Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 11:25 PM EDT

PDB ID	:	3PO2
Title	:	Arrested RNA Polymerase II elongation complex
Authors	:	Cheung, A.C.M.; Cramer, P.
Deposited on	:	2010-11-21
Resolution	:	3.30 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 (i) 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 (1)) were used in the production of this report:

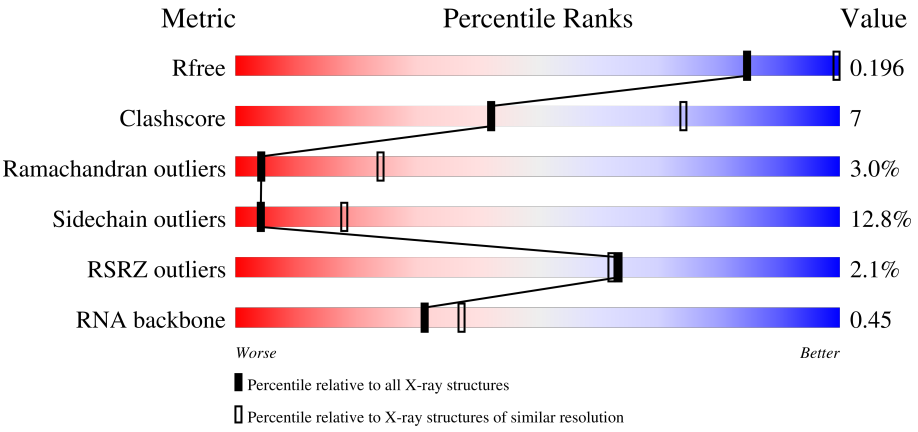
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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 <=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	1733	59% 19% 18%
2	B	1224	68% 20% 8%
3	C	318	57% 23% 16%
4	D	221	62% 17% 19%

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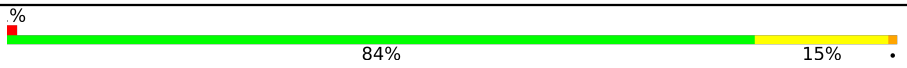
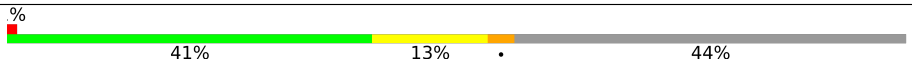
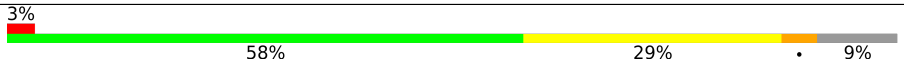
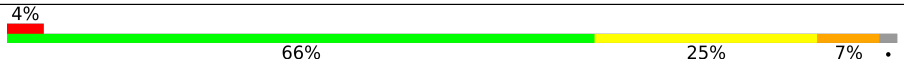
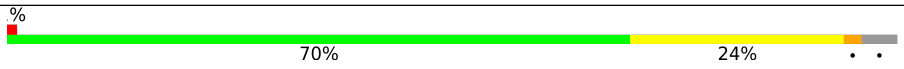
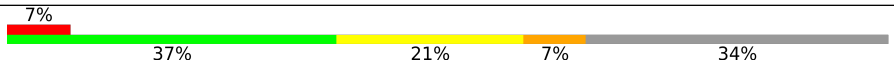
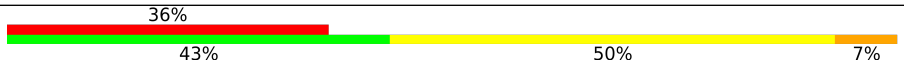
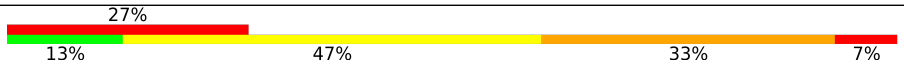
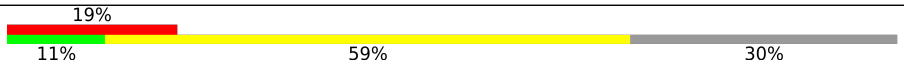
Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	14	
14	P	15	
15	T	27	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32287 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
			Total	C	N	O	S			
1	A	1421	11190	7052	1957	2119	62	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1121	8899	5632	1563	1649	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	180	1440	890	256	291	3	0	0	0

- Molecule 5 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			
5	E	214	1752	1111	309	321	11	0	0	0

- Molecule 6 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			
6	F	87	705	451	119	132	3	0	0	0

- Molecule 7 is a protein called 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 RPABC3.

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 RPABC5.

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 RPABC4.

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 DNA non-template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	14	Total	C	N	O	P	0	0	0
			288	138	57	80	13			

- Molecule 14 is a RNA chain called RNA product strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	15	Total	C	N	O	P	0	0	0
			300	135	45	105	15			

- Molecule 15 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	19	Total	Br	C	N	O	P	0	0	0
			389	1	185	66	118	19			

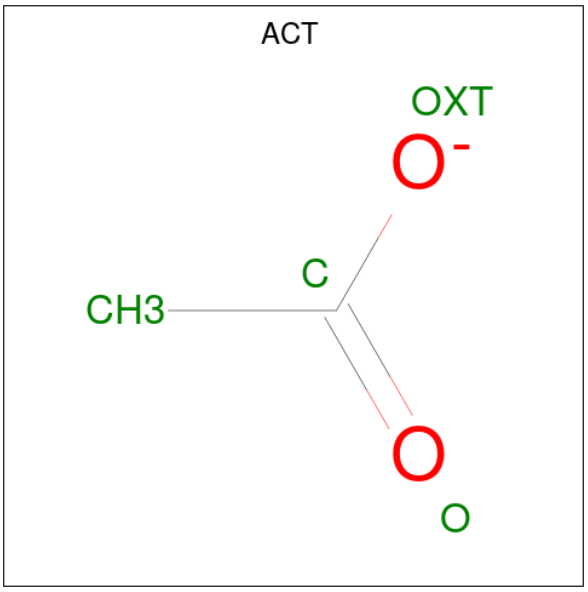
- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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 (three-letter code: MG) (formula: Mg).

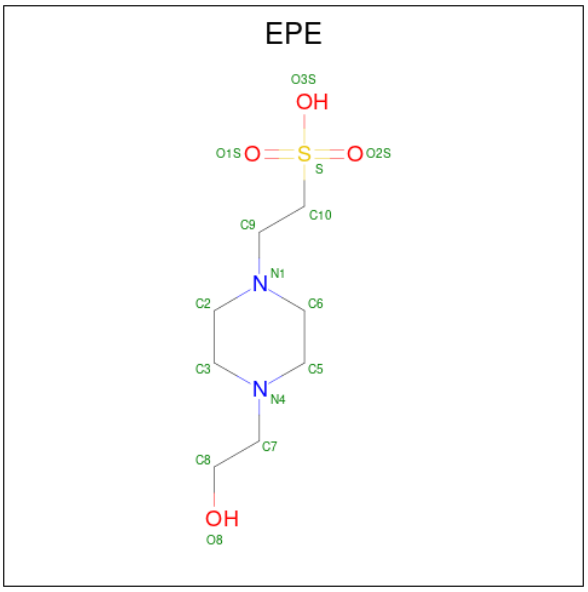
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Mg	0	0
			1	1		

- Molecule 18 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



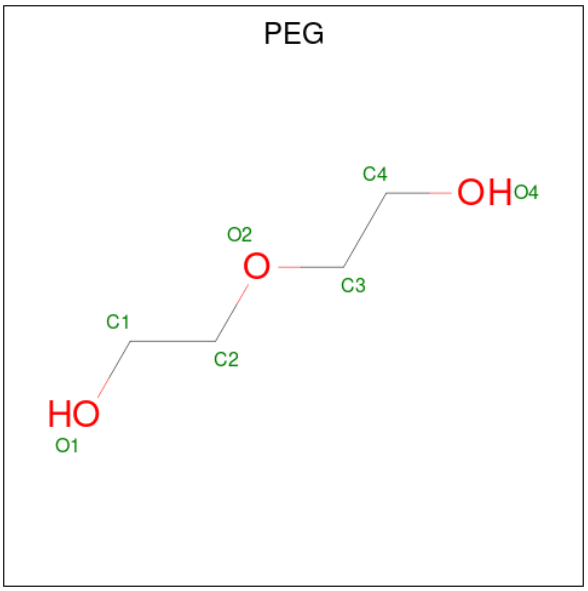
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 19 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 20 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



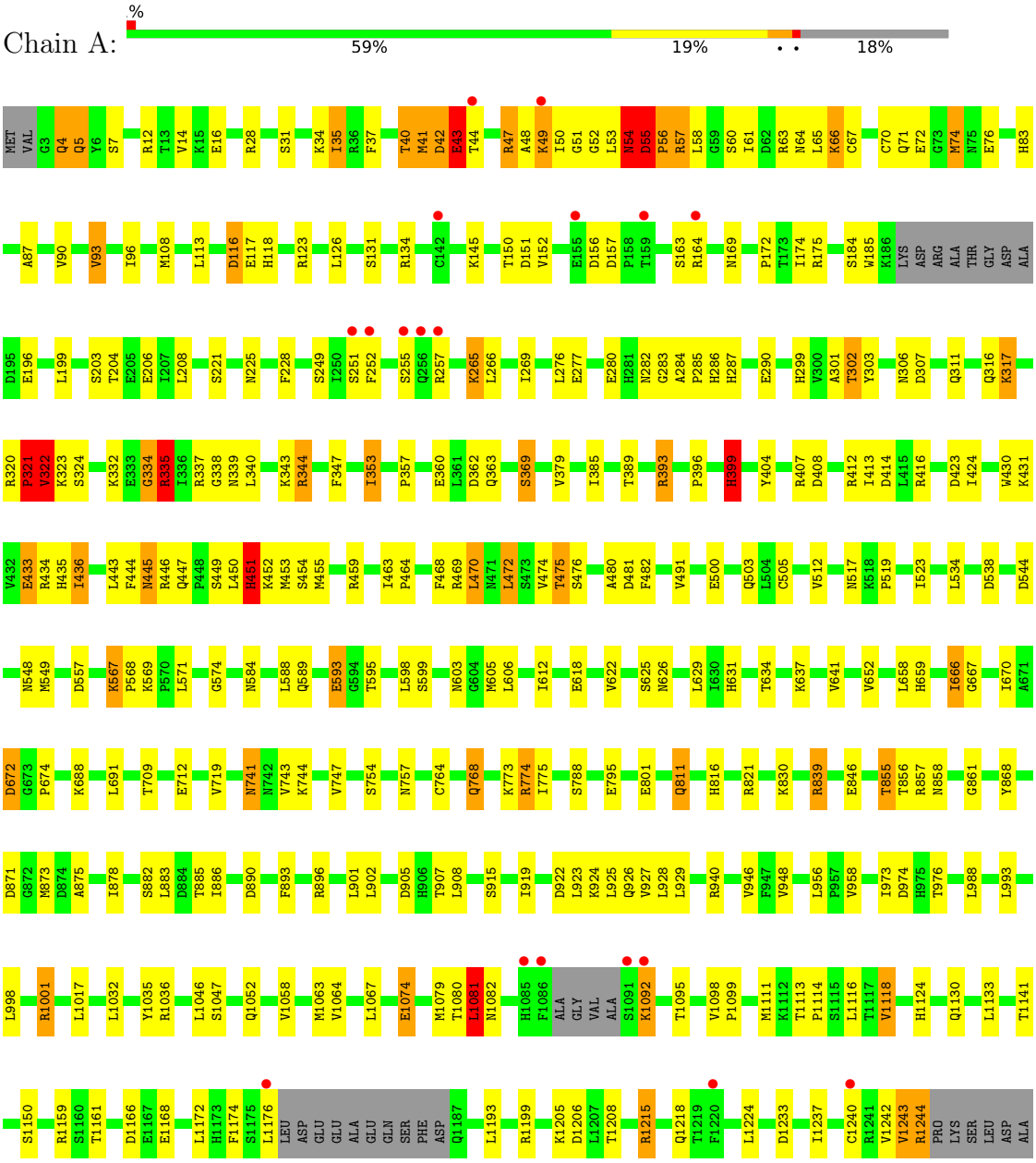
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	G	1	7	4	3	0	0

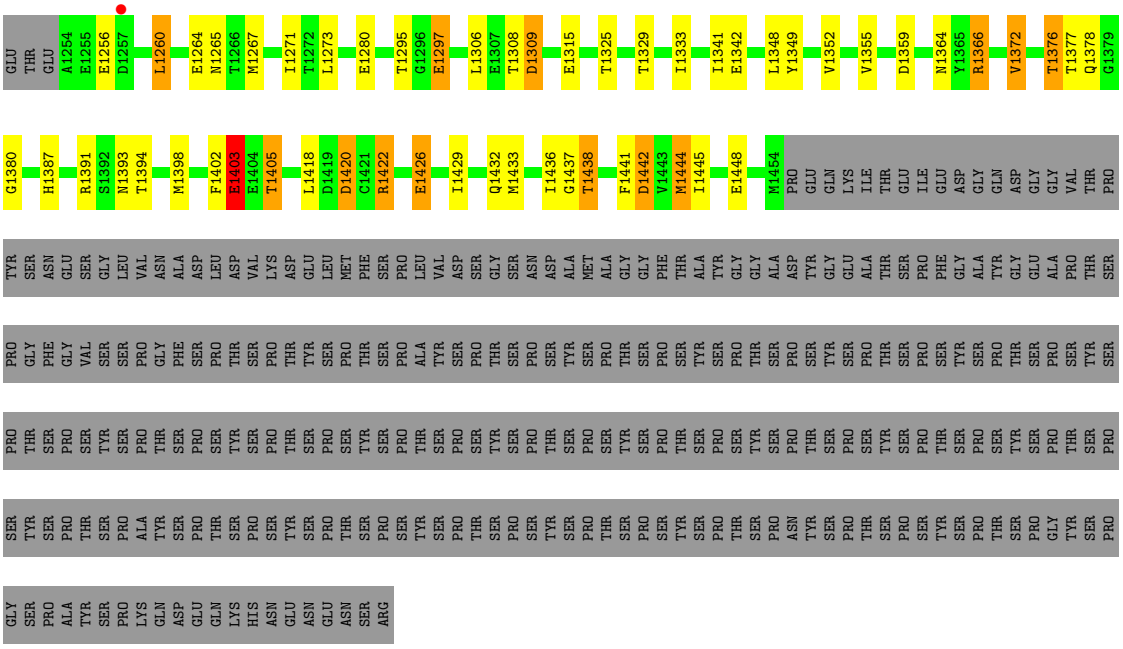
3 Residue-property plots (i)

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

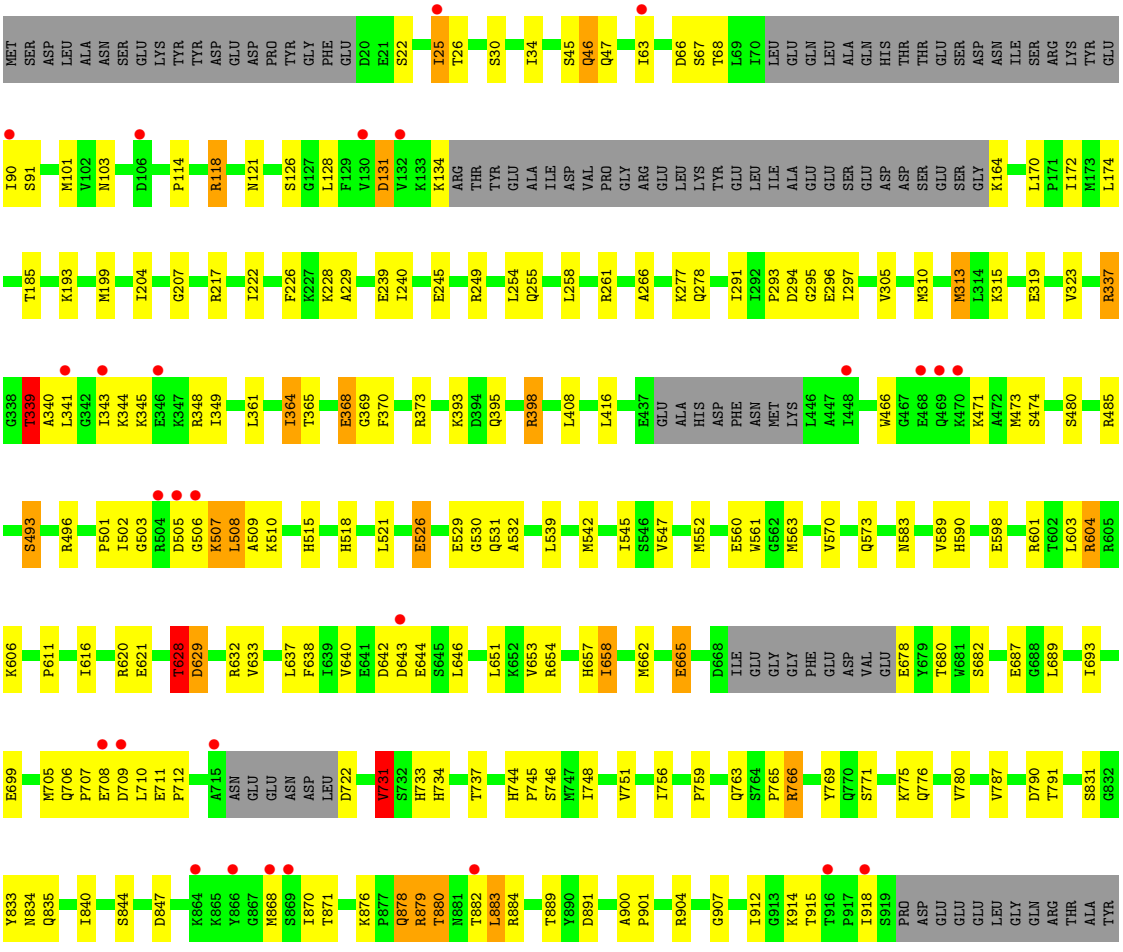
Chain A:

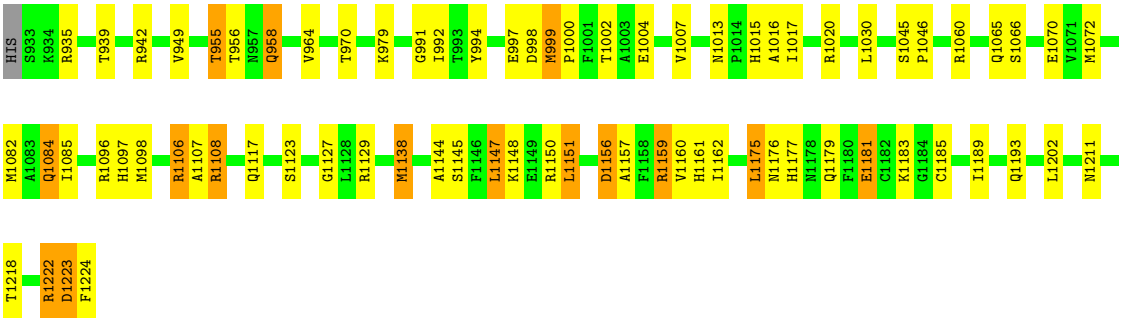




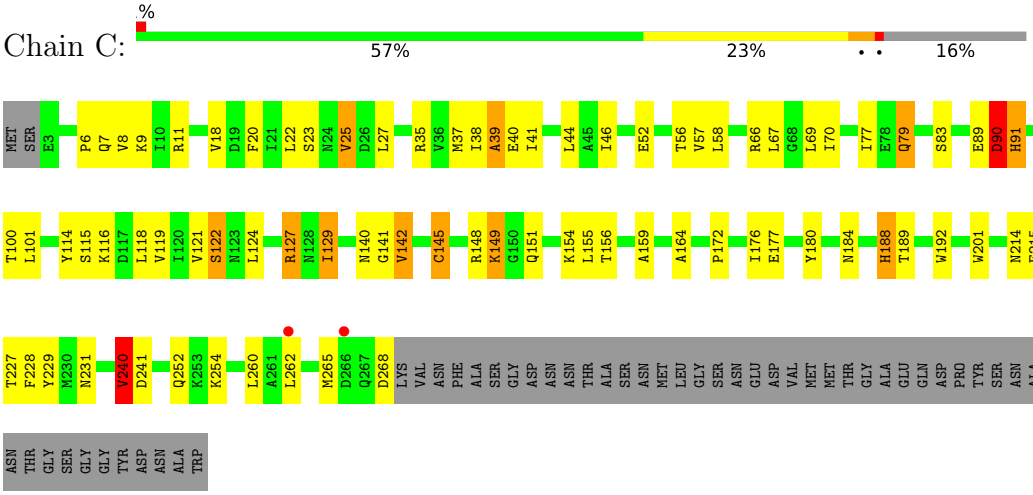
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

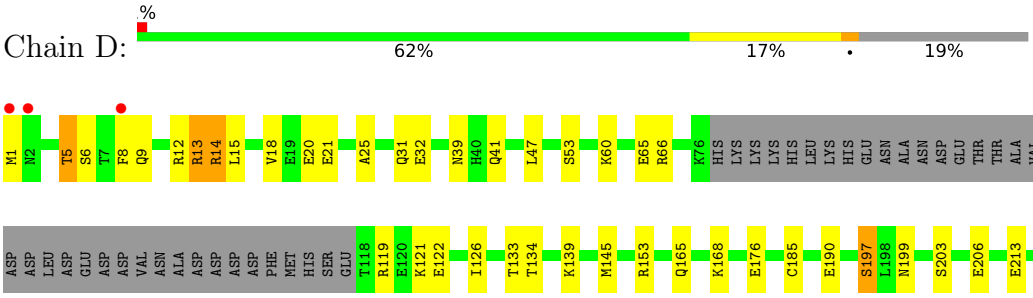




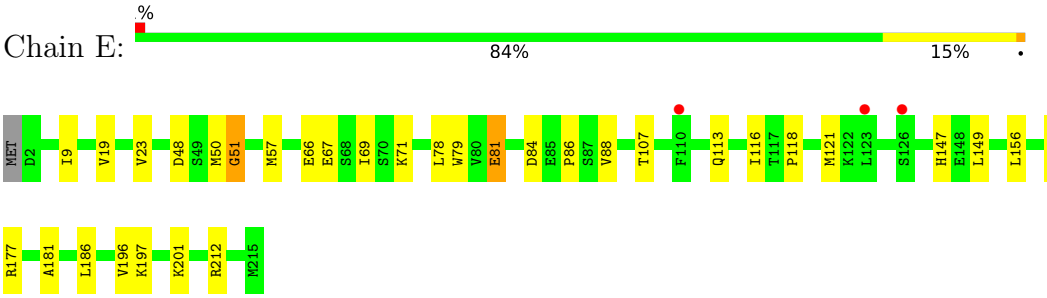
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3



• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

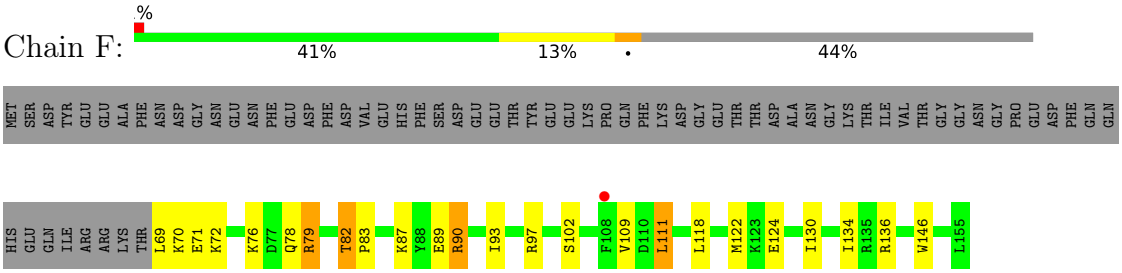


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



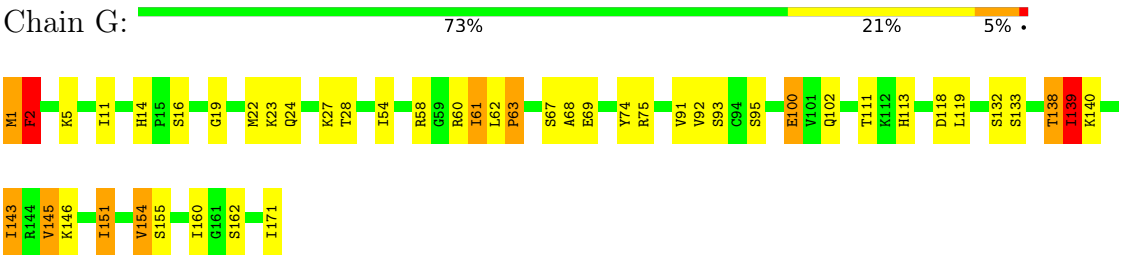
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



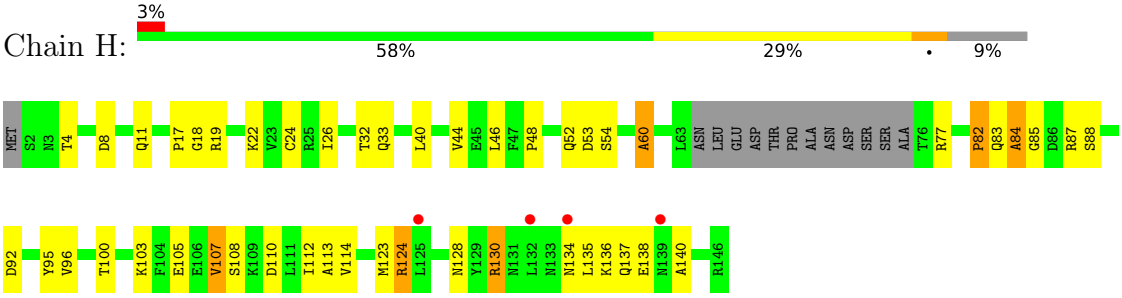
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



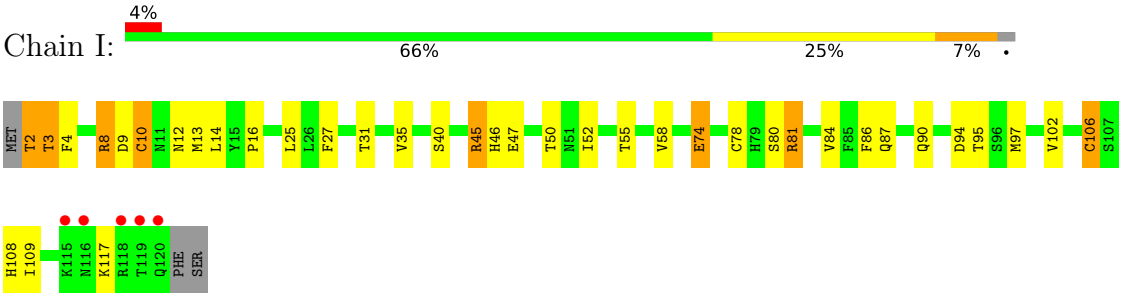
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



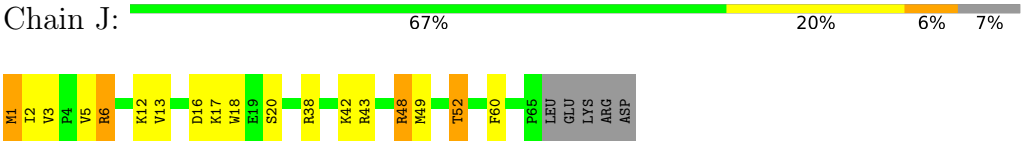
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

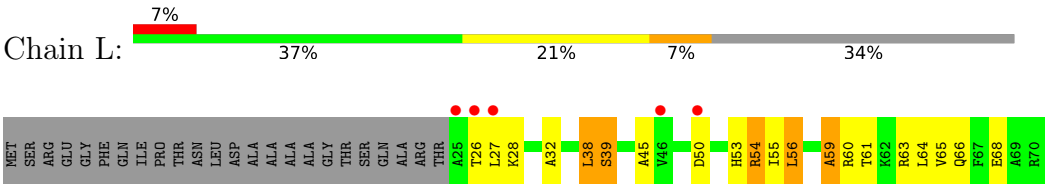
Chain J:



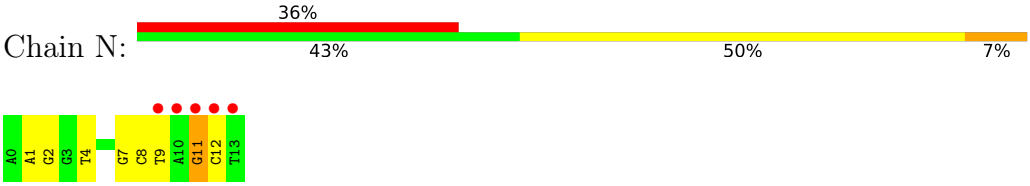
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:

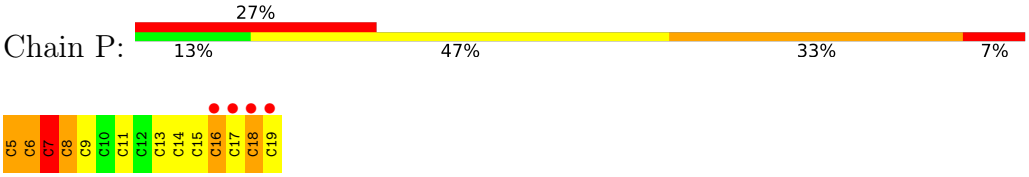
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



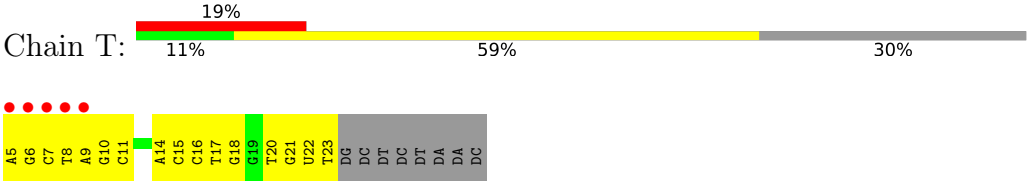
• Molecule 13: DNA non-template strand



• Molecule 14: RNA product strand



• Molecule 15: DNA template strand



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	224.57Å 394.55Å 282.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 3.30 48.98 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.98-3.30) 99.9 (48.98-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.153 , 0.178 0.173 , 0.196	Depositor DCC
R_{free} test set	3690 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	109.2	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 97.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.024 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.028 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	32287	wwPDB-VP
Average B, all atoms (Å^2)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PEG, ZN, EPE, MG, BRU, ACT

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	0.54	1/11391 (0.0%)	0.83	8/15402 (0.1%)
2	B	0.51	0/9072	0.79	2/12233 (0.0%)
3	C	0.50	0/2133	0.79	1/2891 (0.0%)
4	D	0.51	0/1450	0.84	1/1945 (0.1%)
5	E	0.45	0/1788	0.71	0/2406
6	F	0.59	0/717	0.85	0/967
7	G	0.51	0/1368	0.82	1/1844 (0.1%)
8	H	0.47	0/1086	0.81	0/1470
9	I	0.46	0/989	0.78	0/1331
10	J	0.48	0/541	0.84	1/727 (0.1%)
11	K	0.51	0/938	0.72	0/1267
12	L	0.59	0/365	1.05	1/485 (0.2%)
13	N	0.98	0/324	1.87	13/499 (2.6%)
14	P	1.44	2/329 (0.6%)	2.46	34/506 (6.7%)
15	T	1.20	2/411 (0.5%)	2.11	20/630 (3.2%)
All	All	0.55	5/32902 (0.0%)	0.89	82/44603 (0.2%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	PRO	C-N	5.88	1.47	1.34
14	P	5	C	C1'-N1	5.72	1.57	1.48
15	T	23	DT	C1'-N1	5.66	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	21	DG	N3-C4	5.04	1.39	1.35
14	P	6	C	C1'-N1	5.02	1.56	1.48

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	P	5	C	P-O3'-C3'	12.51	134.71	119.70
14	P	7	C	N1-C2-O2	11.87	126.02	118.90
15	T	8	DT	P-O3'-C3'	11.22	133.16	119.70
13	N	11	DG	O4'-C1'-N9	10.82	115.58	108.00
14	P	6	C	N1-C1'-C2'	8.75	125.38	114.00
15	T	20	DT	O4'-C1'-N1	8.61	114.03	108.00
15	T	21	DG	N3-C4-N9	8.41	131.05	126.00
14	P	7	C	C2-N1-C1'	8.19	127.81	118.80
14	P	6	C	P-O3'-C3'	7.92	129.21	119.70
14	P	7	C	N3-C2-O2	-7.83	116.42	121.90
13	N	12	DC	O4'-C1'-N1	7.67	113.37	108.00
14	P	9	C	C2-N3-C4	7.58	123.69	119.90
15	T	5	DA	P-O3'-C3'	7.33	128.50	119.70
13	N	4	DT	O4'-C1'-N1	7.25	113.08	108.00
14	P	6	C	C2-N1-C1'	7.20	126.72	118.80
15	T	11	DC	C2-N3-C4	7.17	123.48	119.90
1	A	55	ASP	N-CA-CB	7.10	123.37	110.60
15	T	15	DC	O4'-C1'-N1	7.01	112.91	108.00
1	A	399	HIS	N-CA-CB	6.99	123.19	110.60
15	T	11	DC	O4'-C1'-N1	6.85	112.79	108.00
1	A	56	PRO	C-N-CA	6.84	138.79	121.70
14	P	9	C	N1-C2-O2	6.80	122.98	118.90
4	D	25	ALA	C-N-CA	6.79	138.67	121.70
13	N	1	DA	O4'-C1'-N9	6.76	112.73	108.00
15	T	6	DG	P-O3'-C3'	6.75	127.81	119.70
13	N	12	DC	O4'-C4'-C3'	-6.68	101.83	104.50
15	T	21	DG	N3-C4-C5	-6.53	125.33	128.60
14	P	7	C	C6-N1-C1'	-6.51	112.99	120.80
14	P	7	C	N1-C1'-C2'	6.50	122.45	114.00
14	P	11	C	O4'-C1'-N1	6.48	113.38	108.20
15	T	23	DT	O4'-C1'-N1	6.45	112.51	108.00
14	P	7	C	P-O3'-C3'	6.40	127.38	119.70
15	T	15	DC	O4'-C4'-C3'	-6.38	101.95	104.50
15	T	11	DC	N1-C2-O2	6.34	122.71	118.90
14	P	6	C	N1-C2-O2	6.28	122.67	118.90
14	P	5	C	O4'-C1'-N1	6.27	113.21	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	P	13	C	O4'-C1'-N1	6.26	113.21	108.20
15	T	16	DC	P-O3'-C3'	6.26	127.22	119.70
15	T	21	DG	N3-C2-N2	6.26	124.28	119.90
14	P	15	C	O4'-C1'-N1	6.22	113.18	108.20
14	P	6	C	C6-N1-C2	-6.12	117.85	120.30
14	P	5	C	N1-C2-O2	6.06	122.54	118.90
1	A	54	ASN	C-N-CA	6.05	136.82	121.70
14	P	5	C	C6-N1-C2	-6.02	117.89	120.30
15	T	9	DA	P-O3'-C3'	6.01	126.91	119.70
14	P	9	C	O4'-C1'-N1	5.99	112.99	108.20
14	P	5	C	N1-C1'-C2'	5.99	121.78	114.00
14	P	9	C	C5-C6-N1	5.93	123.96	121.00
14	P	5	C	C2-N1-C1'	5.89	125.28	118.80
15	T	18	DG	O4'-C1'-N9	5.83	112.08	108.00
7	G	1	MET	C-N-CA	5.80	136.20	121.70
14	P	5	C	C5-C6-N1	5.79	123.89	121.00
13	N	11	DG	C1'-O4'-C4'	-5.78	104.32	110.10
13	N	11	DG	P-O3'-C3'	5.76	126.61	119.70
15	T	14	DA	P-O3'-C3'	5.71	126.56	119.70
3	C	39	ALA	N-CA-C	5.67	126.31	111.00
13	N	2	DG	P-O3'-C3'	5.61	126.44	119.70
15	T	17	DT	C4-C5-C7	5.61	122.36	119.00
2	B	628	THR	C-N-CA	5.59	135.66	121.70
1	A	1403	GLU	N-CA-C	5.54	125.97	111.00
10	J	5	VAL	N-CA-C	-5.52	96.08	111.00
14	P	14	C	O4'-C1'-N1	5.51	112.61	108.20
14	P	18	C	O4'-C1'-N1	5.51	112.61	108.20
13	N	7	DG	O4'-C1'-N9	5.47	111.83	108.00
14	P	6	C	P-O5'-C5'	5.41	129.56	120.90
13	N	9	DT	P-O3'-C3'	5.37	126.14	119.70
14	P	7	C	C5-C6-N1	5.36	123.68	121.00
14	P	9	C	C6-N1-C2	-5.33	118.17	120.30
1	A	1403	GLU	C-N-CA	-5.33	108.38	121.70
13	N	12	DC	C4'-C3'-C2'	-5.32	98.31	103.10
1	A	321	PRO	N-CA-C	5.29	125.85	112.10
15	T	10	DG	P-O3'-C3'	5.27	126.02	119.70
12	L	59	ALA	C-N-CA	5.25	134.84	121.70
13	N	8	DC	O4'-C1'-N1	5.22	111.66	108.00
13	N	8	DC	P-O3'-C3'	5.20	125.94	119.70
2	B	1181	GLU	N-CA-C	5.20	125.03	111.00
14	P	16	C	C4'-C3'-C2'	5.17	107.77	102.60
15	T	21	DG	C6-C5-N7	-5.17	127.30	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	P	6	C	N3-C2-O2	-5.14	118.30	121.90
14	P	7	C	C3'-C2'-C1'	5.13	105.61	101.50
1	A	451	HIS	N-CA-CB	-5.09	101.44	110.60
14	P	6	C	C5-C6-N1	5.04	123.52	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ASP	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11190	0	11255	209	0
2	B	8899	0	8940	117	0
3	C	2095	0	2051	45	0
4	D	1440	0	1456	9	0
5	E	1752	0	1776	13	0
6	F	705	0	731	12	0
7	G	1340	0	1357	23	0
8	H	1068	0	1040	16	0
9	I	971	0	927	19	0
10	J	532	0	542	11	0
11	K	920	0	929	21	0
12	L	363	0	386	6	0
13	N	288	0	159	1	0
14	P	300	0	166	1	0
15	T	389	0	214	1	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	A	4	0	3	0	0
19	D	15	0	17	0	0
20	G	7	0	10	0	0
All	All	32287	0	31959	445	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 7.

All (445) 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)
7:G:151:ILE:CD1	7:G:151:ILE:CG1	1.75	1.58
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.40	1.02
1:A:53:LEU:HD23	1:A:54:ASN:H	1.24	1.02
1:A:1081:LEU:HB2	1:A:1082:ASN:HA	1.43	0.96
10:J:48:ARG:O	10:J:52:THR:HG22	1.67	0.94
1:A:855:THR:HG21	1:A:857:ARG:HE	1.32	0.92
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.51	0.91
10:J:48:ARG:HE	10:J:49:MET:HE2	1.37	0.89
1:A:1081:LEU:HD12	1:A:1082:ASN:HD22	1.38	0.87
11:K:65:HIS:HD2	11:K:67:PHE:H	1.19	0.86
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.56	0.85
1:A:56:PRO:O	1:A:57:ARG:NE	2.10	0.84
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.43	0.82
2:B:900:ALA:HB3	12:L:61:THR:HG23	1.63	0.80
2:B:654:ARG:H	2:B:657:HIS:HD2	1.27	0.79
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.64	0.79
1:A:53:LEU:HD23	1:A:54:ASN:N	1.97	0.78
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.28	0.77
1:A:225:ASN:HD22	1:A:228:PHE:H	1.34	0.75
1:A:55:ASP:N	1:A:56:PRO:HD3	2.01	0.75
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.67	0.75
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.68	0.74
2:B:878:GLN:O	2:B:883:LEU:HD21	1.87	0.74
7:G:1:MET:SD	7:G:2:PHE:N	2.61	0.74
1:A:1079:MET:HB3	1:A:1081:LEU:HD23	1.70	0.74
7:G:111:THR:HG22	7:G:113:HIS:H	1.53	0.73
6:F:118:LEU:O	6:F:122:MET:HG3	1.88	0.73
1:A:875:ALA:HB2	1:A:1366:ARG:HD3	1.70	0.73
2:B:1013:ASN:HD21	2:B:1015:HIS:CD2	2.06	0.73
1:A:855:THR:CG2	1:A:857:ARG:HE	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1013:ASN:HD21	2:B:1015:HIS:HD2	1.37	0.73
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.55	0.72
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.70	0.71
1:A:40:THR:HG22	1:A:41:MET:HG2	1.70	0.71
1:A:472:LEU:O	1:A:475:THR:HB	1.91	0.71
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.56	0.71
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.71	0.71
11:K:65:HIS:CD2	11:K:67:PHE:H	2.06	0.71
3:C:66:ARG:NH2	10:J:3:VAL:O	2.25	0.70
1:A:1079:MET:HB3	1:A:1081:LEU:CD2	2.22	0.69
1:A:1081:LEU:HB2	1:A:1082:ASN:CA	2.19	0.69
2:B:744:HIS:HD2	2:B:746:SER:H	1.39	0.69
12:L:28:LYS:HB2	12:L:39:SER:HA	1.73	0.68
7:G:119:LEU:HD12	7:G:132:SER:HB2	1.76	0.68
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.76	0.68
1:A:316:GLN:HG3	1:A:317:LYS:HG2	1.75	0.67
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.58	0.67
1:A:344:ARG:HH11	1:A:344:ARG:HB3	1.60	0.67
1:A:56:PRO:HD2	1:A:58:LEU:HG	1.76	0.67
3:C:67:LEU:HA	3:C:70:ILE:HD12	1.75	0.67
1:A:347:PHE:H	2:B:1107:ALA:HA	1.60	0.67
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.75	0.66
7:G:14:HIS:CD2	7:G:16:SER:H	2.13	0.66
1:A:1444:MET:HG2	7:G:58:ARG:HB3	1.77	0.66
2:B:339:THR:HG23	2:B:340:ALA:HB2	1.77	0.66
1:A:567:LYS:HB2	8:H:96:VAL:HB	1.78	0.65
3:C:252:GLN:HG2	11:K:95:ILE:HG23	1.77	0.65
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.79	0.65
1:A:64:ASN:HD22	1:A:66:LYS:HB2	1.63	0.64
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.78	0.64
1:A:709:THR:HG23	9:I:94:ASP:HA	1.79	0.64
1:A:444:PHE:HE2	1:A:470:LEU:HD22	1.62	0.64
1:A:399:HIS:O	1:A:435:HIS:HD2	1.81	0.64
2:B:640:VAL:HG22	2:B:651:LEU:HG	1.78	0.64
14:P:7:C:H2'	14:P:8:C:O4'	1.97	0.64
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.79	0.63
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.31	0.63
1:A:1348:LEU:HG	1:A:1372:VAL:HG22	1.81	0.63
1:A:469:ARG:NH2	2:B:991:GLY:O	2.27	0.62
1:A:175:ARG:HH22	1:A:184:SER:HB2	1.64	0.62
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ILE:HD13	1:A:1380:GLY:HA2	1.81	0.62
2:B:706:GLN:H	2:B:710:LEU:HD13	1.65	0.62
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.80	0.62
2:B:1013:ASN:ND2	2:B:1015:HIS:CD2	2.68	0.61
10:J:3:VAL:HG11	10:J:18:TRP:HB2	1.82	0.61
1:A:1267:MET:HA	1:A:1271:ILE:HD12	1.82	0.61
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.99	0.61
3:C:98:VAL:H	3:C:122:SER:HB3	1.64	0.61
8:H:4:THR:HA	8:H:60:ALA:HB2	1.83	0.61
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.81	0.61
2:B:705:MET:H	2:B:710:LEU:HD22	1.65	0.61
3:C:142:VAL:H	10:J:16:ASP:HB3	1.65	0.61
1:A:306:ASN:ND2	1:A:321:PRO:O	2.34	0.61
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.83	0.61
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.81	0.61
1:A:37:PHE:HD1	1:A:52:GLY:HA3	1.67	0.60
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.83	0.60
2:B:310:MET:O	2:B:313:MET:HB2	2.00	0.60
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.84	0.60
2:B:1013:ASN:ND2	2:B:1015:HIS:HD2	2.00	0.60
1:A:316:GLN:HG3	1:A:317:LYS:H	1.67	0.59
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.84	0.59
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.34	0.59
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.48	0.59
1:A:741:ASN:HD22	1:A:744:LYS:H	1.49	0.59
2:B:883:LEU:HB3	2:B:935:ARG:H	1.68	0.59
1:A:1141:THR:HG23	1:A:1205:LYS:HD3	1.84	0.59
2:B:1013:ASN:HD22	2:B:1015:HIS:H	1.50	0.59
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.36	0.59
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.83	0.59
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.84	0.58
1:A:31:SER:OG	1:A:83:HIS:HD2	1.87	0.58
1:A:37:PHE:CD1	1:A:52:GLY:HA3	2.38	0.58
1:A:41:MET:HB3	1:A:49:LYS:HA	1.84	0.58
1:A:14:VAL:H	1:A:1432:GLN:NE2	2.01	0.58
1:A:41:MET:HG3	1:A:42:ASP:H	1.68	0.58
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.86	0.58
9:I:106:CYS:SG	9:I:108:HIS:HB3	2.44	0.58
2:B:1222:ARG:O	2:B:1223:ASP:HB3	2.03	0.58
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.18	0.57
2:B:121:ASN:HD22	2:B:207:GLY:HA3	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.86	0.57
1:A:1124:HIS:HB3	1:A:1130:GLN:HG2	1.86	0.57
1:A:134:ARG:HD2	1:A:221:SER:O	2.04	0.57
1:A:203:SER:OG	1:A:206:GLU:HB2	2.03	0.57
3:C:56:THR:HG22	3:C:58:LEU:H	1.69	0.57
6:F:93:ILE:CD1	6:F:134:ILE:HD11	2.27	0.57
1:A:55:ASP:OD1	1:A:57:ARG:HA	2.05	0.57
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.86	0.57
1:A:534:LEU:O	1:A:574:GLY:HA3	2.04	0.57
1:A:839:ARG:HH22	1:A:1402:PHE:HA	1.68	0.57
2:B:710:LEU:HA	2:B:733:HIS:CB	2.31	0.57
1:A:225:ASN:ND2	1:A:228:PHE:H	2.01	0.57
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.86	0.56
1:A:299:HIS:HA	1:A:302:THR:HG22	1.88	0.56
1:A:339:ASN:HB3	2:B:1117:GLN:NE2	2.17	0.56
1:A:451:HIS:CE1	1:A:1074:GLU:HG2	2.41	0.56
2:B:756:ILE:O	2:B:759:PRO:HD3	2.05	0.56
10:J:6:ARG:HG2	10:J:13:VAL:HG22	1.86	0.56
5:E:86:PRO:HA	5:E:113:GLN:HB2	1.87	0.56
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.88	0.56
1:A:332:LYS:H	1:A:337:ARG:HB2	1.70	0.56
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.87	0.56
12:L:61:THR:HB	12:L:63:ARG:H	1.71	0.56
1:A:568:PRO:HD3	8:H:95:TYR:HA	1.88	0.56
1:A:503:GLN:NE2	6:F:90:ARG:HH22	2.03	0.55
8:H:135:LEU:C	8:H:137:GLN:H	2.09	0.55
2:B:239:GLU:HG2	2:B:255:GLN:HG2	1.88	0.55
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.88	0.55
7:G:143:ILE:HG22	7:G:145:VAL:HG22	1.88	0.55
2:B:637:LEU:HD12	2:B:693:ILE:HD13	1.89	0.55
1:A:593:GLU:HB3	1:A:603:ASN:HD21	1.72	0.55
2:B:507:LYS:HD2	2:B:508:LEU:HD13	1.88	0.55
2:B:901:PRO:O	2:B:949:VAL:O	2.26	0.55
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.89	0.55
6:F:111:LEU:HD12	6:F:111:LEU:H	1.72	0.54
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.90	0.54
13:N:11:DG:H1	15:T:7:DC:H42	1.55	0.54
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.89	0.54
7:G:138:THR:HG22	7:G:139:ILE:H	1.72	0.54
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.43	0.54
1:A:658:LEU:HD23	1:A:659:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:907:THR:HG22	1:A:908:LEU:H	1.71	0.54
2:B:344:LYS:HG3	2:B:348:ARG:HE	1.73	0.53
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.38	0.53
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.91	0.53
3:C:148:ARG:H	3:C:151:GLN:HB2	1.74	0.53
1:A:399:HIS:O	1:A:435:HIS:CD2	2.62	0.53
2:B:654:ARG:H	2:B:657:HIS:CD2	2.17	0.53
2:B:47:GLN:HE21	2:B:408:LEU:HD12	1.74	0.53
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.91	0.53
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.92	0.52
1:A:1215:ARG:HG2	1:A:1273:LEU:HA	1.91	0.52
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.91	0.52
1:A:1081:LEU:CB	1:A:1082:ASN:HA	2.30	0.52
1:A:49:LYS:HG2	1:A:61:ILE:HD12	1.91	0.52
2:B:1082:MET:HA	3:C:189:THR:HA	1.91	0.52
2:B:193:LYS:HB3	2:B:787:VAL:HG11	1.92	0.52
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.75	0.52
2:B:291:ILE:HG22	2:B:297:ILE:HG13	1.91	0.52
1:A:344:ARG:HB3	1:A:344:ARG:NH1	2.25	0.51
9:I:2:THR:O	9:I:3:THR:HG22	2.10	0.51
1:A:316:GLN:HG3	1:A:317:LYS:N	2.25	0.51
1:A:55:ASP:O	1:A:55:ASP:OD2	2.27	0.51
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.45	0.51
1:A:901:LEU:HA	1:A:907:THR:HG23	1.92	0.51
5:E:181:ALA:HA	5:E:186:LEU:HD21	1.93	0.51
1:A:444:PHE:CE2	1:A:470:LEU:HD22	2.44	0.51
1:A:709:THR:HB	1:A:712:GLU:H	1.76	0.51
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.76	0.51
2:B:880:THR:O	2:B:883:LEU:HG	2.11	0.51
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.93	0.51
1:A:1081:LEU:HD13	1:A:1099:PRO:HD2	1.93	0.51
12:L:32:ALA:HB3	12:L:55:ILE:HG21	1.93	0.50
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.76	0.50
3:C:241:ASP:HB3	11:K:109:TRP:CE2	2.46	0.50
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.94	0.50
9:I:74:GLU:HB3	9:I:81:ARG:HD3	1.93	0.50
1:A:463:ILE:HD12	1:A:464:PRO:O	2.11	0.50
3:C:79:GLN:HB3	3:C:127:ARG:HD2	1.94	0.50
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.94	0.50
1:A:35:ILE:HA	1:A:52:GLY:O	2.12	0.50
1:A:1199:ARG:NH2	1:A:1233:ASP:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:254:LYS:HG2	11:K:42:LEU:HD13	1.92	0.50
5:E:66:GLU:HA	5:E:69:ILE:HD12	1.92	0.50
1:A:335:ARG:HH11	1:A:339:ASN:ND2	2.10	0.50
4:D:176:GLU:OE2	4:D:197:SER:HB2	2.10	0.50
10:J:48:ARG:HE	10:J:49:MET:CE	2.18	0.50
7:G:61:ILE:HG13	7:G:68:ALA:HB2	1.94	0.49
8:H:82:PRO:O	8:H:84:ALA:N	2.45	0.49
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.94	0.49
1:A:285:PRO:O	1:A:287:HIS:N	2.43	0.49
9:I:50:THR:HG22	9:I:52:ILE:H	1.77	0.49
2:B:955:THR:HB	12:L:54:ARG:O	2.12	0.49
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.95	0.49
4:D:5:THR:HG21	7:G:74:TYR:OH	2.12	0.49
9:I:8:ARG:NE	9:I:9:ASP:OD1	2.45	0.49
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.44	0.49
1:A:855:THR:HG21	1:A:857:ARG:NE	2.15	0.49
2:B:315:LYS:HG2	9:I:13:MET:HE2	1.95	0.48
2:B:278:GLN:HB3	2:B:337:ARG:HG2	1.95	0.48
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.48
1:A:396:PRO:HG2	1:A:416:ARG:HB3	1.94	0.48
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.48	0.48
2:B:955:THR:OG1	2:B:956:THR:N	2.45	0.48
7:G:92:VAL:HG21	7:G:102:GLN:HB2	1.95	0.48
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.95	0.48
1:A:55:ASP:H	1:A:56:PRO:HD3	1.77	0.48
1:A:56:PRO:CD	1:A:58:LEU:HG	2.43	0.48
1:A:343:LYS:HE3	2:B:1156:ASP:OD2	2.13	0.48
1:A:369:SER:H	11:K:2:ASN:HD21	1.62	0.48
1:A:1308:THR:HG22	1:A:1309:ASP:N	2.28	0.48
2:B:126:SER:OG	2:B:172:ILE:HD11	2.14	0.48
4:D:185:CYS:HB3	4:D:190:GLU:HB3	1.96	0.48
1:A:1387:HIS:HA	1:A:1391:ARG:HH11	1.77	0.48
11:K:107:THR:O	11:K:111:LEU:HG	2.14	0.48
1:A:503:GLN:HE21	6:F:90:ARG:HH22	1.60	0.48
1:A:393:ARG:HH22	1:A:424:ILE:H	1.62	0.48
3:C:22:LEU:O	3:C:227:THR:HA	2.13	0.48
3:C:57:VAL:HG23	3:C:58:LEU:HD13	1.96	0.48
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.94	0.48
7:G:62:LEU:HD21	7:G:69:GLU:HB2	1.95	0.48
2:B:34:ILE:HG12	2:B:542:MET:CE	2.44	0.48
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLY:H	1:A:338:GLY:HA3	1.79	0.47
1:A:362:ASP:OD1	1:A:459:ARG:NH1	2.43	0.47
3:C:91:HIS:HA	3:C:95:CYS:SG	2.54	0.47
1:A:1442:ASP:HB3	1:A:1444:MET:HE1	1.95	0.47
2:B:561:TRP:O	2:B:590:HIS:HE1	1.98	0.47
1:A:49:LYS:NZ	1:A:55:ASP:HB3	2.30	0.47
1:A:93:VAL:HA	1:A:96:ILE:HD12	1.96	0.47
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.95	0.47
2:B:1107:ALA:O	2:B:1108:ARG:HB2	2.14	0.47
4:D:13:ARG:HH22	4:D:18:VAL:HA	1.80	0.47
1:A:255:SER:H	2:B:918:ILE:HD13	1.78	0.47
4:D:13:ARG:HH12	4:D:18:VAL:HB	1.77	0.47
2:B:25:ILE:HD11	2:B:658:ILE:HD13	1.96	0.47
2:B:1106:ARG:HG2	2:B:1127:GLY:HA2	1.97	0.47
2:B:1016:ALA:O	2:B:1020:ARG:HG3	2.15	0.47
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.45	0.47
1:A:55:ASP:N	1:A:56:PRO:CD	2.73	0.46
2:B:1072:MET:HB2	2:B:1085:ILE:HD13	1.97	0.46
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.80	0.46
5:E:79:TRP:HE1	5:E:81:GLU:HG3	1.79	0.46
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.97	0.46
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.97	0.46
8:H:100:THR:HG23	8:H:138:GLU:HA	1.96	0.46
1:A:569:LYS:HD2	3:C:221:TYR:HB2	1.98	0.46
2:B:530:GLY:O	2:B:532:ALA:N	2.45	0.46
4:D:165:GLN:HA	4:D:168:LYS:HD2	1.97	0.46
1:A:1150:SER:HB3	9:I:46:HIS:CB	2.46	0.46
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.97	0.46
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.98	0.46
1:A:1032:LEU:O	1:A:1036:ARG:HD2	2.15	0.46
3:C:180:TYR:OH	3:C:188:HIS:HD2	1.98	0.46
1:A:1172:LEU:C	1:A:1174:PHE:H	2.19	0.46
1:A:1342:GLU:OE2	5:E:212:ARG:NH1	2.48	0.46
12:L:38:LEU:HD22	12:L:56:LEU:HD21	1.98	0.46
1:A:1418:LEU:HD23	2:B:1222:ARG:HE	1.81	0.45
3:C:56:THR:HG22	3:C:57:VAL:N	2.31	0.45
1:A:116:ASP:C	1:A:118:HIS:H	2.19	0.45
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.80	0.45
1:A:754:SER:H	1:A:757:ASN:HD22	1.64	0.45
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.97	0.45
1:A:43:GLU:OE2	1:A:48:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:HIS:HA	1:A:290:GLU:HG2	1.98	0.45
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.80	0.45
2:B:776:GLN:HA	2:B:1096:ARG:NH1	2.32	0.45
3:C:101:LEU:HB2	3:C:118:LEU:HD23	1.99	0.45
1:A:12:ARG:HD3	2:B:1218:THR:HB	1.98	0.45
1:A:53:LEU:CD2	1:A:54:ASN:H	2.12	0.45
1:A:265:LYS:HG2	1:A:303:TYR:HB2	1.97	0.45
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.99	0.45
2:B:604:ARG:HD3	2:B:611:PRO:HA	1.98	0.45
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.82	0.45
1:A:883:LEU:O	1:A:886:ILE:HG22	2.17	0.45
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.98	0.45
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.98	0.45
2:B:114:PRO:HB3	2:B:174:LEU:HD21	1.99	0.45
1:A:404:TYR:CD2	1:A:412:ARG:HG2	2.51	0.45
3:C:37:MET:HA	3:C:41:ILE:HD12	1.98	0.45
3:C:77:ILE:HA	3:C:129:ILE:HD11	1.99	0.45
4:D:66:ARG:HD2	4:D:133:THR:HB	1.97	0.45
1:A:379:VAL:HG22	1:A:431:LYS:HD3	1.99	0.45
1:A:67:CYS:H	1:A:71:GLN:HA	1.82	0.45
1:A:538:ASP:HB3	8:H:22:LYS:HG3	1.98	0.44
1:A:548:ASN:HD21	11:K:47:ARG:HH21	1.65	0.44
1:A:1193:LEU:HB2	1:A:1260:LEU:HD23	1.99	0.44
3:C:11:ARG:NH2	3:C:229:TYR:HD2	2.12	0.44
5:E:147:HIS:CD2	5:E:149:LEU:H	2.35	0.44
1:A:41:MET:HA	1:A:50:ILE:HB	1.99	0.44
1:A:512:VAL:HA	1:A:519:PRO:HA	1.98	0.44
5:E:19:VAL:O	5:E:23:VAL:HG23	2.16	0.44
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.98	0.44
2:B:912:ILE:HB	2:B:939:THR:HB	1.97	0.44
5:E:50:MET:SD	5:E:51:GLY:N	2.90	0.44
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.53	0.44
3:C:124:LEU:HD22	3:C:129:ILE:HG22	2.00	0.44
2:B:294:ASP:H	9:I:12:ASN:HD22	1.65	0.44
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.99	0.44
1:A:672:ASP:HB3	1:A:674:PRO:HD2	1.99	0.44
9:I:16:PRO:HB3	9:I:25:LEU:HD11	2.00	0.44
1:A:339:ASN:CB	2:B:1117:GLN:HE22	2.23	0.44
2:B:345:LYS:HA	2:B:349:ILE:HD13	1.99	0.44
2:B:1177:HIS:HB3	2:B:1179:GLN:NE2	2.32	0.44
1:A:743:VAL:O	1:A:747:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:ARG:HH11	2:B:539:LEU:HB2	1.83	0.44
2:B:844:SER:O	2:B:847:ASP:HB2	2.17	0.44
2:B:889:THR:HG22	2:B:891:ASP:H	1.83	0.44
9:I:78:CYS:SG	9:I:80:SER:HB3	2.58	0.44
1:A:1243:VAL:HG22	1:A:1244:ARG:H	1.83	0.44
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.83	0.44
1:A:123:ARG:HA	1:A:126:LEU:HD12	2.00	0.43
2:B:765:PRO:O	2:B:769:TYR:HD1	2.00	0.43
7:G:60:ARG:NH2	7:G:63:PRO:HD3	2.33	0.43
9:I:45:ARG:NH1	9:I:47:GLU:OE1	2.51	0.43
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.53	0.43
2:B:644:GLU:C	2:B:646:LEU:H	2.16	0.43
2:B:833:TYR:HB3	2:B:992:ILE:CG2	2.48	0.43
7:G:93:SER:OG	7:G:100:GLU:HB2	2.18	0.43
1:A:637:LYS:HB3	1:A:641:VAL:HG11	2.01	0.43
2:B:361:LEU:HB3	2:B:364:ILE:HD12	2.00	0.43
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.98	0.43
3:C:89:GLU:O	3:C:90:ASP:HB3	2.18	0.43
3:C:184:ASN:ND2	3:C:189:THR:O	2.51	0.43
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.84	0.43
1:A:795:GLU:HG2	2:B:731:VAL:HG11	2.00	0.43
1:A:667:GLY:HA2	1:A:670:ILE:HD12	2.01	0.43
1:A:353:ILE:HD12	1:A:482:PHE:CD2	2.54	0.43
1:A:626:ASN:O	1:A:631:HIS:ND1	2.51	0.43
1:A:811:GLN:H	1:A:811:GLN:NE2	2.17	0.43
6:F:136:ARG:HD2	6:F:146:TRP:CD1	2.53	0.43
9:I:87:GLN:HE22	9:I:97:MET:HG2	1.84	0.43
2:B:493:SER:HB3	2:B:775:LYS:HE2	2.00	0.43
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.84	0.43
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.54	0.43
11:K:18:LYS:HE3	11:K:38:GLU:HG2	2.01	0.43
1:A:922:ASP:CG	1:A:925:LEU:HD12	2.39	0.42
7:G:138:THR:O	7:G:140:LYS:N	2.52	0.42
8:H:105:GLU:HB3	8:H:113:ALA:HB3	2.00	0.42
9:I:14:LEU:HB3	9:I:27:PHE:HB3	2.00	0.42
1:A:55:ASP:OD1	1:A:57:ARG:CA	2.67	0.42
1:A:266:LEU:HA	1:A:269:ILE:HD12	2.00	0.42
5:E:118:PRO:HA	5:E:121:MET:HB2	2.00	0.42
1:A:923:LEU:O	1:A:927:VAL:HG23	2.19	0.42
2:B:46:GLN:H	2:B:46:GLN:HG3	1.62	0.42
2:B:644:GLU:C	2:B:646:LEU:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:THR:HG22	2:B:1004:GLU:H	1.83	0.42
7:G:19:GLY:O	7:G:22:MET:HB2	2.19	0.42
1:A:51:GLY:O	1:A:56:PRO:HB3	2.19	0.42
1:A:93:VAL:HG13	1:A:301:ALA:CB	2.50	0.42
2:B:128:LEU:HD21	2:B:170:LEU:HB2	2.02	0.42
2:B:994:TYR:HD1	2:B:999:MET:HE3	1.84	0.42
6:F:82:THR:HG22	6:F:83:PRO:HD2	2.02	0.42
1:A:70:CYS:SG	1:A:72:GLU:HB2	2.59	0.42
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.52	0.42
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.59	0.42
10:J:1:MET:HG3	10:J:60:PHE:CE2	2.47	0.42
1:A:1161:THR:HG21	1:A:1166:ASP:HB2	2.01	0.42
3:C:39:ALA:HA	3:C:164:ALA:HB3	2.01	0.42
1:A:768:GLN:HG2	1:A:816:HIS:HA	2.01	0.42
1:A:956:LEU:HD21	1:A:1017:LEU:HD23	2.01	0.42
3:C:99:LEU:HA	3:C:119:VAL:O	2.20	0.42
11:K:49:GLU:HG3	11:K:94:ILE:HG13	2.01	0.42
1:A:1081:LEU:HD12	1:A:1082:ASN:ND2	2.20	0.42
1:A:1095:THR:HG23	1:A:1113:THR:HG23	2.02	0.42
2:B:515:HIS:H	2:B:518:HIS:CD2	2.38	0.42
7:G:91:VAL:HG23	7:G:143:ILE:HD13	2.02	0.42
7:G:154:VAL:HG23	7:G:155:SER:H	1.83	0.42
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.34	0.41
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.20	0.41
1:A:517:ASN:HD22	1:A:1364:ASN:ND2	2.18	0.41
1:A:605:MET:HE1	1:A:612:ILE:HG23	2.01	0.41
3:C:69:LEU:O	10:J:6:ARG:HD2	2.20	0.41
1:A:42:ASP:O	1:A:44:THR:N	2.53	0.41
1:A:362:ASP:OD1	1:A:459:ARG:HD3	2.20	0.41
1:A:472:LEU:HD21	2:B:835:GLN:HB3	2.01	0.41
1:A:768:GLN:CG	1:A:816:HIS:HA	2.50	0.41
1:A:1433:MET:CE	7:G:63:PRO:HB3	2.50	0.41
2:B:506:GLY:HA3	2:B:507:LYS:HA	1.80	0.41
2:B:745:PRO:O	2:B:748:ILE:HG12	2.20	0.41
7:G:1:MET:HB3	7:G:1:MET:HE3	1.98	0.41
1:A:16:GLU:OE1	4:D:14:ARG:NH2	2.53	0.41
1:A:571:LEU:HD12	8:H:46:LEU:HD11	2.02	0.41
1:A:1081:LEU:HD21	1:A:1098:VAL:HG23	2.02	0.41
2:B:583:ASN:HD21	2:B:628:THR:CG2	2.34	0.41
1:A:151:ASP:HA	1:A:163:SER:HA	2.02	0.41
1:A:605:MET:HE2	1:A:612:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.51	0.41
1:A:1420:ASP:HB3	1:A:1422:ARG:HG2	2.02	0.41
3:C:6:PRO:HB2	11:K:101:LEU:HD13	2.01	0.41
1:A:37:PHE:CD1	1:A:52:GLY:CA	3.03	0.41
1:A:353:ILE:HD12	1:A:482:PHE:HD2	1.86	0.41
1:A:998:LEU:HD23	1:A:1001:ARG:HG3	2.01	0.41
1:A:1150:SER:HB3	9:I:46:HIS:HB3	2.02	0.41
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.55	0.41
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	2.02	0.41
6:F:109:VAL:HG21	6:F:124:GLU:HA	2.02	0.41
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.86	0.41
11:K:49:GLU:HG3	11:K:94:ILE:HG12	2.02	0.41
1:A:282:ASN:O	1:A:284:ALA:N	2.52	0.41
1:A:598:LEU:HD13	8:H:124:ARG:HB2	2.03	0.41
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.54	0.41
2:B:30:SER:O	2:B:34:ILE:HG13	2.20	0.41
2:B:1175:LEU:HG	2:B:1175:LEU:O	2.21	0.41
4:D:126:ILE:HG21	4:D:145:MET:HB3	2.02	0.41
2:B:68:THR:HG23	2:B:91:SER:HB3	2.03	0.41
2:B:1097:HIS:CD2	2:B:1097:HIS:N	2.88	0.41
8:H:114:VAL:HG21	8:H:134:ASN:HD22	1.85	0.41
8:H:130:ARG:H	8:H:130:ARG:HG3	1.54	0.41
1:A:369:SER:HB3	11:K:2:ASN:HD21	1.86	0.41
1:A:774:ARG:H	1:A:774:ARG:HG2	1.60	0.41
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.55	0.41
5:E:156:LEU:HD21	5:E:197:LYS:HB2	2.03	0.41
2:B:398:ARG:HH11	2:B:398:ARG:HB2	1.86	0.40
2:B:521:LEU:HD22	2:B:633:VAL:HG12	2.03	0.40
2:B:766:ARG:NH2	2:B:1020:ARG:HD2	2.35	0.40
3:C:46:ILE:HA	3:C:159:ALA:HA	2.03	0.40
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.21	0.40
1:A:1297:GLU:H	1:A:1297:GLU:HG3	1.54	0.40
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.19	0.40
1:A:1116:LEU:H	1:A:1308:THR:HB	1.85	0.40
2:B:473:MET:HA	2:B:474:SER:HA	1.71	0.40
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.03	0.40
3:C:145:CYS:HA	10:J:2:ILE:CD1	2.50	0.40
11:K:21:ILE:HD13	11:K:84:LYS:HG2	2.03	0.40
1:A:857:ARG:HD3	1:A:861:GLY:O	2.22	0.40
1:A:1243:VAL:HG13	1:A:1244:ARG:H	1.85	0.40
1:A:928:LEU:HD23	1:A:928:LEU:HA	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ILE:HA	2:B:344:LYS:HA	1.91	0.40
2:B:662:MET:HA	2:B:665:GLU:HB2	2.03	0.40
2:B:1138:MET:HB3	2:B:1147:LEU:HG	2.04	0.40
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.57	0.40
7:G:151:ILE:HD11	7:G:160:ILE:CD1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1411/1733 (81%)	1279 (91%)	94 (7%)	38 (3%)	5 26
2	B	1107/1224 (90%)	997 (90%)	74 (7%)	36 (3%)	4 22
3	C	264/318 (83%)	235 (89%)	23 (9%)	6 (2%)	6 29
4	D	176/221 (80%)	157 (89%)	15 (8%)	4 (2%)	6 29
5	E	212/215 (99%)	201 (95%)	9 (4%)	2 (1%)	17 48
6	F	85/155 (55%)	78 (92%)	7 (8%)	0	100 100
7	G	169/171 (99%)	157 (93%)	7 (4%)	5 (3%)	4 24
8	H	129/146 (88%)	105 (81%)	10 (8%)	14 (11%)	0 2
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	5 27
10	J	63/70 (90%)	59 (94%)	2 (3%)	2 (3%)	4 22
11	K	113/120 (94%)	108 (96%)	5 (4%)	0	100 100
12	L	44/70 (63%)	27 (61%)	9 (20%)	8 (18%)	0 1
All	All	3890/4565 (85%)	3501 (90%)	271 (7%)	118 (3%)	4 24

All (118) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	42	ASP
1	A	43	GLU
1	A	54	ASN
1	A	57	ARG
1	A	74	MET
1	A	169	ASN
1	A	286	HIS
1	A	593	GLU
1	A	1243	VAL
1	A	1403	GLU
1	A	1405	THR
2	B	245	GLU
2	B	368	GLU
2	B	509	ALA
2	B	531	GLN
2	B	643	ASP
2	B	879	ARG
2	B	1046	PRO
2	B	1066	SER
2	B	1176	ASN
3	C	91	HIS
4	D	13	ARG
4	D	119	ARG
7	G	139	ILE
7	G	154	VAL
8	H	83	GLN
8	H	84	ALA
8	H	88	SER
10	J	6	ARG
12	L	38	LEU
12	L	39	SER
12	L	50	ASP
12	L	56	LEU
12	L	59	ALA
12	L	60	ARG
1	A	76	GLU
1	A	251	SER
1	A	257	ARG
1	A	283	GLY
1	A	335	ARG
1	A	775	ILE
1	A	1081	LEU

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Mol	Chain	Res	Type
2	B	67	SER
2	B	229	ALA
2	B	277	LYS
2	B	364	ILE
2	B	629	ASP
2	B	712	PRO
2	B	731	VAL
2	B	907	GLY
2	B	958	GLN
2	B	1157	ALA
2	B	1181	GLU
2	B	1223	ASP
3	C	141	GLY
4	D	199	ASN
7	G	63	PRO
8	H	17	PRO
8	H	18	GLY
8	H	85	GLY
8	H	128	ASN
8	H	136	LYS
12	L	45	ALA
1	A	5	GLN
1	A	108	MET
1	A	156	ASP
1	A	321	PRO
1	A	399	HIS
1	A	846	GLU
1	A	1092	LYS
1	A	1377	THR
1	A	1437	GLY
2	B	341	LEU
2	B	369	GLY
2	B	707	PRO
2	B	880	THR
2	B	1185	CYS
2	B	1222	ARG
7	G	2	PHE
8	H	52	GLN
8	H	60	ALA
9	I	10	CYS
9	I	95	THR
1	A	35	ILE

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Mol	Chain	Res	Type
1	A	41	MET
1	A	47	ARG
1	A	1378	GLN
2	B	711	GLU
3	C	142	VAL
4	D	15	LEU
7	G	67	SER
8	H	108	SER
8	H	140	ALA
9	I	3	THR
12	L	26	THR
1	A	322	VAL
1	A	958	VAL
2	B	266	ALA
2	B	339	THR
2	B	526	GLU
2	B	1108	ARG
3	C	90	ASP
5	E	48	ASP
5	E	51	GLY
8	H	107	VAL
10	J	17	LYS
1	A	196	GLU
1	A	334	GLY
3	C	214	ASN
2	B	295	GLY
8	H	82	PRO
1	A	567	LYS
1	A	599	SER
2	B	503	GLY
2	B	1017	ILE
2	B	751	VAL
3	C	240	VAL

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
1	A	1244/1520 (82%)	1081 (87%)	163 (13%)	4 17
2	B	969/1061 (91%)	842 (87%)	127 (13%)	4 17
3	C	234/274 (85%)	205 (88%)	29 (12%)	4 19
4	D	160/200 (80%)	133 (83%)	27 (17%)	2 9
5	E	196/197 (100%)	184 (94%)	12 (6%)	18 48
6	F	77/137 (56%)	66 (86%)	11 (14%)	3 15
7	G	152/152 (100%)	132 (87%)	20 (13%)	4 17
8	H	117/128 (91%)	101 (86%)	16 (14%)	3 16
9	I	113/116 (97%)	99 (88%)	14 (12%)	4 19
10	J	60/65 (92%)	52 (87%)	8 (13%)	4 17
11	K	99/102 (97%)	91 (92%)	8 (8%)	11 36
12	L	40/57 (70%)	33 (82%)	7 (18%)	2 8
All	All	3461/4009 (86%)	3019 (87%)	442 (13%)	4 18

All (442) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	28	ARG
1	A	34	LYS
1	A	40	THR
1	A	43	GLU
1	A	47	ARG
1	A	49	LYS
1	A	60	SER
1	A	63	ARG
1	A	65	LEU
1	A	66	LYS
1	A	74	MET
1	A	90	VAL
1	A	93	VAL
1	A	113	LEU
1	A	116	ASP
1	A	117	GLU
1	A	131	SER
1	A	145	LYS
1	A	150	THR
1	A	152	VAL
1	A	157	ASP

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Mol	Chain	Res	Type
1	A	164	ARG
1	A	174	ILE
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	249	SER
1	A	252	PHE
1	A	265	LYS
1	A	277	GLU
1	A	280	GLU
1	A	302	THR
1	A	307	ASP
1	A	311	GLN
1	A	317	LYS
1	A	320	ARG
1	A	322	VAL
1	A	323	LYS
1	A	324	SER
1	A	335	ARG
1	A	344	ARG
1	A	353	ILE
1	A	369	SER
1	A	385	ILE
1	A	389	THR
1	A	393	ARG
1	A	408	ASP
1	A	423	ASP
1	A	433	GLU
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	447	GLN
1	A	449	SER
1	A	450	LEU
1	A	451	HIS
1	A	452	LYS
1	A	453	MET
1	A	454	SER
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL

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Mol	Chain	Res	Type
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	505	CYS
1	A	523	ILE
1	A	544	ASP
1	A	549	MET
1	A	557	ASP
1	A	584	ASN
1	A	588	LEU
1	A	595	THR
1	A	618	GLU
1	A	622	VAL
1	A	625	SER
1	A	629	LEU
1	A	634	THR
1	A	652	VAL
1	A	666	ILE
1	A	672	ASP
1	A	688	LYS
1	A	691	LEU
1	A	719	VAL
1	A	741	ASN
1	A	764	CYS
1	A	768	GLN
1	A	773	LYS
1	A	774	ARG
1	A	788	SER
1	A	801	GLU
1	A	811	GLN
1	A	821	ARG
1	A	830	LYS
1	A	839	ARG
1	A	855	THR
1	A	856	THR
1	A	858	ASN
1	A	882	SER
1	A	896	ARG
1	A	905	ASP
1	A	915	SER
1	A	919	ILE
1	A	924	LYS

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Mol	Chain	Res	Type
1	A	929	LEU
1	A	948	VAL
1	A	973	ILE
1	A	974	ASP
1	A	976	THR
1	A	988	LEU
1	A	1001	ARG
1	A	1035	TYR
1	A	1047	SER
1	A	1052	GLN
1	A	1064	VAL
1	A	1067	LEU
1	A	1074	GLU
1	A	1080	THR
1	A	1081	LEU
1	A	1092	LYS
1	A	1118	VAL
1	A	1133	LEU
1	A	1159	ARG
1	A	1168	GLU
1	A	1176	LEU
1	A	1206	ASP
1	A	1208	THR
1	A	1215	ARG
1	A	1218	GLN
1	A	1237	ILE
1	A	1242	VAL
1	A	1244	ARG
1	A	1256	GLU
1	A	1260	LEU
1	A	1264	GLU
1	A	1265	ASN
1	A	1280	GLU
1	A	1295	THR
1	A	1297	GLU
1	A	1309	ASP
1	A	1315	GLU
1	A	1325	THR
1	A	1329	THR
1	A	1333	ILE
1	A	1355	VAL
1	A	1359	ASP

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Mol	Chain	Res	Type
1	A	1366	ARG
1	A	1372	VAL
1	A	1376	THR
1	A	1393	ASN
1	A	1394	THR
1	A	1398	MET
1	A	1405	THR
1	A	1420	ASP
1	A	1422	ARG
1	A	1426	GLU
1	A	1438	THR
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1448	GLU
2	B	22	SER
2	B	25	ILE
2	B	26	THR
2	B	45	SER
2	B	46	GLN
2	B	63	ILE
2	B	66	ASP
2	B	90	ILE
2	B	101	MET
2	B	103	ASN
2	B	118	ARG
2	B	131	ASP
2	B	134	LYS
2	B	185	THR
2	B	199	MET
2	B	217	ARG
2	B	222	ILE
2	B	228	LYS
2	B	240	ILE
2	B	249	ARG
2	B	254	LEU
2	B	258	LEU
2	B	261	ARG
2	B	305	VAL
2	B	313	MET
2	B	319	GLU
2	B	323	VAL

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Mol	Chain	Res	Type
2	B	337	ARG
2	B	339	THR
2	B	365	THR
2	B	368	GLU
2	B	393	LYS
2	B	398	ARG
2	B	416	LEU
2	B	466	TRP
2	B	471	LYS
2	B	480	SER
2	B	485	ARG
2	B	493	SER
2	B	501	PRO
2	B	502	ILE
2	B	505	ASP
2	B	507	LYS
2	B	508	LEU
2	B	510	LYS
2	B	529	GLU
2	B	547	VAL
2	B	552	MET
2	B	560	GLU
2	B	563	MET
2	B	570	VAL
2	B	573	GLN
2	B	589	VAL
2	B	598	GLU
2	B	601	ARG
2	B	603	LEU
2	B	604	ARG
2	B	606	LYS
2	B	616	ILE
2	B	620	ARG
2	B	621	GLU
2	B	628	THR
2	B	642	ASP
2	B	658	ILE
2	B	665	GLU
2	B	678	GLU
2	B	680	THR
2	B	682	SER
2	B	687	GLU

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Mol	Chain	Res	Type
2	B	699	GLU
2	B	708	GLU
2	B	709	ASP
2	B	722	ASP
2	B	731	VAL
2	B	734	HIS
2	B	737	THR
2	B	766	ARG
2	B	780	VAL
2	B	790	ASP
2	B	791	THR
2	B	831	SER
2	B	868	MET
2	B	870	ILE
2	B	871	THR
2	B	876	LYS
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	904	ARG
2	B	914	LYS
2	B	915	THR
2	B	942	ARG
2	B	955	THR
2	B	958	GLN
2	B	964	VAL
2	B	970	THR
2	B	979	LYS
2	B	997	GLU
2	B	999	MET
2	B	1007	VAL
2	B	1045	SER
2	B	1060	ARG
2	B	1065	GLN
2	B	1070	GLU
2	B	1084	GLN
2	B	1098	MET
2	B	1106	ARG
2	B	1123	SER
2	B	1129	ARG

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Mol	Chain	Res	Type
2	B	1138	MET
2	B	1145	SER
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1151	LEU
2	B	1156	ASP
2	B	1159	ARG
2	B	1160	VAL
2	B	1162	ILE
2	B	1175	LEU
2	B	1183	LYS
2	B	1189	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1224	PHE
3	C	7	GLN
3	C	9	LYS
3	C	23	SER
3	C	25	VAL
3	C	40	GLU
3	C	52	GLU
3	C	79	GLN
3	C	83	SER
3	C	90	ASP
3	C	100	THR
3	C	115	SER
3	C	116	LYS
3	C	121	VAL
3	C	122	SER
3	C	127	ARG
3	C	129	ILE
3	C	145	CYS
3	C	149	LYS
3	C	154	LYS
3	C	155	LEU
3	C	156	THR
3	C	188	HIS
3	C	215	GLU
3	C	226	ASP
3	C	240	VAL
3	C	260	LEU

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Mol	Chain	Res	Type
3	C	262	LEU
3	C	265	MET
3	C	268	ASP
4	D	1	MET
4	D	5	THR
4	D	6	SER
4	D	8	PHE
4	D	9	GLN
4	D	12	ARG
4	D	14	ARG
4	D	20	GLU
4	D	21	GLU
4	D	31	GLN
4	D	32	GLU
4	D	39	ASN
4	D	41	GLN
4	D	47	LEU
4	D	53	SER
4	D	60	LYS
4	D	65	GLU
4	D	121	LYS
4	D	122	GLU
4	D	134	THR
4	D	139	LYS
4	D	153	ARG
4	D	197	SER
4	D	203	SER
4	D	206	GLU
4	D	213	GLU
4	D	221	TYR
5	E	9	ILE
5	E	57	MET
5	E	67	GLU
5	E	71	LYS
5	E	78	LEU
5	E	81	GLU
5	E	84	ASP
5	E	107	THR
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	196	VAL

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Mol	Chain	Res	Type
6	F	69	LEU
6	F	70	LYS
6	F	71	GLU
6	F	72	LYS
6	F	78	GLN
6	F	79	ARG
6	F	82	THR
6	F	87	LYS
6	F	90	ARG
6	F	102	SER
6	F	111	LEU
7	G	2	PHE
7	G	5	LYS
7	G	11	ILE
7	G	23	LYS
7	G	24	GLN
7	G	28	THR
7	G	61	ILE
7	G	75	ARG
7	G	95	SER
7	G	100	GLU
7	G	118	ASP
7	G	133	SER
7	G	138	THR
7	G	139	ILE
7	G	143	ILE
7	G	145	VAL
7	G	146	LYS
7	G	151	ILE
7	G	162	SER
7	G	171	ILE
8	H	8	ASP
8	H	11	GLN
8	H	19	ARG
8	H	26	ILE
8	H	32	THR
8	H	33	GLN
8	H	53	ASP
8	H	54	SER
8	H	77	ARG
8	H	92	ASP
8	H	103	LYS

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Mol	Chain	Res	Type
8	H	107	VAL
8	H	110	ASP
8	H	112	ILE
8	H	124	ARG
8	H	130	ARG
9	I	2	THR
9	I	4	PHE
9	I	8	ARG
9	I	10	CYS
9	I	31	THR
9	I	35	VAL
9	I	40	SER
9	I	45	ARG
9	I	74	GLU
9	I	81	ARG
9	I	84	VAL
9	I	90	GLN
9	I	106	CYS
9	I	117	LYS
10	J	1	MET
10	J	12	LYS
10	J	20	SER
10	J	38	ARG
10	J	42	LYS
10	J	43	ARG
10	J	48	ARG
10	J	52	THR
11	K	6	ARG
11	K	31	VAL
11	K	34	THR
11	K	47	ARG
11	K	51	LEU
11	K	63	VAL
11	K	103	THR
11	K	114	LEU
12	L	27	LEU
12	L	53	HIS
12	L	54	ARG
12	L	64	LEU
12	L	65	VAL
12	L	66	GLN
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	83	HIS
1	A	118	HIS
1	A	225	ASN
1	A	299	HIS
1	A	339	ASN
1	A	425	GLN
1	A	435	HIS
1	A	447	GLN
1	A	451	HIS
1	A	503	GLN
1	A	515	GLN
1	A	517	ASN
1	A	548	ASN
1	A	603	ASN
1	A	700	ASN
1	A	741	ASN
1	A	757	ASN
1	A	768	GLN
1	A	811	GLN
1	A	858	ASN
1	A	926	GLN
1	A	968	GLN
1	A	975	HIS
1	A	994	GLN
1	A	1082	ASN
1	A	1128	GLN
1	A	1140	HIS
1	A	1211	GLN
1	A	1432	GLN
2	B	47	GLN
2	B	121	ASN
2	B	178	ASN
2	B	465	ASN
2	B	518	HIS
2	B	590	HIS
2	B	657	HIS
2	B	744	HIS
2	B	842	ASN
2	B	862	GLN
2	B	1013	ASN

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Mol	Chain	Res	Type
2	B	1015	HIS
2	B	1040	ASN
2	B	1062	HIS
2	B	1084	GLN
2	B	1112	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1178	ASN
2	B	1179	GLN
3	C	7	GLN
3	C	73	GLN
3	C	112	ASN
3	C	188	HIS
4	D	37	GLN
4	D	39	ASN
4	D	41	GLN
4	D	150	ASN
5	E	147	HIS
6	F	104	ASN
7	G	10	ASN
7	G	14	HIS
7	G	57	GLN
7	G	97	HIS
7	G	122	ASN
7	G	153	GLN
8	H	137	GLN
9	I	12	ASN
9	I	60	GLN
9	I	89	GLN
9	I	116	ASN
11	K	65	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	15/15 (100%)	6 (40%)	2 (13%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	6	C

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Mol	Chain	Res	Type
14	P	7	C
14	P	8	C
14	P	17	C
14	P	18	C
14	P	19	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	5	C
14	P	16	C

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

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	22	14,15	18,21,22	0.77	0	26,30,33	2.20	7 (26%)

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	22	14,15	-	0/7/21/22	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(^{o})	Ideal(^{o})
15	T	22	BRU	C5-C4-N3	5.24	119.37	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	T	22	BRU	C4-N3-C2	-5.20	120.61	127.35
15	T	22	BRU	O4-C4-C5	-4.53	120.16	125.84
15	T	22	BRU	N3-C2-N1	4.25	120.53	114.89
15	T	22	BRU	BR-C5-C4	2.93	121.43	118.03
15	T	22	BRU	O4'-C1'-N1	2.12	111.65	107.86
15	T	22	BRU	C6-C5-C4	-2.06	118.58	120.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	ACT	A	1734	-	3,3,3	0.76	0	3,3,3	1.33	0
19	EPE	D	222	-	15,15,15	0.65	0	18,20,20	2.05	9 (50%)
20	PEG	G	172	-	6,6,6	0.49	0	5,5,5	0.31	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	EPE	D	222	-	-	3/9/19/19	0/1/1/1
20	PEG	G	172	-	-	2/4/4/4	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	D	222	EPE	C5-N4-C3	4.34	118.60	108.83
19	D	222	EPE	O2S-S-C10	3.14	110.69	106.92
19	D	222	EPE	C7-N4-C5	2.99	118.87	111.23
19	D	222	EPE	C7-N4-C3	2.60	117.89	111.23
19	D	222	EPE	O3S-S-C10	2.45	109.73	105.77
19	D	222	EPE	C9-N1-C6	-2.37	105.18	111.23
19	D	222	EPE	O1S-S-C10	-2.27	104.18	106.92
19	D	222	EPE	C6-C5-N4	2.27	115.29	110.64
19	D	222	EPE	C2-C3-N4	2.06	114.88	110.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	D	222	EPE	C10-C9-N1-C2
19	D	222	EPE	C10-C9-N1-C6
19	D	222	EPE	C8-C7-N4-C5
20	G	172	PEG	O1-C1-C2-O2
20	G	172	PEG	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1421/1733 (81%)	-0.01	19 (1%) 77 77	66, 108, 173, 229	0
2	B	1121/1224 (91%)	0.11	27 (2%) 59 56	68, 119, 185, 221	0
3	C	266/318 (83%)	-0.08	2 (0%) 86 86	81, 108, 153, 188	0
4	D	180/221 (81%)	0.07	3 (1%) 70 68	90, 120, 172, 195	0
5	E	214/215 (99%)	-0.00	3 (1%) 75 75	87, 146, 197, 206	0
6	F	87/155 (56%)	-0.27	1 (1%) 80 81	71, 90, 127, 136	0
7	G	171/171 (100%)	0.08	0 100 100	83, 107, 150, 175	0
8	H	133/146 (91%)	0.37	4 (3%) 50 49	111, 154, 193, 214	0
9	I	119/122 (97%)	0.02	5 (4%) 36 34	118, 148, 190, 209	0
10	J	65/70 (92%)	-0.13	0 100 100	90, 107, 150, 161	0
11	K	115/120 (95%)	-0.09	1 (0%) 84 84	75, 108, 144, 161	0
12	L	46/70 (65%)	0.64	5 (10%) 5 5	89, 181, 199, 204	0
13	N	14/14 (100%)	1.24	5 (35%) 0 0	203, 228, 278, 279	0
14	P	15/15 (100%)	0.85	4 (26%) 0 0	151, 172, 214, 227	0
15	T	18/27 (66%)	1.05	5 (27%) 0 0	133, 199, 284, 287	0
All	All	3985/4621 (86%)	0.05	84 (2%) 63 62	66, 115, 186, 287	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	882	THR	8.2
1	A	255	SER	5.8
12	L	27	LEU	5.1
1	A	1176	LEU	5.0
13	N	13	DT	4.8
11	K	115	ALA	4.8
14	P	16	C	4.7

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Mol	Chain	Res	Type	RSRZ
12	L	26	THR	4.6
1	A	256	GLN	4.6
15	T	6	DG	4.3
4	D	8	PHE	4.3
15	T	5	DA	4.1
2	B	708	GLU	3.9
14	P	19	C	3.8
2	B	709	ASP	3.7
2	B	643	ASP	3.7
2	B	468	GLU	3.4
12	L	25	ALA	3.4
8	H	132	LEU	3.4
4	D	1	MET	3.2
2	B	469	GLN	3.2
2	B	343	ILE	3.2
14	P	18	C	3.1
1	A	257	ARG	3.1
2	B	346	GLU	3.0
14	P	17	C	3.0
2	B	470	LYS	3.0
5	E	123	LEU	3.0
1	A	1086	PHE	3.0
15	T	7	DC	2.9
2	B	715	ALA	2.9
8	H	134	ASN	2.9
9	I	119	THR	2.9
1	A	1091	SER	2.9
2	B	918	ILE	2.9
2	B	341	LEU	2.8
13	N	11	DG	2.8
2	B	505	ASP	2.8
8	H	139	ASN	2.8
2	B	869	SER	2.8
1	A	251	SER	2.7
2	B	916	THR	2.7
1	A	1240	CYS	2.7
15	T	8	DT	2.6
5	E	110	PHE	2.6
2	B	506	GLY	2.6
1	A	164	ARG	2.5
1	A	1085	HIS	2.5
15	T	9	DA	2.5

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Mol	Chain	Res	Type	RSRZ
8	H	125	LEU	2.5
13	N	10	DA	2.5
9	I	118	ARG	2.5
2	B	866	TYR	2.5
2	B	132	VAL	2.5
3	C	266	ASP	2.4
12	L	50	ASP	2.4
6	F	108	PHE	2.4
9	I	120	GLN	2.4
1	A	49	LYS	2.4
1	A	159	THR	2.4
9	I	115	LYS	2.4
13	N	12	DC	2.3
2	B	864	LYS	2.3
2	B	448	ILE	2.3
5	E	126	SER	2.3
1	A	44	THR	2.3
1	A	252	PHE	2.2
2	B	25	ILE	2.2
1	A	142	CYS	2.2
1	A	1092	LYS	2.2
2	B	868	MET	2.2
1	A	155	GLU	2.2
9	I	116	ASN	2.2
12	L	46	VAL	2.1
1	A	1220	PHE	2.1
2	B	504	ARG	2.1
4	D	2	ASN	2.1
2	B	106	ASP	2.1
2	B	130	VAL	2.0
2	B	63	ILE	2.0
1	A	1257	ASP	2.0
2	B	90	ILE	2.0
3	C	262	LEU	2.0
13	N	9	DT	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	22	20/21	0.92	0.12	110,169,284,288	0

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, 95^{th} 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
20	PEG	G	172	7/7	0.84	0.85	74,118,300,300	0
18	ACT	A	1734	4/4	0.87	0.33	67,89,129,132	0
16	ZN	L	1071	1/1	0.96	0.03	225,225,225,225	0
19	EPE	D	222	15/15	0.97	0.20	53,72,130,170	0
16	ZN	I	1122	1/1	0.99	0.04	199,199,199,199	0
16	ZN	J	1066	1/1	0.99	0.23	105,105,105,105	0
16	ZN	A	2456	1/1	0.99	0.08	156,156,156,156	0
17	MG	A	2458	1/1	0.99	0.13	78,78,78,78	0
16	ZN	B	2225	1/1	0.99	0.21	99,99,99,99	0
16	ZN	C	1269	1/1	0.99	0.12	93,93,93,93	0
16	ZN	I	1121	1/1	0.99	0.14	124,124,124,124	0
16	ZN	A	2457	1/1	1.00	0.16	94,94,94,94	0

6.5 Other polymers (i)

There are no such residues in this entry.