:C5'	3:A:286:THR:HG23	2.51	0.40
2:P:805:DG:C2'	2:P:806:DT:O5'	2.69	0.40
3:A:65:LYS:O	3:A:68:SER:N	2.55	0.40
3:A:272:PRO:HG3	3:A:351:THR:HG21	2.02	0.40
4:B:206:ARG:HH22	4:B:216:THR:CG2	2.34	0.40
3:A:13:LYS:HG2	3:A:84:THR:C	2.46	0.40
3:A:443:ASP:OD1	3:A:444:GLY:N	2.55	0.40
4:B:13:LYS:CD	4:B:86:ASP:H	2.35	0.40
4:B:255:ASN:HD21	4:B:259:LYS:HE2	1.83	0.40
4:B:278:GLN:O	4:B:299:ALA:HB2	2.22	0.40
3:A:34:LEU:CD1	3:A:62:ALA:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:336:GLN:O	3:A:337:TRP:CD1	2.74	0.40
3:A:385:LYS:HE3	3:A:385:LYS:HB2	1.66	0.40
3:A:475:GLN:HB3	3:A:501:TYR:CE2	2.57	0.40
3:A:495:ILE:O	3:A:533:LEU:HD12	2.22	0.40
4:B:319:TYR:CE2	4:B:383:TRP:HD1	2.40	0.40
4:B:365:VAL:HG12	4:B:393:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	552/558 (99%)	410 (74%)	112 (20%)	30 (5%)	1	9
4	B	410/437 (94%)	278 (68%)	95 (23%)	37 (9%)	0	3
All	All	962/995 (97%)	688 (72%)	207 (22%)	67 (7%)	1	4

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	77	PHE
3	A	154	LYS
3	A	268	SER
3	A	345	PRO
3	A	438	GLU
3	A	471	ASN
4	B	4	PRO
4	B	115	TYR
4	B	125	ARG
4	B	245	VAL
4	B	314	VAL
4	B	425	LEU

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Mol	Chain	Res	Type
3	A	5	ILE
3	A	14	PRO
3	A	334	GLN
3	A	541	GLY
3	A	546	GLU
4	B	45	GLY
4	B	95	PRO
4	B	104	LYS
4	B	282	LEU
4	B	409	THR
3	A	68	SER
3	A	427	TYR
3	A	485	ALA
4	B	93	GLY
4	B	163	SER
4	B	239	TRP
4	B	289	LEU
4	B	383	TRP
4	B	395	LYS
4	B	399	GLU
3	A	121	ASP
3	A	128	THR
3	A	157	PRO
3	A	184	MET
3	A	219	LYS
3	A	298	GLU
3	A	377	THR
3	A	412	PRO
3	A	472	THR
3	A	494	ASN
4	B	98	ALA
4	B	256	ASP
4	B	277	ARG
4	B	286	THR
3	A	66	LYS
3	A	196	GLY
3	A	537	PRO
4	B	61	PHE
4	B	260	LEU
4	B	283	LEU
4	B	368	LEU
4	B	379	SER

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Mol	Chain	Res	Type
4	B	381	VAL
4	B	414	TRP
4	B	424	LYS
3	A	195	ILE
3	A	224	GLU
4	B	123	ASP
4	B	133	PRO
3	A	462	GLY
4	B	148	VAL
4	B	157	PRO
4	B	25	PRO
4	B	170	PRO
4	B	175	ASN

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	
3	A	495/498 (99%)	428 (86%)	67 (14%)	4	18
4	B	376/397 (95%)	340 (90%)	36 (10%)	8	31
All	All	871/895 (97%)	768 (88%)	103 (12%)	5	22

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	7	THR
3	A	14	PRO
3	A	21	VAL
3	A	27	THR
3	A	53	GLU
3	A	58	THR
3	A	83	ARG
3	A	91	GLN
3	A	94	ILE
3	A	100	LEU

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Mol	Chain	Res	Type
3	A	107	THR
3	A	108	VAL
3	A	109	LEU
3	A	118	VAL
3	A	120	LEU
3	A	121	ASP
3	A	135	ILE
3	A	138	GLU
3	A	142	ILE
3	A	150	PRO
3	A	151	GLN
3	A	157	PRO
3	A	165	THR
3	A	179	VAL
3	A	193	LEU
3	A	195	ILE
3	A	197	GLN
3	A	202	ILE
3	A	205	LEU
3	A	206	ARG
3	A	211	ARG
3	A	221	HIS
3	A	228	LEU
3	A	236	PRO
3	A	246	LEU
3	A	250	ASP
3	A	258	CYS
3	A	264	LEU
3	A	268	SER
3	A	270	ILE
3	A	282	LEU
3	A	290	THR
3	A	293	ILE
3	A	294	PRO
3	A	295	LEU
3	A	298	GLU
3	A	309	ILE
3	A	314	VAL
3	A	329	ILE
3	A	340	GLN
3	A	345	PRO
3	A	357	MET

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Mol	Chain	Res	Type
3	A	362	THR
3	A	368	LEU
3	A	386	THR
3	A	411	ILE
3	A	419	THR
3	A	423	VAL
3	A	425	LEU
3	A	428	GLN
3	A	431	LYS
3	A	480	GLN
3	A	515	SER
3	A	517	LEU
3	A	520	GLN
3	A	524	GLN
3	A	547	GLN
4	B	25	PRO
4	B	34	LEU
4	B	46	LYS
4	B	53	GLU
4	B	72	ARG
4	B	100	LEU
4	B	123	ASP
4	B	133	PRO
4	B	139	THR
4	B	184	MET
4	B	189	VAL
4	B	193	LEU
4	B	197	GLN
4	B	200	THR
4	B	201	LYS
4	B	203	GLU
4	B	212	TRP
4	B	233	GLU
4	B	235	HIS
4	B	239	TRP
4	B	240	THR
4	B	242	GLN
4	B	253	THR
4	B	255	ASN
4	B	283	LEU
4	B	289	LEU
4	B	293	ILE

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Mol	Chain	Res	Type
4	B	297	GLU
4	B	324	ASP
4	B	336	GLN
4	B	349	LEU
4	B	350	LYS
4	B	353	LYS
4	B	389	PHE
4	B	426	TRP
4	B	427	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	145	GLN
3	A	161	GLN
3	A	221	HIS
3	A	242	GLN
3	A	255	ASN
3	A	269	GLN
3	A	315	HIS
3	A	332	GLN
3	A	340	GLN
3	A	373	GLN
3	A	407	GLN
3	A	447	ASN
3	A	474	ASN
3	A	480	GLN
3	A	487	GLN
3	A	494	ASN
3	A	500	GLN
3	A	509	GLN
3	A	519	ASN
3	A	547	GLN
4	B	91	GLN
4	B	147	ASN
4	B	174	GLN
4	B	175	ASN
4	B	197	GLN
4	B	242	GLN
4	B	269	GLN
4	B	315	HIS
4	B	330	GLN

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Mol	Chain	Res	Type
4	B	340	GLN
4	B	361	HIS
4	B	394	GLN
4	B	407	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
2	MRG	P	817	2,1	21,24,29	0.57	0	30,35,42	0.66	1 (3%)
2	DDG	P	822	2,1	20,23,24	0.44	0	27,33,36	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MRG	P	817	2,1	-	0/7/21/27	0/3/3/3
2	DDG	P	822	2,1	-	0/7/18/19	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	817	MRG	O3'-C3'-C2'	-3.05	100.28	110.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	817	MRG	3	0
2	P	822	DDG	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	GOL	A	826	-	5,5,5	1.07	0	5,5,5	2.06	2 (40%)
7	GOL	B	439	-	5,5,5	1.02	0	5,5,5	2.05	2 (40%)
6	TNV	A	823	5	26,28,28	1.34	3 (11%)	36,43,43	1.04	2 (5%)
7	GOL	A	825	-	5,5,5	1.22	0	5,5,5	2.07	2 (40%)
7	GOL	B	438	-	5,5,5	0.82	0	5,5,5	2.09	2 (40%)
7	GOL	A	824	-	5,5,5	1.28	0	5,5,5	2.10	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	826	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	B	439	-	-	2/4/4/4	-
6	TNV	A	823	5	-	8/19/22/22	0/2/2/2
7	GOL	A	825	-	-	2/4/4/4	-
7	GOL	B	438	-	-	2/4/4/4	-
7	GOL	A	824	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	823	TNV	PA-O3A	-3.07	1.55	1.58
6	A	823	TNV	C6'-C7'	2.67	1.61	1.51
6	A	823	TNV	C2-N1	2.11	1.37	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	823	TNV	PA-O3A-PB	-3.74	120.17	132.37
7	A	825	GOL	O2-C2-C1	3.12	122.10	109.18
7	B	438	GOL	C3-C2-C1	3.10	123.18	111.80
7	B	439	GOL	O2-C2-C1	3.06	121.84	109.18
7	A	826	GOL	O2-C2-C1	3.05	121.82	109.18
7	A	824	GOL	O2-C2-C1	3.02	121.68	109.18
7	A	824	GOL	C3-C2-C1	3.01	122.84	111.80
7	A	826	GOL	C3-C2-C1	2.92	122.50	111.80
7	A	825	GOL	C3-C2-C1	2.91	122.47	111.80
7	B	438	GOL	O2-C2-C1	2.87	121.07	109.18
7	B	439	GOL	C3-C2-C1	2.85	122.25	111.80
6	A	823	TNV	C6'-N9-C4	2.23	129.00	126.41

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	823	TNV	O9'-C9'-PA-O2A
6	A	823	TNV	O9'-C9'-PA-O3A
6	A	823	TNV	C6'-C7'-O9'-C9'
6	A	823	TNV	N9-C6'-C7'-O9'
6	A	823	TNV	N9-C6'-C7'-C8'
7	A	824	GOL	C1-C2-C3-O3
7	A	825	GOL	O1-C1-C2-C3

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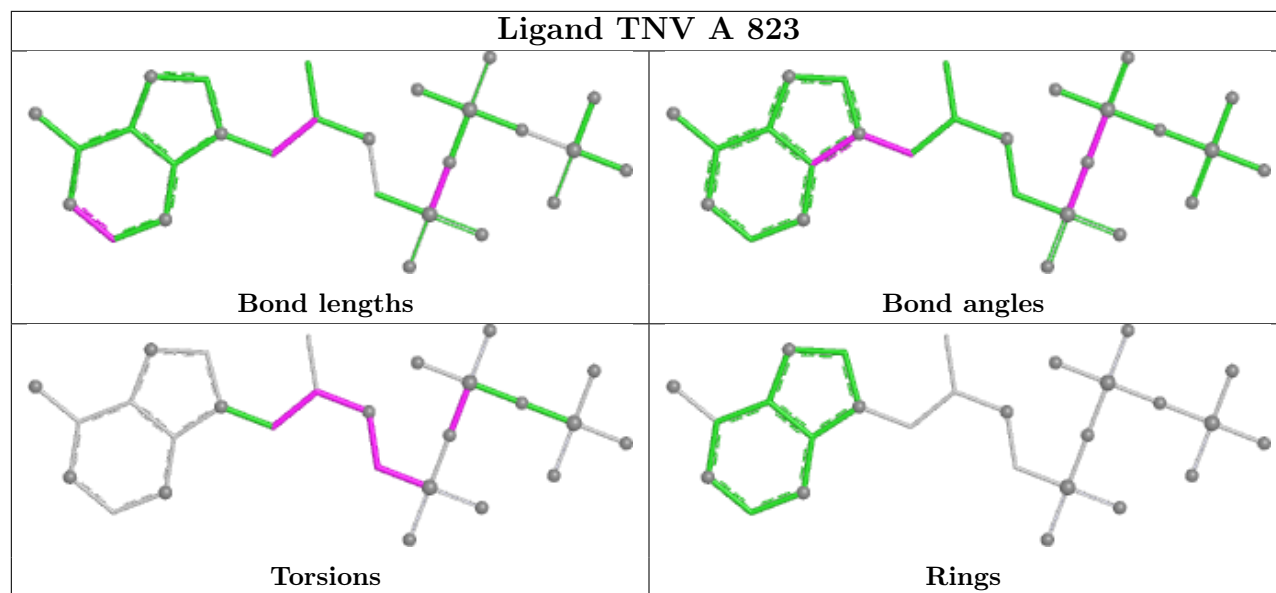
Mol	Chain	Res	Type	Atoms
7	A	825	GOL	C1-C2-C3-O3
7	A	826	GOL	C1-C2-C3-O3
7	B	438	GOL	C1-C2-C3-O3
7	B	439	GOL	O1-C1-C2-C3
7	B	439	GOL	C1-C2-C3-O3
7	B	438	GOL	O1-C1-C2-O2
7	A	826	GOL	O1-C1-C2-C3
7	A	824	GOL	O1-C1-C2-O2
7	A	826	GOL	O1-C1-C2-O2
6	A	823	TNV	O9'-C9'-PA-O1A
6	A	823	TNV	PA-O3A-PB-O2B
6	A	823	TNV	PA-C9'-O9'-C7'

There are no ring outliers.

5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	439	GOL	1	0
6	A	823	TNV	7	0
7	A	825	GOL	1	0
7	B	438	GOL	1	0
7	A	824	GOL	4	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	T	24/27 (88%)	0.51	1 (4%) 40 22	42, 100, 120, 120	0
2	P	18/21 (85%)	0.41	0 100 100	42, 104, 120, 120	0
3	A	554/558 (99%)	0.08	8 (1%) 73 51	13, 71, 119, 120	0
4	B	414/437 (94%)	0.34	18 (4%) 40 21	30, 100, 120, 120	0
All	All	1010/1043 (96%)	0.20	27 (2%) 56 33	13, 86, 120, 120	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	B	4	PRO	4.8
3	A	554	ALA	4.6
3	A	448	ARG	4.2
4	B	3	SER	4.0
4	B	94	ILE	3.8
4	B	88	TRP	3.6
4	B	429	LEU	3.6
3	A	1	PRO	3.4
4	B	426	TRP	3.3
4	B	193	LEU	3.3
3	A	446	ALA	3.1
3	A	495	ILE	3.1
4	B	95	PRO	3.0
3	A	454	LYS	2.9
4	B	318	TYR	2.7
3	A	491	LEU	2.5
3	A	451	LYS	2.5
4	B	97	PRO	2.4
4	B	276	VAL	2.3
4	B	264	LEU	2.3
1	T	725	DG	2.3

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Mol	Chain	Res	Type	RSRZ
4	B	236	PRO	2.3
4	B	423	VAL	2.2
4	B	327	ALA	2.2
4	B	5	ILE	2.2
4	B	200	THR	2.1
4	B	242	GLN	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MRG	P	817	22/27	0.93	0.08	37,60,89,98	0
2	DDG	P	822	21/22	0.97	0.07	39,53,60,74	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

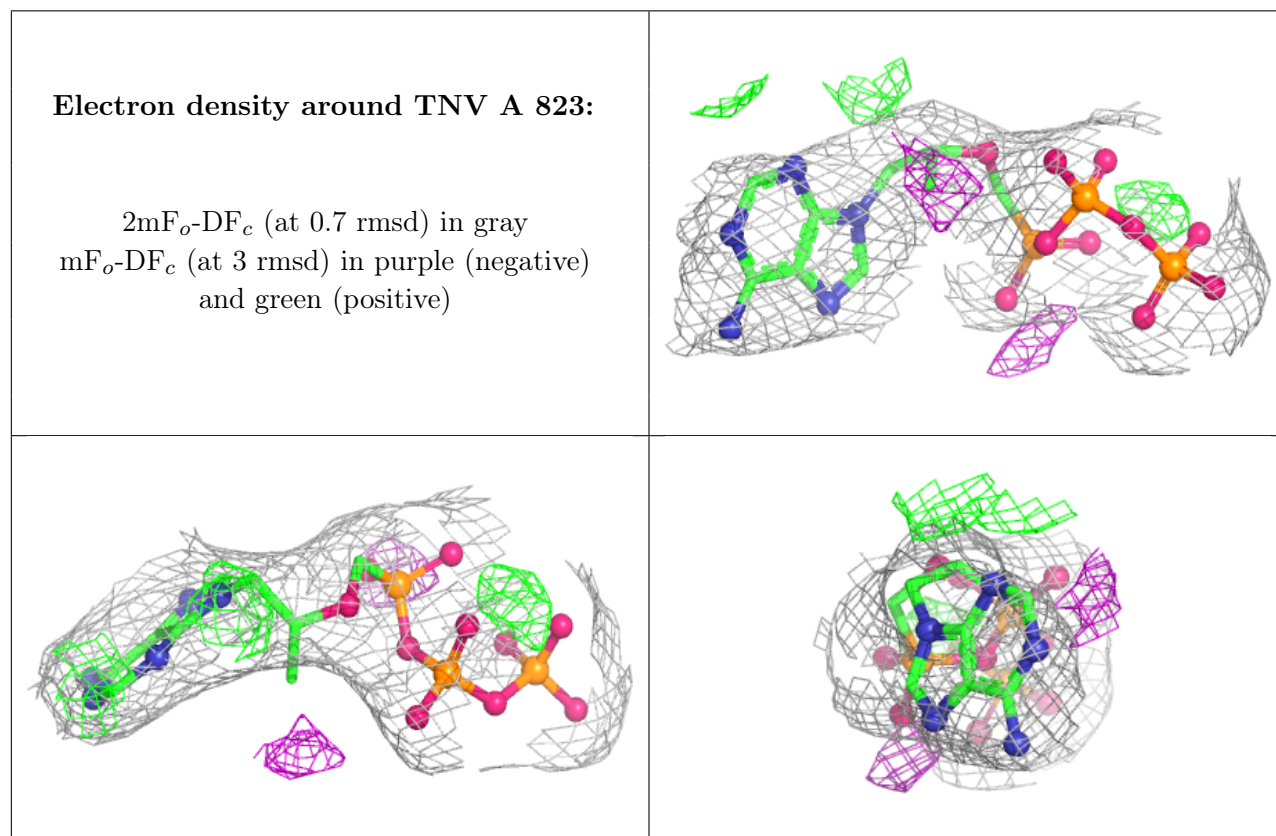
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
7	GOL	B	438	6/6	0.67	0.31	56,70,72,74	6
7	GOL	B	439	6/6	0.72	0.30	63,70,74,75	6
7	GOL	A	825	6/6	0.74	0.30	45,59,68,81	6
7	GOL	A	824	6/6	0.79	0.36	54,58,60,63	6
7	GOL	A	826	6/6	0.88	0.14	36,42,49,50	6
5	MG	A	601	1/1	0.92	0.11	73,73,73,73	0
6	TNV	A	823	27/27	0.97	0.08	34,54,64,71	0
5	MG	A	600	1/1	0.99	0.06	16,16,16,16	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.