



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:43 PM GMT

PDB ID : 3PO3
Title : Arrested RNA Polymerase II reactivation intermediate
Authors : Cheung, A.C.M.; Cramer, P.
Deposited on : 2010-11-21
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

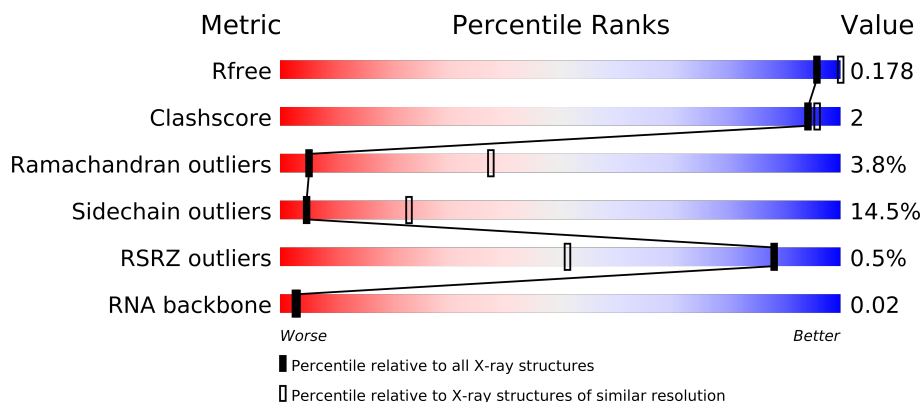
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



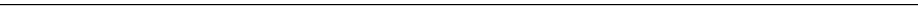





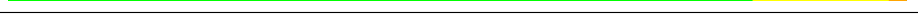



The reported resolution of this entry is 3.30 Å.

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}	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1733	
2	B	1224	
3	C	318	
4	D	221	
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

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Mol	Chain	Length	Quality of chain
13	N	14	
14	P	5	
15	S	178	
16	T	27	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
19	ACT	A	1734	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 33008 atoms, of which 0 are hydrogen and 0 are deuterium.

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	1426	Total	C	N	O	S	0	0	0
			11214	7069	1959	2124	62			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1108	Total	C	N	O	S	0	0	0
			8810	5580	1541	1634	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	177	Total	C	N	O	S	0	0	0
			1417	876	252	287	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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 RPABC2.

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 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	114	Total	C	N	O	S	0	0	0
			919	590	156	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
			364	224	72	64	4			

- Molecule 13 is a DNA chain called DNA non-template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	7	Total	C	N	O	P	0	0	0
			144	69	30	39	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	5	Total	C	N	O	P	0	0	0
			100	45	15	35	5			

- Molecule 15 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	S	164	Total	C	N	O	S	0	0	0
			1294	809	230	247	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	290	ALA	ASP	ENGINEERED MUTATION	UNP P07273
S	291	ALA	GLU	ENGINEERED MUTATION	UNP P07273

- Molecule 16 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	T	13	Total	Br	C	N	O	P	0	0
			266	1	126	44	82	13		

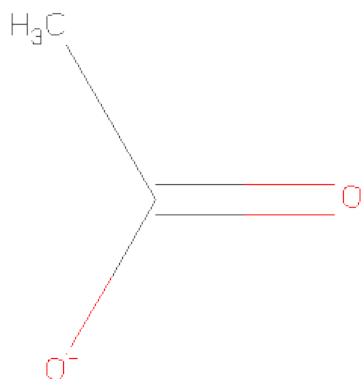
- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

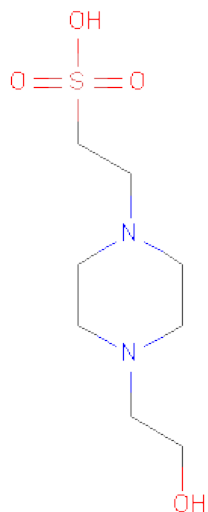
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	1	Total	Mg	0	0
			1	1		

- Molecule 19 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



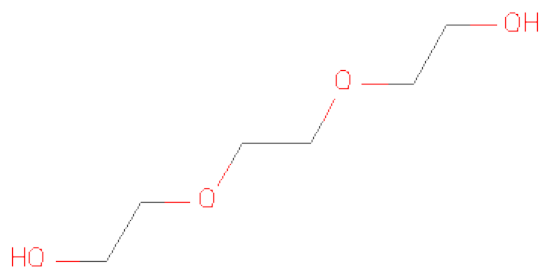
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	C	O	0	0
			4	2	2		
19	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 20 is 4-(2-HYDROXYETHYL)-1-PIPERAZINEETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 21 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).

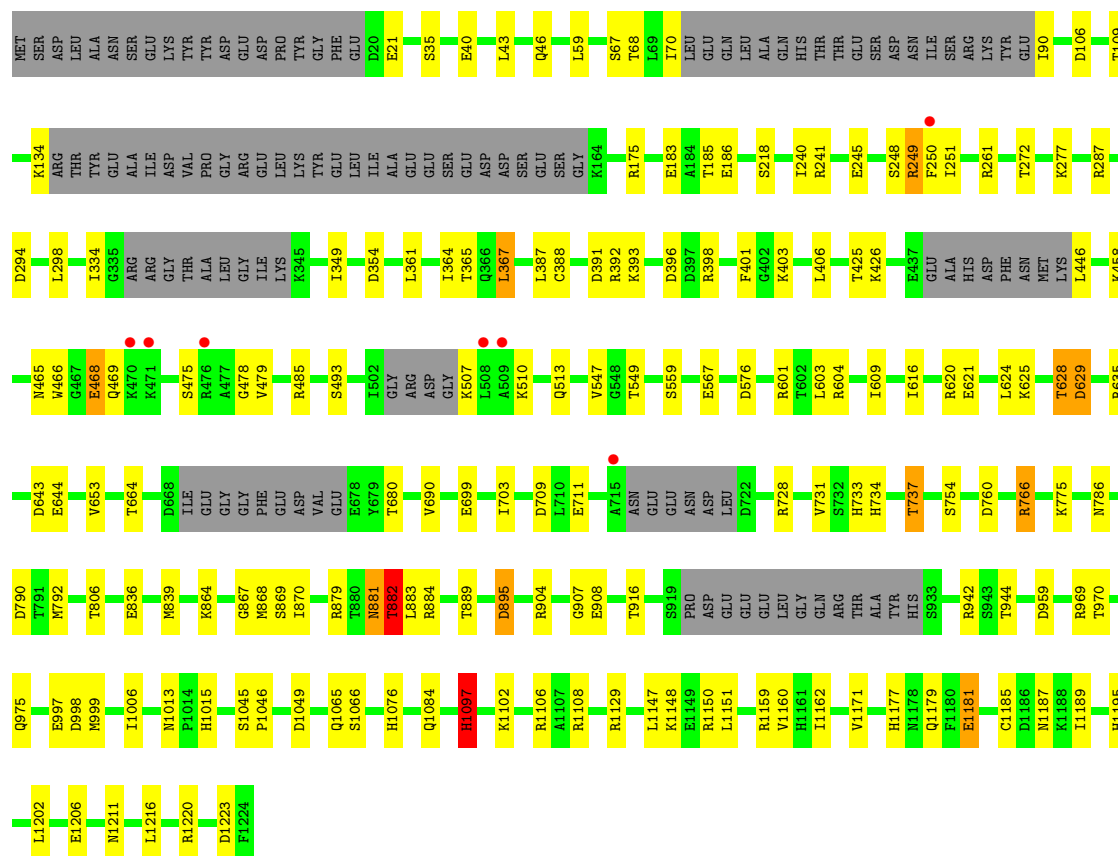


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	L	1	Total	C	O	0	0
			10	6	4		

PRO
ALA
SER
TYR
LEU
SER
PRO
LYS
GLN
ASP
GLU
GLN
LYS
HIS
ASN
GLU
ASN
GLU
ASN
SER
ARG

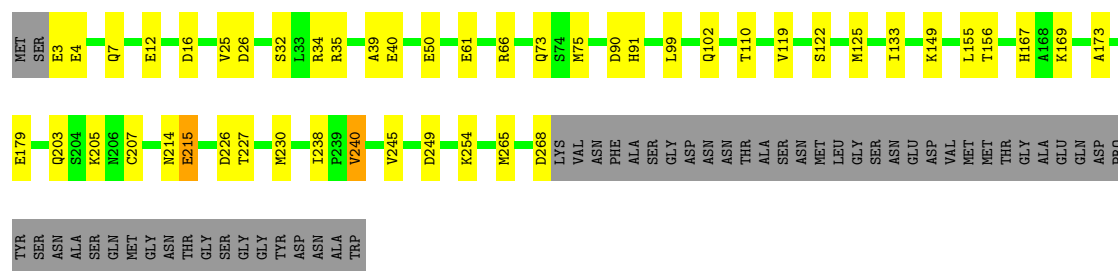
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:



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

Chain C:



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

Chain D:





Y221

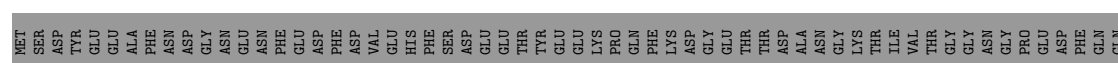
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



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

Chain F:



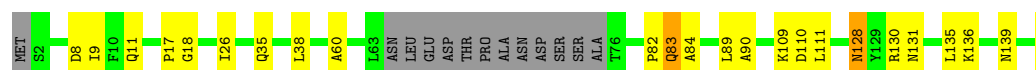
- Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:



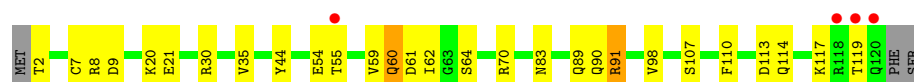
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

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:



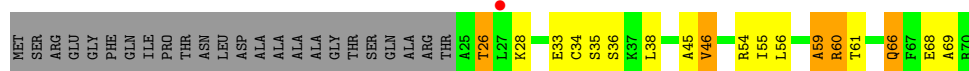
- Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



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

Chain L:



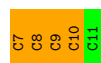
- Molecule 13: DNA non-template strand

Chain N:



- Molecule 14: RNA product strand

Chain P:



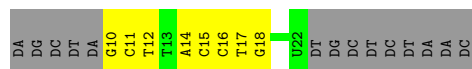
- Molecule 15: Transcription elongation factor S-II

Chain S:



- Molecule 16: DNA template strand

Chain T:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	220.02Å 395.07Å 280.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.97 – 3.30 49.97 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.97-3.30) 99.7 (49.97-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.33Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.161 , 0.189 0.179 , 0.178	Depositor DCC
R_{free} test set	3594 reflections (1.98%)	DCC
Wilson B-factor (Å ²)	111.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 100.9	EDS
Estimated twinning fraction	0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 181822 reflections	Xtriage
F_o , F_c correlation	0.95	EDS
Total number of atoms	33008	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	2/11417 (0.0%)	0.85	7/15442 (0.0%)
2	B	0.51	0/8981	0.79	4/12108 (0.0%)
3	C	0.50	0/2133	0.77	1/2891 (0.0%)
4	D	0.52	0/1427	0.86	2/1914 (0.1%)
5	E	0.44	0/1788	0.71	0/2406
6	F	0.56	0/691	0.77	0/933
7	G	0.55	0/1368	0.82	0/1844
8	H	0.47	0/1086	0.80	0/1470
9	I	0.47	0/989	0.79	0/1331
10	J	0.52	0/541	0.87	1/727 (0.1%)
11	K	0.51	0/937	0.71	0/1265
12	L	0.53	0/366	0.97	1/485 (0.2%)
13	N	0.99	0/162	1.81	6/249 (2.4%)
14	P	1.26	0/109	2.55	10/166 (6.0%)
15	S	0.50	0/1317	0.79	0/1778
16	T	1.16	0/274	1.82	9/421 (2.1%)
All	All	0.53	2/33586 (0.0%)	0.85	41/45430 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	867	ILE	CG1-CD1	5.94	1.91	1.50
1	A	56	PRO	C-N	5.29	1.46	1.34

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	P	8	C	P-O3'-C3'	13.71	136.16	119.70
13	N	6	DA	O4'-C1'-N9	9.07	114.35	108.00
16	T	15	DC	O4'-C1'-N1	8.13	113.69	108.00
14	P	9	C	P-O3'-C3'	7.96	129.25	119.70
16	T	15	DC	O4'-C4'-C3'	-7.65	101.41	106.00
1	A	56	PRO	C-N-CA	7.53	140.53	121.70
13	N	4	DT	O4'-C1'-N1	7.53	113.27	108.00
1	A	3	GLY	C-N-CA	7.33	140.04	121.70
1	A	399	HIS	N-CA-CB	7.27	123.68	110.60
13	N	2	DG	O4'-C1'-N9	7.11	112.98	108.00
4	D	25	ALA	C-N-CA	6.89	138.92	121.70
14	P	7	C	N1-C2-O2	6.55	122.83	118.90
14	P	10	C	P-O3'-C3'	6.47	127.46	119.70
14	P	7	C	C3'-C2'-C1'	6.45	106.66	101.50
16	T	12	DT	P-O3'-C3'	6.34	127.31	119.70
13	N	2	DG	P-O3'-C3'	6.27	127.23	119.70
13	N	3	DG	P-O3'-C3'	6.26	127.21	119.70
16	T	10	DG	P-O3'-C3'	6.25	127.20	119.70
16	T	18	DG	O4'-C1'-N9	6.02	112.22	108.00
1	A	707	GLY	C-N-CA	6.00	136.69	121.70
10	J	5	VAL	N-CA-C	-5.96	94.90	111.00
1	A	451	HIS	CB-CA-C	-5.73	98.93	110.40
14	P	9	C	N1-C2-O2	5.46	122.18	118.90
14	P	7	C	C2-N1-C1'	5.41	124.76	118.80
2	B	882	THR	C-N-CA	5.41	135.23	121.70
16	T	14	DA	O4'-C1'-N9	5.41	111.79	108.00
1	A	568	PRO	N-CA-C	5.40	126.15	112.10
12	L	59	ALA	C-N-CA	5.33	135.03	121.70
4	D	26	THR	N-CA-C	-5.33	96.62	111.00
1	A	1403	GLU	N-CA-C	5.30	125.31	111.00
2	B	628	THR	C-N-CA	5.24	134.79	121.70
2	B	1181	GLU	N-CA-C	5.18	125.00	111.00
16	T	17	DT	C4-C5-C7	5.18	122.11	119.00
13	N	4	DT	P-O3'-C3'	5.18	125.91	119.70
14	P	8	C	N1-C1'-C2'	5.12	120.66	114.00
16	T	16	DC	P-O3'-C3'	5.08	125.80	119.70
16	T	11	DC	P-O3'-C3'	5.06	125.77	119.70
14	P	8	C	C1'-O4'-C4'	-5.02	105.88	109.90
3	C	39	ALA	N-CA-C	5.02	124.55	111.00
14	P	7	C	C6-N1-C2	-5.01	118.30	120.30
2	B	1097	HIS	N-CA-CB	5.00	119.60	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	55	ASP	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11214	0	15	30	0
2	B	8810	0	0	11	0
3	C	2095	0	0	4	0
4	D	1417	0	0	1	0
5	E	1752	0	0	1	0
6	F	679	0	0	2	0
7	G	1340	0	0	2	0
8	H	1068	0	0	1	0
9	I	971	0	0	2	0
10	J	532	0	0	2	0
11	K	919	0	11	0	0
12	L	364	0	0	2	0
13	N	144	0	0	0	0
14	P	100	0	0	0	0
15	S	1294	0	0	4	0
16	T	266	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
17	S	1	0	0	0	0
18	A	1	0	0	0	0
19	A	4	0	3	1	0
19	B	4	0	3	0	0
20	A	15	0	17	2	0
21	L	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	33008	0	63	50	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (50) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:867:ILE:CD1	1:A:867:ILE:CG1	1.91	1.49
7:G:1:MET:SD	7:G:2:PHE:N	2.44	0.91
1:A:567:LYS:O	1:A:569:LYS:N	2.14	0.80
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.26	0.69
9:I:7:CYS:SG	9:I:8:ARG:O	2.53	0.66
1:A:67:CYS:O	1:A:67:CYS:SG	2.53	0.66
1:A:68:GLN:O	1:A:70:CYS:N	2.29	0.66
1:A:55:ASP:OD1	1:A:57:ARG:N	2.30	0.64
1:A:67:CYS:O	1:A:68:GLN:O	2.15	0.63
3:C:66:ARG:NH2	10:J:3:VAL:O	2.33	0.62
7:G:62:LEU:O	7:G:65:ASP:O	2.19	0.61
12:L:34:CYS:O	12:L:36:SER:N	2.37	0.57
4:D:118:THR:O	4:D:121:LYS:NZ	2.38	0.56
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.39	0.56
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.40	0.55
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.40	0.54
1:A:399:HIS:O	1:A:401:GLY:N	2.41	0.54
1:A:306:ASN:ND2	1:A:321:PRO:O	2.43	0.52
15:S:230:THR:C	15:S:232:ASP:N	2.64	0.52
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.44	0.50
1:A:399:HIS:O	1:A:435:HIS:CD2	2.65	0.49
2:B:1013:ASN:ND2	2:B:1015:HIS:CD2	2.81	0.49
1:A:34:LYS:N	20:A:1735:EPE:H101	2.28	0.49
1:A:869:GLY:O	5:E:204:THR:CG2	2.61	0.48
3:C:167:HIS:CD2	3:C:169:LYS:N	2.82	0.48
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.47	0.47
1:A:1345:ARG:NH1	1:A:1373:ASP:OD1	2.47	0.47
10:J:1:MET:N	10:J:54:VAL:O	2.48	0.46
1:A:562:THR:O	1:A:576:GLN:NE2	2.48	0.46
1:A:2:VAL:HG12	2:B:1195:HIS:CD2	2.51	0.46
1:A:942:PHE:CB	19:A:1734:ACT:H1	2.46	0.46
1:A:1172:LEU:O	1:A:1174:PHE:N	2.49	0.45
8:H:82:PRO:O	8:H:84:ALA:N	2.50	0.45
1:A:65:LEU:O	1:A:67:CYS:N	2.50	0.45
2:B:895:ASP:N	2:B:895:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:ARG:NH2	20:A:1735:EPE:O3S	2.51	0.44
2:B:904:ARG:NH2	12:L:66:GLN:O	2.52	0.43
1:A:1035:TYR:N	1:A:1035:TYR:CD2	2.86	0.43
1:A:1436:ILE:O	1:A:1439:GLY:N	2.51	0.43
1:A:471:ASN:OD1	1:A:650:GLN:NE2	2.51	0.43
1:A:780:VAL:N	2:B:699:GLU:OE2	2.52	0.43
1:A:1062:GLU:OE2	6:F:88:TYR:OH	2.38	0.42
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.53	0.42
15:S:185:VAL:O	15:S:189:ASP:N	2.53	0.42
1:A:378:GLU:OE1	1:A:434:ARG:NH1	2.54	0.41
2:B:766:ARG:NH1	15:S:289:ALA:O	2.53	0.41
15:S:239:ALA:N	15:S:240:PRO:CD	2.84	0.40
9:I:59:VAL:C	9:I:61:ASP:N	2.75	0.40
2:B:760:ASP:N	2:B:760:ASP:OD1	2.54	0.40
1:A:503:GLN:NE2	6:F:90:ARG:NH2	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1418/1733 (82%)	1255 (88%)	105 (7%)	58 (4%)	4	35
2	B	1090/1224 (89%)	963 (88%)	92 (8%)	35 (3%)	6	43
3	C	264/318 (83%)	238 (90%)	17 (6%)	9 (3%)	6	42
4	D	173/221 (78%)	153 (88%)	14 (8%)	6 (4%)	6	41
5	E	212/215 (99%)	202 (95%)	8 (4%)	2 (1%)	25	76
6	F	82/155 (53%)	77 (94%)	4 (5%)	1 (1%)	19	71
7	G	169/171 (99%)	154 (91%)	12 (7%)	3 (2%)	13	61
8	H	129/146 (88%)	101 (78%)	18 (14%)	10 (8%)	1	14
9	I	117/122 (96%)	98 (84%)	16 (14%)	3 (3%)	8	50
10	J	63/70 (90%)	54 (86%)	6 (10%)	3 (5%)	4	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	112/120 (93%)	107 (96%)	5 (4%)	0	100	100
12	L	44/70 (63%)	27 (61%)	8 (18%)	9 (20%)	0	1
15	S	162/178 (91%)	129 (80%)	20 (12%)	13 (8%)	1	13
All	All	4035/4743 (85%)	3558 (88%)	325 (8%)	152 (4%)	5	37

All (152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	42	ASP
1	A	65	LEU
1	A	66	LYS
1	A	68	GLN
1	A	69	THR
1	A	74	MET
1	A	254	GLU
1	A	311	GLN
1	A	314	ALA
1	A	410	GLY
1	A	568	PRO
1	A	672	ASP
1	A	708	MET
1	A	709	THR
1	A	1092	LYS
1	A	1122	PRO
1	A	1405	THR
2	B	245	GLU
2	B	249	ARG
2	B	392	ARG
2	B	643	ASP
2	B	731	VAL
2	B	734	HIS
2	B	737	THR
2	B	883	LEU
2	B	1066	SER
2	B	1181	GLU
3	C	90	ASP
3	C	91	HIS
3	C	173	ALA
3	C	215	GLU
4	D	14	ARG

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Mol	Chain	Res	Type
4	D	53	SER
4	D	199	ASN
5	E	104	ASN
7	G	63	PRO
8	H	83	GLN
8	H	139	ASN
9	I	55	THR
9	I	91	ARG
12	L	35	SER
12	L	56	LEU
12	L	59	ALA
12	L	60	ARG
15	S	208	SER
15	S	238	PRO
1	A	43	GLU
1	A	57	ARG
1	A	76	GLU
1	A	166	GLY
1	A	250	ILE
1	A	567	LYS
1	A	593	GLU
1	A	704	ALA
1	A	775	ILE
1	A	1173	HIS
1	A	1256	GLU
2	B	67	SER
2	B	364	ILE
2	B	367	LEU
2	B	629	ASP
2	B	644	GLU
2	B	709	ASP
2	B	867	GLY
2	B	879	ARG
2	B	881	ASN
2	B	1046	PRO
3	C	149	LYS
3	C	227	THR
4	D	16	LYS
4	D	30	GLY
5	E	3	GLN
8	H	18	GLY
10	J	6	ARG

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Mol	Chain	Res	Type
12	L	45	ALA
15	S	166	HIS
15	S	222	ASP
15	S	223	ILE
15	S	237	ALA
15	S	239	ALA
1	A	54	ASN
1	A	332	LYS
1	A	423	ASP
1	A	525	GLN
1	A	543	LEU
1	A	885	THR
1	A	1403	GLU
2	B	468	GLU
2	B	475	SER
2	B	869	SER
2	B	882	THR
2	B	1185	CYS
2	B	1187	ASN
3	C	110	THR
3	C	214	ASN
7	G	133	SER
7	G	134	GLU
8	H	90	ALA
8	H	128	ASN
8	H	131	ASN
12	L	69	ALA
15	S	207	ILE
1	A	5	GLN
1	A	35	ILE
1	A	56	PRO
1	A	62	ASP
1	A	399	HIS
1	A	1255	GLU
1	A	1437	GLY
2	B	478	GLY
6	F	73	ALA
8	H	17	PRO
8	H	60	ALA
8	H	109	LYS
9	I	60	GLN
10	J	2	ILE

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Mol	Chain	Res	Type
12	L	33	GLU
15	S	227	PHE
15	S	295	THR
1	A	71	GLN
1	A	253	ASN
1	A	322	VAL
1	A	331	GLY
1	A	424	ILE
1	A	846	GLU
1	A	1082	ASN
2	B	792	MET
2	B	907	GLY
2	B	1097	HIS
4	D	119	ARG
8	H	35	GLN
10	J	64	ASN
12	L	26	THR
12	L	46	VAL
15	S	167	PRO
15	S	232	ASP
1	A	705	LYS
1	A	958	VAL
2	B	248	SER
2	B	711	GLU
2	B	1108	ARG
15	S	261	ILE
1	A	3	GLY
1	A	283	GLY
2	B	1171	VAL
1	A	55	ASP
2	B	870	ILE
1	A	165	GLY
1	A	310	GLY
3	C	240	VAL
1	A	312	PRO

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	1246/1520 (82%)	1073 (86%)	173 (14%)	5	25
2	B	962/1061 (91%)	832 (86%)	130 (14%)	6	27
3	C	234/274 (85%)	199 (85%)	35 (15%)	4	21
4	D	157/200 (78%)	120 (76%)	37 (24%)	1	4
5	E	196/197 (100%)	178 (91%)	18 (9%)	13	48
6	F	74/137 (54%)	69 (93%)	5 (7%)	22	67
7	G	152/152 (100%)	125 (82%)	27 (18%)	2	13
8	H	117/128 (91%)	103 (88%)	14 (12%)	7	33
9	I	113/116 (97%)	90 (80%)	23 (20%)	2	8
10	J	60/65 (92%)	48 (80%)	12 (20%)	2	9
11	K	99/102 (97%)	87 (88%)	12 (12%)	7	33
12	L	40/57 (70%)	30 (75%)	10 (25%)	1	3
15	S	141/153 (92%)	117 (83%)	24 (17%)	3	15
All	All	3591/4162 (86%)	3071 (86%)	520 (14%)	5	23

All (520) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	18	GLN
1	A	23	SER
1	A	28	ARG
1	A	36	ARG
1	A	39	GLU
1	A	40	THR
1	A	41	MET
1	A	47	ARG
1	A	53	LEU
1	A	55	ASP
1	A	62	ASP
1	A	64	ASN
1	A	68	GLN
1	A	69	THR
1	A	70	CYS
1	A	74	MET
1	A	84	ILE
1	A	93	VAL
1	A	100	LYS

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Mol	Chain	Res	Type
1	A	113	LEU
1	A	120	GLU
1	A	121	LEU
1	A	144	THR
1	A	147	VAL
1	A	149	GLU
1	A	152	VAL
1	A	157	ASP
1	A	186	LYS
1	A	195	ASP
1	A	196	GLU
1	A	199	LEU
1	A	208	LEU
1	A	225	ASN
1	A	232	GLU
1	A	256	GLN
1	A	265	LYS
1	A	302	THR
1	A	313	GLN
1	A	318	SER
1	A	323	LYS
1	A	324	SER
1	A	335	ARG
1	A	344	ARG
1	A	351	THR
1	A	353	ILE
1	A	363	GLN
1	A	381	THR
1	A	383	TYR
1	A	385	ILE
1	A	386	ASP
1	A	406	ILE
1	A	407	ARG
1	A	408	ASP
1	A	409	SER
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	446	ARG
1	A	452	LYS
1	A	454	SER
1	A	461	LYS

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Mol	Chain	Res	Type
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	504	LEU
1	A	505	CYS
1	A	518	LYS
1	A	523	ILE
1	A	537	ARG
1	A	541	ILE
1	A	544	ASP
1	A	549	MET
1	A	567	LYS
1	A	571	LEU
1	A	577	ILE
1	A	595	THR
1	A	618	GLU
1	A	622	VAL
1	A	625	SER
1	A	636	GLU
1	A	644	LYS
1	A	666	ILE
1	A	691	LEU
1	A	693	VAL
1	A	734	GLU
1	A	738	LYS
1	A	739	ASP
1	A	755	PHE
1	A	768	GLN
1	A	769	SER
1	A	774	ARG
1	A	782	ARG
1	A	801	GLU
1	A	806	ARG
1	A	811	GLN
1	A	821	ARG
1	A	830	LYS
1	A	831	THR
1	A	833	GLU
1	A	834	THR
1	A	838	GLN

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Mol	Chain	Res	Type
1	A	855	THR
1	A	878	ILE
1	A	896	ARG
1	A	905	ASP
1	A	915	SER
1	A	918	GLU
1	A	919	ILE
1	A	927	VAL
1	A	929	LEU
1	A	941	LYS
1	A	977	LYS
1	A	983	ILE
1	A	1015	VAL
1	A	1024	SER
1	A	1058	VAL
1	A	1064	VAL
1	A	1067	LEU
1	A	1077	THR
1	A	1081	LEU
1	A	1082	ASN
1	A	1083	THR
1	A	1084	PHE
1	A	1085	HIS
1	A	1094	VAL
1	A	1116	LEU
1	A	1118	VAL
1	A	1129	GLU
1	A	1132	LYS
1	A	1142	THR
1	A	1167	GLU
1	A	1170	ILE
1	A	1172	LEU
1	A	1176	LEU
1	A	1195	LEU
1	A	1205	LYS
1	A	1215	ARG
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1258	HIS
1	A	1259	MET
1	A	1264	GLU

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Mol	Chain	Res	Type
1	A	1274	ARG
1	A	1286	LYS
1	A	1288	ASP
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1309	ASP
1	A	1317	MET
1	A	1325	THR
1	A	1329	THR
1	A	1330	ASN
1	A	1333	ILE
1	A	1334	ASP
1	A	1345	ARG
1	A	1366	ARG
1	A	1370	LEU
1	A	1376	THR
1	A	1382	THR
1	A	1386	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1422	ARG
1	A	1426	GLU
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1454	MET
2	B	21	GLU
2	B	35	SER
2	B	40	GLU
2	B	43	LEU
2	B	46	GLN
2	B	59	LEU
2	B	68	THR
2	B	70	ILE
2	B	90	ILE
2	B	106	ASP
2	B	109	THR
2	B	134	LYS
2	B	175	ARG
2	B	183	GLU
2	B	185	THR

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Mol	Chain	Res	Type
2	B	186	GLU
2	B	218	SER
2	B	240	ILE
2	B	241	ARG
2	B	249	ARG
2	B	250	PHE
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	277	LYS
2	B	287	ARG
2	B	294	ASP
2	B	298	LEU
2	B	334	ILE
2	B	349	ILE
2	B	354	ASP
2	B	361	LEU
2	B	365	THR
2	B	367	LEU
2	B	387	LEU
2	B	388	CYS
2	B	391	ASP
2	B	393	LYS
2	B	396	ASP
2	B	398	ARG
2	B	401	PHE
2	B	403	LYS
2	B	406	LEU
2	B	425	THR
2	B	426	LYS
2	B	446	LEU
2	B	458	LYS
2	B	465	ASN
2	B	466	TRP
2	B	468	GLU
2	B	469	GLN
2	B	479	VAL
2	B	485	ARG
2	B	493	SER
2	B	507	LYS
2	B	510	LYS
2	B	513	GLN

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Mol	Chain	Res	Type
2	B	547	VAL
2	B	549	THR
2	B	559	SER
2	B	567	GLU
2	B	576	ASP
2	B	601	ARG
2	B	603	LEU
2	B	604	ARG
2	B	609	ILE
2	B	616	ILE
2	B	620	ARG
2	B	621	GLU
2	B	624	LEU
2	B	625	LYS
2	B	628	THR
2	B	629	ASP
2	B	635	ARG
2	B	653	VAL
2	B	664	THR
2	B	680	THR
2	B	690	VAL
2	B	703	ILE
2	B	728	ARG
2	B	733	HIS
2	B	737	THR
2	B	754	SER
2	B	766	ARG
2	B	775	LYS
2	B	786	ASN
2	B	790	ASP
2	B	806	THR
2	B	836	GLU
2	B	839	MET
2	B	864	LYS
2	B	868	MET
2	B	881	ASN
2	B	882	THR
2	B	884	ARG
2	B	889	THR
2	B	895	ASP
2	B	908	GLU
2	B	916	THR

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Mol	Chain	Res	Type
2	B	942	ARG
2	B	944	THR
2	B	959	ASP
2	B	970	THR
2	B	975	GLN
2	B	997	GLU
2	B	999	MET
2	B	1006	ILE
2	B	1045	SER
2	B	1049	ASP
2	B	1065	GLN
2	B	1076	HIS
2	B	1084	GLN
2	B	1097	HIS
2	B	1102	LYS
2	B	1106	ARG
2	B	1129	ARG
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1151	LEU
2	B	1160	VAL
2	B	1162	ILE
2	B	1177	HIS
2	B	1179	GLN
2	B	1189	ILE
2	B	1202	LEU
2	B	1211	ASN
2	B	1216	LEU
2	B	1220	ARG
2	B	1223	ASP
3	C	3	GLU
3	C	4	GLU
3	C	7	GLN
3	C	12	GLU
3	C	16	ASP
3	C	25	VAL
3	C	26	ASP
3	C	32	SER
3	C	34	ARG
3	C	40	GLU
3	C	50	GLU

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Mol	Chain	Res	Type
3	C	73	GLN
3	C	75	MET
3	C	99	LEU
3	C	102	GLN
3	C	119	VAL
3	C	122	SER
3	C	125	MET
3	C	133	ILE
3	C	155	LEU
3	C	156	THR
3	C	179	GLU
3	C	203	GLN
3	C	205	LYS
3	C	207	CYS
3	C	215	GLU
3	C	226	ASP
3	C	230	MET
3	C	238	ILE
3	C	240	VAL
3	C	245	VAL
3	C	249	ASP
3	C	254	LYS
3	C	265	MET
3	C	268	ASP
4	D	5	THR
4	D	8	PHE
4	D	9	GLN
4	D	12	ARG
4	D	13	ARG
4	D	14	ARG
4	D	21	GLU
4	D	23	ASN
4	D	28	GLN
4	D	31	GLN
4	D	32	GLU
4	D	35	LEU
4	D	38	ILE
4	D	39	ASN
4	D	46	GLU
4	D	47	LEU
4	D	52	LEU
4	D	53	SER

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Mol	Chain	Res	Type
4	D	60	LYS
4	D	65	GLU
4	D	67	ARG
4	D	74	GLN
4	D	119	ARG
4	D	121	LYS
4	D	123	LEU
4	D	126	ILE
4	D	130	LEU
4	D	137	ASN
4	D	139	LYS
4	D	149	THR
4	D	156	ASP
4	D	168	LYS
4	D	197	SER
4	D	211	LEU
4	D	215	SER
4	D	219	THR
4	D	221	TYR
5	E	3	GLN
5	E	6	GLU
5	E	8	ASN
5	E	70	SER
5	E	78	LEU
5	E	91	LYS
5	E	94	LYS
5	E	104	ASN
5	E	106	GLN
5	E	107	THR
5	E	146	HIS
5	E	152	LYS
5	E	156	LEU
5	E	161	LYS
5	E	173	SER
5	E	174	GLN
5	E	180	ARG
5	E	204	THR
6	F	79	ARG
6	F	87	LYS
6	F	109	VAL
6	F	111	LEU
6	F	115	THR

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Mol	Chain	Res	Type
7	G	2	PHE
7	G	8	SER
7	G	21	ARG
7	G	34	VAL
7	G	37	SER
7	G	39	THR
7	G	45	ILE
7	G	61	ILE
7	G	65	ASP
7	G	73	LYS
7	G	83	LYS
7	G	90	THR
7	G	92	VAL
7	G	96	GLN
7	G	107	LYS
7	G	114	LEU
7	G	133	SER
7	G	134	GLU
7	G	135	ASP
7	G	138	THR
7	G	143	ILE
7	G	145	VAL
7	G	152	SER
7	G	153	GLN
7	G	154	VAL
7	G	165	GLU
7	G	171	ILE
8	H	8	ASP
8	H	9	ILE
8	H	11	GLN
8	H	26	ILE
8	H	38	LEU
8	H	83	GLN
8	H	89	LEU
8	H	110	ASP
8	H	111	LEU
8	H	128	ASN
8	H	130	ARG
8	H	135	LEU
8	H	136	LYS
8	H	146	ARG
9	I	2	THR

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Mol	Chain	Res	Type
9	I	9	ASP
9	I	20	LYS
9	I	21	GLU
9	I	30	ARG
9	I	35	VAL
9	I	44	TYR
9	I	54	GLU
9	I	60	GLN
9	I	62	ILE
9	I	64	SER
9	I	70	ARG
9	I	83	ASN
9	I	89	GLN
9	I	90	GLN
9	I	91	ARG
9	I	98	VAL
9	I	107	SER
9	I	110	PHE
9	I	113	ASP
9	I	114	GLN
9	I	117	LYS
9	I	119	THR
10	J	2	ILE
10	J	3	VAL
10	J	13	VAL
10	J	27	GLU
10	J	28	ASP
10	J	31	ASP
10	J	34	THR
10	J	37	SER
10	J	38	ARG
10	J	47	ARG
10	J	48	ARG
10	J	52	THR
11	K	12	LEU
11	K	20	LYS
11	K	25	THR
11	K	26	LYS
11	K	29	ASN
11	K	31	VAL
11	K	47	ARG
11	K	51	LEU

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Mol	Chain	Res	Type
11	K	54	ARG
11	K	64	GLU
11	K	101	LEU
11	K	103	THR
12	L	26	THR
12	L	28	LYS
12	L	38	LEU
12	L	46	VAL
12	L	54	ARG
12	L	55	ILE
12	L	60	ARG
12	L	61	THR
12	L	66	GLN
12	L	68	GLU
15	S	148	LEU
15	S	149	ARG
15	S	156	LEU
15	S	166	HIS
15	S	172	LEU
15	S	178	ILE
15	S	183	ASN
15	S	202	ILE
15	S	217	LYS
15	S	218	ILE
15	S	220	ASN
15	S	222	ASP
15	S	223	ILE
15	S	228	LEU
15	S	230	THR
15	S	231	CYS
15	S	232	ASP
15	S	234	LYS
15	S	236	LEU
15	S	245	ILE
15	S	262	GLU
15	S	264	SER
15	S	284	LEU
15	S	287	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	5/5 (100%)	3 (60%)	2 (40%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
14	P	8	C
14	P	9	C
14	P	10	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
14	P	7	C
14	P	8	C

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	$\# Z > 2$
16	BRU	T	22	14,16	19,21,22	0.95	1 (5%)	22,30,33	2.92	5 (22%)

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
16	BRU	T	22	14,16	-	0/5/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	22	BRU	C4-C5	2.22	1.43	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	22	BRU	C6-N1-C2	-11.18	119.23	122.41
16	T	22	BRU	N3-C2-N1	6.01	120.99	115.97
16	T	22	BRU	O4'-C1'-N1	3.10	113.51	107.68
16	T	22	BRU	C5-C6-N1	2.23	121.14	119.67
16	T	22	BRU	C4-N3-C2	-2.01	121.27	125.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 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	$\# Z > 2$
19	ACT	A	1734	-	1,3,3	0.83	0	0,3,3	0.00	-
20	EPE	A	1735	-	15,15,15	0.52	0	20,20,20	2.15	8 (40%)
19	ACT	B	1225	-	1,3,3	3.32	1 (100%)	0,3,3	0.00	-
21	PGE	L	71	-	9,9,9	0.48	0	8,8,8	0.32	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	ACT	A	1734	-	-	0/0/0/0	0/0/0/0
20	EPE	A	1735	-	-	0/9/19/19	0/1/1/1
19	ACT	B	1225	-	-	0/0/0/0	0/0/0/0
21	PGE	L	71	-	-	0/7/7/7	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	1225	ACT	CH3-C	3.32	1.53	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	1735	EPE	C5-N4-C3	4.30	119.54	108.86
20	A	1735	EPE	C7-N4-C3	3.61	120.64	111.32
20	A	1735	EPE	C9-C10-S	-3.54	100.39	113.01
20	A	1735	EPE	C7-N4-C5	3.24	119.68	111.32
20	A	1735	EPE	O3S-S-C10	2.85	109.54	105.93
20	A	1735	EPE	C9-N1-C2	-2.84	103.99	111.32
20	A	1735	EPE	C3-C2-N1	2.41	115.35	110.61
20	A	1735	EPE	C5-C6-N1	-2.27	106.14	110.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	1426/1733 (82%)	-0.08	3 (0%) 93 70	67, 109, 163, 215	0
2	B	1108/1224 (90%)	0.01	7 (0%) 86 46	69, 126, 191, 217	0
3	C	266/318 (83%)	-0.15	0 100 100	86, 116, 160, 193	0
4	D	177/221 (80%)	-0.12	1 (0%) 86 46	81, 118, 183, 202	0
5	E	214/215 (99%)	-0.09	0 100 100	88, 141, 188, 203	0
6	F	84/155 (54%)	-0.22	0 100 100	70, 90, 123, 136	0
7	G	171/171 (100%)	-0.06	0 100 100	82, 105, 148, 171	0
8	H	133/146 (91%)	0.15	0 100 100	121, 158, 197, 205	0
9	I	119/122 (97%)	0.07	4 (3%) 43 10	123, 156, 197, 216	0
10	J	65/70 (92%)	-0.09	0 100 100	95, 117, 159, 177	0
11	K	114/120 (95%)	-0.12	0 100 100	85, 112, 157, 173	0
12	L	46/70 (65%)	-0.10	1 (2%) 59 16	93, 158, 183, 202	0
13	N	7/14 (50%)	0.74	1 (14%) 3 1	217, 222, 231, 234	0
14	P	5/5 (100%)	0.00	0 100 100	238, 239, 244, 247	0
15	S	164/178 (92%)	0.28	4 (2%) 56 15	116, 181, 240, 254	0
16	T	13/27 (48%)	0.18	0 100 100	162, 195, 247, 252	0
All	All	4112/4789 (85%)	-0.04	21 (0%) 88 51	67, 119, 191, 254	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	S	157	TYR	4.5
9	I	118	ARG	3.5
2	B	470	LYS	3.3
1	A	69	THR	3.1
2	B	476	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
9	I	119	THR	2.9
1	A	1455	PRO	2.9
2	B	509	ALA	2.8
15	S	163	GLU	2.7
9	I	120	GLN	2.7
2	B	250	PHE	2.6
15	S	162	LYS	2.5
2	B	715	ALA	2.5
2	B	471	LYS	2.4
4	D	13	ARG	2.3
1	A	568	PRO	2.2
2	B	508	LEU	2.2
15	S	179	GLU	2.2
13	N	2	DG	2.2
9	I	55	THR	2.1
12	L	27	LEU	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
16	BRU	T	22	20/21	0.23	1.71	138,213,293,294	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
19	ACT	A	1734	4/4	0.42	5.45	72,95,126,151	0
21	PGE	L	71	10/10	0.26	1.75	116,149,279,292	0
17	ZN	I	1121	1/1	0.14	0.92	130,130,130,130	0
17	ZN	A	2457	1/1	0.19	0.38	87,87,87,87	0
17	ZN	B	2225	1/1	0.22	0.32	94,94,94,94	0
20	EPE	A	1735	15/15	0.21	0.26	25,77,245,245	0
19	ACT	B	1225	4/4	0.18	-0.19	46,51,87,298	0
17	ZN	C	1269	1/1	0.14	-0.45	94,94,94,94	0
17	ZN	L	1071	1/1	0.10	-0.48	158,158,158,158	0
18	MG	A	2458	1/1	0.19	-0.64	83,83,83,83	0
17	ZN	J	1066	1/1	0.24	-0.79	103,103,103,103	0
17	ZN	S	999	1/1	0.06	-1.02	215,215,215,215	0
17	ZN	A	2456	1/1	0.07	-1.79	145,145,145,145	0
17	ZN	I	1122	1/1	0.05	-2.39	186,186,186,186	0

6.5 Other polymers ⓘ

There are no such residues in this entry.