



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 04:40 PM EDT

PDB ID : 7RIX
Title : RNA polymerase II elongation complex with hairpin polyamide Py-Im 1, scaffold 2
Authors : Oh, J.; Dervan, P.B.; Wang, D.
Deposited on : 2021-07-20
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

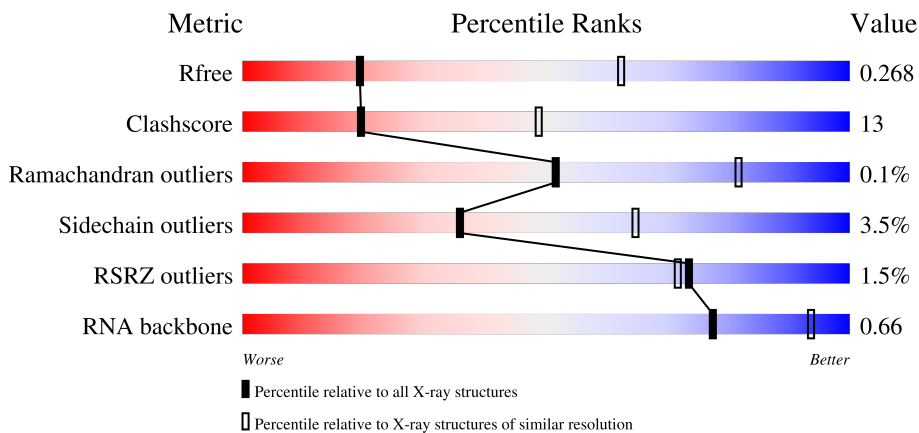
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)
RNA backbone	3102	1006 (3.84-2.96)

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	R	10	 20% 70% 10%
2	T	30	 33% 47% 7% 13%
3	N	20	 30% 40% 30%
4	A	1733	 % 53% 25% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	B	1224	<p>%</p> <p>65% 26% 8%</p>
6	C	318	<p>61% 22% 16%</p>
7	E	215	<p>4%</p> <p>70% 26% ...</p>
8	F	155	<p>%</p> <p>40% 14% 45%</p>
9	H	146	<p>4%</p> <p>64% 23% 9%</p>
10	I	122	<p>72% 24% ..</p>
11	J	70	<p>69% 24% 7%</p>
12	K	120	<p>71% 24% 5%</p>
13	L	70	<p>6%</p> <p>44% 16% 39%</p>

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 29160 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	R	10	215	97	43	66	9	0	0	0

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	T	26	525	252	84	163	26	0	0	0

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	N	14	293	138	63	78	14	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	1384	10828	6831	1896	2041	60	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	1125	8871	5615	1554	1649	53	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	C	267	2101	1320	349	419	13	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	212	1731	1100	305	315	11	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	F	86	684	437	115	129	3	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	H	133	1064	670	179	211	4	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	I	118	952	585	173	184	10	0	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	J	65	532	339	93	94	6	0	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	K	114	919	590	156	171	2	0	0	0

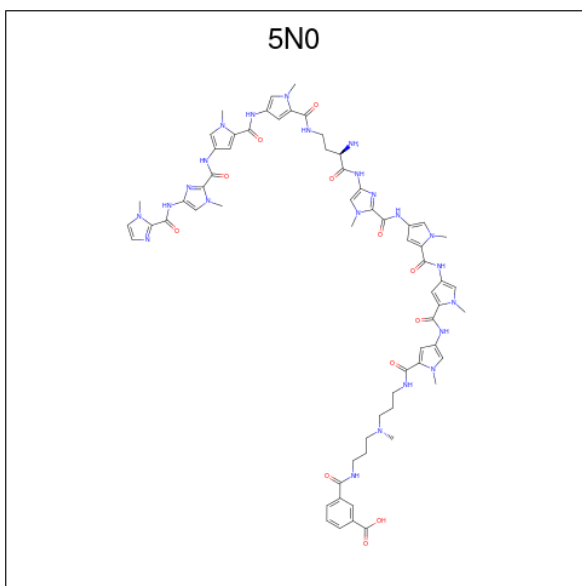
- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	L	43	337	208	66	59	4	0	0	0

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	R	1	Total Mg 1 1	0	0

- Molecule 15 is 3-({3-[(3-[(4-({4-[(4-({(2R)-2-amino-4-[(1-methyl-4-{{1-methyl-4-({1-methyl-4-[(1-methyl-1H-imidazole-2-carbonyl)amino]-1H-imidazole-2-carbonyl}amino)-1H-pyrrole-2-carbonyl]amino}-1H-pyrrole-2-carbonyl)amino]butanoyl}amino)-1-methyl-1H-imidazole-2-carbonyl]amino}-1-methyl-1H-pyrrole-2-carbonyl)amino]-1-methyl-1H-pyrrole-2-carbonyl]amino}propyl)(methyl)amino]propyl}carbamoyl)benzoic acid (three-letter code: 5N0) (formula: C₆₄H₇₅N₂₃O₁₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	T	1	Total C N O 99 64 23 12	0	0

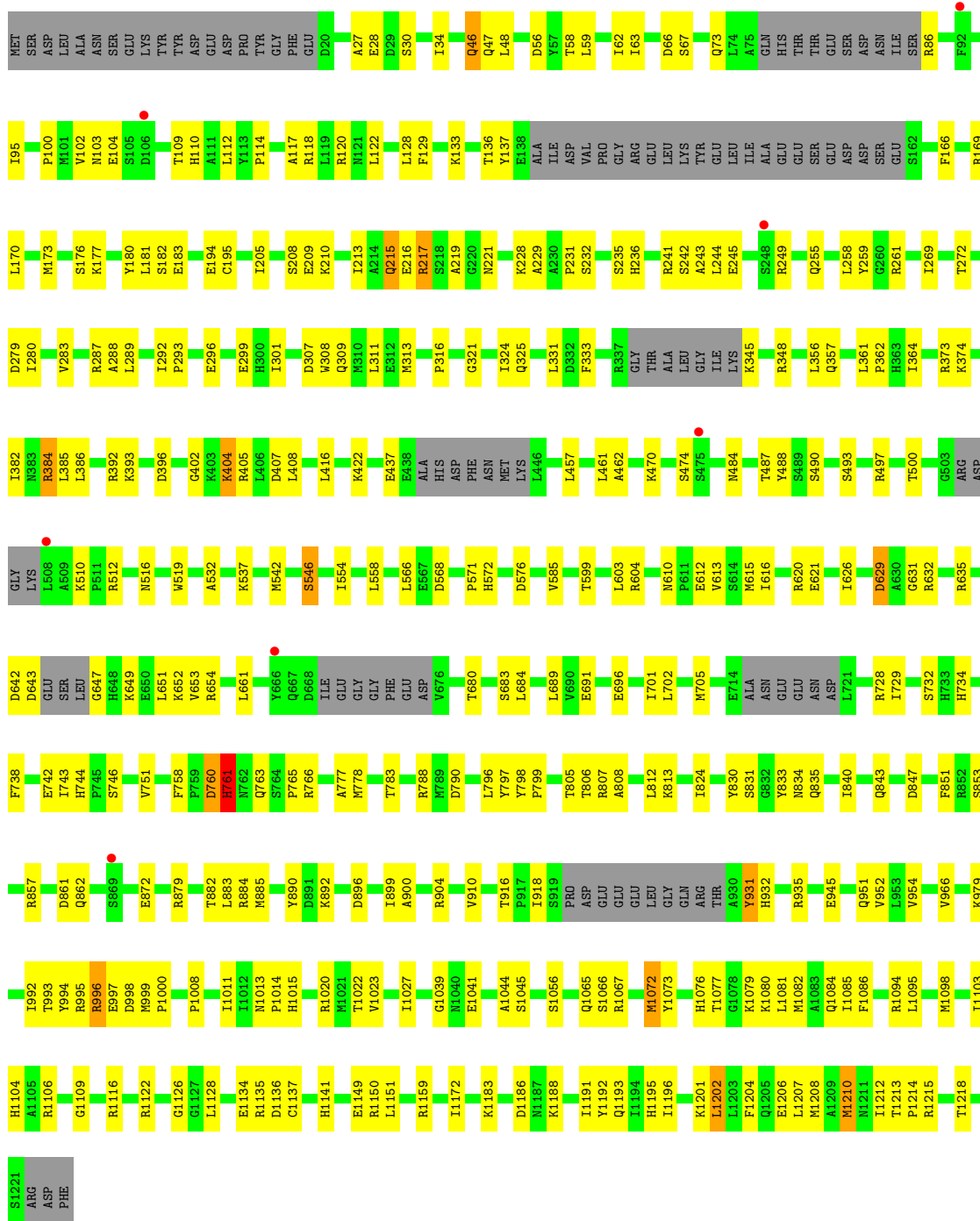
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	2	Total Zn 2 2	0	0
16	B	1	Total Zn 1 1	0	0
16	C	1	Total Zn 1 1	0	0
16	I	2	Total Zn 2 2	0	0
16	J	1	Total Zn 1 1	0	0

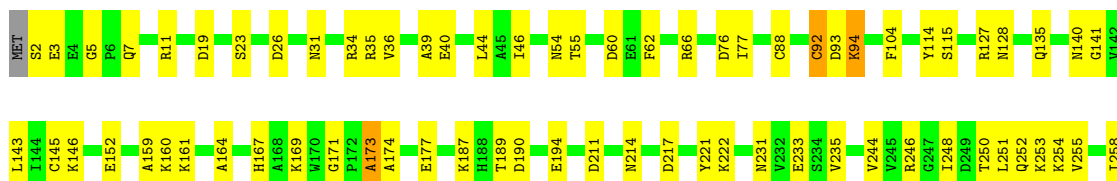
Continued on next page...

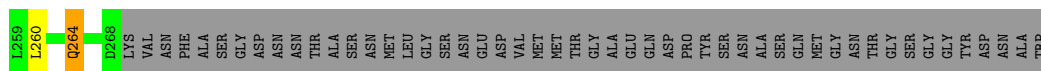
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	L	1	Total	Zn	0	0
			1	1		



● Molecule 6: DNA-directed RNA polymerase II subunit RPB3

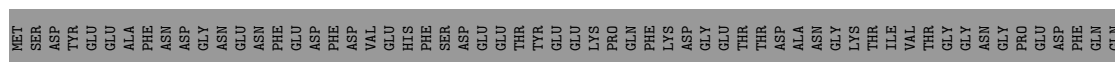




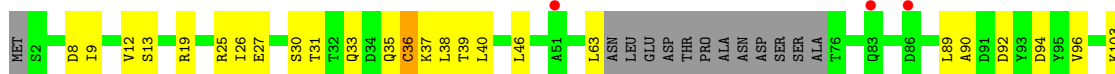
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



- Molecule 10: DNA-directed RNA polymerase II subunit RPB9

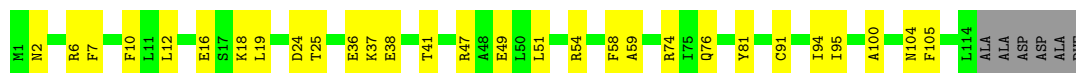


- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5



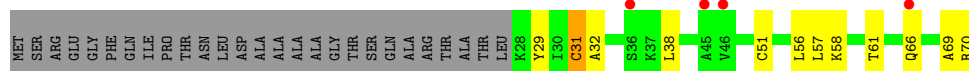
- Molecule 12: DNA-directed RNA polymerase II subunit RPB11

Chain K:  71% 24% 5%



- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  6% 44% 16% 39%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.70Å 222.45Å 194.16Å 90.00° 100.01° 90.00°	Depositor
Resolution (Å)	49.53 – 3.40 49.53 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.53-3.40) 99.9 (49.53-3.40)	Depositor EDS
R_{merge}	0.49	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.40Å)	Xtrriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.222 , 0.268 0.222 , 0.268	Depositor DCC
R_{free} test set	1825 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å ²)	83.3	Xtrriage
Anisotropy	0.554	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	29160	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: ZN, MG, 5N0

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	R	0.40	0/241	1.08	1/375 (0.3%)
2	T	0.83	1/584 (0.2%)	1.23	4/898 (0.4%)
3	N	0.64	0/331	0.85	0/509
4	A	0.39	7/11020 (0.1%)	0.60	20/14907 (0.1%)
5	B	0.32	0/9042	0.52	4/12202 (0.0%)
6	C	0.30	0/2139	0.49	0/2899
7	E	0.44	1/1767 (0.1%)	1.05	7/2378 (0.3%)
8	F	0.28	0/696	0.47	0/943
9	H	0.32	0/1082	0.55	1/1466 (0.1%)
10	I	0.35	0/970	0.51	0/1308
11	J	0.30	0/541	0.49	0/727
12	K	0.29	0/937	0.50	0/1265
13	L	0.31	0/339	0.55	0/450
All	All	0.37	9/29689 (0.0%)	0.63	37/40327 (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
4	A	0	4
5	B	0	1
7	E	0	2
All	All	0	7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	394	ASN	CG-OD1	-12.09	0.97	1.24
4	A	525	GLN	CD-OE1	-11.61	0.98	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	143	ASN	CG-OD1	-11.20	0.99	1.24
4	A	394	ASN	CB-CG	9.47	1.72	1.51
4	A	589	GLN	CB-CG	8.64	1.75	1.52
4	A	589	GLN	CG-CD	7.31	1.67	1.51
4	A	394	ASN	CG-ND2	6.08	1.48	1.32
4	A	525	GLN	CD-NE2	5.78	1.47	1.32
2	T	16	DT	C1'-N1	5.38	1.56	1.49

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	114	ASN	CB-CG-OD1	29.19	179.97	121.60
7	E	143	ASN	CB-CA-C	-19.28	71.84	110.40
5	B	761	HIS	N-CA-CB	-17.18	79.69	110.60
4	A	394	ASN	N-CA-CB	16.51	140.32	110.60
7	E	143	ASN	N-CA-CB	16.34	140.01	110.60
7	E	114	ASN	CB-CG-ND2	-15.13	80.38	116.70
4	A	589	GLN	N-CA-CB	14.41	136.54	110.60
4	A	589	GLN	CG-CD-NE2	-13.87	83.42	116.70
4	A	394	ASN	CB-CA-C	-11.26	87.89	110.40
7	E	143	ASN	CB-CG-OD1	-10.52	100.57	121.60
4	A	589	GLN	CG-CD-OE1	10.44	142.47	121.60
5	B	760	ASP	C-N-CA	10.08	146.90	121.70
4	A	589	GLN	CB-CA-C	-9.93	90.54	110.40
7	E	114	ASN	OD1-CG-ND2	-9.70	99.59	121.90
4	A	393	ARG	C-N-CA	-9.59	97.73	121.70
2	T	18	DA	O4'-C4'-C3'	-9.43	100.34	106.00
4	A	525	GLN	CA-CB-CG	9.10	133.42	113.40
2	T	18	DA	O4'-C1'-N9	8.79	114.15	108.00
4	A	394	ASN	CB-CG-ND2	-8.78	95.62	116.70
4	A	589	GLN	N-CA-C	-7.84	89.83	111.00
4	A	589	GLN	CA-CB-CG	-7.11	97.77	113.40
2	T	18	DA	C1'-O4'-C4'	-6.62	103.48	110.10
5	B	761	HIS	ND1-CG-CD2	-6.43	96.99	106.00
1	R	10	C	C6-N1-C2	-6.34	117.76	120.30
4	A	525	GLN	N-CA-C	-6.29	94.01	111.00
4	A	266	LEU	CB-CG-CD2	6.28	121.68	111.00
4	A	525	GLN	OE1-CD-NE2	-6.17	107.72	121.90
5	B	761	HIS	CB-CA-C	6.16	122.72	110.40
4	A	525	GLN	O-C-N	-6.09	112.96	122.70
4	A	394	ASN	CB-CG-OD1	6.08	133.77	121.60
4	A	472	LEU	CB-CG-CD2	-6.03	100.76	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	398	GLU	C-N-CA	6.00	136.71	121.70
7	E	114	ASN	N-CA-C	5.94	127.04	111.00
4	A	525	GLN	CG-CD-NE2	-5.90	102.54	116.70
9	H	142	LEU	CB-CG-CD2	5.65	120.61	111.00
4	A	589	GLN	OE1-CD-NE2	-5.60	109.02	121.90
2	T	18	DA	C4'-C3'-C2'	-5.49	98.16	103.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	394	ASN	Sidechain
4	A	524	VAL	Peptide
4	A	525	GLN	Sidechain
4	A	589	GLN	Sidechain
5	B	761	HIS	Sidechain
7	E	143	ASN	Mainchain,Sidechain

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	R	215	0	111	5	0
2	T	525	0	297	23	0
3	N	293	0	156	11	0
4	A	10828	0	10876	348	0
5	B	8871	0	8829	235	0
6	C	2101	0	2056	61	0
7	E	1731	0	1758	39	0
8	F	684	0	692	17	0
9	H	1064	0	1029	31	0
10	I	952	0	898	17	0
11	J	532	0	542	11	0
12	K	919	0	929	25	0
13	L	337	0	353	9	0
14	R	1	0	0	0	0
15	T	99	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
All	All	29160	0	28526	736	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 13.

All (736) 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)
4:A:589:GLN:CG	4:A:589:GLN:CB	1.75	1.55
2:T:17:DG:H1'	2:T:18:DA:H5'	1.25	1.18
5:B:213:ILE:O	5:B:215:GLN:NE2	1.88	1.05
4:A:589:GLN:CG	4:A:589:GLN:CA	2.43	0.97
5:B:857:ARG:NH1	5:B:945:GLU:OE2	2.08	0.85
5:B:996:ARG:HH12	6:C:173:ALA:HB1	1.45	0.81
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.13	0.81
4:A:90:VAL:HG21	4:A:296:LEU:HD12	1.62	0.81
4:A:738:LYS:NZ	6:C:194:GLU:O	2.13	0.81
5:B:996:ARG:NH2	6:C:173:ALA:O	2.13	0.81
4:A:472:LEU:HD13	5:B:835:GLN:NE2	1.96	0.80
4:A:848:ILE:HG21	4:A:1370:LEU:HD21	1.64	0.79
4:A:589:GLN:CG	4:A:589:GLN:HA	2.11	0.79
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.65	0.77
11:J:9:SER:OG	11:J:48:ARG:NH2	2.17	0.77
9:H:33:GLN:HB3	9:H:35:GLN:HE22	1.50	0.76
2:T:26:DG:H2''	2:T:27:DA:H5''	1.67	0.75
4:A:55:ASP:O	4:A:57:ARG:N	2.22	0.73
4:A:1100:ARG:NH2	4:A:1351:GLU:OE2	2.21	0.73
4:A:1329:THR:HG22	4:A:1331:SER:H	1.52	0.72
5:B:629:ASP:O	5:B:632:ARG:NH1	2.22	0.72
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.21	0.72
5:B:46:GLN:HB2	5:B:408:LEU:HD21	1.70	0.72
7:E:127:ILE:HG22	7:E:129:PRO:HD2	1.72	0.72
4:A:526:ASP:OD1	5:B:1013:ASN:ND2	2.23	0.71
7:E:24:LYS:NZ	7:E:32:GLN:OE1	2.23	0.71
2:T:8:DT:H2''	2:T:9:DC:H2'	1.71	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:620:ARG:HD3	10:I:68:LEU:HD11	1.73	0.70
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.24	0.70
4:A:1276:VAL:HB	4:A:1279:ILE:HD13	1.74	0.70
5:B:661:LEU:HD11	5:B:684:LEU:HD11	1.73	0.70
5:B:219:ALA:HB2	5:B:405:ARG:HD3	1.73	0.69
5:B:824:ILE:HG22	5:B:1008:PRO:HA	1.72	0.69
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.22	0.69
5:B:766:ARG:HG3	5:B:1022:THR:HG22	1.73	0.69
5:B:1076:HIS:O	6:C:31:ASN:ND2	2.26	0.69
3:N:11:DG:H2''	3:N:12:DA:H5'	1.74	0.69
2:T:7:DC:H2''	2:T:8:DT:H5''	1.75	0.68
5:B:287:ARG:NH1	5:B:324:ILE:O	2.27	0.68
2:T:19:DG:H2'	2:T:20:DC:H6	1.59	0.68
4:A:239:LEU:HD12	4:A:240:PRO:HD2	1.76	0.67
4:A:898:ARG:O	4:A:1029:ARG:NH1	2.27	0.67
4:A:12:ARG:HD2	5:B:1218:THR:HG21	1.76	0.67
4:A:262:LEU:O	4:A:266:LEU:HD13	1.93	0.67
4:A:91:PHE:H	4:A:297:GLN:HE22	1.42	0.67
4:A:60:SER:OG	4:A:66:LYS:O	2.12	0.67
5:B:788:ARG:NH1	5:B:790:ASP:OD2	2.28	0.67
4:A:961:ARG:HH11	4:A:1025:ARG:HH22	1.42	0.67
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.27	0.67
4:A:888:GLY:O	4:A:940:ARG:NH2	2.27	0.67
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.26	0.67
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.76	0.67
4:A:663:SER:O	4:A:742:ASN:ND2	2.28	0.66
5:B:758:PHE:O	5:B:761:HIS:HB2	1.94	0.66
10:I:80:SER:OG	10:I:103:CYS:SG	2.53	0.66
4:A:100:LYS:O	4:A:104:GLU:N	2.27	0.66
4:A:562:THR:O	4:A:576:GLN:NE2	2.29	0.66
5:B:232:SER:O	5:B:261:ARG:NH2	2.28	0.66
5:B:995:ARG:NH1	5:B:997:GLU:OE1	2.29	0.66
5:B:1020:ARG:HB2	5:B:1022:THR:HG23	1.78	0.66
5:B:1067:ARG:NE	6:C:194:GLU:OE2	2.28	0.66
6:C:54:ASN:ND2	6:C:60:ASP:OD1	2.28	0.66
5:B:843:GLN:HG2	5:B:993:THR:HB	1.77	0.65
5:B:66:ASP:OD2	5:B:422:LYS:NZ	2.28	0.65
5:B:216:GLU:OE1	5:B:537:LYS:NZ	2.29	0.65
5:B:643:ASP:O	5:B:647:GLY:N	2.29	0.65
4:A:1239:ARG:HH12	4:A:1241:ARG:HH12	1.43	0.65
5:B:242:SER:HB2	5:B:362:PRO:HD2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:34:LYS:HG2	4:A:83:HIS:HE1	1.60	0.65
10:I:50:THR:HG22	10:I:52:ILE:H	1.62	0.65
4:A:1397:LEU:HB2	4:A:1426:GLU:HG3	1.78	0.65
5:B:205:ILE:HG13	5:B:461:LEU:HB3	1.77	0.65
4:A:42:ASP:OD2	4:A:46:THR:OG1	2.14	0.65
6:C:169:LYS:NZ	13:L:69:ALA:O	2.25	0.65
8:F:82:THR:O	8:F:136:ARG:NH1	2.26	0.65
4:A:490:HIS:HB3	5:B:1150:ARG:NH1	2.12	0.65
5:B:612:GLU:O	5:B:632:ARG:NH2	2.30	0.65
3:N:12:DA:H2''	3:N:13:DG:C8	2.32	0.64
4:A:901:LEU:N	4:A:926:GLN:OE1	2.30	0.64
9:H:103:LYS:HB3	9:H:115:TYR:HD1	1.61	0.64
10:I:71:SER:OG	10:I:83:ASN:OD1	2.16	0.64
4:A:246:VAL:HG12	4:A:328:ARG:HH22	1.61	0.64
2:T:19:DG:H2'	2:T:20:DC:C6	2.31	0.64
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.79	0.64
4:A:167:CYS:SG	4:A:169:ASN:ND2	2.61	0.64
11:J:10:CYS:SG	11:J:43:ARG:NH2	2.69	0.64
10:I:59:VAL:H	10:I:62:ILE:HD13	1.63	0.63
5:B:103:ASN:ND2	5:B:109:THR:OG1	2.31	0.63
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.31	0.63
5:B:287:ARG:HG2	5:B:292:ILE:HA	1.80	0.63
5:B:208:SER:OG	5:B:210:LYS:NZ	2.31	0.63
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.81	0.63
6:C:254:LYS:NZ	12:K:38:GLU:OE1	2.32	0.63
7:E:78:LEU:HD21	7:E:109:ILE:HD13	1.81	0.63
2:T:17:DG:H1'	2:T:18:DA:C5'	2.15	0.63
11:J:13:VAL:O	11:J:17:LYS:NZ	2.30	0.63
2:T:25:DC:OP1	5:B:857:ARG:NH2	2.31	0.62
5:B:763:GLN:HG2	5:B:765:PRO:HD2	1.79	0.62
4:A:79:GLY:HA3	4:A:243:PRO:HG3	1.82	0.62
5:B:680:THR:O	5:B:683:SER:OG	2.13	0.62
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.62	0.62
5:B:56:ASP:OD2	5:B:177:LYS:NZ	2.28	0.62
5:B:299:GLU:OE1	5:B:572:HIS:ND1	2.28	0.62
4:A:444:PHE:HE2	4:A:470:LEU:HD23	1.64	0.62
5:B:100:PRO:O	5:B:180:TYR:OH	2.18	0.62
4:A:782:ARG:NH2	5:B:701:ILE:O	2.33	0.62
9:H:37:LYS:NZ	9:H:126:GLU:OE1	2.29	0.61
9:H:118:PHE:CZ	9:H:142:LEU:HD12	2.35	0.61
4:A:884:ASP:HB3	4:A:896:ARG:HH22	1.66	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1132:LYS:HD3	4:A:1135:ARG:NH1	2.15	0.61
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.81	0.61
4:A:1094:VAL:HA	4:A:1113:THR:HG21	1.82	0.61
5:B:1082:MET:HA	6:C:189:THR:HA	1.82	0.61
4:A:1239:ARG:HH22	4:A:1241:ARG:HH22	1.48	0.61
4:A:541:ILE:HD12	4:A:577:ILE:HG21	1.83	0.61
4:A:879:GLU:OE1	4:A:962:ARG:NH2	2.33	0.61
5:B:255:GLN:H	5:B:272:THR:HG22	1.66	0.61
4:A:808:LEU:O	5:B:728:ARG:NH1	2.34	0.61
4:A:1444:MET:HG3	8:F:133:VAL:HG13	1.82	0.61
5:B:487:THR:OG1	5:B:777:ALA:O	2.19	0.61
12:K:58:PHE:HB3	12:K:76:GLN:HB3	1.83	0.60
5:B:102:VAL:CG1	5:B:112:LEU:HD22	2.30	0.60
7:E:197:LYS:HE2	7:E:199:ILE:HD11	1.84	0.60
2:T:11:DG:H2''	2:T:12:DG:C8	2.36	0.60
4:A:765:VAL:HG22	4:A:800:VAL:HB	1.82	0.60
5:B:103:ASN:OD1	5:B:169:ARG:NH2	2.32	0.60
9:H:25:ARG:HD2	9:H:39:THR:HG22	1.83	0.60
4:A:443:LEU:HB2	4:A:501:LEU:HD11	1.84	0.60
4:A:147:VAL:HG22	4:A:170:THR:HG22	1.84	0.59
5:B:840:ILE:HB	5:B:1011:ILE:HB	1.85	0.59
5:B:979:LYS:HG2	5:B:1095:LEU:HD12	1.84	0.59
10:I:111:THR:HG22	10:I:113:ASP:H	1.67	0.59
2:T:12:DG:H2''	2:T:13:DT:H5''	1.85	0.59
2:T:13:DT:H2'	2:T:14:DC:C6	2.37	0.59
4:A:1021:LEU:HD11	4:A:1025:ARG:HH11	1.67	0.59
4:A:404:TYR:HD2	4:A:412:ARG:HG2	1.68	0.59
4:A:353:ILE:HG21	4:A:487:MET:HG3	1.85	0.59
4:A:472:LEU:HD13	5:B:835:GLN:CD	2.23	0.59
4:A:746:MET:SD	5:B:1015:HIS:ND1	2.72	0.59
9:H:103:LYS:HB3	9:H:115:TYR:CD1	2.38	0.59
5:B:345:LYS:HA	5:B:348:ARG:HD3	1.83	0.59
4:A:526:ASP:OD1	5:B:835:GLN:HG2	2.03	0.58
4:A:1281:ARG:NH2	4:A:1309:ASP:OD1	2.31	0.58
4:A:378:GLU:OE2	4:A:387:ARG:NH2	2.35	0.58
4:A:549:MET:HE1	4:A:656:TRP:HD1	1.68	0.58
4:A:881:GLN:HA	4:A:961:ARG:HH22	1.66	0.58
1:R:9:G:O2'	4:A:485:ASP:OD1	2.21	0.58
4:A:446:ARG:NH1	4:A:447:GLN:O	2.31	0.58
6:C:40:GLU:OE1	6:C:254:LYS:HE2	2.04	0.58
5:B:104:GLU:OE1	5:B:120:ARG:NH1	2.29	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:466:SER:HB3	5:B:1103:ILE:HD11	1.86	0.58
4:A:34:LYS:HG2	4:A:83:HIS:CE1	2.39	0.58
4:A:119:ASN:OD1	4:A:122:MET:N	2.34	0.58
5:B:705:MET:HE3	5:B:742:GLU:HG3	1.86	0.58
6:C:31:ASN:O	6:C:35:ARG:HG3	2.04	0.58
4:A:1400:CYS:HB2	4:A:1405:THR:HG23	1.85	0.57
5:B:59:LEU:HG	5:B:95:ILE:HD13	1.86	0.57
5:B:173:MET:O	5:B:176:SER:OG	2.16	0.57
5:B:373:ARG:HA	5:B:566:LEU:HD23	1.85	0.57
8:F:111:LEU:HD23	8:F:111:LEU:H	1.68	0.57
4:A:1155:ASP:OD2	4:A:1161:THR:OG1	2.17	0.57
6:C:246:ARG:O	6:C:250:THR:OG1	2.18	0.57
4:A:1438:THR:HG23	8:F:92:ARG:HB2	1.86	0.57
5:B:519:TRP:CZ2	5:B:705:MET:HE1	2.38	0.57
7:E:47:CYS:HA	7:E:53:PRO:HA	1.85	0.57
9:H:27:GLU:OE2	9:H:39:THR:OG1	2.22	0.57
4:A:336:ILE:HD13	4:A:340:LEU:HD12	1.85	0.57
6:C:94:LYS:HA	6:C:127:ARG:HH22	1.69	0.57
4:A:526:ASP:HB2	5:B:835:GLN:OE1	2.05	0.57
5:B:416:LEU:HD23	5:B:457:LEU:HD23	1.86	0.57
4:A:713:SER:O	4:A:717:ASN:ND2	2.35	0.57
4:A:961:ARG:NH1	4:A:1025:ARG:HH22	2.03	0.57
4:A:1206:ASP:OD1	4:A:1274:ARG:NH1	2.36	0.56
5:B:744:HIS:ND1	5:B:746:SER:OG	2.37	0.56
8:F:79:ARG:NH1	8:F:145:ASP:O	2.37	0.56
2:T:8:DT:H1'	2:T:9:DC:H5'	1.87	0.56
4:A:54:ASN:HB3	4:A:247:ARG:HH22	1.71	0.56
12:K:51:LEU:CD1	12:K:59:ALA:HB3	2.35	0.56
4:A:28:ARG:HH22	4:A:85:ASP:HB3	1.70	0.56
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.87	0.56
4:A:1140:HIS:HA	4:A:1275:GLY:HA3	1.88	0.56
4:A:514:PRO:HB3	4:A:875:ALA:HB3	1.87	0.56
4:A:901:LEU:HA	4:A:907:THR:HG23	1.88	0.56
4:A:1350:LYS:O	4:A:1354:ASN:ND2	2.32	0.56
5:B:216:GLU:OE1	5:B:500:THR:OG1	2.21	0.56
5:B:384:ARG:NH2	5:B:621:GLU:OE2	2.39	0.56
5:B:470:LYS:O	5:B:474:SER:OG	2.23	0.56
5:B:546:SER:OG	5:B:631:GLY:N	2.38	0.56
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.06	0.56
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.37	0.56
3:N:10:DA:H2''	3:N:11:DG:C8	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:77:ILE:HG13	6:C:161:LYS:HE3	1.88	0.56
4:A:445:ASN:OD1	4:A:446:ARG:N	2.38	0.56
4:A:544:ASP:N	4:A:544:ASP:OD1	2.38	0.56
5:B:604:ARG:NH1	5:B:691:GLU:OE2	2.33	0.56
4:A:867:ILE:HG22	4:A:872:GLY:N	2.21	0.55
4:A:939:ASP:OD2	4:A:1023:ARG:NH1	2.38	0.55
4:A:899:VAL:HG13	4:A:929:LEU:HD13	1.89	0.55
6:C:66:ARG:NH1	6:C:143:LEU:O	2.39	0.55
9:H:12:VAL:HG13	9:H:26:ILE:HD11	1.87	0.55
4:A:329:LEU:HA	4:A:335:ARG:H	1.70	0.55
5:B:1103:ILE:O	5:B:1122:ARG:NH2	2.39	0.55
4:A:568:PRO:HB2	9:H:46:LEU:HD22	1.88	0.55
4:A:598:LEU:O	9:H:122:LEU:HD12	2.05	0.55
5:B:896:ASP:OD2	13:L:29:TYR:OH	2.20	0.55
7:E:81:GLU:HB3	7:E:96:PHE:HE1	1.71	0.55
4:A:877:HIS:CD2	4:A:1056:SER:HA	2.41	0.55
4:A:899:VAL:CG1	4:A:929:LEU:HD13	2.36	0.55
4:A:113:LEU:HD23	4:A:113:LEU:H	1.72	0.55
5:B:27:ALA:O	5:B:30:SER:OG	2.21	0.55
10:I:10:CYS:SG	10:I:31:THR:OG1	2.63	0.55
4:A:541:ILE:HD13	4:A:549:MET:HE1	1.87	0.55
5:B:307:ASP:OD1	5:B:392:ARG:NH1	2.38	0.55
6:C:2:SER:OG	12:K:104:ASN:OD1	2.24	0.55
7:E:124:VAL:HG13	7:E:132:ILE:HB	1.88	0.55
1:R:3:C:H2'	1:R:4:G:H8	1.72	0.55
4:A:846:GLU:HA	4:A:1066:VAL:HG22	1.89	0.55
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.89	0.55
4:A:42:ASP:HB2	4:A:50:ILE:HG23	1.89	0.54
4:A:269:ILE:HG12	4:A:299:HIS:HB3	1.88	0.54
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.42	0.54
4:A:90:VAL:HG13	4:A:297:GLN:CD	2.28	0.54
4:A:1130:GLN:O	4:A:1134:ILE:HG12	2.07	0.54
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.89	0.54
5:B:996:ARG:NH1	6:C:173:ALA:HB1	2.20	0.54
6:C:252:GLN:HG3	12:K:95:ILE:HG23	1.88	0.54
4:A:146:MET:HG3	4:A:147:VAL:HG23	1.89	0.54
4:A:737:LEU:HD11	4:A:758:ILE:HG21	1.89	0.54
4:A:452:LYS:O	5:B:1141:HIS:NE2	2.41	0.54
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.43	0.54
6:C:258:ILE:HG23	12:K:19:LEU:HD11	1.89	0.54
4:A:494:SER:O	4:A:498:ARG:HG3	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:579:SER:HB3	4:A:611:GLN:HA	1.89	0.54
9:H:36:CYS:SG	9:H:130:ARG:NH2	2.80	0.54
4:A:1138:ILE:HG23	4:A:1282:VAL:HG21	1.90	0.54
5:B:1056:SER:HB3	5:B:1066:SER:HB3	1.89	0.53
4:A:903:ASN:O	4:A:907:THR:OG1	2.25	0.53
5:B:652:LYS:HB3	5:B:689:LEU:HD22	1.90	0.53
5:B:872:GLU:HG2	5:B:916:THR:HB	1.90	0.53
4:A:351:THR:OG1	4:A:352:VAL:N	2.42	0.53
4:A:517:ASN:O	4:A:517:ASN:ND2	2.38	0.53
4:A:1351:GLU:O	4:A:1355:VAL:HG13	2.09	0.53
5:B:63:ILE:O	5:B:67:SER:HB3	2.08	0.53
7:E:46:TYR:CE2	7:E:58:MET:HA	2.44	0.53
11:J:37:SER:OG	11:J:47:ARG:NH2	2.41	0.53
4:A:534:LEU:O	4:A:574:GLY:HA3	2.08	0.53
5:B:235:SER:OG	5:B:236:HIS:ND1	2.37	0.53
4:A:153:PRO:HA	4:A:161:LEU:HB2	1.90	0.53
4:A:392:VAL:HG13	4:A:415:LEU:HD11	1.91	0.53
5:B:896:ASP:OD2	13:L:58:LYS:NZ	2.41	0.53
4:A:332:LYS:HA	4:A:337:ARG:NH2	2.23	0.53
5:B:778:MET:HE1	5:B:1094:ARG:HD3	1.90	0.53
6:C:2:SER:OG	6:C:3:GLU:N	2.41	0.53
12:K:16:GLU:OE1	12:K:37:LYS:NZ	2.25	0.53
4:A:589:GLN:CB	4:A:589:GLN:NE2	2.72	0.52
4:A:1161:THR:HG21	4:A:1166:ASP:HB2	1.91	0.52
5:B:195:CYS:HG	5:B:783:THR:HG1	1.55	0.52
4:A:672:ASP:N	4:A:672:ASP:OD1	2.39	0.52
4:A:993:LEU:HD22	4:A:1046:LEU:HG	1.91	0.52
4:A:1345:ARG:HG2	4:A:1372:VAL:HG12	1.90	0.52
8:F:101:ILE:HD13	8:F:120:ILE:HG22	1.91	0.52
4:A:848:ILE:HB	4:A:1065:GLY:HA3	1.90	0.52
4:A:1005:GLU:O	4:A:1009:ASN:ND2	2.42	0.52
5:B:931:TYR:HD2	5:B:932:HIS:H	1.57	0.52
12:K:91:CYS:O	12:K:95:ILE:HG13	2.09	0.52
4:A:567:LYS:HB3	4:A:568:PRO:HD3	1.90	0.52
4:A:1120:LEU:O	4:A:1323:ASP:HB2	2.10	0.52
3:N:12:DA:OP2	3:N:12:DA:H2'	2.09	0.52
4:A:284:ALA:HB3	4:A:289:ILE:HD11	1.91	0.52
5:B:245:GLU:O	5:B:249:ARG:NH2	2.42	0.52
9:H:92:ASP:OD1	9:H:92:ASP:N	2.36	0.52
4:A:111:GLY:HA3	4:A:213:HIS:O	2.09	0.52
4:A:780:VAL:HG13	4:A:789:LYS:HE2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:979:SER:OG	4:A:980:ASP:N	2.42	0.52
4:A:929:LEU:HD11	4:A:983:ILE:HD13	1.92	0.52
5:B:308:TRP:HA	5:B:311:LEU:HD12	1.92	0.52
5:B:805:THR:OG1	5:B:1041:GLU:OE1	2.26	0.52
7:E:20:LYS:NZ	7:E:34:GLU:O	2.42	0.52
4:A:306:ASN:ND2	4:A:313:GLN:OE1	2.43	0.52
4:A:550:LEU:HD23	4:A:556:TRP:CZ2	2.43	0.52
4:A:1341:ILE:HD13	4:A:1380:GLY:HA2	1.92	0.52
5:B:1186:ASP:OD1	5:B:1188:LYS:NZ	2.34	0.52
6:C:244:VAL:O	6:C:248:ILE:HG13	2.10	0.52
8:F:77:ASP:OD1	8:F:77:ASP:N	2.43	0.52
3:N:9:DC:H2''	3:N:10:DA:C8	2.44	0.52
10:I:60:GLN:OE1	10:I:107:SER:OG	2.24	0.52
4:A:904:THR:OG1	4:A:905:ASP:OD1	2.26	0.51
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.09	0.51
6:C:251:LEU:O	6:C:255:VAL:HG23	2.10	0.51
7:E:26:ARG:NH2	7:E:133:GLU:OE1	2.28	0.51
12:K:100:ALA:O	12:K:104:ASN:ND2	2.43	0.51
4:A:151:ASP:OD1	4:A:164:ARG:N	2.38	0.51
5:B:301:ILE:HD13	5:B:382:ILE:HG21	1.91	0.51
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.11	0.51
5:B:840:ILE:HG12	5:B:992:ILE:HG22	1.92	0.51
5:B:1077:THR:HG22	5:B:1079:LYS:H	1.74	0.51
5:B:616:ILE:HD11	5:B:696:GLU:HB3	1.92	0.51
4:A:453:MET:HB3	4:A:477:PRO:HB3	1.91	0.51
5:B:259:TYR:OH	5:B:279:ASP:OD2	2.24	0.51
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.44	0.51
1:R:7:A:O2'	1:R:8:G:H5'	2.10	0.51
4:A:98:LYS:O	4:A:102:VAL:HG12	2.10	0.51
3:N:8:DC:H2''	3:N:9:DC:C6	2.45	0.51
5:B:117:ALA:HA	5:B:122:LEU:HB2	1.91	0.51
5:B:1191:ILE:HD12	5:B:1191:ILE:O	2.11	0.51
5:B:209:GLU:OE2	5:B:788:ARG:NH2	2.44	0.51
2:T:16:DT:H2'	2:T:17:DG:N3	2.26	0.51
5:B:63:ILE:HG13	5:B:95:ILE:HD12	1.92	0.51
4:A:74:MET:O	5:B:1116:ARG:NH2	2.43	0.51
4:A:824:LEU:HD21	5:B:765:PRO:HB3	1.93	0.51
5:B:309:GLN:HE22	10:I:50:THR:HG21	1.76	0.51
4:A:35:ILE:O	4:A:84:ILE:HD13	2.11	0.50
4:A:42:ASP:HA	4:A:50:ILE:HG13	1.94	0.50
4:A:870:GLU:HG2	7:E:208:TYR:CD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:913:LEU:N	4:A:978:PRO:HB3	2.26	0.50
5:B:102:VAL:HG11	5:B:112:LEU:HD22	1.92	0.50
2:T:16:DT:H2'	2:T:17:DG:C2	2.46	0.50
4:A:451:HIS:HB3	4:A:453:MET:H	1.76	0.50
4:A:1140:HIS:HE1	4:A:1142:THR:HG23	1.76	0.50
4:A:1267:MET:HA	4:A:1271:ILE:HD13	1.92	0.50
4:A:1420:ASP:OD2	4:A:1422:ARG:NH2	2.45	0.50
4:A:109:HIS:HB2	4:A:167:CYS:SG	2.51	0.50
4:A:569:LYS:HD2	4:A:571:LEU:HD11	1.93	0.50
4:A:1398:MET:N	4:A:1426:GLU:OE2	2.38	0.50
5:B:487:THR:O	5:B:490:SER:OG	2.27	0.50
12:K:12:LEU:HD12	12:K:12:LEU:H	1.75	0.50
4:A:549:MET:CE	4:A:656:TRP:HD1	2.23	0.50
4:A:664:THR:OG1	5:B:1014:PRO:HB3	2.11	0.50
5:B:992:ILE:HG12	5:B:994:TYR:CE2	2.47	0.50
5:B:1072:MET:HE2	5:B:1085:ILE:HG13	1.93	0.50
5:B:73:GLN:N	5:B:86:ARG:O	2.44	0.50
5:B:830:TYR:O	5:B:831:SER:OG	2.25	0.50
4:A:778:GLY:HA3	5:B:516:ASN:HB2	1.94	0.50
4:A:800:VAL:HG13	4:A:812:GLU:HB3	1.93	0.50
4:A:873:MET:HG3	4:A:957:PRO:HG3	1.93	0.50
5:B:1094:ARG:NH1	5:B:1098:MET:SD	2.79	0.50
6:C:145:CYS:SG	6:C:146:LYS:N	2.85	0.50
10:I:44:TYR:CE1	10:I:46:HIS:HB2	2.46	0.50
4:A:208:LEU:HD23	4:A:235:ILE:HG12	1.93	0.49
4:A:747:VAL:HG21	4:A:758:ILE:HD11	1.94	0.49
5:B:615:MET:HG2	5:B:626:ILE:HG23	1.93	0.49
5:B:904:ARG:NH1	13:L:66:GLN:O	2.45	0.49
5:B:48:LEU:HD23	5:B:173:MET:SD	2.53	0.49
5:B:892:LYS:NZ	5:B:904:ARG:O	2.29	0.49
4:A:266:LEU:HD11	4:A:303:TYR:CE1	2.48	0.49
4:A:569:LYS:HZ3	6:C:222:LYS:HD3	1.77	0.49
5:B:847:ASP:HB3	6:C:167:HIS:CE1	2.48	0.49
4:A:237:THR:OG1	4:A:238:CYS:N	2.45	0.49
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.11	0.49
5:B:705:MET:CE	5:B:742:GLU:HG3	2.42	0.49
4:A:90:VAL:HG13	4:A:297:GLN:NE2	2.26	0.49
7:E:169:ARG:HB3	8:F:140:ASP:HB3	1.93	0.49
4:A:1025:ARG:HA	4:A:1030:ARG:HH11	1.77	0.49
5:B:851:PHE:HB3	5:B:1094:ARG:HD2	1.94	0.49
4:A:323:LYS:NZ	4:A:328:ARG:HE	2.10	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:840:ARG:NH2	4:A:1106:ASN:OD1	2.45	0.49
4:A:944:ARG:NH2	4:A:1296:GLY:O	2.34	0.49
4:A:1002:GLY:O	4:A:1008:GLN:NE2	2.42	0.49
4:A:1062:GLU:OE2	8:F:88:TYR:OH	2.29	0.49
4:A:1373:ASP:O	4:A:1377:THR:N	2.39	0.49
6:C:92:CYS:SG	6:C:94:LYS:N	2.80	0.49
10:I:98:VAL:HG11	10:I:113:ASP:HB2	1.94	0.49
7:E:94:LYS:HA	7:E:97:VAL:HG22	1.95	0.48
7:E:127:ILE:HB	7:E:130:ALA:HB3	1.94	0.48
3:N:11:DG:H2'	3:N:12:DA:C8	2.48	0.48
6:C:135:GLN:NE2	6:C:235:VAL:O	2.46	0.48
1:R:3:C:H2'	1:R:4:G:C8	2.48	0.48
4:A:356:ASP:HB3	4:A:359:LEU:HG	1.94	0.48
4:A:471:ASN:O	4:A:474:VAL:HG12	2.13	0.48
4:A:543:LEU:O	4:A:547:LEU:HD12	2.13	0.48
6:C:26:ASP:OD1	6:C:26:ASP:N	2.44	0.48
9:H:40:LEU:HD13	9:H:123:MET:HB2	1.94	0.48
4:A:57:ARG:O	4:A:68:GLN:HB2	2.14	0.48
4:A:311:GLN:N	4:A:312:PRO:HD3	2.28	0.48
4:A:1155:ASP:HB3	4:A:1241:ARG:HH21	1.77	0.48
5:B:114:PRO:HG2	5:B:181:LEU:HD11	1.94	0.48
11:J:3:VAL:HG11	11:J:18:TRP:HB2	1.96	0.48
4:A:589:GLN:CB	4:A:589:GLN:CD	2.77	0.48
4:A:1428:VAL:HG13	5:B:1151:LEU:HD23	1.95	0.48
10:I:5:ARG:NH2	10:I:36:GLU:OE2	2.47	0.48
4:A:350:ARG:HD3	5:B:1128:LEU:HD11	1.95	0.48
4:A:748:MET:HE2	9:H:19:ARG:HH22	1.79	0.48
4:A:874:ASP:HB3	4:A:877:HIS:NE2	2.29	0.48
4:A:1363:VAL:HB	4:A:1368:MET:HE2	1.95	0.48
7:E:115:ASN:OD1	7:E:116:ILE:N	2.46	0.48
2:T:19:DG:O4'	4:A:835:GLY:HA3	2.13	0.48
4:A:464:PRO:HG2	4:A:465:TYR:HD1	1.79	0.48
4:A:771:GLU:OE2	5:B:510:LYS:NZ	2.32	0.48
5:B:554:ILE:O	5:B:558:LEU:HG	2.14	0.48
5:B:576:ASP:OD1	5:B:576:ASP:N	2.46	0.48
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.95	0.48
6:C:92:CYS:SG	6:C:93:ASP:N	2.87	0.48
4:A:635:ARG:NE	4:A:877:HIS:HB3	2.29	0.48
4:A:928:LEU:HD23	4:A:928:LEU:HA	1.72	0.48
5:B:1072:MET:HE1	5:B:1085:ILE:HG21	1.96	0.48
6:C:115:SER:OG	6:C:141:GLY:HA3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:751:VAL:HG23	5:B:812:LEU:HD22	1.96	0.48
4:A:840:ARG:NE	4:A:1384:VAL:O	2.43	0.47
5:B:118:ARG:NH2	5:B:194:GLU:OE2	2.46	0.47
11:J:48:ARG:O	11:J:52:THR:OG1	2.24	0.47
4:A:665:GLY:HA2	5:B:1086:PHE:CG	2.49	0.47
4:A:1376:THR:HG22	7:E:212:ARG:HH12	1.78	0.47
6:C:44:LEU:HD12	6:C:160:LYS:O	2.14	0.47
4:A:545:GLN:O	4:A:549:MET:HG3	2.14	0.47
4:A:582:ILE:HG22	4:A:610:GLY:HA2	1.96	0.47
5:B:599:THR:O	5:B:603:LEU:HG	2.15	0.47
6:C:11:ARG:NH2	6:C:19:ASP:OD1	2.47	0.47
4:A:1051:ALA:O	4:A:1055:ARG:HG3	2.15	0.47
4:A:1135:ARG:HA	4:A:1138:ILE:HG22	1.97	0.47
4:A:1199:ARG:NH2	4:A:1231:ASP:O	2.47	0.47
5:B:393:LYS:HA	5:B:393:LYS:HD2	1.70	0.47
7:E:157:SER:N	7:E:160:GLU:OE1	2.40	0.47
12:K:18:LYS:NZ	12:K:36:GLU:O	2.40	0.47
4:A:666:ILE:HD11	5:B:1027:ILE:HG12	1.95	0.47
4:A:1323:ASP:OD1	4:A:1325:THR:OG1	2.31	0.47
5:B:616:ILE:CD1	5:B:696:GLU:HB3	2.44	0.47
5:B:1204:PHE:O	5:B:1208:MET:HG3	2.13	0.47
4:A:323:LYS:HD3	4:A:328:ARG:HG3	1.96	0.47
4:A:635:ARG:HE	4:A:877:HIS:HA	1.79	0.47
4:A:1229:SER:OG	4:A:1230:GLU:N	2.47	0.47
5:B:313:MET:O	5:B:316:PRO:HD2	2.14	0.47
4:A:12:ARG:HG3	5:B:1192:TYR:CD2	2.50	0.47
4:A:44:THR:OG1	4:A:46:THR:HG23	2.15	0.47
4:A:1140:HIS:CE1	4:A:1142:THR:HG23	2.50	0.47
4:A:1166:ASP:HA	4:A:1169:ILE:HD13	1.97	0.47
5:B:843:GLN:CG	5:B:993:THR:HB	2.44	0.47
2:T:19:DG:H5'	4:A:832:ALA:HA	1.97	0.47
4:A:172:PRO:HB3	4:A:185:TRP:CG	2.50	0.47
4:A:414:ASP:OD2	4:A:416:ARG:NH2	2.48	0.47
5:B:1065:GLN:OE1	5:B:1067:ARG:N	2.48	0.47
6:C:46:ILE:HA	6:C:159:ALA:HA	1.96	0.47
4:A:9:ALA:O	5:B:1193:GLN:NE2	2.48	0.46
4:A:449:SER:HB3	5:B:1137:CYS:SG	2.55	0.46
4:A:1363:VAL:HB	4:A:1368:MET:CE	2.45	0.46
4:A:1409:LEU:HD23	5:B:1207:LEU:HD21	1.97	0.46
5:B:58:THR:O	5:B:62:ILE:HG13	2.14	0.46
5:B:892:LYS:O	5:B:899:ILE:HG13	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:13:DT:HI'	15:T:101:5N0:C15	2.46	0.46
4:A:1004:ASN:ND2	7:E:167:ARG:HD2	2.31	0.46
4:A:29:ALA:O	5:B:1183:LYS:HG2	2.15	0.46
4:A:42:ASP:N	4:A:49:LYS:HA	2.31	0.46
4:A:464:PRO:O	12:K:2:ASN:HB3	2.15	0.46
4:A:1030:ARG:NE	4:A:1034:GLU:OE1	2.38	0.46
4:A:1080:THR:OG1	4:A:1081:LEU:N	2.48	0.46
6:C:62:PHE:HE2	6:C:66:ARG:HD2	1.79	0.46
7:E:78:LEU:HD23	7:E:107:THR:HB	1.97	0.46
4:A:332:LYS:HA	4:A:337:ARG:HH21	1.78	0.46
4:A:1364:ASN:OD1	4:A:1366:ARG:HG2	2.15	0.46
5:B:136:THR:HG22	5:B:137:TYR:H	1.81	0.46
5:B:1084:GLN:NE2	6:C:190:ASP:O	2.35	0.46
4:A:885:THR:HG23	4:A:1024:SER:HB3	1.98	0.46
5:B:882:THR:OG1	5:B:885:MET:SD	2.73	0.46
4:A:556:TRP:CH2	4:A:558:GLY:HA2	2.51	0.46
9:H:63:LEU:HB3	9:H:90:ALA:HB2	1.97	0.46
4:A:586:ILE:HD11	4:A:637:LYS:HG2	1.98	0.46
4:A:886:ILE:HD11	4:A:943:LEU:HB3	1.96	0.46
4:A:1436:ILE:HG22	4:A:1437:GLY:H	1.81	0.46
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.97	0.46
5:B:299:GLU:HG3	5:B:571:PRO:HG2	1.96	0.46
5:B:758:PHE:CE2	5:B:1044:ALA:HA	2.51	0.46
10:I:72:ASP:O	10:I:81:ARG:NH2	2.33	0.46
4:A:303:TYR:CZ	4:A:325:ILE:HD11	2.51	0.46
4:A:1157:ASP:OD1	4:A:1160:SER:N	2.48	0.46
5:B:402:GLY:O	5:B:405:ARG:NH1	2.49	0.46
6:C:66:ARG:NH2	11:J:3:VAL:O	2.41	0.46
9:H:115:TYR:OH	9:H:124:ARG:NH1	2.48	0.46
4:A:567:LYS:HB2	9:H:96:VAL:HB	1.98	0.46
4:A:930:ASP:O	4:A:934:LYS:HD3	2.15	0.46
5:B:861:ASP:OD1	5:B:862:GLN:N	2.48	0.46
6:C:36:VAL:HG23	12:K:41:THR:HG21	1.98	0.46
4:A:350:ARG:HD2	4:A:488:ASN:OD1	2.15	0.46
4:A:960:ILE:HG23	4:A:964:ILE:HD13	1.98	0.46
4:A:1322:ILE:O	4:A:1324:PRO:HD3	2.16	0.46
5:B:129:PHE:HE2	5:B:166:PHE:HB2	1.81	0.46
12:K:47:ARG:NH1	12:K:51:LEU:HD22	2.31	0.46
4:A:335:ARG:NH1	5:B:1202:LEU:HD13	2.31	0.45
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.50	0.45
9:H:8:ASP:OD1	9:H:129:TYR:OH	2.23	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:8:ASP:OD2	9:H:9:ILE:N	2.46	0.45
4:A:369:SER:OG	12:K:2:ASN:ND2	2.45	0.45
5:B:807:ARG:H	5:B:1045:SER:HB3	1.81	0.45
4:A:18:GLN:O	5:B:1215:ARG:HB2	2.17	0.45
5:B:46:GLN:HG3	5:B:47:GLN:H	1.81	0.45
12:K:47:ARG:O	12:K:51:LEU:HD13	2.16	0.45
5:B:289:LEU:HD21	5:B:356:LEU:HD12	1.98	0.45
12:K:24:ASP:OD1	12:K:25:THR:N	2.50	0.45
4:A:315:LEU:HA	4:A:321:PRO:HA	1.98	0.45
5:B:182:SER:OG	5:B:183:GLU:OE2	2.35	0.45
4:A:28:ARG:HH12	4:A:85:ASP:HB3	1.82	0.45
4:A:896:ARG:NH2	4:A:897:TYR:OH	2.50	0.45
4:A:939:ASP:O	4:A:943:LEU:HG	2.16	0.45
4:A:1219:THR:HG21	4:A:1271:ILE:HD11	1.98	0.45
4:A:444:PHE:CE2	4:A:470:LEU:HD23	2.48	0.45
4:A:490:HIS:HB3	5:B:1150:ARG:HH11	1.78	0.45
4:A:515:GLN:HB2	4:A:1071:SER:HB3	1.98	0.45
4:A:531:ILE:HD12	4:A:649:ILE:HD11	1.99	0.45
4:A:1281:ARG:HB3	4:A:1309:ASP:HB2	1.99	0.45
7:E:143:ASN:ND2	7:E:187:TYR:OH	2.50	0.45
6:C:211:ASP:OD1	6:C:211:ASP:N	2.44	0.45
4:A:328:ARG:HD3	5:B:1206:GLU:OE1	2.16	0.45
5:B:778:MET:CE	5:B:1094:ARG:HD3	2.47	0.45
9:H:35:GLN:N	9:H:35:GLN:OE1	2.50	0.45
9:H:111:LEU:HD23	9:H:111:LEU:HA	1.82	0.45
2:T:9:DC:H2"	2:T:10:DT:C7	2.46	0.44
4:A:569:LYS:NZ	6:C:221:TYR:O	2.45	0.44
4:A:775:ILE:HG21	4:A:815:PHE:CE2	2.52	0.44
4:A:900:ASP:O	4:A:907:THR:OG1	2.34	0.44
6:C:76:ASP:OD2	6:C:128:ASN:N	2.41	0.44
4:A:62:ASP:HB3	4:A:64:ASN:ND2	2.33	0.44
4:A:348:SER:HB2	5:B:1128:LEU:HB2	1.98	0.44
4:A:447:GLN:HE22	4:A:488:ASN:ND2	2.16	0.44
4:A:802:ASN:OD1	5:B:729:ILE:N	2.34	0.44
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.99	0.44
4:A:1132:LYS:HB2	4:A:1132:LYS:HE2	1.61	0.44
7:E:190:LEU:HD13	7:E:190:LEU:HA	1.84	0.44
4:A:1027:ALA:HB3	4:A:1030:ARG:HB2	1.98	0.44
5:B:885:MET:HE3	5:B:885:MET:HB3	1.85	0.44
7:E:98:ILE:HD13	7:E:98:ILE:HA	1.87	0.44
4:A:455:MET:HE1	5:B:1134:GLU:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:952:VAL:HG22	5:B:966:VAL:HG22	1.98	0.44
5:B:1039:GLY:O	11:J:32:GLU:HB2	2.18	0.44
9:H:13:SER:OG	9:H:27:GLU:O	2.23	0.44
4:A:203:SER:O	4:A:207:ILE:HG13	2.17	0.44
4:A:571:LEU:HD22	9:H:46:LEU:HD11	1.98	0.44
4:A:881:GLN:NE2	4:A:958:VAL:O	2.40	0.44
6:C:46:ILE:HD12	6:C:46:ILE:H	1.82	0.44
4:A:1027:ALA:O	4:A:1031:VAL:HG23	2.17	0.44
5:B:1104:HIS:NE2	5:B:1126:GLY:O	2.48	0.44
6:C:114:TYR:HB3	6:C:141:GLY:H	1.83	0.44
9:H:30:SER:OG	9:H:36:CYS:O	2.24	0.44
13:L:38:LEU:HD22	13:L:56:LEU:HD21	1.99	0.44
4:A:53:LEU:HD12	4:A:53:LEU:HA	1.78	0.44
4:A:380:VAL:HG21	4:A:427:GLN:O	2.18	0.44
5:B:834:ASN:HB3	5:B:840:ILE:HG13	1.99	0.44
7:E:66:GLU:O	7:E:69:ILE:HG12	2.18	0.44
4:A:547:LEU:HD23	12:K:58:PHE:CD1	2.53	0.44
8:F:90:ARG:O	8:F:94:LEU:HG	2.18	0.44
2:T:9:DC:H2"	2:T:10:DT:H71	2.00	0.43
4:A:131:SER:HB3	4:A:223:GLY:HA2	2.00	0.43
4:A:1303:GLU:CD	4:A:1326:ARG:HH12	2.18	0.43
12:K:47:ARG:NH1	12:K:51:LEU:CD2	2.81	0.43
12:K:49:GLU:HG2	12:K:94:ILE:HG13	1.99	0.43
3:N:14:DA:H2"	3:N:15:DG:C8	2.53	0.43
4:A:357:PRO:HD2	5:B:833:TYR:CZ	2.52	0.43
4:A:379:VAL:HG22	4:A:431:LYS:HG2	1.99	0.43
4:A:601:LYS:HB2	4:A:603:ASN:ND2	2.33	0.43
4:A:1116:LEU:O	4:A:1308:THR:HG23	2.19	0.43
5:B:128:LEU:HD21	5:B:170:LEU:HB2	1.98	0.43
5:B:1172:ILE:HD13	5:B:1172:ILE:HA	1.85	0.43
6:C:253:LYS:HB2	6:C:253:LYS:HE3	1.69	0.43
3:N:14:DA:H2"	3:N:15:DG:H8	1.82	0.43
4:A:515:GLN:HE21	4:A:1071:SER:HA	1.82	0.43
4:A:1215:ARG:O	4:A:1219:THR:OG1	2.31	0.43
5:B:229:ALA:HB1	5:B:231:PRO:HD2	1.99	0.43
5:B:512:ARG:NH2	5:B:532:ALA:H	2.16	0.43
6:C:244:VAL:HG11	12:K:105:PHE:CZ	2.52	0.43
4:A:1135:ARG:HD3	4:A:1282:VAL:HG12	2.00	0.43
4:A:1239:ARG:HH22	4:A:1241:ARG:NH2	2.14	0.43
7:E:55:ARG:HA	7:E:58:MET:HG3	2.01	0.43
4:A:298:PHE:HE1	4:A:312:PRO:HB2	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:607:ILE:HA	4:A:612:ILE:HA	2.00	0.43
4:A:804:TYR:O	5:B:761:HIS:HD2	2.02	0.43
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.29	0.43
6:C:88:CYS:HB3	6:C:92:CYS:HB3	2.01	0.43
4:A:122:MET:HE1	4:A:138:ILE:HG12	1.99	0.43
4:A:531:ILE:CD1	4:A:649:ILE:HD11	2.49	0.43
4:A:836:TYR:OH	4:A:1403:GLU:OE2	2.27	0.43
5:B:34:ILE:HG12	5:B:542:MET:HE3	2.01	0.43
5:B:954:VAL:N	13:L:56:LEU:O	2.44	0.43
5:B:221:ASN:OD1	5:B:243:ALA:N	2.35	0.43
5:B:1213:THR:OG1	5:B:1215:ARG:NH2	2.52	0.43
6:C:260:LEU:O	6:C:264:GLN:NE2	2.51	0.43
4:A:246:VAL:O	4:A:328:ARG:NH1	2.41	0.43
4:A:494:SER:OG	5:B:1149:GLU:OE2	2.32	0.43
4:A:1445:ILE:H	4:A:1445:ILE:HG13	1.68	0.43
7:E:201:LYS:H	7:E:201:LYS:HG3	1.63	0.43
13:L:31:CYS:SG	13:L:32:ALA:N	2.91	0.43
4:A:122:MET:O	4:A:126:LEU:HG	2.19	0.43
4:A:184:SER:O	4:A:199:LEU:N	2.52	0.43
8:F:85:MET:HG3	8:F:89:GLU:HG3	2.01	0.43
9:H:130:ARG:H	9:H:130:ARG:HD2	1.83	0.43
4:A:1068:ALA:O	4:A:1072:ILE:HG13	2.19	0.43
4:A:1112:LYS:HE3	4:A:1112:LYS:HB3	1.83	0.43
4:A:1386:ARG:HD3	4:A:1403:GLU:OE1	2.19	0.43
7:E:101:GLN:HB2	7:E:127:ILE:HG12	1.99	0.43
3:N:13:DG:H2''	3:N:14:DA:H5''	2.00	0.42
4:A:53:LEU:O	4:A:55:ASP:N	2.46	0.42
4:A:451:HIS:HB3	4:A:453:MET:N	2.34	0.42
5:B:28:GLU:OE1	5:B:807:ARG:NH2	2.34	0.42
5:B:102:VAL:HG13	5:B:112:LEU:HB2	2.00	0.42
4:A:399:HIS:CD2	4:A:400:PRO:HA	2.54	0.42
8:F:128:LYS:NZ	8:F:149:GLU:O	2.44	0.42
4:A:67:CYS:HB3	4:A:70:CYS:HB3	2.01	0.42
4:A:335:ARG:NH1	5:B:1206:GLU:OE2	2.52	0.42
4:A:1303:GLU:OE2	4:A:1326:ARG:NH1	2.43	0.42
7:E:162:ARG:HE	7:E:162:ARG:HB2	1.62	0.42
7:E:196:VAL:HG23	7:E:198:ILE:HD11	2.01	0.42
4:A:456:MET:HB2	4:A:478:TYR:OH	2.19	0.42
4:A:1021:LEU:HD11	4:A:1025:ARG:NH1	2.33	0.42
5:B:653:VAL:O	5:B:654:ARG:HD3	2.19	0.42
6:C:7:GLN:HB2	6:C:23:SER:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:265:LYS:HG3	4:A:303:TYR:HB2	2.02	0.42
5:B:404:LYS:O	5:B:405:ARG:HD2	2.20	0.42
5:B:879:ARG:HD3	5:B:885:MET:HE2	2.01	0.42
6:C:114:TYR:CG	6:C:140:ASN:HB3	2.54	0.42
6:C:214:ASN:HB2	6:C:217:ASP:CG	2.39	0.42
5:B:288:ALA:HB1	5:B:331:LEU:HD23	2.02	0.42
5:B:649:LYS:NZ	5:B:738:PHE:O	2.35	0.42
5:B:806:THR:HG22	5:B:808:ALA:H	1.84	0.42
7:E:28:TYR:HE1	7:E:78:LEU:HG	1.85	0.42
7:E:133:GLU:HB3	7:E:135:PHE:HE1	1.84	0.42
9:H:9:ILE:O	9:H:31:THR:HG22	2.19	0.42
11:J:57:ILE:O	11:J:61:LEU:HG	2.19	0.42
4:A:152:VAL:O	4:A:162:VAL:N	2.53	0.42
4:A:555:ASP:OD1	4:A:644:LYS:HD2	2.19	0.42
4:A:951:GLU:O	4:A:954:TRP:NE1	2.42	0.42
4:A:1341:ILE:HG22	7:E:182:ASP:OD2	2.20	0.42
4:A:1390:ASN:O	4:A:1399:ARG:HG2	2.19	0.42
5:B:732:SER:HB3	5:B:734:HIS:CE1	2.55	0.42
5:B:1081:LEU:HD23	5:B:1081:LEU:HA	1.78	0.42
6:C:104:PHE:CD1	6:C:152:GLU:HB3	2.54	0.42
6:C:171:GLY:C	6:C:173:ALA:H	2.23	0.42
10:I:92:ARG:NH2	10:I:93:LYS:H	2.18	0.42
4:A:54:ASN:HB2	4:A:244:PRO:HG3	2.01	0.42
4:A:556:TRP:CZ3	4:A:558:GLY:HA2	2.55	0.42
4:A:1155:ASP:HB3	4:A:1241:ARG:NH2	2.34	0.42
4:A:1156:PRO:O	4:A:1158:PRO:HD3	2.19	0.42
4:A:1199:ARG:HG2	4:A:1236:LEU:HD23	2.02	0.42
4:A:1436:ILE:O	4:A:1440:ALA:N	2.52	0.42
5:B:493:SER:OG	5:B:497:ARG:NH2	2.51	0.42
5:B:1196:ILE:HD11	5:B:1201:LYS:HB2	2.02	0.42
4:A:289:ILE:N	4:A:289:ILE:CD1	2.83	0.42
4:A:449:SER:OG	5:B:1134:GLU:HG3	2.19	0.42
4:A:584:ASN:HA	4:A:610:GLY:HA3	2.00	0.42
4:A:1207:LEU:HD23	4:A:1207:LEU:HA	1.78	0.42
5:B:997:GLU:CD	6:C:39:ALA:HB2	2.40	0.42
9:H:142:LEU:HD22	9:H:144:ILE:HD12	2.01	0.42
4:A:110:CYS:HB3	4:A:167:CYS:HB2	2.02	0.42
4:A:569:LYS:NZ	6:C:222:LYS:HA	2.35	0.42
4:A:834:THR:HG21	4:A:1077:THR:HA	2.01	0.42
4:A:998:LEU:HD13	4:A:1001:ARG:HG3	2.01	0.42
4:A:1338:VAL:HG12	4:A:1339:LEU:HD23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:258:LEU:HB2	5:B:385:LEU:HD21	2.02	0.42
5:B:356:LEU:HD13	5:B:356:LEU:HA	1.88	0.42
6:C:5:GLY:O	6:C:7:GLN:NE2	2.47	0.42
4:A:472:LEU:HD13	5:B:835:GLN:HE22	1.80	0.41
4:A:553:VAL:HG13	4:A:648:ASN:HB3	2.02	0.41
4:A:683:ILE:HD13	4:A:683:ILE:HA	1.90	0.41
4:A:907:THR:HG22	4:A:908:LEU:H	1.85	0.41
4:A:1063:MET:HG3	4:A:1436:ILE:HG23	2.02	0.41
8:F:97:ARG:HA	8:F:97:ARG:HD2	1.68	0.41
4:A:266:LEU:CD1	4:A:303:TYR:CE1	3.03	0.41
4:A:1325:THR:O	7:E:148:GLU:HG3	2.20	0.41
4:A:1370:LEU:O	4:A:1374:VAL:HG23	2.21	0.41
8:F:82:THR:HG22	8:F:84:TYR:H	1.85	0.41
9:H:31:THR:C	9:H:33:GLN:H	2.22	0.41
9:H:110:ASP:C	9:H:128:ASN:HD22	2.23	0.41
2:T:17:DG:C6	2:T:18:DA:C2	3.08	0.41
4:A:40:THR:HA	4:A:53:LEU:HD23	2.00	0.41
4:A:259:GLU:OE1	4:A:260:ASP:N	2.45	0.41
4:A:587:HIS:HA	4:A:607:ILE:O	2.20	0.41
4:A:758:ILE:O	4:A:762:SER:OG	2.34	0.41
7:E:185:ALA:HA	7:E:190:LEU:HD23	2.02	0.41
2:T:27:DA:H5''	2:T:27:DA:H8	1.84	0.41
4:A:31:SER:HG	4:A:83:HIS:HD1	1.67	0.41
4:A:697:ALA:HA	4:A:702:LEU:HD23	2.02	0.41
4:A:744:LYS:HE3	4:A:748:MET:HE3	2.01	0.41
5:B:244:LEU:HD12	5:B:244:LEU:H	1.85	0.41
5:B:361:LEU:N	5:B:362:PRO:HD3	2.36	0.41
10:I:68:LEU:HA	10:I:69:PRO:HD3	1.89	0.41
4:A:1208:THR:OG1	4:A:1211:GLN:HG3	2.20	0.41
5:B:309:GLN:OE1	5:B:392:ARG:NH2	2.53	0.41
5:B:408:LEU:HD12	5:B:408:LEU:HA	1.70	0.41
5:B:484:ASN:OD1	5:B:490:SER:HB2	2.21	0.41
5:B:488:TYR:HE2	5:B:813:LYS:HB2	1.85	0.41
5:B:743:ILE:H	5:B:743:ILE:HG12	1.71	0.41
6:C:174:ALA:HB3	6:C:233:GLU:O	2.20	0.41
4:A:1352:VAL:O	4:A:1355:VAL:HG22	2.20	0.41
5:B:357:GLN:HA	5:B:374:LYS:NZ	2.36	0.41
5:B:783:THR:HG1	5:B:783:THR:H	1.64	0.41
5:B:883:LEU:HD12	5:B:884:ARG:H	1.84	0.41
6:C:55:THR:OG1	6:C:152:GLU:N	2.40	0.41
9:H:40:LEU:HD13	9:H:123:MET:HE3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:5:A:H2'	1:R:6:G:H8	1.85	0.41
4:A:890:ASP:OD2	4:A:940:ARG:NH1	2.54	0.41
5:B:210:LYS:HE2	5:B:462:ALA:HA	2.02	0.41
7:E:78:LEU:HD22	7:E:79:TRP:N	2.35	0.41
9:H:26:ILE:HD12	9:H:26:ILE:HA	1.86	0.41
10:I:29:CYS:SG	10:I:31:THR:OG1	2.67	0.41
2:T:17:DG:C6	2:T:18:DA:H2	2.38	0.41
4:A:304:MET:SD	5:B:1210:MET:HG3	2.60	0.41
4:A:396:PRO:HB3	4:A:403:LYS:HG2	2.02	0.41
4:A:406:ILE:HB	4:A:431:LYS:HB2	2.03	0.41
4:A:779:PHE:CE1	4:A:785:PRO:HD3	2.56	0.41
5:B:635:ARG:NH1	5:B:742:GLU:OE2	2.46	0.41
5:B:702:LEU:HD12	5:B:702:LEU:HA	1.94	0.41
12:K:7:PHE:HA	12:K:10:PHE:CE2	2.56	0.41
4:A:573:SER:O	4:A:577:ILE:HG22	2.21	0.41
4:A:676:MET:O	4:A:680:THR:HG22	2.21	0.41
4:A:714:PHE:O	4:A:718:VAL:HG23	2.20	0.41
5:B:280:ILE:HD13	5:B:280:ILE:HA	1.91	0.41
5:B:283:VAL:CG2	5:B:321:GLY:HA3	2.51	0.41
5:B:760:ASP:C	5:B:761:HIS:CG	2.92	0.41
5:B:918:ILE:HD13	5:B:935:ARG:HH11	1.84	0.41
7:E:94:LYS:HA	7:E:94:LYS:HD3	1.86	0.41
7:E:117:THR:HG23	7:E:120:ALA:H	1.86	0.41
8:F:101:ILE:HD13	8:F:120:ILE:CG2	2.49	0.41
10:I:47:GLU:OE1	10:I:50:THR:HG23	2.21	0.41
4:A:466:SER:HB3	5:B:1103:ILE:CD1	2.51	0.41
4:A:37:PHE:CD1	4:A:52:GLY:HA3	2.55	0.40
5:B:364:ILE:HD13	5:B:585:VAL:HG13	2.03	0.40
5:B:1106:ARG:NE	5:B:1109:GLY:H	2.19	0.40
7:E:41:ASP:OD1	7:E:41:ASP:N	2.53	0.40
11:J:5:VAL:HG12	11:J:6:ARG:HG2	2.02	0.40
4:A:270:LEU:HD23	4:A:270:LEU:HA	1.96	0.40
4:A:913:LEU:HD22	4:A:915:SER:H	1.85	0.40
4:A:1206:ASP:O	4:A:1274:ARG:NH1	2.51	0.40
5:B:384:ARG:HA	5:B:384:ARG:HD2	1.92	0.40
5:B:1212:ILE:O	5:B:1214:PRO:HD3	2.22	0.40
4:A:392:VAL:CG1	4:A:424:ILE:HG12	2.51	0.40
4:A:453:MET:HE2	4:A:453:MET:HB2	1.92	0.40
4:A:575:LYS:HB3	4:A:612:ILE:HD11	2.04	0.40
5:B:807:ARG:HA	5:B:807:ARG:HD2	1.92	0.40
7:E:48:ASP:N	7:E:52:ARG:O	2.40	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:123:LYS:HA	8:F:123:LYS:HD3	1.80	0.40
11:J:48:ARG:H	11:J:48:ARG:HG3	1.76	0.40
2:T:16:DT:C2'	2:T:17:DG:C2	3.04	0.40
4:A:598:LEU:HA	4:A:598:LEU:HD23	1.84	0.40
4:A:1100:ARG:O	4:A:1104:ILE:HG13	2.22	0.40
5:B:1073:TYR:CE2	5:B:1080:LYS:HG2	2.56	0.40
6:C:167:HIS:CD2	13:L:70:ARG:HB3	2.56	0.40
8:F:103:MET:O	8:F:105:ALA:N	2.54	0.40
3:N:9:DC:C4	3:N:10:DA:C6	3.10	0.40
4:A:903:ASN:OD1	4:A:905:ASP:N	2.51	0.40
5:B:228:LYS:HA	5:B:228:LYS:HD2	1.86	0.40
7:E:98:ILE:O	7:E:102:GLU:HG3	2.22	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	
4	A	1370/1733 (79%)	1287 (94%)	83 (6%)	0	100	100
5	B	1105/1224 (90%)	1050 (95%)	55 (5%)	0	100	100
6	C	265/318 (83%)	254 (96%)	10 (4%)	1 (0%)	34	67
7	E	210/215 (98%)	200 (95%)	9 (4%)	1 (0%)	29	61
8	F	84/155 (54%)	80 (95%)	4 (5%)	0	100	100
9	H	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
10	I	116/122 (95%)	112 (97%)	4 (3%)	0	100	100
11	J	63/70 (90%)	61 (97%)	2 (3%)	0	100	100
12	K	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
13	L	41/70 (59%)	41 (100%)	0	0	100	100
All	All	3495/4173 (84%)	3313 (95%)	180 (5%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	E	114	ASN
6	C	173	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	1194/1520 (79%)	1147 (96%)	47 (4%)	32	61
5	B	956/1061 (90%)	930 (97%)	26 (3%)	44	70
6	C	235/274 (86%)	230 (98%)	5 (2%)	53	76
7	E	193/197 (98%)	185 (96%)	8 (4%)	30	59
8	F	73/137 (53%)	69 (94%)	4 (6%)	21	51
9	H	116/128 (91%)	108 (93%)	8 (7%)	15	45
10	I	110/116 (95%)	106 (96%)	4 (4%)	35	63
11	J	60/65 (92%)	59 (98%)	1 (2%)	60	80
12	K	99/102 (97%)	97 (98%)	2 (2%)	55	77
13	L	37/57 (65%)	34 (92%)	3 (8%)	11	38
All	All	3073/3657 (84%)	2965 (96%)	108 (4%)	36	65

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	22	PHE
4	A	36	ARG
4	A	68	GLN
4	A	83	HIS
4	A	113	LEU
4	A	167	CYS
4	A	185	TRP
4	A	261	ASP
4	A	265	LYS
4	A	270	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	290	GLU
4	A	323	LYS
4	A	337	ARG
4	A	356	ASP
4	A	383	TYR
4	A	412	ARG
4	A	419	LYS
4	A	446	ARG
4	A	455	MET
4	A	470	LEU
4	A	515	GLN
4	A	517	ASN
4	A	547	LEU
4	A	551	TYR
4	A	584	ASN
4	A	598	LEU
4	A	618	GLU
4	A	629	LEU
4	A	688	LYS
4	A	764	CYS
4	A	782	ARG
4	A	821	ARG
4	A	905	ASP
4	A	979	SER
4	A	984	LYS
4	A	992	ASP
4	A	1025	ARG
4	A	1030	ARG
4	A	1100	ARG
4	A	1206	ASP
4	A	1215	ARG
4	A	1217	LYS
4	A	1257	ASP
4	A	1309	ASP
4	A	1315	GLU
4	A	1366	ARG
4	A	1399	ARG
5	B	46	GLN
5	B	110	HIS
5	B	133	LYS
5	B	215	GLN
5	B	217	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	241	ARG
5	B	325	GLN
5	B	333	PHE
5	B	384	ARG
5	B	396	ASP
5	B	404	LYS
5	B	437	GLU
5	B	546	SER
5	B	568	ASP
5	B	629	ASP
5	B	642	ASP
5	B	651	LEU
5	B	853	SER
5	B	931	TYR
5	B	951	GLN
5	B	996	ARG
5	B	999	MET
5	B	1072	MET
5	B	1195	HIS
5	B	1202	LEU
5	B	1210	MET
6	C	34	ARG
6	C	92	CYS
6	C	94	LYS
6	C	187	LYS
6	C	264	GLN
7	E	29	PHE
7	E	48	ASP
7	E	52	ARG
7	E	101	GLN
7	E	110	PHE
7	E	114	ASN
7	E	123	LEU
7	E	192	ARG
8	F	90	ARG
8	F	111	LEU
8	F	114	GLU
8	F	123	LYS
9	H	36	CYS
9	H	38	LEU
9	H	89	LEU
9	H	94	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	H	110	ASP
9	H	111	LEU
9	H	130	ARG
9	H	131	ASN
10	I	4	PHE
10	I	7	CYS
10	I	8	ARG
10	I	44	TYR
11	J	7	CYS
12	K	54	ARG
12	K	81	TYR
13	L	31	CYS
13	L	51	CYS
13	L	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	297	GLN
4	A	1140	HIS
5	B	103	ASN
5	B	761	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	9	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 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
15	5N0	T	101	-	93,107,107	2.34	32 (34%)	94,153,153	1.47	11 (11%)

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
15	5N0	T	101	-	-	8/51/92/92	0/9/9/9

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	101	5N0	C49-N23	6.35	1.47	1.33
15	T	101	5N0	C22-N10	6.31	1.47	1.33
15	T	101	5N0	C56-N25	6.25	1.47	1.33
15	T	101	5N0	C26-N14	5.16	1.47	1.35
15	T	101	5N0	C5-N3	4.81	1.48	1.35
15	T	101	5N0	C43-N21	4.51	1.47	1.35
15	T	101	5N0	C10-N6	4.44	1.47	1.35
15	T	101	5N0	C31-N17	4.36	1.47	1.35
15	T	101	5N0	C30-C31	4.33	1.56	1.53
15	T	101	5N0	C16-N8	4.28	1.47	1.35
15	T	101	5N0	C37-N19	4.25	1.47	1.35
15	T	101	5N0	C6-C10	4.18	1.56	1.53
15	T	101	5N0	C4-C5	4.06	1.56	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	101	5N0	C9-N3	3.70	1.48	1.40
15	T	101	5N0	C21-N8	3.36	1.48	1.41
15	T	101	5N0	C36-N17	3.35	1.48	1.41
15	T	101	5N0	C14-N6	3.32	1.48	1.41
15	T	101	5N0	C42-N19	3.23	1.48	1.41
15	T	101	5N0	C48-N21	3.19	1.48	1.41
15	T	101	5N0	C29-N14	2.93	1.46	1.40
15	T	101	5N0	C59-C63	2.64	1.55	1.49
15	T	101	5N0	C2-N1	-2.63	1.33	1.37
15	T	101	5N0	C57-C56	2.63	1.55	1.50
15	T	101	5N0	O5-C26	-2.24	1.18	1.23
15	T	101	5N0	O9-C49	-2.16	1.18	1.23
15	T	101	5N0	O8-C43	-2.16	1.18	1.23
15	T	101	5N0	C30-N15	-2.06	1.31	1.34
15	T	101	5N0	O10-C56	-2.06	1.19	1.23
15	T	101	5N0	O7-C37	-2.06	1.19	1.23
15	T	101	5N0	O1-C5	-2.05	1.19	1.23
15	T	101	5N0	O6-C31	-2.03	1.19	1.23
15	T	101	5N0	O2-C10	-2.01	1.19	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	101	5N0	C4-C5-N3	6.51	120.76	113.69
15	T	101	5N0	C6-C10-N6	5.26	119.40	113.69
15	T	101	5N0	C19-N9-C17	3.26	112.11	108.65
15	T	101	5N0	C24-C25-C26	-3.08	104.17	110.85
15	T	101	5N0	C30-C31-N17	2.51	116.41	113.69
15	T	101	5N0	O9-C49-N23	-2.34	117.95	122.61
15	T	101	5N0	O11-C63-C59	2.15	120.42	114.85
15	T	101	5N0	C3-N2-C4	2.09	109.12	104.01
15	T	101	5N0	C42-N19-C37	-2.06	121.23	126.58
15	T	101	5N0	C48-N21-C43	-2.02	121.33	126.58
15	T	101	5N0	O4-C22-N10	-2.01	118.61	122.61

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	101	5N0	C23-C24-C25-N11
15	T	101	5N0	C23-C24-C25-C26
15	T	101	5N0	C58-C59-C63-O12

Continued on next page...

Continued from previous page...

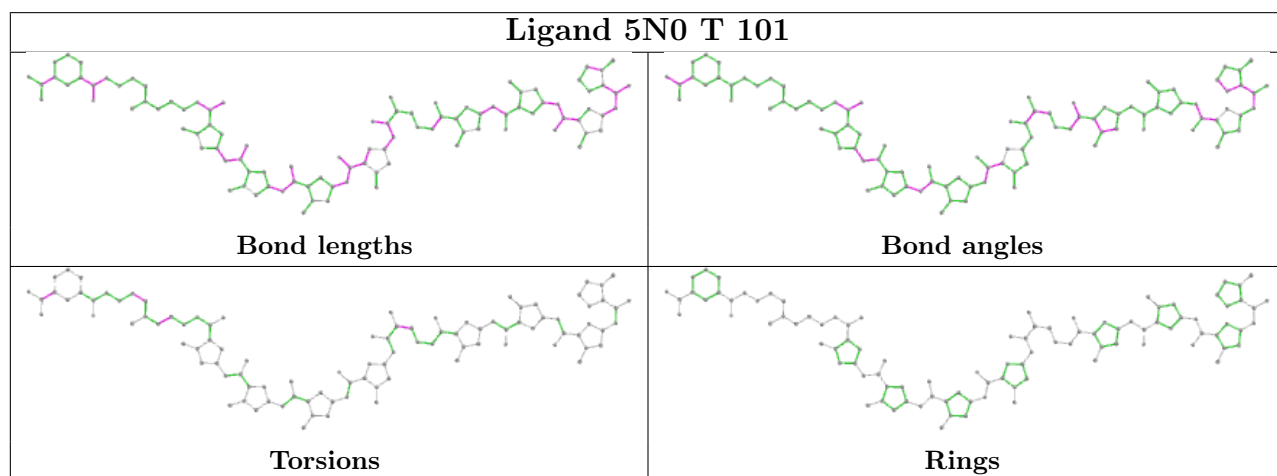
Mol	Chain	Res	Type	Atoms
15	T	101	5N0	C60-C59-C63-O11
15	T	101	5N0	C60-C59-C63-O12
15	T	101	5N0	C58-C59-C63-O11
15	T	101	5N0	C50-C51-C52-N24
15	T	101	5N0	N24-C53-C54-C55

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	101	5N0	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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	R	10/10 (100%)	-0.22	0 100 100	88, 106, 162, 167	0
2	T	26/30 (86%)	-0.19	0 100 100	85, 221, 326, 353	0
3	N	14/20 (70%)	-0.16	0 100 100	216, 233, 327, 332	0
4	A	1384/1733 (79%)	-0.06	25 (1%) 68 67	45, 92, 164, 197	0
5	B	1125/1224 (91%)	-0.08	7 (0%) 89 89	42, 76, 133, 172	0
6	C	267/318 (83%)	-0.25	0 100 100	51, 81, 113, 144	0
7	E	212/215 (98%)	0.05	9 (4%) 36 35	70, 126, 177, 186	0
8	F	86/155 (55%)	-0.30	2 (2%) 60 59	64, 94, 133, 173	0
9	H	133/146 (91%)	0.28	6 (4%) 33 33	85, 121, 157, 189	0
10	I	118/122 (96%)	-0.20	0 100 100	58, 96, 123, 147	0
11	J	65/70 (92%)	-0.29	0 100 100	49, 70, 104, 119	0
12	K	114/120 (95%)	-0.18	0 100 100	57, 85, 114, 130	0
13	L	43/70 (61%)	0.44	4 (9%) 8 10	60, 136, 178, 187	0
All	All	3597/4233 (84%)	-0.07	53 (1%) 73 72	42, 89, 160, 353	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	144	THR	4.7
4	A	114	LEU	4.7
7	E	83	CYS	4.5
13	L	45	ALA	4.4
4	A	103	CYS	4.3
7	E	93	MET	4.1
7	E	110	PHE	3.9
4	A	65	LEU	3.6
9	H	139	ASN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	B	106	ASP	3.4
4	A	111	GLY	3.3
5	B	869	SER	3.2
4	A	108	MET	3.2
7	E	121	MET	3.1
9	H	86	ASP	3.1
7	E	118	PRO	3.1
9	H	83	GLN	3.0
9	H	51	ALA	3.0
4	A	182	VAL	3.0
7	E	128	PRO	2.9
7	E	123	LEU	2.9
4	A	200	ARG	2.8
4	A	201	VAL	2.8
4	A	150	THR	2.8
4	A	69	THR	2.8
4	A	163	SER	2.7
4	A	286	HIS	2.5
4	A	62	ASP	2.5
7	E	122	LYS	2.4
8	F	104	ASN	2.4
9	H	130	ARG	2.4
5	B	92	PHE	2.3
7	E	82	PHE	2.3
13	L	46	VAL	2.3
4	A	105	CYS	2.3
8	F	69	LEU	2.3
4	A	141	LEU	2.2
5	B	475	SER	2.2
4	A	183	GLY	2.2
4	A	323	LYS	2.2
5	B	666	TYR	2.1
4	A	161	LEU	2.1
4	A	199	LEU	2.1
9	H	133	ASN	2.1
5	B	508	LEU	2.1
13	L	36	SER	2.1
4	A	66	LYS	2.1
4	A	181	LEU	2.1
4	A	1192	LEU	2.1
4	A	1126	ALA	2.1
4	A	142	CYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	L	66	GLN	2.1
5	B	248	SER	2.0

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

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

6.3 Carbohydrates [i](#)

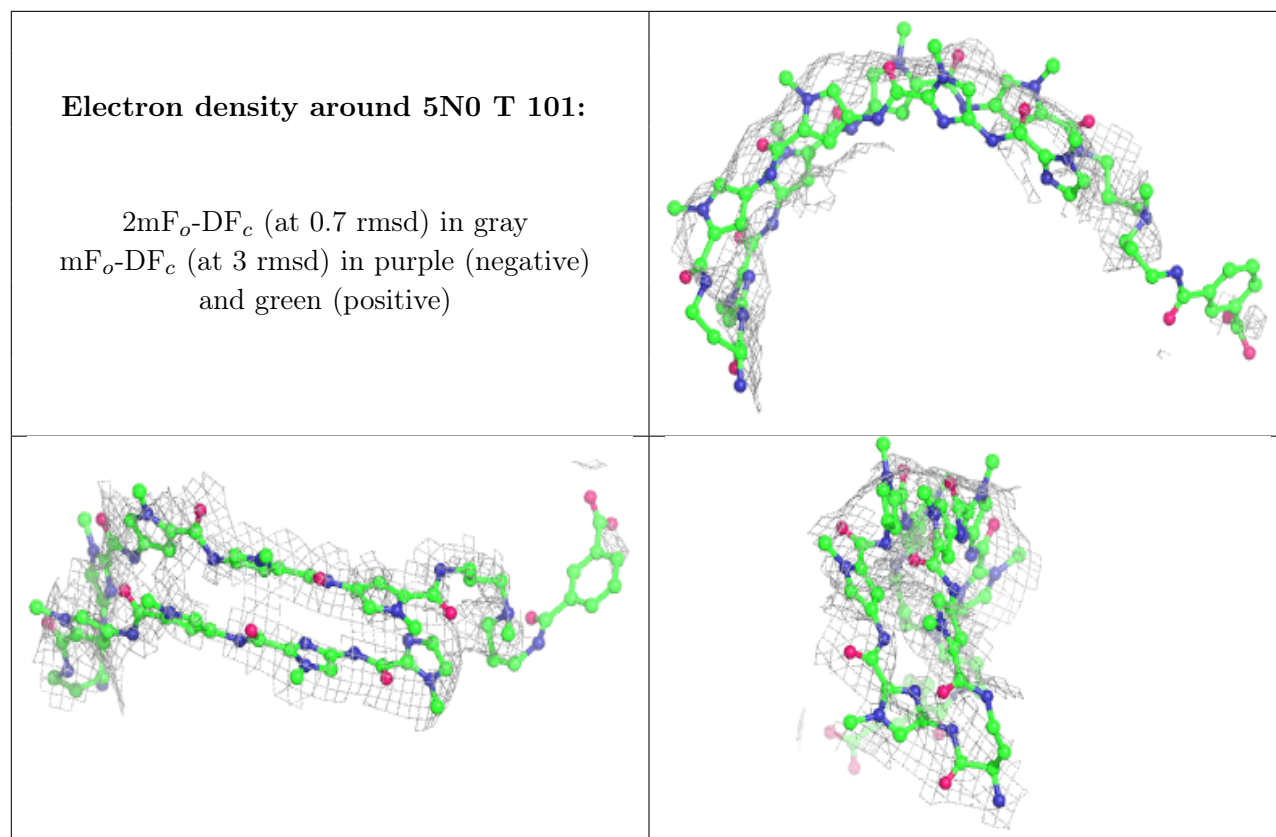
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
15	5N0	T	101	99/99	0.81	0.35	192,229,259,262	0
16	ZN	A	1801	1/1	0.86	0.10	206,206,206,206	0
16	ZN	B	1301	1/1	0.88	0.09	164,164,164,164	0
14	MG	R	2001	1/1	0.96	0.08	111,111,111,111	0
16	ZN	I	201	1/1	0.96	0.12	97,97,97,97	0
16	ZN	A	1802	1/1	0.97	0.10	132,132,132,132	0
16	ZN	L	101	1/1	0.97	0.04	153,153,153,153	0
16	ZN	J	101	1/1	0.98	0.19	62,62,62,62	0
16	ZN	C	401	1/1	0.98	0.13	81,81,81,81	0
16	ZN	I	202	1/1	0.99	0.14	89,89,89,89	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 [i](#)

There are no such residues in this entry.