



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:03 PM UTC

PDB ID : 4A3J / pdb_00004a3j
Title : RNA Polymerase II initial transcribing complex with a 2nt DNA-RNA hybrid and soaked with GMPCPP
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
Resolution : 3.70 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

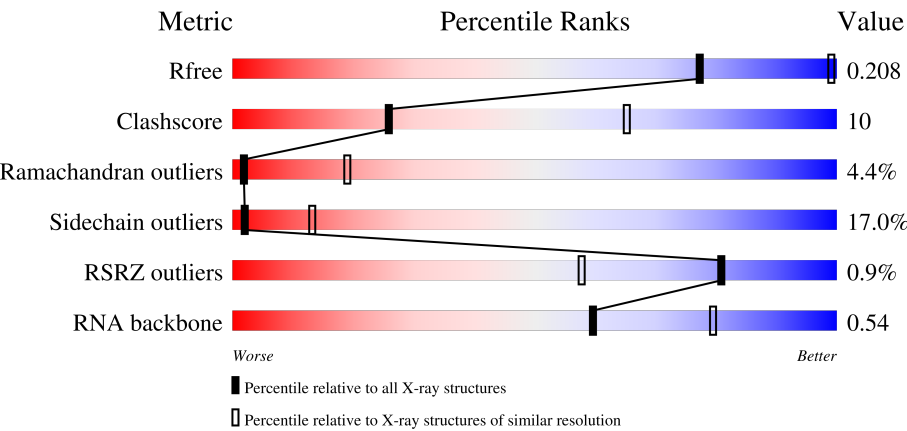
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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.



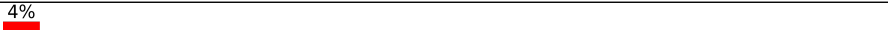
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1732	% 50% 24% 7% • 18%
2	B	1224	% 58% 26% 6% • 9%
3	C	318	49% 27% 6% • 16%
4	D	221	% 41% 30% 9% • 19%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	2	
15	T	27	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31802 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1425	Total	C	N	O	S	0	0	0
			11197	7051	1958	2126	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*GP*TP*AP*GP*AP*AP*AP*GP*CP*TP*AP*GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	9	Total	C	N	O	P	0	0	0
			184	89	37	50	8			

- Molecule 14 is a RNA chain called 5'-R(*CP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	2	Total	C	N	O	P	0	0	0
			42	19	8	13	2			

- Molecule 15 is a DNA chain called 5'-D(*AP*GP*CP*TP*AP*GP*CP*TP*TP*TP*CP*BRUP*AP*CP*CP*TP*GP*AP*AP*CP*AP*AP*CP*TP*AP*AP*CP)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	16	Total	Br	C	N	O	P	0	0	0
			325	1	155	57	96	16			

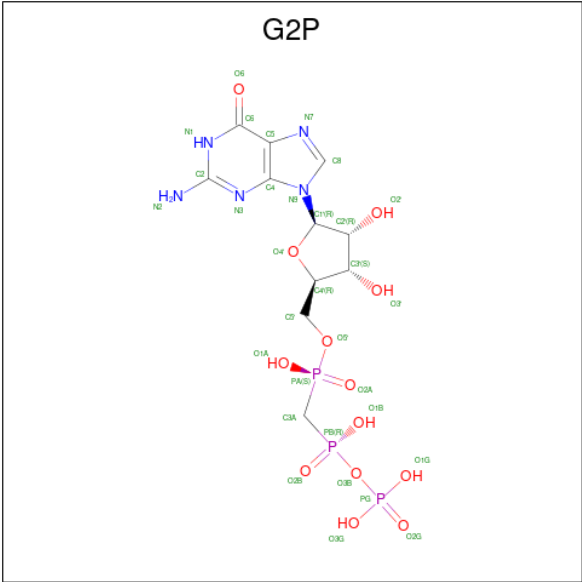
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

- Molecule 18 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃).

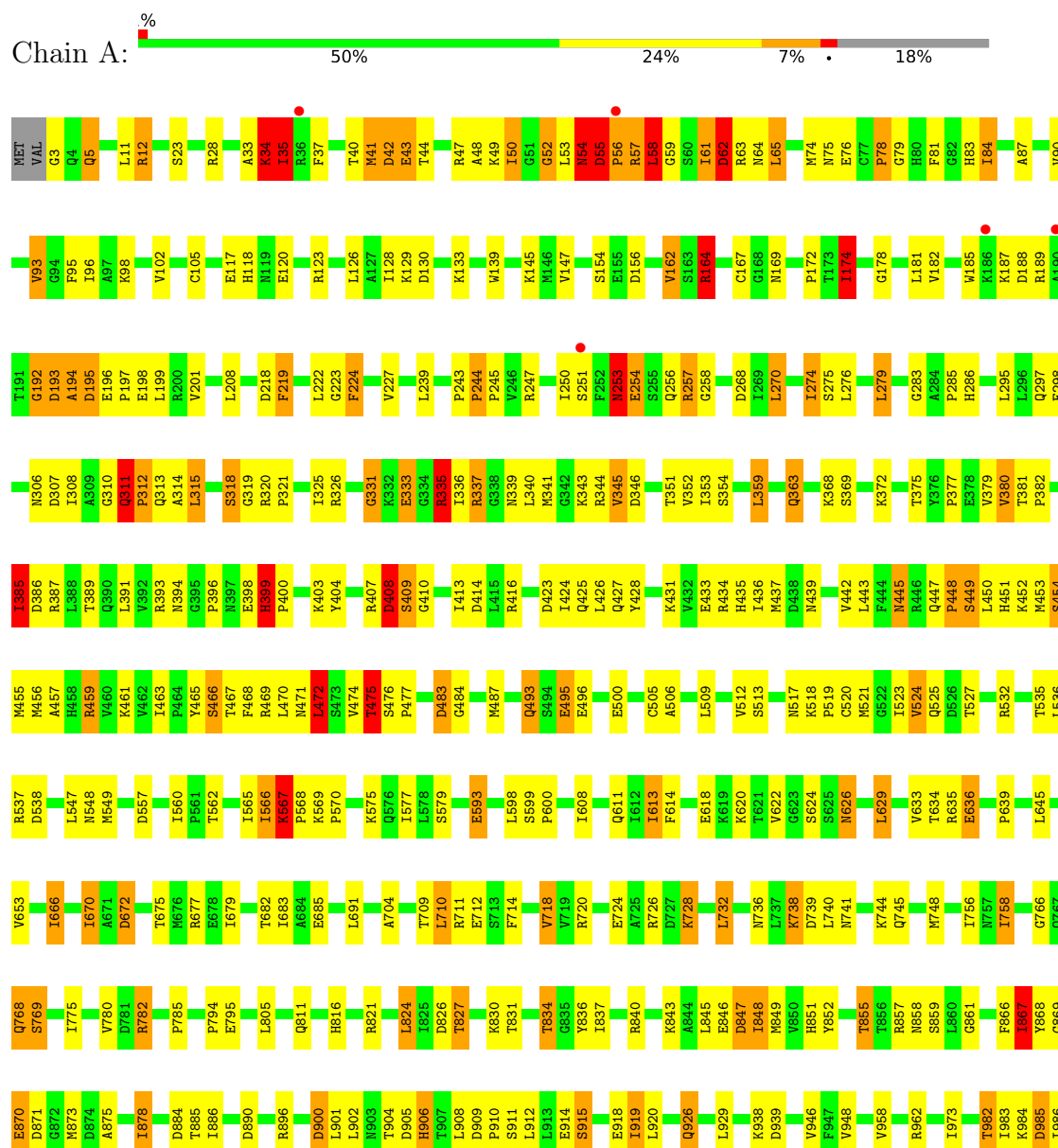


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	T	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

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: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1

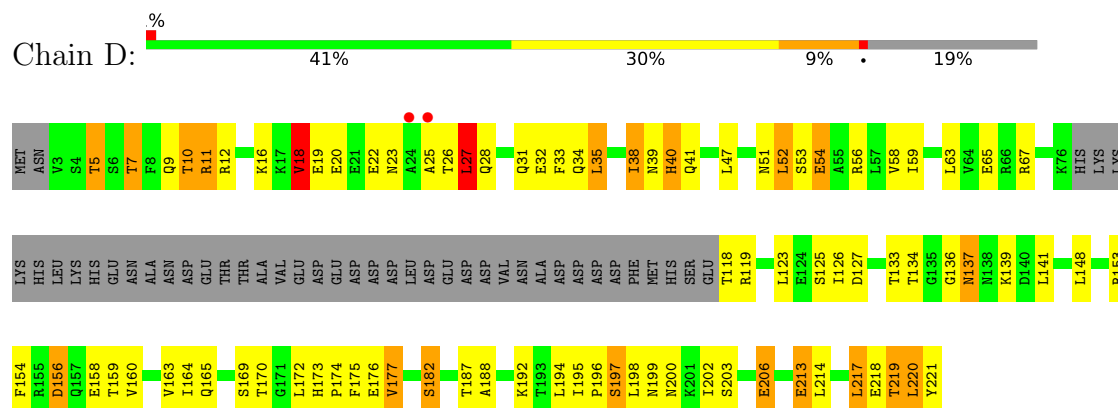




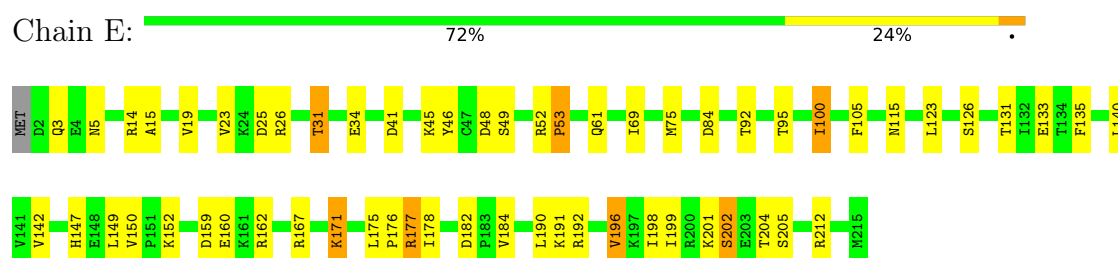
RET	GLU	ARG	MET
R261	SER	LYS	ARG
E262	GLY	TYR	LYS
G263	K164	GLU	TYR
S264		I90	GLU
			ALA
T268	I167		ASN
I269	G168	I95	SER
	R169	Y96	GLU
			LYS
T272	L170	P100	TYR
L273	P171	M101	TYR
	I172	V102	ASP
			GLU
L276			GLU
G277	N178	V108	ASP
G278		T109	PRO
D279	L181	H110	PRO
I280			TYR
G281	E186	A111	GLY
I282	S187	L112	PHE
	D188	T113	GLU
	L189	P114	
I291	Y190		GLU
		A117	D20
D294	E194	R118	E21
G295	C195		S22
E296	P196		I25
I297		N121	S35
L298	F197		
E299	D198	S126	R39
H300		G127	E40
		L128	F40
V305	I204	F129	K41
R306	L205	V130	
D307	G206	D131	
V308	N207		V44
Q309	G207		S45
M310	L212	K134	Q46
		ARG	Q47
E312	S213	THR	L48
M313	I222	TYR	
L314	V223	GLU	V55
K315		ALA	
P316	A229	ILE	T58
		ASP	
		VAL	I63
D320	A238		
G321	E239	PRO	L69
F322	I240	GLY	I70
V323		ARG	
I324	L244	GLU	LEU
		LEU	GLU
		LYS	GLN
R327	G247	TYR	ALA
		GLU	ALA
R336	F250	LEU	HIS
R337	I251	ILE	THR
G338		ALA	THR
T339	L254	GLU	THR
A340	Q255	GLU	SER
L341	V256	SER	ASP
G342	K257	GLU	ASP
	L258	ASP	ILE
I343	K344	SER	SER
K245	G259		



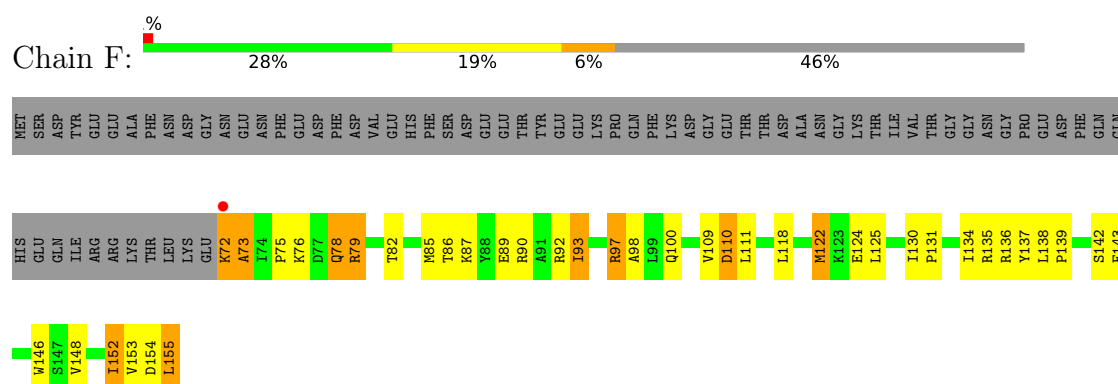
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4



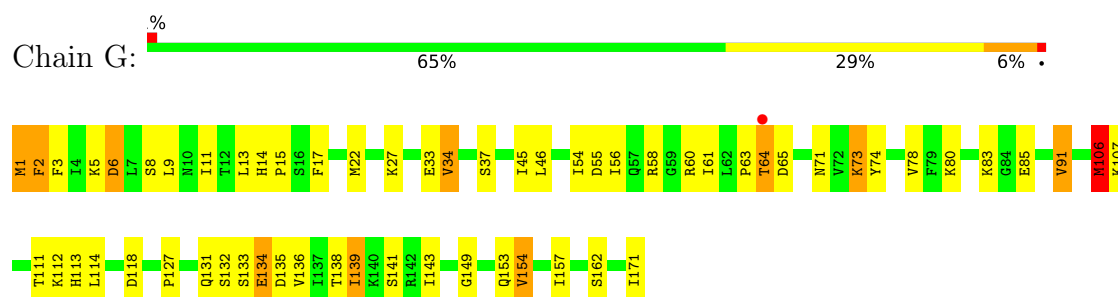
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

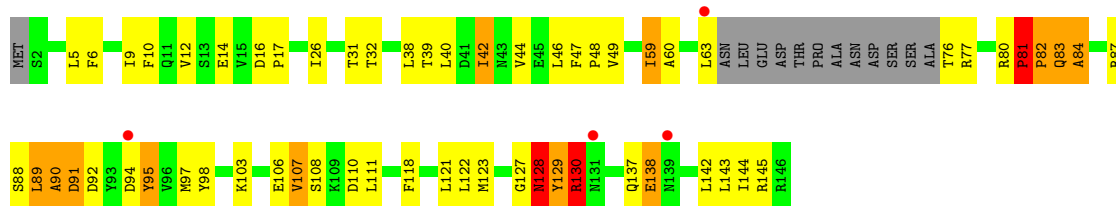


• Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7



• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3





• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9

Chain I: 75% 18% . . .



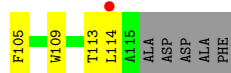
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J: 51% 23% 14% 7%



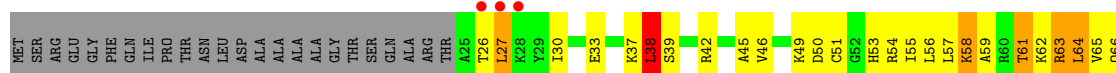
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11

Chain K: 64% 23% 8%



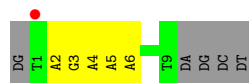
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L: 4% 26% 31% 7% 34%



• Molecule 13: 5'-D(*GP*TP*AP*GP*AP*AP*AP*GP*CP*TP*AP*GP*CP*TP)-3'

Chain N: 7% 29% 36% 36%



• Molecule 14: 5'-R(*CP*AP)-3'

Chain P:  50% 50%

 C9 A10

• Molecule 15: 5'-D(*AP*GP*CP*TP*AP*GP*CP*TP*TP*TP*CP*BRUP*AP*CP*CP *TP*GP*AP*AP*CP*AP*AP*CP*TP*AP*AP*CP)-3'

Chain T:  4% 52% 41%

 DA DG DC DT AB U15 A16 C17 A23 DA DA DC DT DA DA DC

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	223.29Å 392.79Å 282.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.70 50.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (50.00-3.70) 97.2 (50.00-3.70)	Depositor EDS
R_{merge}	0.65	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.67Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.157 , 0.194 0.180 , 0.208	Depositor DCC
R_{free} test set	2526 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	117.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 110.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.040 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.057 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31802	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BRU, G2P, ZN, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.92	9/11397 (0.1%)	1.61	165/15415 (1.1%)
2	B	0.88	0/9029	1.52	107/12171 (0.9%)
3	C	0.86	0/2133	1.49	22/2891 (0.8%)
4	D	0.89	1/1444 (0.1%)	1.67	27/1935 (1.4%)
5	E	0.82	0/1788	1.47	16/2406 (0.7%)
6	F	0.94	0/691	1.49	9/933 (1.0%)
7	G	0.87	1/1368 (0.1%)	1.41	14/1844 (0.8%)
8	H	0.90	1/1086 (0.1%)	1.53	17/1470 (1.2%)
9	I	0.82	0/989	1.41	8/1331 (0.6%)
10	J	0.85	0/541	1.61	10/727 (1.4%)
11	K	0.85	0/938	1.47	5/1267 (0.4%)
12	L	0.92	0/365	1.50	3/485 (0.6%)
13	N	0.59	0/207	0.70	0/318
14	P	1.12	1/46 (2.2%)	0.71	0/69
15	T	0.53	0/340	0.58	0/519
All	All	0.89	13/32362 (0.0%)	1.53	403/43781 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	ASN	CA-C	7.42	1.62	1.52
1	A	867	ILE	CG1-CD1	6.26	1.76	1.51
14	P	9	C	C1'-N1	6.12	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	C-N	6.09	1.42	1.33
1	A	56	PRO	CA-C	5.88	1.60	1.52
1	A	1454	MET	CA-C	5.66	1.59	1.52
4	D	18	VAL	CA-C	5.60	1.59	1.52
1	A	52	GLY	C-N	5.41	1.41	1.33
7	G	1	MET	C-N	5.41	1.41	1.33
1	A	1398	MET	SD-CE	5.37	1.93	1.79
1	A	452	LYS	CA-C	5.32	1.59	1.52
1	A	57	ARG	CA-C	5.31	1.59	1.52
8	H	16	ASP	CA-C	5.29	1.57	1.52

All (403) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	92	ASP	N-CA-C	-10.12	99.26	112.41
4	D	26	THR	N-CA-C	-9.67	98.22	111.56
1	A	42	ASP	CA-CB-CG	9.60	122.20	112.60
1	A	483	ASP	CA-CB-CG	9.15	121.75	112.60
2	B	1007	VAL	N-CA-CB	-9.06	105.58	111.83
1	A	34	LYS	CA-C-N	8.82	137.58	121.70
1	A	34	LYS	C-N-CA	8.82	137.58	121.70
1	A	886	ILE	N-CA-C	8.81	119.61	110.36
10	J	5	VAL	N-CA-C	-8.69	97.42	108.89
1	A	56	PRO	CA-C-N	8.54	137.85	121.54
1	A	56	PRO	C-N-CA	8.54	137.85	121.54
2	B	340	ALA	CA-C-N	8.52	137.81	121.54
2	B	340	ALA	C-N-CA	8.52	137.81	121.54
8	H	81	PRO	N-CA-C	8.46	121.03	110.70
2	B	881	ASN	CA-C-N	8.44	137.67	121.54
2	B	881	ASN	C-N-CA	8.44	137.67	121.54
1	A	341	MET	CA-C-N	8.13	127.87	121.61
1	A	341	MET	C-N-CA	8.13	127.87	121.61
8	H	129	TYR	N-CA-C	7.93	119.70	111.14
1	A	452	LYS	N-CA-C	-7.88	102.77	111.36
4	D	41	GLN	N-CA-C	-7.83	102.81	113.30
1	A	998	LEU	N-CA-C	7.82	122.19	109.76
2	B	296	GLU	N-CA-C	-7.76	101.67	112.45
1	A	218	ASP	CA-CB-CG	7.67	120.27	112.60
4	D	31	GLN	N-CA-C	-7.64	103.03	111.36
1	A	54	ASN	CA-CB-CG	7.49	120.08	112.60
2	B	881	ASN	N-CA-C	7.48	121.72	111.17
1	A	724	GLU	N-CA-C	-7.41	102.90	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	169	SER	CA-C-N	7.29	130.37	120.38
4	D	169	SER	C-N-CA	7.29	130.37	120.38
1	A	622	VAL	N-CA-CB	-7.24	103.92	112.39
1	A	57	ARG	CA-C-N	7.22	135.32	121.54
1	A	57	ARG	C-N-CA	7.22	135.32	121.54
1	A	194	ALA	CA-C-N	7.19	134.64	121.70
1	A	194	ALA	C-N-CA	7.19	134.64	121.70
2	B	41	LYS	N-CA-C	7.18	118.75	111.07
12	L	62	LYS	N-CA-C	-7.12	103.25	112.23
4	D	188	ALA	N-CA-C	-7.09	103.89	112.54
3	C	26	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	724	GLU	CA-C-N	7.07	129.97	120.65
1	A	724	GLU	C-N-CA	7.07	129.97	120.65
2	B	479	VAL	N-CA-C	-7.01	104.02	110.82
10	J	16	ASP	CA-CB-CG	7.01	119.61	112.60
2	B	943	SER	CA-C-N	6.99	129.64	120.28
2	B	943	SER	C-N-CA	6.99	129.64	120.28
1	A	5	GLN	N-CA-C	6.96	119.94	110.55
1	A	472	LEU	N-CA-C	6.95	119.70	111.71
1	A	445	ASN	CA-CB-CG	6.92	119.52	112.60
2	B	339	THR	CA-C-N	6.87	134.66	121.54
2	B	339	THR	C-N-CA	6.87	134.66	121.54
7	G	34	VAL	N-CA-C	6.84	116.99	110.42
5	E	126	SER	N-CA-C	6.79	118.68	111.28
7	G	33	GLU	CA-C-N	6.78	129.10	120.56
7	G	33	GLU	C-N-CA	6.78	129.10	120.56
2	B	1184	GLY	CA-C-N	6.75	134.43	121.54
2	B	1184	GLY	C-N-CA	6.75	134.43	121.54
1	A	223	GLY	CA-C-N	6.71	134.36	121.54
1	A	223	GLY	C-N-CA	6.71	134.36	121.54
6	F	154	ASP	CA-CB-CG	6.68	119.28	112.60
1	A	3	GLY	CA-C-N	6.66	130.29	120.90
1	A	3	GLY	C-N-CA	6.66	130.29	120.90
1	A	35	ILE	N-CA-CB	6.63	122.77	111.50
1	A	399	HIS	N-CA-CB	6.62	122.16	110.37
6	F	87	LYS	CA-C-N	6.62	129.44	120.44
6	F	87	LYS	C-N-CA	6.62	129.44	120.44
1	A	408	ASP	N-CA-C	-6.61	104.16	111.36
2	B	1006	ILE	N-CA-CB	6.61	117.92	110.72
1	A	34	LYS	N-CA-C	-6.61	97.51	108.34
4	D	31	GLN	CA-C-N	6.61	129.13	120.28
4	D	31	GLN	C-N-CA	6.61	129.13	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	213	PRO	N-CA-C	6.58	122.53	113.65
8	H	16	ASP	N-CA-C	6.54	121.31	107.91
8	H	138	GLU	N-CA-C	-6.52	104.25	111.36
9	I	93	LYS	CA-C-N	6.51	130.59	120.82
9	I	93	LYS	C-N-CA	6.51	130.59	120.82
6	F	72	LYS	CA-C-N	6.48	133.91	121.54
6	F	72	LYS	C-N-CA	6.48	133.91	121.54
2	B	276	ILE	CA-C-N	6.43	129.53	120.28
2	B	276	ILE	C-N-CA	6.43	129.53	120.28
1	A	890	ASP	CA-C-N	6.42	129.17	120.44
1	A	890	ASP	C-N-CA	6.42	129.17	120.44
1	A	54	ASN	CA-C-N	6.40	137.43	121.80
1	A	54	ASN	C-N-CA	6.40	137.43	121.80
5	E	171	LYS	N-CA-C	-6.39	99.88	110.17
3	C	136	ASP	CA-CB-CG	6.38	118.98	112.60
1	A	381	THR	CB-CA-C	6.36	118.45	108.84
2	B	489	SER	CA-C-N	6.35	129.08	120.38
2	B	489	SER	C-N-CA	6.35	129.08	120.38
2	B	1009	ASP	N-CA-C	-6.35	105.67	113.41
4	D	39	ASN	CA-CB-CG	6.34	118.94	112.60
2	B	1169	MET	CA-C-N	6.34	129.63	120.38
2	B	1169	MET	C-N-CA	6.34	129.63	120.38
3	C	183	TRP	N-CA-C	-6.32	96.80	107.99
1	A	311	GLN	N-CA-C	6.32	123.78	109.81
2	B	703	ILE	N-CA-C	6.32	117.39	108.36
1	A	244	PRO	N-CA-C	6.29	118.38	110.70
1	A	193	ASP	CA-C-N	6.28	133.00	121.70
1	A	193	ASP	C-N-CA	6.28	133.00	121.70
2	B	707	PRO	CA-C-N	6.27	130.23	120.82
2	B	707	PRO	C-N-CA	6.27	130.23	120.82
2	B	1013	ASN	N-CA-C	6.26	117.53	109.65
1	A	452	LYS	CA-C-N	6.26	133.78	121.58
1	A	452	LYS	C-N-CA	6.26	133.78	121.58
5	E	5	ASN	N-CA-C	-6.25	104.00	111.69
2	B	1130	PHE	N-CA-C	-6.18	100.34	109.11
4	D	18	VAL	CA-C-N	6.17	132.81	121.70
4	D	18	VAL	C-N-CA	6.17	132.81	121.70
1	A	219	PHE	CA-CB-CG	6.17	119.97	113.80
1	A	1436	ILE	N-CA-CB	-6.17	102.86	111.25
1	A	193	ASP	CA-CB-CG	6.14	118.75	112.60
1	A	535	THR	N-CA-C	6.14	119.81	112.93
2	B	55	VAL	CA-C-N	6.14	128.79	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	VAL	C-N-CA	6.14	128.79	120.38
3	C	121	VAL	CB-CA-C	6.12	117.55	110.88
2	B	879	ARG	CA-C-N	6.12	133.23	121.54
2	B	879	ARG	C-N-CA	6.12	133.23	121.54
1	A	794	PRO	CA-C-N	6.11	129.07	120.28
1	A	794	PRO	C-N-CA	6.11	129.07	120.28
1	A	346	ASP	CA-CB-CG	6.09	118.69	112.60
2	B	1155	SER	CA-C-N	6.07	133.13	121.54
2	B	1155	SER	C-N-CA	6.07	133.13	121.54
1	A	557	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	285	PRO	CA-C-N	6.07	133.13	121.54
1	A	285	PRO	C-N-CA	6.07	133.13	121.54
1	A	1419	ASP	CA-C-N	6.06	128.40	120.28
1	A	1419	ASP	C-N-CA	6.06	128.40	120.28
2	B	647	GLY	CA-C-N	6.05	131.30	121.74
2	B	647	GLY	C-N-CA	6.05	131.30	121.74
5	E	199	ILE	N-CA-C	6.05	115.44	106.85
5	E	196	VAL	N-CA-CB	6.05	119.48	111.25
3	C	39	ALA	N-CA-C	6.03	120.83	112.45
1	A	1226	VAL	N-CA-C	6.03	117.16	108.48
4	D	170	THR	N-CA-C	6.02	118.62	111.33
1	A	884	ASP	CA-C-N	6.01	128.66	120.54
1	A	884	ASP	C-N-CA	6.01	128.66	120.54
11	K	25	THR	CA-C-N	6.01	128.66	120.54
11	K	25	THR	C-N-CA	6.01	128.66	120.54
2	B	736	THR	N-CA-C	-5.99	104.49	112.94
4	D	219	THR	CA-C-N	5.99	132.98	121.54
4	D	219	THR	C-N-CA	5.99	132.98	121.54
2	B	694	ASP	CA-CB-CG	5.98	118.58	112.60
2	B	693	ILE	N-CA-C	5.97	116.21	107.37
10	J	18	TRP	N-CA-C	5.96	117.45	111.07
1	A	325	ILE	N-CA-C	-5.96	104.70	110.72
3	C	135	GLN	CA-C-N	5.96	129.57	120.82
3	C	135	GLN	C-N-CA	5.96	129.57	120.82
1	A	75	ASN	N-CA-C	-5.95	101.48	110.28
2	B	895	ASP	N-CA-C	5.94	119.35	111.75
2	B	916	THR	CB-CA-C	5.93	116.61	109.31
5	E	147	HIS	CA-C-N	5.93	130.61	121.19
5	E	147	HIS	C-N-CA	5.93	130.61	121.19
10	J	17	LYS	N-CA-C	5.93	119.61	112.38
2	B	343	ILE	CA-C-N	5.92	132.86	121.54
2	B	343	ILE	C-N-CA	5.92	132.86	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	49	LYS	CA-C-N	5.92	132.85	121.54
12	L	49	LYS	C-N-CA	5.92	132.85	121.54
7	G	6	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	1340	GLY	CA-C-N	5.91	132.60	121.97
1	A	1340	GLY	C-N-CA	5.91	132.60	121.97
1	A	423	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	1403	GLU	N-CA-C	5.90	123.38	110.80
1	A	636	GLU	CB-CG-CD	5.90	122.63	112.60
2	B	294	ASP	CA-CB-CG	5.90	118.50	112.60
2	B	190	TYR	CA-C-N	5.89	128.77	120.28
2	B	190	TYR	C-N-CA	5.89	128.77	120.28
3	C	56	THR	N-CA-C	5.89	117.66	110.41
1	A	718	VAL	CA-C-N	5.88	128.82	120.53
1	A	718	VAL	C-N-CA	5.88	128.82	120.53
1	A	1406	VAL	CA-C-N	5.87	128.14	120.28
1	A	1406	VAL	C-N-CA	5.87	128.14	120.28
2	B	222	ILE	N-CA-C	5.86	116.31	107.75
8	H	130	ARG	CA-C-N	5.84	128.11	120.28
8	H	130	ARG	C-N-CA	5.84	128.11	120.28
7	G	61	ILE	CA-C-N	5.84	128.59	120.65
7	G	61	ILE	C-N-CA	5.84	128.59	120.65
1	A	939	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	1231	ASP	CA-C-N	5.82	128.54	120.63
1	A	1231	ASP	C-N-CA	5.82	128.54	120.63
2	B	1125	ASP	CA-CB-CG	5.81	118.41	112.60
11	K	113	THR	CB-CA-C	5.81	120.30	111.76
1	A	985	ASP	CA-CB-CG	5.80	118.40	112.60
10	J	64	ASN	N-CA-C	5.79	122.61	109.81
1	A	758	ILE	CA-C-N	5.79	128.35	120.54
1	A	758	ILE	C-N-CA	5.79	128.35	120.54
2	B	433	GLN	CA-C-N	5.79	128.61	120.28
2	B	433	GLN	C-N-CA	5.79	128.61	120.28
1	A	93	VAL	N-CA-C	5.78	119.15	111.17
1	A	562	THR	CB-CA-C	5.78	118.69	109.62
1	A	1373	ASP	CA-C-N	5.78	127.84	120.56
1	A	1373	ASP	C-N-CA	5.78	127.84	120.56
2	B	188	ASP	CA-CB-CG	5.78	118.38	112.60
8	H	128	ASN	CA-C-N	5.77	128.29	120.44
8	H	128	ASN	C-N-CA	5.77	128.29	120.44
1	A	174	ILE	N-CA-C	5.77	117.06	109.21
1	A	1403	GLU	CA-C-N	-5.77	113.37	122.95
1	A	1403	GLU	C-N-CA	-5.77	113.37	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	710	LEU	N-CA-C	-5.75	104.91	111.07
1	A	858	ASN	CA-C-N	5.73	127.96	120.28
1	A	858	ASN	C-N-CA	5.73	127.96	120.28
1	A	993	LEU	CA-C-N	5.73	128.23	120.38
1	A	993	LEU	C-N-CA	5.73	128.23	120.38
1	A	399	HIS	CA-CB-CG	-5.72	108.08	113.80
1	A	495	GLU	CA-C-N	5.72	130.26	120.71
1	A	495	GLU	C-N-CA	5.72	130.26	120.71
11	K	2	ASN	CA-C-N	5.71	128.33	120.39
11	K	2	ASN	C-N-CA	5.71	128.33	120.39
2	B	198	ASP	CA-C-N	5.70	131.12	121.14
2	B	198	ASP	C-N-CA	5.70	131.12	121.14
1	A	78	PRO	N-CA-C	-5.70	103.25	111.22
1	A	345	VAL	N-CA-C	5.69	117.61	108.85
9	I	52	ILE	N-CA-CB	5.68	117.48	111.00
1	A	847	ASP	N-CA-C	5.68	119.69	112.87
2	B	681	TRP	N-CA-C	-5.66	104.50	111.40
1	A	35	ILE	CB-CA-C	5.63	122.87	111.60
1	A	1117	THR	CB-CA-C	5.62	120.83	111.51
2	B	516	ASN	CA-C-N	5.59	128.05	120.38
2	B	516	ASN	C-N-CA	5.59	128.05	120.38
2	B	629	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	466	SER	N-CA-C	5.59	121.08	113.37
2	B	364	ILE	N-CA-CB	5.58	120.44	111.23
1	A	399	HIS	N-CA-C	5.57	122.11	109.81
1	A	1325	THR	N-CA-C	-5.57	106.84	113.97
1	A	375	THR	N-CA-C	5.54	117.93	108.90
4	D	54	GLU	N-CA-C	-5.54	104.63	111.33
8	H	137	GLN	CA-C-N	5.54	128.15	120.29
8	H	137	GLN	C-N-CA	5.54	128.15	120.29
2	B	307	ASP	CA-C-N	5.53	127.95	120.38
2	B	307	ASP	C-N-CA	5.53	127.95	120.38
2	B	1065	GLN	CB-CA-C	5.53	118.55	110.26
2	B	1099	VAL	N-CA-CB	5.53	117.38	110.47
1	A	532	ARG	N-CA-C	-5.52	104.90	111.03
2	B	607	GLY	CA-C-N	5.52	128.43	120.38
2	B	607	GLY	C-N-CA	5.52	128.43	120.38
7	G	55	ASP	CA-CB-CG	5.51	118.11	112.60
7	G	63	PRO	CA-C-N	-5.51	112.73	122.26
7	G	63	PRO	C-N-CA	-5.51	112.73	122.26
2	B	186	GLU	CA-C-N	5.50	127.97	120.54
2	B	186	GLU	C-N-CA	5.50	127.97	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	56	ILE	N-CA-C	5.50	116.16	110.82
2	B	48	LEU	N-CA-C	5.50	117.08	111.14
7	G	141	SER	N-CA-C	5.48	117.36	110.24
9	I	83	ASN	CA-C-N	5.48	129.95	122.34
9	I	83	ASN	C-N-CA	5.48	129.95	122.34
2	B	964	VAL	N-CA-C	5.47	116.16	108.17
1	A	769	SER	N-CA-C	5.47	117.70	109.23
3	C	82	TYR	N-CA-C	-5.47	101.55	109.59
1	A	1344	GLY	CA-C-N	5.47	127.55	120.44
1	A	1344	GLY	C-N-CA	5.47	127.55	120.44
3	C	40	GLU	N-CA-C	5.46	120.05	113.17
1	A	319	GLY	CA-C-N	5.46	127.98	120.39
1	A	319	GLY	C-N-CA	5.46	127.98	120.39
1	A	1308	THR	CA-C-N	5.46	129.34	120.23
1	A	1308	THR	C-N-CA	5.46	129.34	120.23
5	E	160	GLU	CA-C-N	5.45	128.04	120.63
5	E	160	GLU	C-N-CA	5.45	128.04	120.63
1	A	728	LYS	CA-C-N	5.44	127.57	120.28
1	A	728	LYS	C-N-CA	5.44	127.57	120.28
2	B	1211	ASN	N-CA-C	5.44	119.50	112.86
6	F	89	GLU	CA-C-N	5.43	127.87	120.54
6	F	89	GLU	C-N-CA	5.43	127.87	120.54
2	B	650	GLU	CA-C-N	5.43	128.81	121.05
2	B	650	GLU	C-N-CA	5.43	128.81	121.05
4	D	25	ALA	CA-C-N	5.43	132.38	122.50
4	D	25	ALA	C-N-CA	5.43	132.38	122.50
8	H	10	PHE	CA-CB-CG	5.42	119.22	113.80
9	I	112	SER	N-CA-C	-5.41	106.26	112.92
10	J	52	THR	CB-CA-C	5.40	119.11	110.09
1	A	1424	VAL	CA-C-N	5.40	127.46	120.44
1	A	1424	VAL	C-N-CA	5.40	127.46	120.44
1	A	1360	GLY	CA-C-N	5.39	128.75	120.82
1	A	1360	GLY	C-N-CA	5.39	128.75	120.82
5	E	25	ASP	CA-CB-CG	5.38	117.98	112.60
8	H	111	LEU	N-CA-C	5.38	118.02	109.96
2	B	484	ASN	CA-CB-CG	5.37	117.97	112.60
4	D	156	ASP	N-CA-C	5.37	118.50	109.95
1	A	35	ILE	CA-C-N	5.36	131.90	122.42
1	A	35	ILE	C-N-CA	5.36	131.90	122.42
2	B	1140	ALA	CA-C-N	5.36	128.45	120.31
2	B	1140	ALA	C-N-CA	5.36	128.45	120.31
3	C	77	ILE	CA-C-N	5.35	127.45	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	77	ILE	C-N-CA	5.35	127.45	120.28
2	B	880	THR	CA-C-N	5.35	130.41	122.82
2	B	880	THR	C-N-CA	5.35	130.41	122.82
1	A	677	ARG	CA-C-N	5.34	127.43	120.28
1	A	677	ARG	C-N-CA	5.34	127.43	120.28
1	A	1376	THR	N-CA-C	5.34	116.79	110.97
2	B	568	ASP	CA-CB-CG	5.33	117.94	112.60
2	B	1156	ASP	N-CA-C	5.33	122.15	110.80
5	E	95	THR	CA-C-N	5.33	127.36	120.44
5	E	95	THR	C-N-CA	5.33	127.36	120.44
2	B	95	ILE	N-CA-CB	5.33	117.38	110.99
1	A	379	VAL	N-CA-CB	5.32	116.52	110.72
2	B	320	ASP	CA-CB-CG	5.32	117.92	112.60
10	J	9	SER	N-CA-C	5.32	116.76	111.07
6	F	122	MET	CA-C-N	5.31	127.34	120.44
6	F	122	MET	C-N-CA	5.31	127.34	120.44
1	A	1258	HIS	CA-C-N	5.30	127.38	120.28
1	A	1258	HIS	C-N-CA	5.30	127.38	120.28
1	A	484	GLY	CA-C-N	5.30	128.23	120.71
1	A	484	GLY	C-N-CA	5.30	128.23	120.71
1	A	557	ASP	N-CA-C	5.29	117.79	111.71
2	B	1133	MET	CA-C-N	5.29	127.80	120.29
2	B	1133	MET	C-N-CA	5.29	127.80	120.29
2	B	918	ILE	N-CA-C	5.29	115.47	107.75
1	A	1072	ILE	CA-C-N	5.29	125.81	119.94
1	A	1072	ILE	C-N-CA	5.29	125.81	119.94
1	A	47	ARG	CA-C-N	5.28	131.63	121.54
1	A	47	ARG	C-N-CA	5.28	131.63	121.54
1	A	672	ASP	CA-CB-CG	5.28	117.88	112.60
4	D	38	ILE	N-CA-C	5.28	115.58	107.77
2	B	222	ILE	CA-C-N	5.28	129.10	121.18
2	B	222	ILE	C-N-CA	5.28	129.10	121.18
2	B	327	ARG	CA-C-N	5.27	127.61	120.65
2	B	327	ARG	C-N-CA	5.27	127.61	120.65
1	A	1132	LYS	CA-C-N	5.27	127.29	120.44
1	A	1132	LYS	C-N-CA	5.27	127.29	120.44
1	A	192	GLY	CA-C-N	5.26	131.60	121.54
1	A	192	GLY	C-N-CA	5.26	131.60	121.54
10	J	8	PHE	CA-CB-CG	5.24	119.04	113.80
1	A	1373	ASP	CA-CB-CG	5.24	117.83	112.60
8	H	83	GLN	CA-C-N	5.23	131.54	121.54
8	H	83	GLN	C-N-CA	5.23	131.54	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	64	THR	CB-CA-C	5.23	118.75	109.65
1	A	475	THR	CB-CA-C	5.23	119.05	110.95
2	B	338	GLY	CA-C-N	5.23	131.11	121.70
2	B	338	GLY	C-N-CA	5.23	131.11	121.70
3	C	248	ILE	CA-C-N	5.23	127.28	120.28
3	C	248	ILE	C-N-CA	5.23	127.28	120.28
1	A	398	GLU	CB-CG-CD	5.23	121.48	112.60
1	A	626	ASN	N-CA-C	5.22	119.14	112.87
3	C	181	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	55	ASP	N-CA-CB	5.22	119.66	110.37
1	A	653	VAL	N-CA-CB	5.22	116.66	110.55
1	A	467	THR	CB-CA-C	-5.21	101.20	109.80
1	A	1414	ALA	N-CA-C	5.21	116.65	111.07
2	B	1011	ILE	N-CA-CB	5.21	119.83	111.23
1	A	938	LYS	CA-C-N	5.21	127.57	120.54
1	A	938	LYS	C-N-CA	5.21	127.57	120.54
1	A	333	GLU	CB-CG-CD	5.20	121.44	112.60
1	A	1029	ARG	CA-C-N	5.20	127.51	120.65
1	A	1029	ARG	C-N-CA	5.20	127.51	120.65
2	B	322	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	848	ILE	N-CA-CB	5.19	116.19	110.53
4	D	7	THR	CA-C-N	5.19	128.20	120.31
4	D	7	THR	C-N-CA	5.19	128.20	120.31
2	B	847	ASP	CA-CB-CG	5.18	117.78	112.60
10	J	2	ILE	N-CA-CB	5.18	119.78	111.23
2	B	69	LEU	N-CA-C	5.18	116.54	109.18
4	D	137	ASN	CA-CB-CG	5.17	117.77	112.60
2	B	945	GLU	N-CA-C	5.16	117.46	110.35
1	A	1222	ASN	CA-C-N	5.15	127.49	120.54
1	A	1222	ASN	C-N-CA	5.15	127.49	120.54
1	A	253	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	224	PHE	CA-CB-CG	-5.14	108.66	113.80
1	A	33	ALA	CA-C-N	5.14	130.02	122.77
1	A	33	ALA	C-N-CA	5.14	130.02	122.77
2	B	117	ALA	CA-C-N	5.14	127.12	120.44
2	B	117	ALA	C-N-CA	5.14	127.12	120.44
2	B	885	MET	N-CA-C	5.13	117.48	110.55
1	A	268	ASP	CA-CB-CG	5.13	117.73	112.60
7	G	153	GLN	N-CA-C	5.13	118.49	107.67
8	H	94	ASP	CA-CB-CG	5.13	117.73	112.60
2	B	222	ILE	CB-CA-C	5.12	118.05	110.77
2	B	628	THR	N-CA-C	-5.12	106.44	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	177	ARG	N-CA-C	5.12	117.84	109.59
5	E	123	LEU	CA-C-N	5.12	124.43	120.33
5	E	123	LEU	C-N-CA	5.12	124.43	120.33
2	B	828	ALA	CA-C-N	5.12	129.50	122.84
2	B	828	ALA	C-N-CA	5.12	129.50	122.84
2	B	947	GLY	N-CA-C	5.12	117.75	110.74
1	A	575	LYS	CA-C-N	5.11	127.44	120.54
1	A	575	LYS	C-N-CA	5.11	127.44	120.54
2	B	1156	ASP	CA-C-N	5.10	131.28	121.54
2	B	1156	ASP	C-N-CA	5.10	131.28	121.54
2	B	825	VAL	N-CA-C	5.10	115.25	108.11
3	C	140	ASN	CA-CB-CG	5.09	117.69	112.60
7	G	106	MET	N-CA-C	5.09	118.31	110.42
1	A	900	ASP	CA-CB-CG	5.08	117.68	112.60
3	C	62	PHE	CA-C-N	5.08	126.97	120.56
3	C	62	PHE	C-N-CA	5.08	126.97	120.56
1	A	1232	ASN	CA-C-N	5.08	128.32	121.05
1	A	1232	ASN	C-N-CA	5.08	128.32	121.05
2	B	902	GLY	CA-C-N	5.08	131.12	121.97
2	B	902	GLY	C-N-CA	5.08	131.12	121.97
3	C	231	ASN	CA-C-N	5.08	128.79	121.18
3	C	231	ASN	C-N-CA	5.08	128.79	121.18
10	J	60	PHE	CA-CB-CG	5.08	118.88	113.80
4	D	158	GLU	CA-C-N	5.06	127.33	120.65
4	D	158	GLU	C-N-CA	5.06	127.33	120.65
3	C	120	ILE	N-CA-CB	5.06	116.43	110.82
5	E	53	PRO	N-CA-C	5.05	118.42	110.80
1	A	1266	THR	N-CA-C	-5.05	105.78	111.28
9	I	94	ASP	CA-C-N	5.04	131.17	121.54
9	I	94	ASP	C-N-CA	5.04	131.17	121.54
1	A	331	GLY	CA-C-N	5.03	131.15	121.54
1	A	331	GLY	C-N-CA	5.03	131.15	121.54
1	A	310	GLY	CA-C-N	5.03	134.06	121.80
1	A	310	GLY	C-N-CA	5.03	134.06	121.80
1	A	1064	VAL	N-CA-C	5.02	119.06	112.04
4	D	33	PHE	CA-CB-CG	-5.01	108.78	113.80
8	H	59	ILE	CB-CA-C	5.01	119.51	111.29
4	D	136	GLY	CA-C-N	5.01	127.49	120.28
4	D	136	GLY	C-N-CA	5.01	127.49	120.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11197	0	11257	235	0
2	B	8859	0	8901	172	0
3	C	2095	0	2051	59	0
4	D	1434	0	1460	33	0
5	E	1752	0	1776	23	0
6	F	679	0	701	25	0
7	G	1340	0	1357	33	0
8	H	1068	0	1040	29	0
9	I	971	0	927	11	0
10	J	532	0	542	20	0
11	K	920	0	929	26	0
12	L	363	0	386	10	0
13	N	184	0	103	4	0
14	P	42	0	22	0	0
15	T	325	0	179	2	0
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
17	A	1	0	0	0	0
18	T	32	0	14	0	0
All	All	31802	0	31645	603	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 10.

All (603) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.76	1.62
1:A:53:LEU:HD23	1:A:54:ASN:H	1.12	1.15
1:A:855:THR:HG21	1:A:857:ARG:HE	1.23	1.01
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	2.04	0.93
1:A:55:ASP:HA	1:A:58:LEU:HB2	1.51	0.92
7:G:1:MET:HE1	7:G:80:LYS:O	1.72	0.88
2:B:986:GLN:HE22	2:B:1022:THR:HG21	1.36	0.87
3:C:148:ARG:H	3:C:151:GLN:HG3	1.40	0.86
1:A:53:LEU:HD23	1:A:54:ASN:N	1.91	0.86
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.60	0.82
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.42	0.82
12:L:61:THR:HG21	12:L:63:ARG:HE	1.43	0.82
3:C:147:LEU:HB3	3:C:151:GLN:HB2	1.61	0.81
3:C:66:ARG:NH2	10:J:3:VAL:O	2.15	0.79
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.64	0.79
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.64	0.78
2:B:338:GLY:HA2	2:B:339:THR:HB	1.65	0.77
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.66	0.77
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.65	0.76
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.50	0.76
5:E:19:VAL:O	5:E:23:VAL:HG23	1.86	0.76
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.68	0.75
10:J:48:ARG:O	10:J:52:THR:HG22	1.87	0.75
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.66	0.74
1:A:49:LYS:HD2	1:A:55:ASP:HB3	1.71	0.73
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.69	0.73
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.69	0.73
4:D:220:LEU:H	4:D:220:LEU:HD12	1.53	0.73
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.69	0.73
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.71	0.72
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.71	0.72
1:A:62:ASP:HB3	1:A:65:LEU:HB2	1.71	0.71
2:B:882:THR:HG1	2:B:935:ARG:N	1.88	0.71
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.72	0.71
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.89	0.71
1:A:1077:THR:HG22	1:A:1081:LEU:HD12	1.72	0.71
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.72	0.71
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.31	0.71
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.73	0.71
1:A:868:TYR:CD2	1:A:1058:VAL:HG11	2.26	0.70
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.27	0.70
2:B:313:MET:HE2	2:B:386:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.72	0.69
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.73	0.69
6:F:118:LEU:O	6:F:122:MET:HG3	1.94	0.68
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.76	0.68
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.74	0.68
8:H:127:GLY:HA3	8:H:130:ARG:HH21	1.58	0.68
1:A:41:MET:HB2	1:A:49:LYS:HA	1.76	0.67
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.76	0.67
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.76	0.66
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.78	0.66
1:A:866:PHE:O	1:A:867:ILE:HD12	1.96	0.66
1:A:1100:ARG:O	1:A:1104:ILE:HG13	1.96	0.66
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.10	0.65
4:D:40:HIS:ND1	7:G:6:ASP:HB3	2.12	0.65
8:H:82:PRO:C	8:H:84:ALA:H	2.02	0.65
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.76	0.65
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.79	0.64
2:B:542:MET:HB3	2:B:636:PRO:HD2	1.79	0.64
2:B:776:GLN:HA	2:B:1096:ARG:HH11	1.61	0.64
1:A:670:ILE:HG13	1:A:805:LEU:HD21	1.77	0.64
1:A:682:THR:HG23	1:A:728:LYS:HE3	1.79	0.64
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.80	0.64
1:A:1308:THR:HG22	1:A:1309:ASP:H	1.62	0.64
4:D:18:VAL:HG22	4:D:20:GLU:H	1.63	0.64
2:B:916:THR:HB	2:B:935:ARG:HG3	1.80	0.64
7:G:34:VAL:O	7:G:37:SER:HB3	1.98	0.63
3:C:148:ARG:N	3:C:151:GLN:HG3	2.13	0.63
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.79	0.63
1:A:870:GLU:O	5:E:205:SER:HB3	1.98	0.63
8:H:89:LEU:C	8:H:91:ASP:H	2.05	0.63
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.80	0.63
3:C:50:GLU:HB3	12:L:64:LEU:HD22	1.79	0.63
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.29	0.62
3:C:125:MET:SD	3:C:125:MET:N	2.73	0.62
8:H:47:PHE:HB3	8:H:95:TYR:CD2	2.35	0.62
1:A:855:THR:CG2	1:A:857:ARG:HE	2.07	0.62
1:A:54:ASN:HB3	1:A:247:ARG:HH12	1.64	0.62
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.80	0.62
4:D:35:LEU:HD11	4:D:173:HIS:HB3	1.82	0.62
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.35	0.61
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:HD3	2:B:1156:ASP:HB2	1.82	0.61
2:B:338:GLY:HA2	2:B:339:THR:CB	2.30	0.61
2:B:296:GLU:O	2:B:300:HIS:HD2	1.83	0.61
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.83	0.61
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.36	0.61
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.31	0.60
2:B:797:TYR:HB2	2:B:852:ARG:O	2.01	0.60
2:B:1006:ILE:HG23	10:J:43:ARG:HD2	1.83	0.60
3:C:98:VAL:H	3:C:122:SER:HB3	1.66	0.60
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.84	0.60
3:C:43:THR:HG22	3:C:44:LEU:H	1.64	0.60
1:A:672:ASP:HB2	1:A:736:ASN:ND2	2.17	0.60
1:A:855:THR:HG21	1:A:857:ARG:NE	2.05	0.60
9:I:72:ASP:O	9:I:81:ARG:HG2	2.01	0.60
1:A:824:LEU:HD11	2:B:765:PRO:HB3	1.84	0.60
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.67	0.60
3:C:46:ILE:HD13	3:C:67:LEU:O	2.02	0.60
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.84	0.59
3:C:142:VAL:HG22	10:J:15:GLY:HA3	1.84	0.59
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.84	0.59
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.83	0.59
1:A:1442:ASP:HB2	6:F:137:TYR:HE1	1.67	0.59
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.84	0.59
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.84	0.59
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.85	0.58
1:A:827:THR:O	1:A:831:THR:HB	2.03	0.58
7:G:8:SER:HB2	7:G:71:ASN:HD21	1.68	0.58
2:B:642:ASP:HA	2:B:649:LYS:HA	1.86	0.58
2:B:705:MET:H	2:B:710:LEU:HD12	1.68	0.58
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.86	0.58
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.86	0.58
3:C:3:GLU:HB3	3:C:7:GLN:HE22	1.69	0.58
1:A:194:ALA:HA	1:A:195:ASP:C	2.28	0.58
8:H:95:TYR:HE1	8:H:97:MET:HG3	1.67	0.58
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.86	0.57
10:J:48:ARG:HE	10:J:49:MET:HE2	1.69	0.57
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.04	0.57
2:B:620:ARG:HD2	9:I:62:ILE:HD11	1.85	0.57
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	2.04	0.57
1:A:672:ASP:HB2	1:A:736:ASN:HD21	1.69	0.57
1:A:53:LEU:CD2	1:A:54:ASN:H	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ASP:OD1	1:A:416:ARG:HB2	2.05	0.57
7:G:114:LEU:HD12	7:G:162:SER:HB2	1.86	0.57
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.86	0.57
2:B:261:ARG:H	2:B:264:SER:HB3	1.70	0.56
11:K:18:LYS:HE3	11:K:38:GLU:HG2	1.87	0.56
1:A:472:LEU:O	1:A:475:THR:HB	2.06	0.56
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.87	0.56
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.88	0.56
2:B:35:SER:HA	2:B:811:TYR:HE1	1.69	0.56
13:N:5:DA:H2"	13:N:6:DA:C8	2.40	0.56
2:B:363:HIS:HD2	2:B:585:VAL:HG22	1.70	0.56
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.88	0.56
7:G:8:SER:HB3	7:G:73:LYS:HD2	1.87	0.56
3:C:100:THR:CG2	3:C:119:VAL:HG13	2.36	0.56
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.85	0.56
1:A:512:VAL:HA	1:A:519:PRO:HA	1.87	0.56
1:A:513:SER:HB2	1:A:520:CYS:HB3	1.87	0.56
1:A:714:PHE:O	1:A:718:VAL:HG23	2.07	0.55
2:B:35:SER:HA	2:B:811:TYR:CE1	2.41	0.55
3:C:125:MET:HE3	3:C:125:MET:HA	1.88	0.55
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.42	0.55
6:F:72:LYS:HE3	6:F:142:SER:HB3	1.87	0.55
1:A:614:PHE:HB3	8:H:122:LEU:HD21	1.89	0.55
2:B:806:THR:HG22	2:B:808:ALA:H	1.72	0.55
2:B:512:ARG:NH1	2:B:531:GLN:O	2.38	0.55
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.89	0.55
1:A:453:MET:O	1:A:456:MET:HE2	2.07	0.55
3:C:124:LEU:HD22	3:C:129:ILE:HG22	1.89	0.55
8:H:95:TYR:CE1	8:H:97:MET:HG3	2.41	0.55
1:A:982:THR:HB	1:A:985:ASP:H	1.72	0.54
2:B:840:ILE:HG21	2:B:994:TYR:HD2	1.71	0.54
3:C:165:LYS:O	11:K:6:ARG:NH1	2.40	0.54
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.37	0.54
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.88	0.54
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.71	0.54
11:K:42:LEU:HG	11:K:46:ILE:CD1	2.38	0.54
1:A:254:GLU:HB3	2:B:935:ARG:HH21	1.71	0.54
4:D:47:LEU:HD21	7:G:3:PHE:CD1	2.43	0.54
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.08	0.54
8:H:47:PHE:HB3	8:H:95:TYR:HD2	1.70	0.54
1:A:1324:PRO:HB2	5:E:142:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:HG22	3:C:44:LEU:N	2.23	0.54
6:F:100:GLN:HG2	7:G:15:PRO:HB3	1.90	0.54
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.42	0.54
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.38	0.54
1:A:565:ILE:O	1:A:570:PRO:HA	2.08	0.54
1:A:900:ASP:HB3	1:A:906:HIS:HB2	1.90	0.54
7:G:9:LEU:HD22	7:G:34:VAL:HG23	1.90	0.54
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.89	0.53
1:A:353:ILE:HD13	1:A:487:MET:CE	2.38	0.53
1:A:915:SER:HB2	1:A:919:ILE:HD13	1.89	0.53
3:C:172:PRO:O	3:C:235:VAL:HG23	2.08	0.53
11:K:42:LEU:HG	11:K:46:ILE:HD11	1.88	0.53
11:K:87:LEU:O	11:K:91:CYS:HB2	2.08	0.53
5:E:19:VAL:HG22	5:E:140:LEU:HD22	1.90	0.53
1:A:741:ASN:HB3	1:A:744:LYS:HB2	1.90	0.53
1:A:1317:MET:HG3	1:A:1327:ILE:HG21	1.90	0.53
1:A:1224:LEU:HD23	1:A:1226:VAL:HG22	1.89	0.53
1:A:1172:LEU:C	1:A:1174:PHE:H	2.17	0.53
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.91	0.52
2:B:315:LYS:N	2:B:316:PRO:HD2	2.24	0.52
2:B:344:LYS:HB3	2:B:347:LYS:HB2	1.90	0.52
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.90	0.52
2:B:983:ARG:HD2	2:B:1091:TYR:HD2	1.74	0.52
3:C:100:THR:HG22	3:C:119:VAL:HG13	1.91	0.52
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.90	0.52
2:B:880:THR:HB	2:B:934:LYS:HD2	1.92	0.52
2:B:1037:LEU:HD21	2:B:1064:TYR:HE2	1.75	0.52
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.92	0.52
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.91	0.52
9:I:82:GLU:HB3	9:I:104:LEU:HB2	1.92	0.52
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.90	0.52
3:C:105:GLY:HA3	3:C:149:LYS:O	2.10	0.52
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.44	0.52
1:A:345:VAL:HG12	2:B:1155:SER:HB2	1.92	0.52
1:A:451:HIS:HB2	1:A:454:SER:HB2	1.92	0.52
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.43	0.52
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.91	0.52
1:A:1077:THR:CG2	1:A:1081:LEU:HD12	2.41	0.51
3:C:62:PHE:O	3:C:66:ARG:HG3	2.09	0.51
1:A:55:ASP:H	1:A:56:PRO:HD3	1.75	0.51
1:A:495:GLU:HG3	6:F:98:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:291:ILE:HD12	2:B:291:ILE:H	1.75	0.51
2:B:1181:GLU:HG3	2:B:1188:LYS:HG2	1.92	0.51
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.91	0.51
4:D:172:LEU:HB2	4:D:177:VAL:HG22	1.92	0.51
1:A:359:LEU:HD13	1:A:363:GLN:HG3	1.93	0.51
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.93	0.51
8:H:5:LEU:HB2	8:H:59:ILE:HG22	1.93	0.51
1:A:63:ARG:HG3	1:A:74:MET:HG3	1.92	0.51
1:A:547:LEU:HD22	11:K:58:PHE:CD2	2.45	0.51
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.44	0.51
4:D:40:HIS:CB	7:G:73:LYS:HE3	2.40	0.51
7:G:1:MET:CG	7:G:2:PHE:H	2.23	0.51
9:I:101:PHE:HE1	9:I:112:SER:HB3	1.73	0.51
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.92	0.51
1:A:1379:GLY:HA2	5:E:177:ARG:O	2.11	0.51
2:B:1002:THR:HG22	2:B:1072:MET:HE2	1.92	0.51
1:A:831:THR:O	1:A:834:THR:HG22	2.11	0.51
3:C:18:VAL:HG22	11:K:109:TRP:HZ3	1.76	0.51
2:B:766:ARG:HH21	2:B:1020:ARG:HG2	1.75	0.51
1:A:182:VAL:HB	1:A:201:VAL:HG23	1.92	0.50
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.72	0.50
1:A:449:SER:HA	1:A:454:SER:HB3	1.92	0.50
1:A:1229:SER:HB3	1:A:1237:ILE:H	1.76	0.50
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.10	0.50
2:B:365:THR:HG21	2:B:370:PHE:CD2	2.47	0.50
3:C:114:TYR:HB2	3:C:116:LYS:HG2	1.93	0.50
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.93	0.50
2:B:658:ILE:HG23	2:B:662:MET:HE2	1.92	0.50
7:G:91:VAL:HG22	7:G:143:ILE:HD12	1.93	0.50
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.47	0.50
1:A:982:THR:H	1:A:985:ASP:HB2	1.76	0.50
3:C:97:VAL:HG11	3:C:130:GLY:HA3	1.93	0.50
7:G:1:MET:CG	7:G:2:PHE:N	2.75	0.50
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.44	0.50
1:A:857:ARG:HD3	1:A:861:GLY:O	2.11	0.50
2:B:336:ARG:HH21	2:B:337:ARG:HH21	1.58	0.50
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.12	0.50
1:A:548:ASN:HD21	11:K:47:ARG:HE	1.60	0.50
1:A:1451:VAL:O	1:A:1454:MET:HE2	2.12	0.50
5:E:198:ILE:HD11	5:E:212:ARG:HB2	1.94	0.50
7:G:83:LYS:HD3	7:G:149:GLY:HA2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:LEU:HA	1:A:321:PRO:HA	1.93	0.50
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.93	0.50
13:N:2:DA:H4'	13:N:3:DG:OP1	2.12	0.50
2:B:96:TYR:HB2	2:B:129:PHE:HB2	1.94	0.49
4:D:18:VAL:HG22	4:D:19:GLU:HA	1.93	0.49
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.47	0.49
5:E:15:ALA:O	5:E:19:VAL:HG23	2.11	0.49
8:H:63:LEU:C	8:H:90:ALA:HB3	2.37	0.49
1:A:471:ASN:O	1:A:474:VAL:HG12	2.13	0.49
2:B:840:ILE:CG2	2:B:994:TYR:HD2	2.25	0.49
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.94	0.49
1:A:447:GLN:HA	1:A:448:PRO:C	2.37	0.49
7:G:111:THR:HG22	7:G:113:HIS:H	1.77	0.49
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.95	0.49
2:B:792:MET:H	2:B:857:ARG:HA	1.78	0.49
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.94	0.49
1:A:351:THR:HG22	1:A:468:PHE:CD2	2.48	0.49
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.93	0.49
6:F:134:ILE:HG22	6:F:136:ARG:HG3	1.95	0.49
1:A:37:PHE:HD2	1:A:52:GLY:CA	2.20	0.49
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.46	0.49
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.95	0.49
2:B:579:ARG:HA	2:B:589:VAL:HG12	1.94	0.48
13:N:5:DA:H2''	13:N:6:DA:H8	1.76	0.48
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.47	0.48
7:G:106:MET:HG2	7:G:107:LYS:N	2.25	0.48
1:A:78:PRO:HB3	2:B:1201:LYS:HE3	1.95	0.48
1:A:709:THR:HB	1:A:712:GLU:H	1.78	0.48
8:H:40:LEU:HB2	8:H:123:MET:HG3	1.95	0.48
1:A:337:ARG:NH2	15:T:17:DC:OP1	2.46	0.48
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.94	0.48
4:D:159:THR:O	4:D:163:VAL:HG23	2.14	0.48
1:A:1220:PHE:HE2	1:A:1267:MET:HG3	1.78	0.48
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.96	0.48
4:D:54:GLU:O	4:D:58:VAL:HG23	2.13	0.48
4:D:220:LEU:H	4:D:220:LEU:CD1	2.22	0.48
10:J:48:ARG:HE	10:J:49:MET:CE	2.27	0.48
1:A:1135:ARG:HG2	1:A:1282:VAL:HG12	1.95	0.48
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.79	0.48
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.95	0.48
9:I:50:THR:HG22	9:I:52:ILE:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:LEU:O	1:A:633:VAL:HG23	2.14	0.48
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.94	0.48
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.95	0.48
2:B:1037:LEU:HD21	2:B:1064:TYR:CE2	2.48	0.48
4:D:7:THR:HG21	7:G:5:LYS:HZ2	1.79	0.48
1:A:275:SER:O	1:A:279:LEU:HB2	2.14	0.48
1:A:326:ARG:HG3	1:A:1406:VAL:HG11	1.95	0.48
3:C:196:ASP:HB3	3:C:199:LYS:HB2	1.96	0.48
8:H:142:LEU:HG	8:H:144:ILE:HD11	1.95	0.48
1:A:58:LEU:HB3	1:A:59:GLY:H	1.47	0.48
1:A:704:ALA:HB2	1:A:710:LEU:HA	1.96	0.48
6:F:97:ARG:HD2	6:F:97:ARG:HA	1.55	0.48
1:A:98:LYS:O	1:A:102:VAL:HG23	2.13	0.47
1:A:352:VAL:HB	2:B:1099:VAL:HG23	1.95	0.47
1:A:506:ALA:HB3	1:A:509:LEU:HD12	1.96	0.47
2:B:711:GLU:HB2	2:B:712:PRO:HD3	1.96	0.47
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.96	0.47
2:B:792:MET:HE2	2:B:857:ARG:NH2	2.30	0.47
2:B:273:LEU:HD12	2:B:280:ILE:HD12	1.96	0.47
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.97	0.47
8:H:81:PRO:CB	8:H:82:PRO:HD3	2.44	0.47
11:K:35:PHE:O	11:K:70:ARG:HA	2.14	0.47
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.97	0.47
1:A:306:ASN:OD1	1:A:314:ALA:HB3	2.15	0.47
2:B:542:MET:HG2	2:B:747:MET:HE3	1.96	0.47
2:B:1071:VAL:HG13	2:B:1084:GLN:HG3	1.97	0.47
5:E:159:ASP:HA	5:E:162:ARG:NH1	2.29	0.47
7:G:14:HIS:CD2	7:G:15:PRO:HD2	2.50	0.47
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.97	0.47
1:A:257:ARG:HB3	1:A:258:GLY:H	1.52	0.47
1:A:1438:THR:O	6:F:92:ARG:HD2	2.15	0.47
1:A:404:TYR:HB2	1:A:433:GLU:HB2	1.97	0.47
1:A:1444:MET:HE2	1:A:1444:MET:HB2	1.74	0.47
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.97	0.47
3:C:43:THR:CG2	3:C:44:LEU:H	2.27	0.47
7:G:106:MET:HG3	7:G:157:ILE:O	2.15	0.47
1:A:537:ARG:HG2	8:H:121:LEU:HD23	1.95	0.47
1:A:851:HIS:HB3	6:F:139:PRO:HD3	1.96	0.47
1:A:1116:LEU:HB2	1:A:1308:THR:OG1	2.15	0.47
2:B:879:ARG:HG3	2:B:883:LEU:HD23	1.97	0.46
4:D:18:VAL:HG22	4:D:20:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.97	0.46
1:A:709:THR:HG22	1:A:711:ARG:H	1.79	0.46
2:B:101:MET:HE3	2:B:169:ARG:HH22	1.80	0.46
1:A:219:PHE:HA	1:A:222:LEU:HD12	1.98	0.46
1:A:396:PRO:HB3	1:A:403:LYS:HA	1.97	0.46
8:H:127:GLY:CA	8:H:130:ARG:HH21	2.25	0.46
2:B:797:TYR:HB3	2:B:798:TYR:HD1	1.81	0.46
3:C:36:VAL:HG21	3:C:251:LEU:HD13	1.97	0.46
13:N:4:DA:H2''	13:N:5:DA:C8	2.51	0.46
1:A:738:LYS:HB2	1:A:740:LEU:HG	1.98	0.46
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.51	0.46
2:B:580:VAL:HG13	2:B:624:LEU:HD23	1.97	0.46
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.98	0.46
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.96	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.80	0.46
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.49	0.46
3:C:6:PRO:HB2	11:K:101:LEU:HD23	1.98	0.46
3:C:124:LEU:O	3:C:127:ARG:HG2	2.16	0.46
6:F:76:LYS:HA	6:F:79:ARG:CD	2.42	0.46
1:A:709:THR:HG23	9:I:94:ASP:HA	1.98	0.46
1:A:908:LEU:HB3	1:A:912:LEU:HD12	1.98	0.46
2:B:295:GLY:H	2:B:298:LEU:HD12	1.81	0.46
2:B:765:PRO:O	2:B:769:TYR:HD1	1.99	0.46
10:J:2:ILE:HD12	10:J:57:ILE:HD13	1.98	0.46
4:D:5:THR:HG21	7:G:74:TYR:OH	2.16	0.46
1:A:909:ASP:C	1:A:911:SER:H	2.23	0.45
11:K:55:LYS:HB3	11:K:81:TYR:CE2	2.51	0.45
1:A:524:VAL:HG12	1:A:525:GLN:H	1.81	0.45
1:A:726:ARG:CD	1:A:766:GLY:HA3	2.45	0.45
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.81	0.45
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.83	0.45
2:B:825:VAL:HG13	2:B:1010:LEU:HB3	1.98	0.45
3:C:58:LEU:HD12	3:C:145:CYS:SG	2.56	0.45
1:A:826:ASP:HB2	1:A:830:LYS:HD2	1.97	0.45
1:A:1283:VAL:HB	1:A:1307:GLU:HB2	1.98	0.45
3:C:46:ILE:HD12	3:C:46:ILE:H	1.81	0.45
4:D:213:GLU:O	4:D:217:LEU:HD12	2.16	0.45
7:G:138:THR:HG22	7:G:139:ILE:H	1.82	0.45
1:A:382:PRO:HA	1:A:428:TYR:HE1	1.81	0.45
1:A:869:GLY:O	5:E:204:THR:HG21	2.17	0.45
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:823:ALA:O	2:B:825:VAL:HG23	2.16	0.45
3:C:164:ALA:HA	3:C:167:HIS:O	2.16	0.45
10:J:30:LEU:HD21	10:J:38:ARG:HH12	1.81	0.45
3:C:3:GLU:HB3	3:C:7:GLN:NE2	2.32	0.45
7:G:138:THR:HG22	7:G:139:ILE:N	2.32	0.45
10:J:32:GLU:CD	10:J:32:GLU:H	2.24	0.45
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.41	0.45
1:A:1450:LEU:HD12	6:F:131:PRO:HG3	1.99	0.45
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.98	0.45
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.99	0.45
8:H:6:PHE:HB3	8:H:59:ILE:HB	1.98	0.45
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.17	0.45
1:A:477:PRO:HG3	1:A:521:MET:HE2	1.99	0.45
1:A:567:LYS:HA	1:A:568:PRO:C	2.41	0.45
4:D:56:ARG:HB2	4:D:148:LEU:HB3	1.99	0.45
1:A:915:SER:O	1:A:918:GLU:HG3	2.17	0.45
10:J:9:SER:OG	10:J:48:ARG:NH2	2.49	0.45
1:A:1004:ASN:CG	5:E:167:ARG:HD2	2.42	0.44
11:K:6:ARG:O	11:K:9:LEU:HD12	2.16	0.44
1:A:185:TRP:HE3	1:A:185:TRP:H	1.65	0.44
2:B:295:GLY:O	2:B:299:GLU:HB2	2.18	0.44
2:B:778:MET:HB3	2:B:779:GLY:H	1.64	0.44
3:C:232:VAL:HG21	3:C:244:VAL:HG22	1.98	0.44
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.42	0.44
2:B:640:VAL:HA	2:B:651:LEU:HA	2.00	0.44
2:B:800:GLN:HB3	10:J:52:THR:HG23	1.99	0.44
8:H:47:PHE:CB	8:H:95:TYR:HD2	2.29	0.44
1:A:42:ASP:O	1:A:44:THR:N	2.51	0.44
2:B:1138:MET:HE3	2:B:1138:MET:HA	1.99	0.44
3:C:92:CYS:SG	3:C:94:LYS:HB2	2.57	0.44
5:E:176:PRO:O	5:E:212:ARG:HA	2.18	0.44
2:B:1201:LYS:HE2	2:B:1205:GLN:HE22	1.82	0.44
5:E:178:ILE:HB	5:E:212:ARG:HB3	1.99	0.44
7:G:131:GLN:HA	7:G:136:VAL:HG22	2.00	0.44
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.17	0.44
2:B:291:ILE:HD12	2:B:291:ILE:N	2.33	0.44
1:A:1407:GLU:CD	1:A:1407:GLU:H	2.25	0.44
2:B:356:LEU:HA	2:B:360:PHE:HB3	2.00	0.44
2:B:485:ARG:NH1	2:B:491:THR:HG21	2.33	0.44
4:D:52:LEU:H	4:D:182:SER:HB3	1.82	0.44
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:61:THR:HG21	12:L:63:ARG:NE	2.22	0.44
1:A:780:VAL:O	1:A:782:ARG:HD3	2.18	0.44
1:A:849:MET:HB3	1:A:1063:MET:SD	2.57	0.44
1:A:1120:LEU:HD23	1:A:1124:HIS:O	2.18	0.44
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.83	0.44
4:D:198:LEU:O	4:D:200:ASN:N	2.51	0.44
6:F:111:LEU:HD12	6:F:111:LEU:H	1.82	0.44
8:H:89:LEU:O	8:H:91:ASP:N	2.48	0.44
1:A:95:PHE:CE1	1:A:1414:ALA:HB2	2.53	0.44
1:A:675:THR:HG21	1:A:736:ASN:HB2	2.00	0.44
2:B:789:MET:HE2	2:B:953:LEU:HB3	2.00	0.44
4:D:18:VAL:HG13	4:D:19:GLU:HA	2.00	0.44
4:D:59:ILE:HG21	4:D:141:LEU:HD11	1.99	0.44
11:K:59:ALA:HA	11:K:74:ARG:O	2.18	0.43
1:A:41:MET:CB	1:A:49:LYS:HA	2.45	0.43
1:A:50:ILE:C	1:A:52:GLY:H	2.26	0.43
1:A:354:SER:O	1:A:469:ARG:HA	2.18	0.43
1:A:387:ARG:NH1	1:A:437:MET:HE1	2.33	0.43
2:B:902:GLY:O	12:L:65:VAL:HG11	2.17	0.43
10:J:14:VAL:HG13	10:J:50:ILE:HD11	2.00	0.43
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.99	0.43
2:B:583:ASN:ND2	2:B:628:THR:HG22	2.20	0.43
2:B:879:ARG:HB3	2:B:880:THR:H	1.51	0.43
11:K:8:GLU:O	11:K:37:LYS:HD3	2.18	0.43
1:A:442:VAL:O	1:A:457:ALA:HA	2.18	0.43
1:A:1215:ARG:O	1:A:1218:GLN:HG2	2.18	0.43
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.83	0.43
2:B:247:GLY:H	2:B:418:LYS:NZ	2.17	0.43
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.01	0.43
4:D:154:PHE:HB2	4:D:160:VAL:HG22	2.01	0.43
8:H:80:ARG:HG2	11:K:57:LEU:HD22	1.99	0.43
12:L:61:THR:HB	12:L:63:ARG:HG2	1.99	0.43
1:A:399:HIS:HB3	1:A:400:PRO:HD3	2.00	0.43
1:A:867:ILE:CD1	1:A:867:ILE:CB	2.83	0.43
2:B:446:LEU:HD12	2:B:448:ILE:HD11	2.01	0.43
1:A:49:LYS:HD3	1:A:61:ILE:HG13	2.00	0.43
1:A:984:LYS:O	1:A:988:LEU:HB2	2.18	0.43
2:B:918:ILE:HG12	2:B:935:ARG:NH2	2.32	0.43
4:D:202:ILE:HD11	4:D:206:GLU:HB3	2.01	0.43
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.84	0.43
1:A:466:SER:HB2	2:B:1099:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1386:ARG:CD	15:T:15:BRU:H2''	2.48	0.43
2:B:101:MET:HA	2:B:112:LEU:H	1.83	0.43
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.82	0.43
2:B:1173:ALA:HB1	2:B:1175:LEU:HD23	2.01	0.43
3:C:101:LEU:HD12	3:C:118:LEU:HG	1.99	0.43
6:F:109:VAL:HG22	6:F:110:ASP:N	2.34	0.43
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.99	0.43
2:B:581:PHE:HB2	2:B:625:LYS:HG2	2.00	0.43
2:B:911:ILE:HD11	2:B:941:LEU:HD13	2.00	0.43
2:B:957:ASN:HB3	2:B:961:LEU:H	1.82	0.43
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.34	0.43
4:D:27:LEU:HD23	4:D:197:SER:HB3	2.00	0.43
4:D:63:LEU:O	4:D:133:THR:HG21	2.18	0.43
1:A:105:CYS:SG	1:A:139:TRP:HA	2.58	0.43
1:A:1142:THR:HG22	1:A:1271:ILE:O	2.19	0.43
2:B:167:ILE:HG22	2:B:167:ILE:O	2.18	0.43
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	2.01	0.43
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.92	0.43
1:A:847:ASP:HB3	1:A:1398:MET:HE1	2.01	0.43
1:A:859:SER:HB3	1:A:1394:THR:HG22	2.00	0.43
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.52	0.43
2:B:981:ALA:HB2	2:B:987:LYS:HA	2.00	0.43
3:C:149:LYS:HE2	10:J:64:ASN:O	2.18	0.43
11:K:12:LEU:HA	11:K:37:LYS:HG3	2.00	0.43
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	2.01	0.42
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.01	0.42
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	2.00	0.42
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.73	0.42
2:B:46:GLN:H	2:B:46:GLN:HG3	1.65	0.42
2:B:952:VAL:HB	12:L:58:LYS:HB2	2.02	0.42
6:F:85:MET:O	6:F:155:LEU:HD11	2.19	0.42
1:A:675:THR:HG23	1:A:732:LEU:HD22	2.01	0.42
2:B:100:PRO:HG3	2:B:172:ILE:HD12	2.02	0.42
2:B:842:ASN:HB2	2:B:1009:ASP:HA	2.01	0.42
7:G:45:ILE:HA	7:G:78:VAL:HG12	2.01	0.42
9:I:55:THR:HG21	9:I:109:ILE:HG21	2.01	0.42
2:B:701:ILE:HD11	2:B:703:ILE:HD11	2.01	0.42
2:B:911:ILE:HG23	2:B:966:VAL:HG11	2.01	0.42
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.83	0.42
10:J:57:ILE:O	10:J:60:PHE:HB2	2.19	0.42
1:A:81:PHE:HE1	2:B:1205:GLN:HG2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:TYR:CE2	1:A:1058:VAL:HG11	2.54	0.42
1:A:1159:ARG:HE	1:A:1174:PHE:HE2	1.66	0.42
1:A:1442:ASP:HB2	6:F:137:TYR:CE1	2.51	0.42
2:B:254:LEU:HD12	2:B:272:THR:O	2.19	0.42
7:G:127:PRO:HB2	7:G:139:ILE:HD13	2.00	0.42
8:H:47:PHE:CB	8:H:95:TYR:CD2	3.02	0.42
2:B:464:GLY:HA2	2:B:480:SER:HB3	2.01	0.42
3:C:67:LEU:HD11	3:C:155:LEU:HD13	2.01	0.42
5:E:46:TYR:O	5:E:53:PRO:HA	2.20	0.42
1:A:270:LEU:HD12	1:A:274:ILE:HD11	2.01	0.42
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.60	0.42
6:F:93:ILE:HG21	6:F:148:VAL:HG11	2.01	0.42
1:A:568:PRO:HG2	8:H:46:LEU:HD12	2.02	0.42
5:E:26:ARG:HH22	5:E:133:GLU:CD	2.28	0.42
1:A:408:ASP:C	1:A:410:GLY:H	2.28	0.42
2:B:130:VAL:HG23	2:B:167:ILE:HD13	2.02	0.42
3:C:4:GLU:HB3	3:C:5:GLY:H	1.51	0.42
1:A:519:PRO:O	1:A:624:SER:HB2	2.19	0.42
2:B:343:ILE:O	2:B:344:LYS:HB2	2.19	0.42
2:B:773:MET:HE1	2:B:981:ALA:HB1	2.00	0.42
6:F:152:ILE:H	6:F:152:ILE:HG13	1.62	0.42
1:A:174:ILE:H	1:A:174:ILE:HG13	1.71	0.41
1:A:837:ILE:HG21	1:A:1101:LEU:HD21	2.02	0.41
2:B:383:ASN:O	2:B:387:LEU:HB2	2.20	0.41
7:G:132:SER:C	7:G:134:GLU:H	2.28	0.41
1:A:311:GLN:O	1:A:312:PRO:C	2.63	0.41
1:A:445:ASN:HB2	1:A:455:MET:HG2	2.01	0.41
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.19	0.41
1:A:1375:MET:HE3	1:A:1384:VAL:HG23	2.01	0.41
2:B:101:MET:HB3	2:B:109:THR:HG22	2.02	0.41
2:B:1119:VAL:HG23	2:B:1126:GLY:HA2	2.01	0.41
2:B:1208:MET:HA	2:B:1212:ILE:O	2.20	0.41
1:A:1404:GLU:HB3	1:A:1407:GLU:HB2	2.02	0.41
2:B:405:ARG:HE	2:B:629:ASP:CG	2.28	0.41
2:B:785:TYR:HE2	10:J:60:PHE:CE2	2.38	0.41
4:D:153:ARG:HH12	4:D:214:LEU:HD13	1.85	0.41
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.55	0.41
8:H:110:ASP:HB3	8:H:128:ASN:HB2	2.02	0.41
12:L:38:LEU:O	12:L:39:SER:HB3	2.19	0.41
1:A:84:ILE:HG13	1:A:239:LEU:HB3	2.02	0.41
1:A:130:ASP:HB3	1:A:133:LYS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ILE:HG13	1:A:732:LEU:HD13	2.03	0.41
1:A:1444:MET:HG2	7:G:58:ARG:HB3	2.02	0.41
2:B:882:THR:CG2	2:B:935:ARG:HA	2.50	0.41
2:B:996:ARG:NH2	3:C:174:ALA:O	2.53	0.41
1:A:63:ARG:HA	1:A:74:MET:CG	2.51	0.41
1:A:79:GLY:HA3	1:A:243:PRO:HG2	2.01	0.41
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.50	0.41
1:A:834:THR:CG2	1:A:1077:THR:HG23	2.50	0.41
1:A:946:VAL:HG22	5:E:201:LYS:HB3	2.01	0.41
1:A:1208:THR:H	1:A:1211:GLN:HG2	1.86	0.41
3:C:100:THR:HG23	3:C:119:VAL:HG13	2.02	0.41
7:G:111:THR:HB	7:G:114:LEU:HD23	2.03	0.41
1:A:335:ARG:HA	1:A:339:ASN:HB2	2.02	0.41
1:A:1121:GLU:HG2	1:A:1124:HIS:CE1	2.56	0.41
3:C:69:LEU:HD23	10:J:6:ARG:HD3	2.02	0.41
1:A:35:ILE:O	1:A:84:ILE:HG22	2.21	0.41
1:A:95:PHE:HE1	1:A:1414:ALA:HB2	1.86	0.41
2:B:126:SER:HB2	2:B:172:ILE:HD11	2.02	0.41
2:B:852:ARG:HH22	12:L:70:ARG:C	2.28	0.41
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.56	0.41
1:A:118:HIS:CD2	1:A:164:ARG:HB3	2.56	0.41
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.56	0.41
1:A:335:ARG:HD3	2:B:1202:LEU:HD13	2.02	0.41
2:B:102:VAL:HG13	2:B:112:LEU:HB2	2.02	0.41
2:B:398:ARG:HB2	2:B:398:ARG:HH11	1.86	0.41
3:C:18:VAL:HG22	11:K:109:TRP:CZ3	2.54	0.41
3:C:45:ALA:HA	3:C:72:LEU:HD12	2.03	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.56	0.41
4:D:10:THR:HG22	4:D:12:ARG:HH12	1.86	0.41
4:D:194:LEU:O	4:D:196:PRO:HD3	2.20	0.41
5:E:202:SER:HB3	5:E:205:SER:H	1.86	0.41
1:A:55:ASP:N	1:A:56:PRO:HD3	2.35	0.41
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.86	0.41
2:B:258:LEU:HB2	2:B:385:LEU:HD21	2.03	0.41
1:A:579:SER:HB3	1:A:611:GLN:HA	2.03	0.40
3:C:44:LEU:HB2	3:C:77:ILE:HD13	2.02	0.40
3:C:248:ILE:HD13	11:K:102:LYS:HA	2.04	0.40
8:H:98:TYR:C	8:H:118:PHE:HD1	2.29	0.40
1:A:12:ARG:O	2:B:1194:ILE:HG22	2.21	0.40
2:B:295:GLY:N	2:B:298:LEU:HD12	2.37	0.40
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.23	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:THR:HG23	2:B:1046:PRO:HD3	2.03	0.40
2:B:856:PHE:CE1	2:B:969:ARG:HG3	2.56	0.40
4:D:195:ILE:HG22	4:D:198:LEU:HG	2.03	0.40
5:E:100:ILE:HG13	5:E:105:PHE:HD2	1.86	0.40
12:L:27:LEU:HA	12:L:39:SER:HB2	2.03	0.40
12:L:57:LEU:HD23	12:L:57:LEU:HA	1.93	0.40
1:A:244:PRO:O	1:A:245:PRO:C	2.65	0.40
2:B:485:ARG:HD2	2:B:491:THR:HG23	2.04	0.40
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.21	0.40
2:B:776:GLN:O	2:B:1095:LEU:HA	2.22	0.40
8:H:42:ILE:HG23	8:H:95:TYR:HE2	1.85	0.40
1:A:413:ILE:HD13	1:A:424:ILE:HD11	2.03	0.40
1:A:439:ASN:OD1	1:A:459:ARG:HG2	2.22	0.40
1:A:745:GLN:HA	1:A:748:MET:HE3	2.04	0.40
1:A:901:LEU:HB2	1:A:926:GLN:HG2	2.03	0.40
1:A:1208:THR:HB	1:A:1211:GLN:H	1.86	0.40
2:B:70:ILE:HD13	2:B:429:PHE:HZ	1.87	0.40
2:B:244:LEU:HD11	2:B:250:PHE:HD2	1.86	0.40
2:B:310:MET:HE2	2:B:386:LEU:HB2	2.04	0.40
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.51	0.40
4:D:23:ASN:HA	4:D:28:GLN:O	2.20	0.40
6:F:76:LYS:HG2	6:F:79:ARG:CZ	2.51	0.40
1:A:636:GLU:OE1	1:A:962:ARG:NH1	2.54	0.40
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	2.04	0.40
1:A:1444:MET:HE1	6:F:135:ARG:HB2	2.03	0.40
2:B:484:ASN:HB3	2:B:486:TYR:CE2	2.57	0.40
2:B:952:VAL:HG13	2:B:966:VAL:HG22	2.02	0.40
3:C:186:LEU:HB3	3:C:188:HIS:CD2	2.56	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	
1	A	1417/1732 (82%)	1205 (85%)	143 (10%)	69 (5%)	1	17
2	B	1095/1224 (90%)	940 (86%)	109 (10%)	46 (4%)	2	20
3	C	264/318 (83%)	238 (90%)	20 (8%)	6 (2%)	5	30
4	D	174/221 (79%)	151 (87%)	9 (5%)	14 (8%)	1	9
5	E	212/215 (99%)	189 (89%)	19 (9%)	4 (2%)	6	33
6	F	82/155 (53%)	75 (92%)	6 (7%)	1 (1%)	10	40
7	G	169/171 (99%)	150 (89%)	16 (10%)	3 (2%)	6	34
8	H	129/146 (88%)	99 (77%)	19 (15%)	11 (8%)	0	8
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	4	28
10	J	63/70 (90%)	56 (89%)	3 (5%)	4 (6%)	1	14
11	K	113/120 (94%)	105 (93%)	8 (7%)	0	100	100
12	L	44/70 (63%)	27 (61%)	8 (18%)	9 (20%)	0	1
All	All	3879/4564 (85%)	3333 (86%)	376 (10%)	170 (4%)	2	19

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	48	ALA
1	A	58	LEU
1	A	189	ARG
1	A	193	ASP
1	A	195	ASP
1	A	286	HIS
1	A	311	GLN
1	A	335	ARG
1	A	399	HIS
1	A	448	PRO
1	A	775	ILE
1	A	1341	ILE
1	A	1403	GLU
2	B	340	ALA
2	B	341	LEU
2	B	344	LYS
2	B	473	MET
2	B	707	PRO
2	B	711	GLU
2	B	731	VAL
2	B	751	VAL

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Mol	Chain	Res	Type
2	B	1157	ALA
2	B	1185	CYS
3	C	161	LYS
4	D	18	VAL
4	D	53	SER
4	D	199	ASN
4	D	220	LEU
8	H	81	PRO
10	J	6	ARG
10	J	13	VAL
1	A	54	ASN
1	A	55	ASP
1	A	57	ARG
1	A	61	ILE
1	A	76	GLU
1	A	167	CYS
1	A	251	SER
1	A	257	ARG
1	A	318	SER
1	A	449	SER
1	A	870	GLU
1	A	1405	THR
2	B	108	VAL
2	B	229	ALA
2	B	338	GLY
2	B	339	THR
2	B	369	GLY
2	B	449	ASN
2	B	772	ALA
2	B	792	MET
2	B	867	GLY
2	B	879	ARG
2	B	880	THR
2	B	883	LEU
2	B	1046	PRO
2	B	1066	SER
2	B	1167	GLY
2	B	1176	ASN
4	D	27	LEU
4	D	52	LEU
4	D	119	ARG
4	D	174	PRO

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Mol	Chain	Res	Type
6	F	73	ALA
7	G	139	ILE
7	G	154	VAL
8	H	17	PRO
8	H	82	PRO
8	H	90	ALA
8	H	128	ASN
9	I	3	THR
9	I	95	THR
12	L	37	LYS
12	L	45	ALA
12	L	50	ASP
1	A	62	ASP
1	A	169	ASN
1	A	409	SER
1	A	426	LEU
1	A	465	TYR
1	A	600	PRO
1	A	846	GLU
1	A	852	TYR
1	A	1124	HIS
1	A	1173	HIS
1	A	1255	GLU
1	A	1438	THR
2	B	58	THR
2	B	282	ILE
2	B	343	ILE
2	B	364	ILE
2	B	368	GLU
2	B	1069	PHE
2	B	1143	ALA
2	B	1156	ASP
2	B	1175	LEU
3	C	4	GLU
3	C	240	VAL
4	D	11	ARG
5	E	3	GLN
5	E	45	LYS
5	E	49	SER
7	G	2	PHE
8	H	32	THR
8	H	60	ALA

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Mol	Chain	Res	Type
8	H	83	GLN
8	H	84	ALA
8	H	108	SER
12	L	26	THR
12	L	53	HIS
12	L	59	ALA
1	A	164	ARG
1	A	196	GLU
1	A	253	ASN
1	A	333	GLU
1	A	569	LYS
1	A	593	GLU
1	A	1002	GLY
1	A	1242	VAL
2	B	713	ALA
2	B	734	HIS
2	B	764	SER
2	B	882	THR
2	B	891	ASP
2	B	1155	SER
2	B	1223	ASP
3	C	149	LYS
3	C	214	ASN
4	D	16	LYS
4	D	22	GLU
4	D	40	HIS
5	E	48	ASP
9	I	105	SER
12	L	63	ARG
1	A	224	PHE
1	A	254	GLU
1	A	312	PRO
1	A	958	VAL
2	B	466	TRP
4	D	192	LYS
10	J	2	ILE
10	J	57	ILE
1	A	40	THR
1	A	156	ASP
1	A	331	GLY
1	A	336	ILE
1	A	910	PRO

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Mol	Chain	Res	Type
1	A	1327	ILE
2	B	901	PRO
4	D	218	GLU
12	L	38	LEU
1	A	283	GLY
1	A	567	LYS
1	A	986	ILE
1	A	1123	GLY
8	H	107	VAL
1	A	385	ILE
1	A	639	PRO
1	A	35	ILE
1	A	178	GLY
1	A	380	VAL
1	A	599	SER
2	B	247	GLY
1	A	128	ILE
12	L	46	VAL
1	A	192	GLY
1	A	197	PRO
2	B	870	ILE
3	C	77	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1243/1519 (82%)	1015 (82%)	228 (18%)	2	11
2	B	966/1061 (91%)	804 (83%)	162 (17%)	2	13
3	C	234/274 (85%)	192 (82%)	42 (18%)	2	12
4	D	160/200 (80%)	127 (79%)	33 (21%)	1	8
5	E	196/197 (100%)	172 (88%)	24 (12%)	5	22
6	F	74/137 (54%)	61 (82%)	13 (18%)	2	12
7	G	152/152 (100%)	137 (90%)	15 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	117/128 (91%)	95 (81%)	22 (19%)	1	10
9	I	113/116 (97%)	105 (93%)	8 (7%)	13	40
10	J	60/65 (92%)	50 (83%)	10 (17%)	2	14
11	K	99/102 (97%)	83 (84%)	16 (16%)	2	14
12	L	40/57 (70%)	26 (65%)	14 (35%)	0	1
All	All	3454/4008 (86%)	2867 (83%)	587 (17%)	2	13

All (587) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	23	SER
1	A	28	ARG
1	A	34	LYS
1	A	41	MET
1	A	43	GLU
1	A	50	ILE
1	A	58	LEU
1	A	62	ASP
1	A	64	ASN
1	A	65	LEU
1	A	84	ILE
1	A	93	VAL
1	A	96	ILE
1	A	117	GLU
1	A	120	GLU
1	A	123	ARG
1	A	126	LEU
1	A	129	LYS
1	A	145	LYS
1	A	147	VAL
1	A	162	VAL
1	A	164	ARG
1	A	174	ILE
1	A	188	ASP
1	A	199	LEU
1	A	208	LEU
1	A	227	VAL
1	A	250	ILE
1	A	253	ASN

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Mol	Chain	Res	Type
1	A	256	GLN
1	A	270	LEU
1	A	274	ILE
1	A	279	LEU
1	A	295	LEU
1	A	307	ASP
1	A	308	ILE
1	A	313	GLN
1	A	315	LEU
1	A	318	SER
1	A	320	ARG
1	A	335	ARG
1	A	337	ARG
1	A	340	LEU
1	A	344	ARG
1	A	359	LEU
1	A	363	GLN
1	A	369	SER
1	A	385	ILE
1	A	386	ASP
1	A	389	THR
1	A	391	LEU
1	A	393	ARG
1	A	394	ASN
1	A	408	ASP
1	A	409	SER
1	A	425	GLN
1	A	427	GLN
1	A	431	LYS
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	450	LEU
1	A	454	SER
1	A	459	ARG
1	A	461	LYS
1	A	463	ILE
1	A	470	LEU
1	A	472	LEU
1	A	475	THR
1	A	476	SER
1	A	483	ASP

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Mol	Chain	Res	Type
1	A	493	GLN
1	A	496	GLU
1	A	500	GLU
1	A	505	CYS
1	A	517	ASN
1	A	518	LYS
1	A	523	ILE
1	A	524	VAL
1	A	527	THR
1	A	536	LEU
1	A	538	ASP
1	A	549	MET
1	A	560	ILE
1	A	566	ILE
1	A	567	LYS
1	A	577	ILE
1	A	593	GLU
1	A	598	LEU
1	A	613	ILE
1	A	618	GLU
1	A	620	LYS
1	A	626	ASN
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	645	LEU
1	A	666	ILE
1	A	670	ILE
1	A	683	ILE
1	A	685	GLU
1	A	691	LEU
1	A	720	ARG
1	A	732	LEU
1	A	738	LYS
1	A	739	ASP
1	A	756	ILE
1	A	758	ILE
1	A	768	GLN
1	A	769	SER
1	A	782	ARG
1	A	795	GLU
1	A	811	GLN

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Mol	Chain	Res	Type
1	A	821	ARG
1	A	824	LEU
1	A	827	THR
1	A	834	THR
1	A	843	LYS
1	A	848	ILE
1	A	855	THR
1	A	867	ILE
1	A	878	ILE
1	A	885	THR
1	A	896	ARG
1	A	904	THR
1	A	905	ASP
1	A	906	HIS
1	A	914	GLU
1	A	915	SER
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	929	LEU
1	A	948	VAL
1	A	973	ILE
1	A	982	THR
1	A	983	ILE
1	A	988	LEU
1	A	998	LEU
1	A	999	VAL
1	A	1001	ARG
1	A	1006	ILE
1	A	1009	ASN
1	A	1024	SER
1	A	1029	ARG
1	A	1033	GLN
1	A	1036	ARG
1	A	1047	SER
1	A	1050	GLU
1	A	1062	GLU
1	A	1064	VAL
1	A	1067	LEU
1	A	1079	MET
1	A	1080	THR
1	A	1094	VAL

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Mol	Chain	Res	Type
1	A	1096	SER
1	A	1098	VAL
1	A	1100	ARG
1	A	1116	LEU
1	A	1118	VAL
1	A	1120	LEU
1	A	1124	HIS
1	A	1133	LEU
1	A	1134	ILE
1	A	1142	THR
1	A	1145	SER
1	A	1147	THR
1	A	1170	ILE
1	A	1173	HIS
1	A	1175	SER
1	A	1176	LEU
1	A	1188	GLN
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1222	ASN
1	A	1223	ASP
1	A	1226	VAL
1	A	1237	ILE
1	A	1238	ILE
1	A	1242	VAL
1	A	1243	VAL
1	A	1255	GLU
1	A	1256	GLU
1	A	1257	ASP
1	A	1260	LEU
1	A	1270	ASN
1	A	1274	ARG
1	A	1276	VAL
1	A	1289	ARG
1	A	1291	VAL
1	A	1293	SER
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1309	ASP
1	A	1316	VAL

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Mol	Chain	Res	Type
1	A	1319	VAL
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1334	ASP
1	A	1336	MET
1	A	1341	ILE
1	A	1351	GLU
1	A	1371	LEU
1	A	1376	THR
1	A	1378	GLN
1	A	1382	THR
1	A	1387	HIS
1	A	1391	ARG
1	A	1393	ASN
1	A	1394	THR
1	A	1403	GLU
1	A	1420	ASP
1	A	1422	ARG
1	A	1424	VAL
1	A	1426	GLU
1	A	1432	GLN
1	A	1436	ILE
1	A	1442	ASP
1	A	1443	VAL
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1453	TYR
1	A	1454	MET
2	B	20	ASP
2	B	22	SER
2	B	25	ILE
2	B	35	SER
2	B	44	VAL
2	B	46	GLN
2	B	58	THR
2	B	63	ILE
2	B	110	HIS
2	B	118	ARG
2	B	128	LEU
2	B	134	LYS

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Mol	Chain	Res	Type
2	B	170	LEU
2	B	178	ASN
2	B	194	GLU
2	B	205	ILE
2	B	218	SER
2	B	222	ILE
2	B	223	VAL
2	B	240	ILE
2	B	251	ILE
2	B	261	ARG
2	B	262	GLU
2	B	268	THR
2	B	272	THR
2	B	278	GLN
2	B	294	ASP
2	B	305	VAL
2	B	309	GLN
2	B	312	GLU
2	B	313	MET
2	B	324	ILE
2	B	337	ARG
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	347	LYS
2	B	348	ARG
2	B	357	GLN
2	B	361	LEU
2	B	364	ILE
2	B	365	THR
2	B	368	GLU
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	446	LEU
2	B	453	ILE
2	B	470	LYS
2	B	476	ARG
2	B	485	ARG

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Mol	Chain	Res	Type
2	B	487	THR
2	B	491	THR
2	B	502	ILE
2	B	531	GLN
2	B	538	ASN
2	B	544	CYS
2	B	545	ILE
2	B	547	VAL
2	B	549	THR
2	B	552	MET
2	B	554	ILE
2	B	566	LEU
2	B	567	GLU
2	B	570	VAL
2	B	574	SER
2	B	580	VAL
2	B	582	VAL
2	B	595	ARG
2	B	603	LEU
2	B	609	ILE
2	B	612	GLU
2	B	616	ILE
2	B	620	ARG
2	B	628	THR
2	B	635	ARG
2	B	637	LEU
2	B	644	GLU
2	B	653	VAL
2	B	655	LYS
2	B	658	ILE
2	B	664	THR
2	B	678	GLU
2	B	680	THR
2	B	693	ILE
2	B	694	ASP
2	B	696	GLU
2	B	708	GLU
2	B	734	HIS
2	B	736	THR
2	B	737	THR
2	B	748	ILE
2	B	766	ARG

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Mol	Chain	Res	Type
2	B	780	VAL
2	B	787	VAL
2	B	790	ASP
2	B	795	ILE
2	B	797	TYR
2	B	839	MET
2	B	841	MET
2	B	844	SER
2	B	858	SER
2	B	868	MET
2	B	871	THR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	885	MET
2	B	904	ARG
2	B	934	LYS
2	B	939	THR
2	B	942	ARG
2	B	944	THR
2	B	945	GLU
2	B	946	ASN
2	B	953	LEU
2	B	970	THR
2	B	972	LYS
2	B	975	GLN
2	B	976	ILE
2	B	979	LYS
2	B	986	GLN
2	B	995	ARG
2	B	997	GLU
2	B	1006	ILE
2	B	1007	VAL
2	B	1010	LEU
2	B	1020	ARG
2	B	1022	THR
2	B	1028	GLU
2	B	1031	LEU
2	B	1045	SER
2	B	1050	ILE
2	B	1053	GLU
2	B	1058	LEU

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Mol	Chain	Res	Type
2	B	1065	GLN
2	B	1071	VAL
2	B	1072	MET
2	B	1113	VAL
2	B	1122	ARG
2	B	1123	SER
2	B	1128	LEU
2	B	1129	ARG
2	B	1133	MET
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1149	GLU
2	B	1156	ASP
2	B	1160	VAL
2	B	1172	ILE
2	B	1175	LEU
2	B	1179	GLN
2	B	1183	LYS
2	B	1188	LYS
2	B	1190	ASP
2	B	1193	GLN
2	B	1202	LEU
2	B	1212	ILE
3	C	3	GLU
3	C	4	GLU
3	C	11	ARG
3	C	12	GLU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	27	LEU
3	C	44	LEU
3	C	48	SER
3	C	49	VAL
3	C	52	GLU
3	C	55	THR
3	C	79	GLN
3	C	89	GLU
3	C	93	ASP
3	C	100	THR
3	C	115	SER

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Mol	Chain	Res	Type
3	C	119	VAL
3	C	121	VAL
3	C	123	ASN
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	137	LYS
3	C	142	VAL
3	C	147	LEU
3	C	148	ARG
3	C	161	LYS
3	C	197	SER
3	C	215	GLU
3	C	226	ASP
3	C	228	PHE
3	C	230	MET
3	C	233	GLU
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	262	LEU
3	C	268	ASP
4	D	5	THR
4	D	9	GLN
4	D	10	THR
4	D	11	ARG
4	D	18	VAL
4	D	27	LEU
4	D	32	GLU
4	D	34	GLN
4	D	35	LEU
4	D	38	ILE
4	D	51	ASN
4	D	65	GLU
4	D	67	ARG
4	D	118	THR
4	D	123	LEU
4	D	125	SER
4	D	126	ILE
4	D	127	ASP

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Mol	Chain	Res	Type
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	156	ASP
4	D	164	ILE
4	D	165	GLN
4	D	177	VAL
4	D	182	SER
4	D	187	THR
4	D	197	SER
4	D	206	GLU
4	D	213	GLU
4	D	217	LEU
4	D	219	THR
4	D	221	TYR
5	E	14	ARG
5	E	31	THR
5	E	41	ASP
5	E	52	ARG
5	E	61	GLN
5	E	69	ILE
5	E	75	MET
5	E	84	ASP
5	E	92	THR
5	E	100	ILE
5	E	115	ASN
5	E	131	THR
5	E	149	LEU
5	E	150	VAL
5	E	152	LYS
5	E	171	LYS
5	E	175	LEU
5	E	182	ASP
5	E	184	VAL
5	E	190	LEU
5	E	191	LYS
5	E	192	ARG
5	E	196	VAL
5	E	202	SER
6	F	78	GLN
6	F	79	ARG
6	F	82	THR

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Mol	Chain	Res	Type
6	F	86	THR
6	F	90	ARG
6	F	93	ILE
6	F	97	ARG
6	F	110	ASP
6	F	125	LEU
6	F	138	LEU
6	F	152	ILE
6	F	153	VAL
6	F	155	LEU
7	G	11	ILE
7	G	22	MET
7	G	46	LEU
7	G	64	THR
7	G	65	ASP
7	G	73	LYS
7	G	91	VAL
7	G	106	MET
7	G	112	LYS
7	G	118	ASP
7	G	133	SER
7	G	134	GLU
7	G	135	ASP
7	G	154	VAL
7	G	171	ILE
8	H	9	ILE
8	H	12	VAL
8	H	14	GLU
8	H	26	ILE
8	H	31	THR
8	H	39	THR
8	H	42	ILE
8	H	49	VAL
8	H	76	THR
8	H	77	ARG
8	H	88	SER
8	H	89	LEU
8	H	91	ASP
8	H	95	TYR
8	H	103	LYS
8	H	106	GLU
8	H	107	VAL

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Mol	Chain	Res	Type
8	H	129	TYR
8	H	130	ARG
8	H	138	GLU
8	H	143	LEU
8	H	145	ARG
9	I	8	ARG
9	I	21	GLU
9	I	31	THR
9	I	50	THR
9	I	51	ASN
9	I	52	ILE
9	I	62	ILE
9	I	92	ARG
10	J	3	VAL
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	22	LEU
10	J	23	ASN
10	J	42	LYS
10	J	48	ARG
10	J	52	THR
10	J	56	LEU
11	K	1	MET
11	K	5	ASP
11	K	12	LEU
11	K	18	LYS
11	K	21	ILE
11	K	25	THR
11	K	29	ASN
11	K	33	ILE
11	K	37	LYS
11	K	47	ARG
11	K	51	LEU
11	K	63	VAL
11	K	91	CYS
11	K	101	LEU
11	K	102	LYS
11	K	114	LEU
12	L	27	LEU
12	L	30	ILE
12	L	33	GLU

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Mol	Chain	Res	Type
12	L	38	LEU
12	L	42	ARG
12	L	51	CYS
12	L	54	ARG
12	L	55	ILE
12	L	56	LEU
12	L	58	LYS
12	L	61	THR
12	L	64	LEU
12	L	66	GLN
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	54	ASN
1	A	64	ASN
1	A	71	GLN
1	A	209	ASN
1	A	281	HIS
1	A	311	GLN
1	A	358	ASN
1	A	397	ASN
1	A	510	GLN
1	A	545	GLN
1	A	548	ASN
1	A	584	ASN
1	A	640	GLN
1	A	654	ASN
1	A	660	ASN
1	A	742	ASN
1	A	760	GLN
1	A	811	GLN
1	A	968	GLN
1	A	969	GLN
1	A	994	GLN
1	A	1070	GLN
1	A	1106	ASN
1	A	1124	HIS
1	A	1128	GLN
1	A	1232	ASN

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Mol	Chain	Res	Type
1	A	1312	ASN
1	A	1390	ASN
1	A	1427	ASN
2	B	178	ASN
2	B	224	GLN
2	B	300	HIS
2	B	325	GLN
2	B	357	GLN
2	B	363	HIS
2	B	366	GLN
2	B	400	HIS
2	B	449	ASN
2	B	484	ASN
2	B	538	ASN
2	B	706	GLN
2	B	763	GLN
2	B	975	GLN
2	B	986	GLN
2	B	1025	HIS
2	B	1177	HIS
2	B	1193	GLN
2	B	1195	HIS
3	C	7	GLN
3	C	91	HIS
3	C	102	GLN
3	C	151	GLN
3	C	184	ASN
3	C	224	GLN
3	C	231	ASN
4	D	150	ASN
4	D	216	ASN
5	E	3	GLN
5	E	8	ASN
5	E	99	HIS
5	E	174	GLN
7	G	71	ASN
7	G	102	GLN
8	H	131	ASN
8	H	134	ASN
8	H	139	ASN
9	I	46	HIS
9	I	51	ASN

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Mol	Chain	Res	Type
9	I	60	GLN
9	I	83	ASN
9	I	89	GLN
9	I	108	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	1/2 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
15	BRU	T	15	13,15	18,21,22	0.87	0	25,30,33	2.07	7 (28%)

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	BRU	T	15	13,15	-	2/7/21/22	0/2/2/2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	15	BRU	C4-N3-C2	-4.73	121.14	127.34
15	T	15	BRU	O4-C4-C5	-4.34	120.26	125.80
15	T	15	BRU	N3-C2-N1	3.98	120.07	114.89
15	T	15	BRU	C5-C4-N3	3.59	117.47	113.34
15	T	15	BRU	O4'-C1'-N1	3.39	113.89	107.86
15	T	15	BRU	C1'-N1-C2	2.45	122.45	117.66
15	T	15	BRU	BR-C5-C4	2.29	120.66	118.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	T	15	BRU	C3'-C4'-C5'-O5'
15	T	15	BRU	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	T	15	BRU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
18	G2P	T	1024	-	30,34,34	1.80	6 (20%)	46,54,54	2.10	5 (10%)

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
18	G2P	T	1024	-	-	2/19/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	1024	G2P	C6-N1	4.12	1.46	1.38
18	T	1024	G2P	PB-O3B	3.95	1.62	1.58
18	T	1024	G2P	C4-N3	3.40	1.42	1.34
18	T	1024	G2P	C8-N9	2.84	1.43	1.37
18	T	1024	G2P	C2-N3	2.50	1.39	1.33
18	T	1024	G2P	C2-N2	2.28	1.39	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	1024	G2P	PB-O3B-PG	11.75	174.55	132.45
18	T	1024	G2P	O2A-PA-C3A	3.09	117.19	109.05
18	T	1024	G2P	O1G-PG-O2G	2.46	120.42	110.83
18	T	1024	G2P	O3G-PG-O1G	-2.42	98.74	107.80
18	T	1024	G2P	O2B-PB-C3A	2.09	114.56	109.05

There are no chirality outliers.

All (2) torsion outliers are listed below:

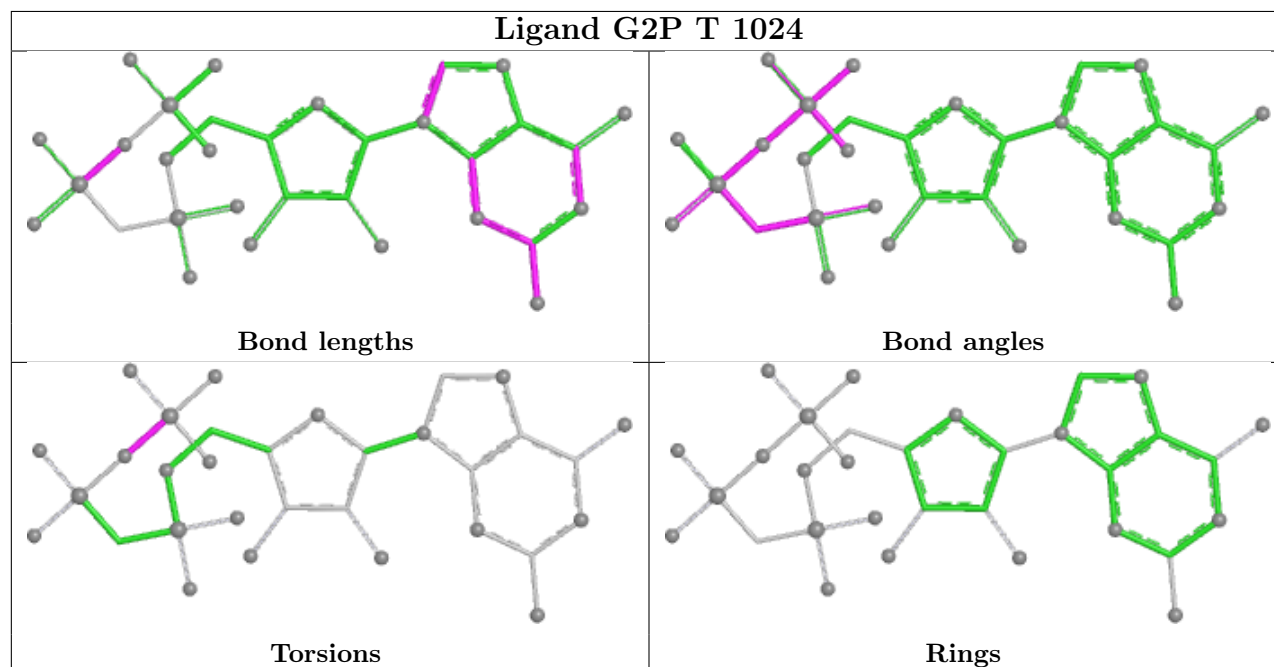
Mol	Chain	Res	Type	Atoms
18	T	1024	G2P	PB-O3B-PG-O1G
18	T	1024	G2P	PB-O3B-PG-O3G

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.74
1	B	351:TYR	C	352:ALA	N	3.20

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	1425/1732 (82%)	-0.38	9 (0%) 85 66	68, 122, 180, 239	0
2	B	1115/1224 (91%)	-0.25	13 (1%) 76 51	71, 135, 194, 224	0
3	C	266/318 (83%)	-0.54	0 100 100	89, 120, 158, 195	0
4	D	178/221 (80%)	-0.24	2 (1%) 78 53	95, 134, 183, 201	0
5	E	214/215 (99%)	-0.35	0 100 100	97, 158, 205, 214	0
6	F	84/155 (54%)	-0.64	1 (1%) 76 51	75, 103, 132, 149	0
7	G	171/171 (100%)	-0.38	1 (0%) 85 66	94, 119, 151, 181	0
8	H	133/146 (91%)	0.05	4 (3%) 52 32	135, 163, 198, 220	0
9	I	119/122 (97%)	-0.21	0 100 100	123, 168, 204, 216	0
10	J	65/70 (92%)	-0.49	1 (1%) 72 46	101, 117, 161, 173	0
11	K	115/120 (95%)	-0.63	1 (0%) 81 58	87, 119, 157, 171	0
12	L	46/70 (65%)	0.34	3 (6%) 25 18	110, 185, 203, 208	0
13	N	9/14 (64%)	0.71	1 (11%) 10 11	236, 246, 283, 284	0
14	P	2/2 (100%)	-0.01	0 100 100	216, 216, 216, 220	0
15	T	15/27 (55%)	0.54	1 (6%) 24 17	191, 217, 273, 276	0
All	All	3957/4607 (85%)	-0.32	37 (0%) 81 58	68, 129, 194, 284	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	446	LEU	4.4
12	L	27	LEU	4.4
2	B	708	GLU	4.1
4	D	24	ALA	3.8
2	B	134	LYS	3.7
2	B	709	ASP	3.7
1	A	1081	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	251	SER	3.5
8	H	63	LEU	3.4
1	A	1243	VAL	3.4
2	B	509	ALA	3.2
1	A	186	LYS	3.2
7	G	64	THR	3.2
2	B	502	ILE	3.1
6	F	72	LYS	3.0
12	L	28	LYS	2.9
13	N	1	DT	2.9
1	A	56	PRO	2.8
11	K	114	LEU	2.7
15	T	23	DA	2.5
2	B	584	GLY	2.5
1	A	1254	ALA	2.5
8	H	94	ASP	2.4
1	A	1092	LYS	2.4
10	J	65	PRO	2.4
2	B	383	ASN	2.3
2	B	251	ILE	2.3
2	B	70	ILE	2.3
4	D	25	ALA	2.2
1	A	190	ALA	2.2
12	L	26	THR	2.2
1	A	36	ARG	2.2
2	B	710	LEU	2.1
8	H	131	ASN	2.1
2	B	883	LEU	2.1
2	B	1224	PHE	2.0
8	H	139	ASN	2.0

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

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	BRU	T	15	20/21	0.85	0.11	214,225,227,233	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

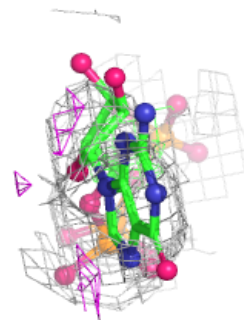
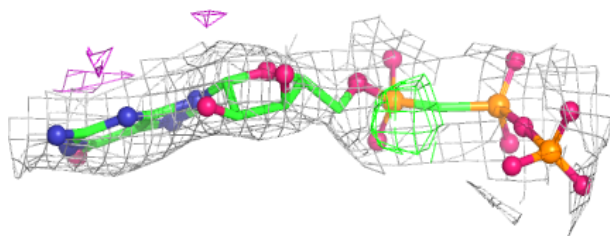
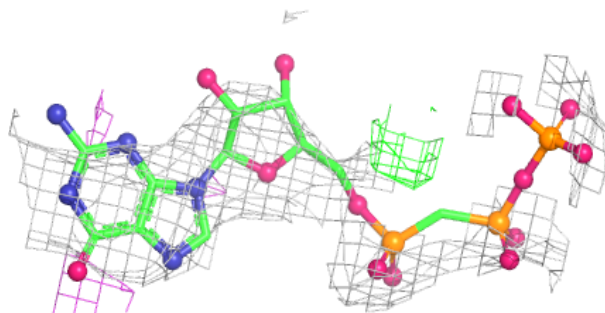
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	G2P	T	1024	32/32	0.85	0.11	221,226,247,248	0
16	ZN	L	1071	1/1	0.99	0.03	194,194,194,194	0
17	MG	A	2458	1/1	0.99	0.03	100,100,100,100	0
16	ZN	I	1122	1/1	0.99	0.05	217,217,217,217	0
16	ZN	I	1121	1/1	1.00	0.04	142,142,142,142	0
16	ZN	A	2456	1/1	1.00	0.02	157,157,157,157	0
16	ZN	J	1066	1/1	1.00	0.04	95,95,95,95	0
16	ZN	A	2457	1/1	1.00	0.01	82,82,82,82	0
16	ZN	B	2225	1/1	1.00	0.03	97,97,97,97	0
16	ZN	C	1269	1/1	1.00	0.02	96,96,96,96	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G2P T 1024:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.