



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 15, 2025 – 07:05 pm BST

PDB ID : 9EWC / pdb\_00009ewc  
Title : DNA Polymerase Lambda I493R 528-530 NEY, TTP:At Ca<sup>2+</sup> Ground State Ternary Complex  
Authors : Nourisson, A.; Haouz, A.; Missouri, S.; Delarue, M.  
Deposited on : 2024-04-03  
Resolution : 3.67 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

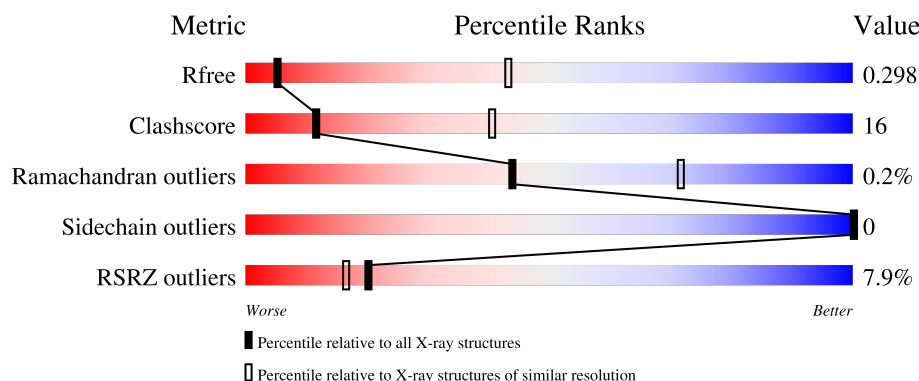
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.67 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.





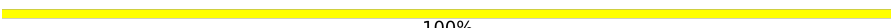
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1132 (3.80-3.56)
Clashscore	180529	1194 (3.80-3.56)
Ramachandran outliers	177936	1173 (3.80-3.56)
Sidechain outliers	177891	1170 (3.80-3.56)
RSRZ outliers	164620	1132 (3.80-3.56)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	330	<div> <div>7%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
1	C	330	<div> <div>7%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
2	E	11	<div> <div>64%</div> <div>36%</div> </div>
2	F	11	<div> <div>18%</div> <div>64%</div> <div>36%</div> </div>
3	G	6	<div> <div>50%</div> <div>100%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	I	6	 17% 83%
4	H	4	 25% 75%
4	J	4	 100%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5410 atoms, of which 6 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 polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2308	1438	417	443	10			
1	C	317	Total	C	N	O	S	0	1	0
			2231	1379	412	433	7			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLY	-	expression tag	UNP Q9UGP5
A	463	LYS	-	linker	UNP Q9UGP5
A	464	GLY	-	linker	UNP Q9UGP5
A	470	GLU	-	linker	UNP Q9UGP5
A	471	THR	-	linker	UNP Q9UGP5
A	492	ARG	ILE	engineered mutation	UNP Q9UGP5
A	528	ASN	SER	engineered mutation	UNP Q9UGP5
A	530	TYR	HIS	engineered mutation	UNP Q9UGP5
A	543	ALA	CYS	conflict	UNP Q9UGP5
C	241	GLY	-	expression tag	UNP Q9UGP5
C	463	LYS	-	linker	UNP Q9UGP5
C	464	GLY	-	linker	UNP Q9UGP5
C	470	GLU	-	linker	UNP Q9UGP5
C	471	THR	-	linker	UNP Q9UGP5
C	492	ARG	ILE	engineered mutation	UNP Q9UGP5
C	528	ASN	SER	engineered mutation	UNP Q9UGP5
C	530	TYR	HIS	engineered mutation	UNP Q9UGP5
C	543	ALA	CYS	conflict	UNP Q9UGP5

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	P	0	0	0
			224	107	43	64	10			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	11	Total	C	N	O	P	0	0	0
			224	107	43	64	10			

- Molecule 3 is a DNA chain called DNA primer strand upstream.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			
3	I	6	Total	C	N	O	P	0	0	0
			119	58	23	33	5			

- Molecule 4 is a DNA chain called DNA primer strand downstream (5'P).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			
4	J	4	Total	C	N	O	P	0	0	0
			83	38	16	25	4			

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		
5	C	1	Total	Na	0	0
			1	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ca	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	H	O	0	0
			10	2	6	2		

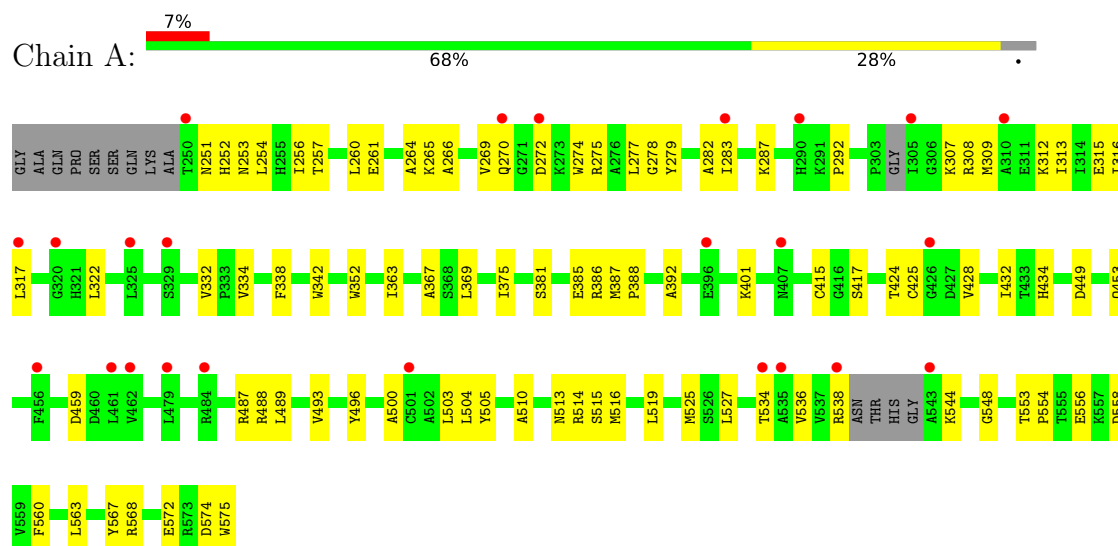
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	3	Total	O	0	0
			3	3		
8	C	1	Total	O	0	0
			1	1		
8	F	1	Total	O	0	0
			1	1		

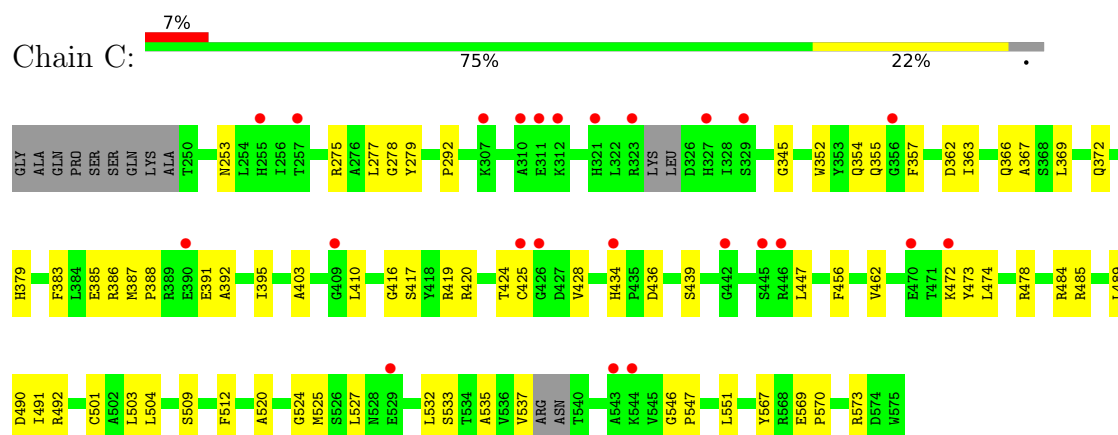
### 3 Residue-property plots

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

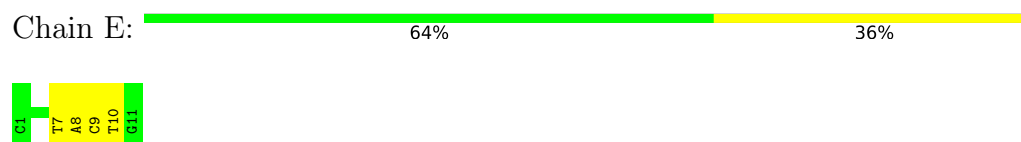
#### • Molecule 1: DNA polymerase lambda



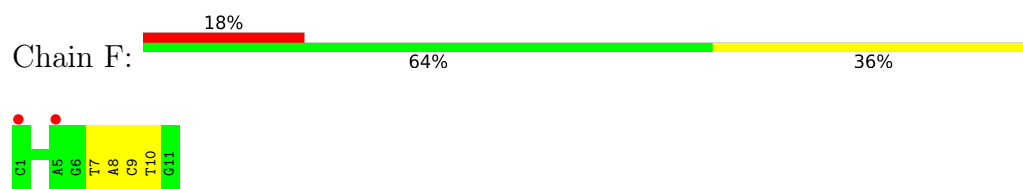
#### • Molecule 1: DNA polymerase lambda



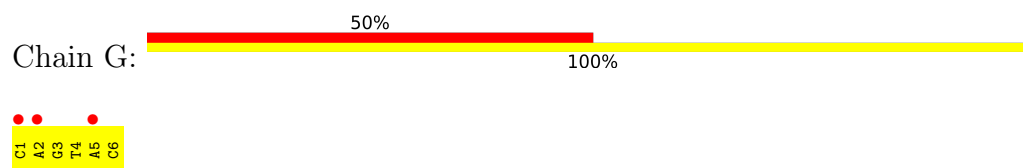
#### • Molecule 2: DNA template strand



- Molecule 2: DNA template strand



- Molecule 3: DNA primer strand upstream



- Molecule 3: DNA primer strand upstream



- Molecule 4: DNA primer strand downstream (5'P)



- Molecule 4: DNA primer strand downstream (5'P)





## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.90Å 149.90Å 272.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	60.26 – 3.67 60.26 – 3.67	Depositor EDS
% Data completeness (in resolution range)	45.5 (60.26-3.67) 45.4 (60.26-3.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 3.67Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.240 , 0.293 0.241 , 0.298	Depositor DCC
$R_{free}$ test set	12547 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	-73.8	Xtriage
Anisotropy	-12.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5410	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CA, NA

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	0.17	0/2353	0.49	0/3193
1	C	0.18	0/2275	0.52	0/3101
2	E	0.34	0/251	0.69	0/386
2	F	0.36	0/251	0.69	0/386
3	G	0.25	0/133	0.60	0/203
3	I	0.22	0/133	0.52	0/203
4	H	0.25	0/92	0.50	0/138
4	J	0.23	0/92	0.55	0/138
All	All	0.20	0/5580	0.53	0/7748

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2308	0	2115	71	0
1	C	2231	0	1908	67	0
2	E	224	0	125	5	0
2	F	224	0	125	3	0
3	G	119	0	69	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	119	0	69	5	0
4	H	83	0	45	4	0
4	J	83	0	45	4	0
5	A	2	0	0	0	0
5	C	1	0	0	0	0
6	A	1	0	0	0	0
7	C	4	6	6	3	0
8	A	3	0	0	0	0
8	C	1	0	0	0	0
8	F	1	0	0	0	0
All	All	5404	6	4507	156	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 16.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:GLU:HG3	1:C:570:PRO:HD2	1.39	1.03
1:A:504:LEU:HD11	1:A:516:MET:HE2	1.48	0.93
1:A:261:GLU:HG3	1:A:283:ILE:HD13	1.55	0.87
1:A:315:GLU:HG2	1:A:322:LEU:HD12	1.58	0.85
1:A:265:LYS:O	1:A:269:VAL:HG13	1.80	0.80
2:F:9:DC:H2'	2:F:10:DT:H71	1.65	0.79
1:A:315:GLU:HG2	1:A:322:LEU:CD1	2.12	0.79
1:A:568:ARG:HH11	1:A:572:GLU:HB3	1.49	0.77
1:A:261:GLU:CG	1:A:283:ILE:HD13	2.16	0.75
1:A:538:ARG:HA	1:A:544:LYS:HA	1.69	0.74
1:A:417:SER:HB2	1:A:425:CYS:SG	2.29	0.73
1:C:474:LEU:HD13	1:C:490:ASP:OD1	1.89	0.73
1:C:385:GLU:HG3	1:C:485:ARG:NH1	2.03	0.72
1:C:420:ARG:NH1	1:C:509:SER:HB3	2.04	0.71
2:E:7:DT:H2'	2:E:8:DA:C8	2.26	0.71
1:A:342:TRP:CH2	3:G:5:DA:H4'	2.26	0.70
1:C:387:MET:HE3	1:C:392:ALA:HB2	1.73	0.70
1:A:515:SER:O	1:A:519:LEU:HG	1.91	0.69
1:C:537:VAL:CG2	1:C:546:GLY:HA3	2.23	0.68
1:C:357:PHE:HE1	1:C:366:GLN:HB2	1.58	0.68
1:A:264:ALA:HB2	1:A:279:TYR:HB3	1.74	0.68
2:E:9:DC:C6	2:E:10:DT:H72	2.29	0.67
1:A:387:MET:HB2	1:A:487:ARG:CZ	2.24	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:TRP:O	1:C:357:PHE:HB2	1.95	0.66
1:C:410:LEU:HD23	1:C:434:HIS:HB2	1.79	0.65
1:A:266:ALA:O	1:A:269:VAL:HG22	1.96	0.65
1:A:428:VAL:O	1:A:489:LEU:HD12	1.96	0.65
1:A:254:LEU:HA	1:A:257:THR:OG1	1.97	0.64
1:C:489:LEU:HD21	1:C:491:ILE:HD11	1.80	0.64
1:C:428:VAL:O	1:C:489:LEU:HD12	1.98	0.63
2:F:7:DT:H2'	2:F:8:DA:C8	2.33	0.63
1:A:309:MET:HG3	4:H:1:DG:O3'	1.98	0.63
1:A:253:ASN:O	1:A:257:THR:HG23	2.00	0.61
1:A:387:MET:HG2	1:A:388:PRO:O	2.00	0.61
1:C:357:PHE:HD1	1:C:362:ASP:HB3	1.66	0.61
1:A:504:LEU:HD11	1:A:516:MET:CE	2.29	0.60
1:A:363:ILE:HA	1:A:367:ALA:HB3	1.84	0.59
1:A:415:CYS:SG	1:A:503:LEU:CD1	2.90	0.59
1:C:417:SER:HB2	1:C:425:CYS:SG	2.41	0.59
1:C:462:VAL:HB	1:C:474:LEU:HB2	1.84	0.59
1:C:527:LEU:HD13	1:C:532:LEU:HB2	1.85	0.59
2:E:9:DC:H2'	2:E:10:DT:H72	1.84	0.59
1:A:252:HIS:HB3	1:A:292:PRO:HG3	1.86	0.58
3:I:4:DT:H2''	3:I:5:DA:C8	2.39	0.57
1:A:500:ALA:HB2	1:A:554:PRO:O	2.03	0.57
3:G:5:DA:H2'	3:G:6:DC:C6	2.39	0.57
1:A:375:ILE:HD13	1:A:459:ASP:HB3	1.86	0.57
1:A:251:ASN:CG	1:A:287:LYS:HG2	2.30	0.56
1:A:386:ARG:CB	1:A:424:THR:HB	2.35	0.56
1:C:391:GLU:OE1	7:C:601:EDO:H12	2.06	0.56
2:F:9:DC:C2'	2:F:10:DT:H71	2.36	0.56
1:C:472:LYS:HD2	1:C:492:ARG:HH22	1.70	0.56
1:C:357:PHE:CE1	1:C:366:GLN:HB2	2.40	0.55
1:C:387:MET:SD	1:C:391:GLU:HB2	2.47	0.55
1:C:537:VAL:HG21	1:C:546:GLY:HA3	1.87	0.55
3:I:5:DA:H2'	3:I:6:DC:C6	2.43	0.54
1:C:403:ALA:HB2	1:C:447:LEU:HD22	1.88	0.53
1:A:352:TRP:NE1	1:A:367:ALA:HB1	2.23	0.53
1:A:277:LEU:HD21	1:A:514:ARG:NH1	2.23	0.53
1:C:387:MET:HB2	7:C:601:EDO:H22	1.89	0.53
1:A:415:CYS:SG	1:A:503:LEU:HD13	2.48	0.53
1:C:387:MET:CG	1:C:391:GLU:HB2	2.38	0.53
1:C:278:GLY:HA3	4:J:1:DG:H1'	1.91	0.53
1:C:504:LEU:HD21	1:C:527:LEU:HD21	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:ALA:HB1	1:C:525:MET:O	2.09	0.53
1:A:266:ALA:O	1:A:270:GLN:HG3	2.09	0.52
1:C:527:LEU:CD1	1:C:532:LEU:HB2	2.40	0.52
1:A:272:ASP:HB3	1:A:275:ARG:HB2	1.92	0.52
1:A:256:ILE:O	1:A:260:LEU:HG	2.11	0.51
1:C:372:GLN:OE1	2:E:10:DT:H4'	2.10	0.51
1:C:253:ASN:HD21	1:C:292:PRO:HA	1.75	0.51
1:C:354:GLN:O	1:C:355:GLN:HB2	2.11	0.51
1:C:387:MET:HG3	1:C:391:GLU:HB2	1.93	0.51
1:C:410:LEU:CD2	1:C:434:HIS:HB2	2.41	0.51
1:A:342:TRP:CH2	1:A:488:ARG:CZ	2.95	0.50
1:A:363:ILE:HA	1:A:367:ALA:CB	2.40	0.50
1:A:510:ALA:O	1:A:514:ARG:HG3	2.12	0.50
1:A:387:MET:HE3	1:A:392:ALA:HB2	1.93	0.50
1:C:387:MET:HG2	1:C:388:PRO:O	2.11	0.50
1:C:533:SER:HA	1:C:551:LEU:HG	1.93	0.50
1:C:509:SER:N	1:C:512:PHE:HB3	2.27	0.50
1:A:363:ILE:CG2	1:A:369:LEU:HD21	2.41	0.49
2:E:9:DC:H2'	2:E:10:DT:C7	2.43	0.49
1:A:387:MET:O	1:A:424:THR:HA	2.13	0.49
1:C:403:ALA:CB	1:C:447:LEU:HD22	2.41	0.49
1:A:449:ASP:O	1:A:453:GLN:HG2	2.14	0.48
1:A:316:ILE:HG12	1:A:322:LEU:HB2	1.96	0.48
1:C:420:ARG:HH12	1:C:509:SER:HB3	1.77	0.47
1:A:334:VAL:HG12	1:A:338:PHE:CE2	2.49	0.47
1:A:505:TYR:HD1	1:A:513:ASN:ND2	2.12	0.47
1:A:574:ASP:O	1:A:575:TRP:C	2.57	0.47
1:A:525:MET:HG2	1:A:534:THR:HA	1.96	0.47
1:C:345:GLY:H	3:I:4:DT:H5''	1.78	0.47
1:A:500:ALA:HB3	1:A:553:THR:O	2.15	0.47
1:C:387:MET:CE	1:C:392:ALA:HB2	2.42	0.47
1:A:269:VAL:HG21	1:A:332:VAL:HG13	1.97	0.46
1:C:403:ALA:HB2	1:C:447:LEU:CD2	2.44	0.46
1:C:473:TYR:HB3	1:C:491:ILE:O	2.15	0.46
1:C:537:VAL:HG23	1:C:546:GLY:HA3	1.94	0.46
1:A:316:ILE:HD11	1:A:322:LEU:HD22	1.98	0.46
1:A:312:LYS:HG3	1:A:322:LEU:HD11	1.98	0.45
1:C:379:HIS:HB2	1:C:383:PHE:CE2	2.51	0.45
1:C:363:ILE:HA	1:C:367:ALA:CB	2.46	0.45
1:C:387:MET:HB2	7:C:601:EDO:C2	2.47	0.45
1:C:504:LEU:CD2	1:C:527:LEU:HD21	2.46	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ARG:NH1	1:A:572:GLU:HB3	2.26	0.45
1:C:275:ARG:O	1:C:279:TYR:HD1	2.00	0.45
1:A:274:TRP:HB3	4:H:1:DG:C6	2.52	0.45
1:A:313:ILE:O	1:A:317:LEU:HG	2.17	0.45
1:A:556:GLU:HB3	1:A:567:TYR:HE1	1.82	0.45
1:C:277:LEU:C	1:C:277:LEU:HD23	2.42	0.45
1:C:512:PHE:CZ	1:C:573:ARG:HD3	2.53	0.44
1:A:352:TRP:CZ2	1:A:369:LEU:HD23	2.53	0.44
1:C:567:TYR:HE2	1:C:569:GLU:OE2	2.01	0.44
1:A:282:ALA:HB3	1:A:309:MET:HE1	1.99	0.44
1:A:363:ILE:HG22	1:A:369:LEU:HD21	1.98	0.44
3:G:1:DC:H2'	3:G:2:DA:C8	2.53	0.43
1:A:307:LYS:HD3	1:A:308:ARG:HG2	2.00	0.43
1:A:575:TRP:H	1:A:575:TRP:HD1	1.66	0.43
1:A:527:LEU:HD22	1:A:563:LEU:HD11	2.00	0.43
1:C:379:HIS:HB2	1:C:383:PHE:CZ	2.53	0.43
1:C:501:CYS:O	1:C:504:LEU:HB3	2.19	0.43
4:J:1:DG:H2'	4:J:2:DC:C6	2.52	0.43
1:A:434:HIS:O	1:A:496:TYR:HB2	2.18	0.43
1:A:556:GLU:O	1:A:560:PHE:HD2	2.01	0.43
1:A:387:MET:HE2	1:A:387:MET:HB3	1.96	0.43
1:C:416:GLY:O	1:C:420:ARG:HG3	2.19	0.43
1:C:417:SER:HA	1:C:420:ARG:HE	1.84	0.43
1:C:357:PHE:CD1	1:C:362:ASP:HB3	2.51	0.42
1:C:387:MET:O	1:C:424:THR:HA	2.19	0.42
4:J:3:DC:H2''	4:J:4:DG:C8	2.54	0.42
1:A:278:GLY:HA3	4:H:1:DG:H1'	2.01	0.42
3:I:4:DT:H2''	3:I:5:DA:H8	1.84	0.42
3:G:3:DG:H2'	3:G:4:DT:H71	2.01	0.42
1:A:554:PRO:HD2	1:A:558:ASP:OD2	2.20	0.42
4:H:3:DC:H2''	4:H:4:DG:C8	2.55	0.42
1:A:575:TRP:H	1:A:575:TRP:CD1	2.38	0.42
1:C:386:ARG:CB	1:C:424:THR:HB	2.49	0.42
1:C:417:SER:HB2	1:C:425:CYS:HB3	2.01	0.42
3:I:1:DC:H2'	3:I:2:DA:C8	2.55	0.42
1:A:272:ASP:OD2	1:A:275:ARG:HG3	2.21	0.41
1:C:434:HIS:ND1	1:C:436:ASP:OD1	2.52	0.41
1:C:524:GLY:O	1:C:535:ALA:HB2	2.20	0.41
1:C:478:ARG:NH1	1:C:484:ARG:HB2	2.35	0.41
4:J:2:DC:H2''	4:J:3:DC:C6	2.56	0.41
1:A:381:SER:O	1:A:385:GLU:HG2	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ARG:NH2	1:C:503:LEU:HD21	2.36	0.41
1:A:432:ILE:O	1:A:493:VAL:HA	2.21	0.40
1:C:395:ILE:HG23	1:C:456:PHE:HZ	1.87	0.40
1:C:434:HIS:CG	1:C:439:SER:HB2	2.56	0.40
1:A:342:TRP:CZ3	3:G:5:DA:H5''	2.55	0.40
1:A:401:LYS:HE2	1:A:401:LYS:HB3	1.97	0.40
1:A:536:VAL:HA	1:A:548:GLY:HA2	2.02	0.40
1:C:352:TRP:CZ2	1:C:369:LEU:HD23	2.56	0.40
1:C:363:ILE:HA	1:C:367:ALA:HB3	2.03	0.40
1:C:509:SER:H	1:C:512:PHE:HB3	1.86	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	310/330 (94%)	299 (96%)	11 (4%)	0	100	100
1	C	312/330 (94%)	299 (96%)	12 (4%)	1 (0%)	37	67
All	All	622/660 (94%)	598 (96%)	23 (4%)	1 (0%)	44	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	547	PRO

### 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	217/274 (79%)	217 (100%)	0	100	100
1	C	188/274 (69%)	188 (100%)	0	100	100
All	All	405/548 (74%)	405 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	486	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
7	EDO	C	601	-	3,3,3	0.28	0	2,2,2	0.62	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
7	EDO	C	601	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	601	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	601	EDO	3	0

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	316/330 (95%)	0.70	24 (7%) 21 17	9, 30, 57, 82	0
1	C	317/330 (96%)	0.68	24 (7%) 21 17	6, 28, 63, 80	1 (0%)
2	E	11/11 (100%)	0.81	0 100 100	25, 37, 55, 64	0
2	F	11/11 (100%)	1.33	2 (18%) 4 6	43, 51, 59, 70	0
3	G	6/6 (100%)	1.56	3 (50%) 0 0	36, 43, 83, 90	0
3	I	6/6 (100%)	0.95	0 100 100	27, 29, 46, 54	0
4	H	4/4 (100%)	0.70	0 100 100	42, 49, 62, 66	0
4	J	4/4 (100%)	0.75	0 100 100	35, 38, 39, 42	0
All	All	675/702 (96%)	0.72	53 (7%) 20 16	6, 31, 62, 90	1 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	321	HIS	4.6
1	A	543	ALA	3.9
1	C	445	SER	3.5
1	C	255	HIS	3.5
1	C	409	GLY	3.3
1	C	543	ALA	3.2
1	A	290	HIS	3.2
3	G	5	DA	3.0
1	C	327	HIS	3.0
1	C	257	THR	3.0
1	A	305	ILE	2.8
1	A	270	GLN	2.8
1	C	329	SER	2.8
1	C	307	LYS	2.8
1	C	310	ALA	2.7
1	C	426	GLY	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	325	LEU	2.6
1	C	529	GLU	2.6
1	A	538	ARG	2.6
1	A	501	CYS	2.6
1	A	426	GLY	2.5
1	C	425	CYS	2.5
1	A	317	LEU	2.5
1	C	544	LYS	2.5
2	F	5	DA	2.4
1	C	472	LYS	2.4
1	C	470	GLU	2.4
1	A	461	LEU	2.4
1	C	446	ARG	2.4
1	C	442	GLY	2.3
1	A	534	THR	2.3
1	A	272	ASP	2.3
1	A	407	ASN	2.3
1	A	310	ALA	2.3
1	C	311	GLU	2.2
1	C	356	GLY	2.2
1	C	390	GLU	2.2
1	A	462	VAL	2.2
1	C	323	ARG	2.2
1	A	479	LEU	2.2
1	A	329	SER	2.2
1	A	396	GLU	2.2
1	C	312	LYS	2.2
1	A	283	ILE	2.1
1	A	456	PHE	2.1
3	G	1	DC	2.1
1	A	484	ARG	2.1
1	A	535	ALA	2.1
1	C	434	HIS	2.0
1	A	250	THR	2.0
1	A	320	GLY	2.0
2	F	1	DC	2.0
3	G	2	DA	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NA	A	602	1/1	0.83	0.45	0,0,0,0	0
5	NA	A	601	1/1	0.84	0.18	16,16,16,16	0
5	NA	C	602	1/1	0.97	0.24	0,0,0,0	0
7	EDO	C	601	4/4	0.97	0.07	4,8,9,11	0
6	CA	A	603	1/1	0.98	0.06	22,22,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.