



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 02:03 AM EDT

PDB ID : 1RZT
Title : Crystal structure of DNA polymerase lambda complexed with a two nucleotide gap DNA molecule
Authors : Pedersen, L.C.; Garcia-Diaz, M.; Bebenek, K.; Krahn, J.M.; Blanco, L.; Kunkel, T.A.
Deposited on : unknown
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

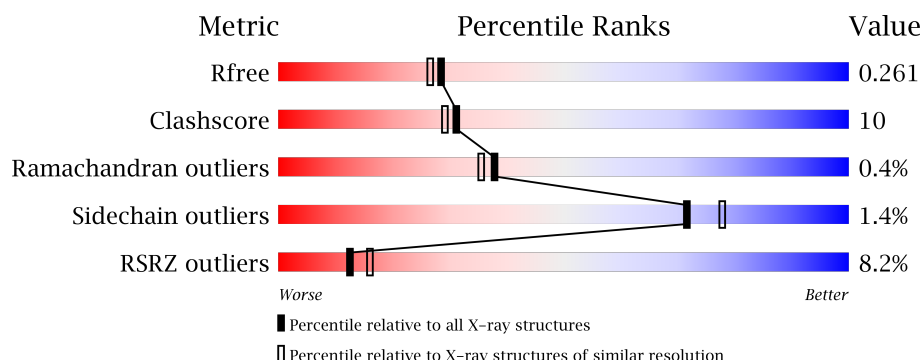
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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. 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	B	11	
1	F	11	
1	J	11	
1	N	11	
2	C	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	G	5	 100%
2	K	5	 80% 20%
2	O	5	 80% 20%
3	D	4	 75% 25%
3	H	4	 75% 25%
3	L	4	 50% 50%
3	P	4	 25% 25% 50%
4	A	331	 3% 86% 13% .
4	E	331	 12% 72% 27% .
4	I	331	 13% 74% 24% .
4	M	331	 6% 84% 14% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NA	A	2001	-	-	-	X
5	NA	A	2008	-	-	-	X
6	EDO	M	2801	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12863 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 DNA chain called 5'-D(*CP*GP*GP*CP*AP*AP*CP*GP*CP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	11	Total	C	N	O	P	0	0	0
			221	105	45	61	10			
1	F	11	Total	C	N	O	P	0	0	0
			221	105	45	61	10			
1	J	11	Total	C	N	O	P	0	0	0
			221	105	45	61	10			
1	N	11	Total	C	N	O	P	0	0	0
			221	105	45	61	10			

- Molecule 2 is a DNA chain called 5'-D(*GP*TP*GP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	P	0	0	0
			102	49	20	29	4			
2	G	5	Total	C	N	O	P	0	0	0
			102	49	20	29	4			
2	K	5	Total	C	N	O	P	0	0	0
			102	49	20	29	4			
2	O	5	Total	C	N	O	P	0	0	0
			102	49	20	29	4			

- Molecule 3 is a DNA chain called 5'-D(P*GP*CP*CP*G)-3'.

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

- Molecule 4 is a protein called DNA polymerase lambda.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	327	Total	C	N	O	S	0	1	0
			2565	1608	468	477	12			
4	E	326	Total	C	N	O	S	0	0	0
			2544	1597	465	470	12			
4	I	326	Total	C	N	O	S	0	0	0
			2529	1589	461	467	12			
4	M	327	Total	C	N	O	S	0	0	0
			2561	1607	468	474	12			

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	2	Total	Na	0	0
			2	2		
5	E	1	Total	Na	0	0
			1	1		
5	B	1	Total	Na	0	0
			1	1		
5	I	1	Total	Na	0	0
			1	1		
5	A	2	Total	Na	0	0
			2	2		
5	F	1	Total	Na	0	0
			1	1		
5	M	2	Total	Na	0	0
			2	2		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	24	Total	O	0	0
			24	24		
7	C	14	Total	O	0	0
			14	14		
7	D	5	Total	O	0	0
			5	5		
7	F	21	Total	O	0	0
			21	21		
7	G	4	Total	O	0	0
			4	4		
7	H	4	Total	O	0	0
			4	4		
7	J	20	Total	O	0	0
			20	20		
7	K	11	Total	O	0	0
			11	11		
7	L	6	Total	O	0	0
			6	6		
7	N	34	Total	O	0	0
			34	34		
7	O	16	Total	O	0	0
			16	16		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	6	Total 6	O 6	0	0
7	A	289	Total 289	O 289	0	0
7	E	109	Total 109	O 109	0	0
7	I	134	Total 134	O 134	0	0
7	M	329	Total 329	O 329	0	0

3 Residue-property plots


These plots are drawn for all protein, RNA and DNA 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: 5'-D(*CP*GP*GP*CP*AP*AP*CP*GP*CP*AP*C)-3'

Chain B: 



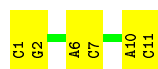
- Molecule 1: 5'-D(*CP*GP*GP*CP*AP*AP*CP*GP*CP*AP*C)-3'

Chain F: 



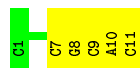
- Molecule 1: 5'-D(*CP*GP*GP*CP*AP*AP*CP*GP*CP*AP*C)-3'

Chain J: 




- Molecule 1: 5'-D(*CP*GP*GP*CP*AP*AP*CP*GP*CP*AP*C)-3'

Chain N: 



- Molecule 2: 5'-D(*GP*TP*GP*CP*G)-3'

Chain C: 




- Molecule 2: 5'-D(*GP*TP*GP*CP*G)-3'

Chain G: 

There are no outlier residues recorded for this chain.

- Molecule 2: 5'-D(*GP*TP*GP*CP*G)-3'

Chain K:  80% 20%




- Molecule 2: 5'-D(*GP*TP*GP*CP*G)-3'

Chain O:  80% 20%

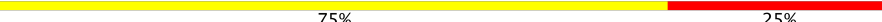


- Molecule 3: 5'-D(P*GP*CP*CP*G)-3'

Chain D:  75% 25%



- Molecule 3: 5'-D(P*GP*CP*CP*G)-3'

Chain H:  75% 25%




- Molecule 3: 5'-D(P*GP*CP*CP*G)-3'

Chain L:  50% 50%




- Molecule 3: 5'-D(P*GP*CP*CP*G)-3'

Chain P:  25% 25% 50%



- Molecule 4: DNA polymerase lambda

Chain A:  3% 86% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	191.32Å 99.03Å 104.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.10 24.55 – 2.09	Depositor EDS
% Data completeness (in resolution range)	93.2 (19.92-2.10) 92.5 (24.55-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.227 , 0.260 0.228 , 0.261	Depositor DCC
R_{free} test set	2701 reflections (2.49%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12863	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	B	0.42	0/248	0.69	0/380
1	F	0.30	0/248	0.67	0/380
1	J	0.33	0/248	0.67	0/380
1	N	0.37	0/248	0.70	0/380
2	C	0.40	0/114	0.67	0/175
2	G	0.27	0/114	0.58	0/175
2	K	0.33	0/114	0.62	0/175
2	O	0.40	0/114	0.58	0/175
3	D	0.93	1/92 (1.1%)	0.77	0/138
3	H	0.98	1/92 (1.1%)	0.75	0/138
3	L	0.96	1/92 (1.1%)	0.73	0/138
3	P	1.01	1/92 (1.1%)	0.93	0/138
4	A	0.36	0/2618	0.59	0/3536
4	E	0.31	0/2597	0.54	0/3508
4	I	0.31	0/2582	0.54	0/3490
4	M	0.34	0/2614	0.59	0/3529
All	All	0.37	4/12227 (0.0%)	0.59	0/16835

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
3	D	0	1
3	H	0	1
3	P	0	2
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1	DG	OP3-P	-7.49	1.52	1.61
3	L	1	DG	OP3-P	-7.22	1.52	1.61
3	D	1	DG	OP3-P	-7.19	1.52	1.61
3	H	1	DG	OP3-P	-7.18	1.52	1.61

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	1	DG	Sidechain
3	H	1	DG	Sidechain
3	P	2	DC	Sidechain
3	P	3	DC	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	221	0	123	5	0
1	F	221	0	123	6	0
1	J	221	0	123	6	0
1	N	221	0	123	5	0
2	C	102	0	58	1	0
2	G	102	0	58	0	0
2	K	102	0	58	1	0
2	O	102	0	58	1	0
3	D	83	0	45	2	0
3	H	83	0	45	3	0
3	L	83	0	45	1	0
3	P	83	0	45	2	0
4	A	2565	0	2535	34	0
4	E	2544	0	2518	74	0
4	I	2529	0	2489	64	0
4	M	2561	0	2543	39	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
5	J	2	0	0	0	0
5	M	2	0	0	0	0
6	M	4	0	6	0	0
7	A	289	0	0	2	0
7	B	24	0	0	0	0
7	C	14	0	0	0	0
7	D	5	0	0	0	0
7	E	109	0	0	0	0
7	F	21	0	0	0	0
7	G	4	0	0	0	0
7	H	4	0	0	0	0
7	I	134	0	0	0	0
7	J	20	0	0	1	0
7	K	11	0	0	0	0
7	L	6	0	0	0	0
7	M	329	0	0	0	0
7	N	34	0	0	0	0
7	O	16	0	0	0	0
7	P	6	0	0	0	0
All	All	12863	0	10995	236	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (236) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:519:LEU:HD13	4:M:565:LEU:HD11	1.36	1.05
4:A:519:LEU:HD21	4:A:565:LEU:HD21	1.41	1.01
4:A:519:LEU:HD23	4:A:565:LEU:HD11	1.48	0.96
4:I:252:HIS:HB3	4:I:292:PRO:HG3	1.50	0.94
4:E:410:LEU:HD11	4:E:443:ILE:HD13	1.55	0.85
4:E:387:MET:HE2	4:E:391:GLU:HB3	1.59	0.85
4:M:308:ARG:HG3	4:M:308:ARG:HH11	1.45	0.82
4:A:519:LEU:CD2	4:A:565:LEU:HD11	2.10	0.82
4:A:387:MET:HE1	4:A:395:ILE:HD12	1.65	0.76
4:A:266:ALA:O	4:A:270:GLN:HG2	1.85	0.76
1:F:9:DC:H5'	4:E:465:GLU:HG3	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:251:ASN:OD1	4:I:287:LYS:HA	1.86	0.74
1:B:10:DA:H2''	1:B:11:DC:H5'	1.69	0.74
4:I:519:LEU:HD13	4:I:565:LEU:HD11	1.69	0.74
4:M:387:MET:HE1	4:M:395:ILE:HD12	1.69	0.73
4:I:288:SER:HB3	4:I:575:TRP:HZ3	1.52	0.73
4:M:519:LEU:CD1	4:M:565:LEU:HD11	2.18	0.73
4:M:442:GLY:O	4:M:446:ARG:HD3	1.89	0.71
4:I:261:GLU:HG2	4:I:283:ILE:HD13	1.72	0.71
4:I:470:GLN:HG2	4:I:494:VAL:HG12	1.73	0.71
4:E:252:HIS:HB3	4:E:292:PRO:HG3	1.72	0.71
4:M:519:LEU:HD11	4:M:565:LEU:HD21	1.72	0.70
4:E:291:LYS:HD2	4:E:298:GLU:OE2	1.94	0.69
4:I:346:THR:O	4:I:350:GLN:HB2	1.94	0.68
4:M:308:ARG:HG3	4:M:308:ARG:NH1	2.06	0.68
4:E:549:ARG:HG2	4:E:549:ARG:HH11	1.59	0.67
4:I:296:TYR:N	4:I:314:ILE:HD11	2.10	0.66
4:E:539:ASN:HD21	4:E:543:CYS:HB2	1.61	0.65
4:E:539:ASN:ND2	4:E:543:CYS:HB2	2.11	0.65
4:I:501:CYS:SG	4:I:531:ALA:HA	2.36	0.65
4:E:251:ASN:ND2	4:E:287:LYS:HG2	2.12	0.65
4:I:387:MET:HE2	4:I:391:GLU:HB3	1.79	0.65
4:M:440:HIS:HA	4:M:443:ILE:HD12	1.77	0.65
4:E:501:CYS:SG	4:E:531:ALA:HA	2.38	0.64
4:E:385:GLU:HG3	4:E:485:ARG:NH1	2.14	0.62
4:M:387:MET:CE	4:M:395:ILE:HD12	2.29	0.62
4:A:387:MET:CE	4:A:395:ILE:HD12	2.28	0.62
4:I:557:LYS:CG	4:I:567:TYR:CD2	2.83	0.62
4:M:549:ARG:HG2	4:M:549:ARG:HH11	1.64	0.62
4:E:385:GLU:CD	4:E:485:ARG:HH12	2.02	0.61
4:A:519:LEU:HD21	4:A:565:LEU:CD2	2.26	0.61
4:E:519:LEU:HD11	4:E:565:LEU:HD21	1.82	0.61
4:I:308:ARG:HH11	4:I:308:ARG:HG3	1.66	0.61
4:I:557:LYS:HG3	4:I:567:TYR:CD2	2.36	0.60
4:M:538:ARG:HB2	4:M:543:CYS:N	2.16	0.60
4:E:275:ARG:NH1	4:E:275:ARG:HB2	2.16	0.60
4:E:364:ARG:HB2	4:E:377:LEU:HD21	1.84	0.60
4:M:518:ALA:O	4:M:522:THR:HG23	2.01	0.60
4:E:410:LEU:HD21	4:E:443:ILE:CD1	2.32	0.59
4:E:296:TYR:HB2	4:E:314:ILE:HG13	1.83	0.59
4:I:265:LYS:HD3	4:I:336:GLU:OE2	2.02	0.59
4:A:323:ARG:HH11	4:A:323:ARG:HG2	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:DC:H2''	1:B:2:DG:C8	2.37	0.59
4:E:332:VAL:HB	4:E:333:PRO:HD3	1.84	0.59
4:M:439:SER:O	4:M:443:ILE:HD11	2.02	0.59
4:E:519:LEU:HD13	4:E:565:LEU:HD11	1.83	0.59
4:I:296:TYR:HB2	4:I:314:ILE:HG13	1.84	0.58
4:M:410:LEU:HD11	4:M:443:ILE:HD13	1.83	0.58
1:B:10:DA:H2''	1:B:11:DC:C5'	2.33	0.58
4:I:266:ALA:O	4:I:270:GLN:HG3	2.04	0.58
1:F:10:DA:H2''	1:F:11:DC:C5'	2.34	0.58
4:E:359:SER:HB2	4:E:361:GLU:OE1	2.02	0.57
1:N:10:DA:H2''	1:N:11:DC:C5'	2.34	0.57
4:A:387:MET:HE2	4:A:391:GLU:HB3	1.87	0.57
4:E:279:TYR:O	4:E:283:ILE:HG13	2.05	0.57
1:F:10:DA:H2''	1:F:11:DC:H5'	1.87	0.57
4:M:501:CYS:SG	4:M:531:ALA:HA	2.45	0.57
4:E:434:HIS:CG	4:E:439:SER:HB2	2.40	0.57
4:M:410:LEU:HD21	4:M:443:ILE:CD1	2.35	0.57
1:N:10:DA:H1'	1:N:11:DC:H5''	1.85	0.57
4:E:269:VAL:O	4:E:346:THR:HG22	2.05	0.57
4:I:334:VAL:HG21	4:I:353:TYR:CD2	2.40	0.56
4:M:387:MET:HE1	4:M:392:ALA:HA	1.87	0.56
4:A:251:ASN:HD21	4:A:254:LEU:HA	1.70	0.56
4:I:557:LYS:HG2	4:I:567:TYR:CD2	2.41	0.56
4:E:519:LEU:CD1	4:E:565:LEU:HD21	2.35	0.56
1:F:1:DC:H2''	1:F:2:DG:C8	2.40	0.56
4:I:331:SER:O	4:I:334:VAL:HG22	2.05	0.56
4:M:277:LEU:HD11	4:M:281:LYS:HE3	1.88	0.55
4:M:519:LEU:CD1	4:M:565:LEU:HD21	2.36	0.55
4:E:378:LYS:HE3	4:E:379:HIS:NE2	2.20	0.55
4:I:256:ILE:HD13	4:I:313:ILE:HG23	1.89	0.55
4:I:470:GLN:CG	4:I:494:VAL:HG12	2.36	0.55
4:I:536:VAL:HG13	4:I:546:GLY:O	2.07	0.55
4:I:456:PHE:HE1	4:I:479:LEU:HD23	1.73	0.54
1:N:10:DA:H2''	1:N:11:DC:H5'	1.88	0.54
4:E:305:ILE:HG23	4:E:309:MET:HB3	1.90	0.54
4:I:261:GLU:CG	4:I:283:ILE:HD13	2.38	0.54
1:J:10:DA:H1'	1:J:11:DC:H5''	1.88	0.54
4:A:277:LEU:HG	4:A:281:LYS:HE3	1.89	0.54
4:I:387:MET:HE1	4:I:395:ILE:HD12	1.90	0.54
4:I:386:ARG:HB3	4:I:424:THR:HB	1.89	0.54
4:M:434:HIS:ND1	4:M:435:PRO:HD2	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:470:GLN:HG2	4:E:494:VAL:HG12	1.89	0.53
4:E:272:ASP:OD2	4:E:275:ARG:NH1	2.42	0.53
4:I:267:TYR:CZ	4:I:275:ARG:HD3	2.44	0.53
4:I:382:ASP:OD1	4:I:485:ARG:HD3	2.09	0.53
4:M:286:LEU:HD13	4:M:305:ILE:HD11	1.91	0.53
4:A:281:LYS:HE2	7:A:2133:HOH:O	2.08	0.53
4:A:367:ALA:O	4:I:566:PRO:HB3	2.08	0.53
4:I:569:GLU:HG3	4:I:570:PRO:HD2	1.91	0.53
4:M:305:ILE:HG23	4:M:309:MET:HB3	1.91	0.52
4:E:538:ARG:HA	4:E:543:CYS:O	2.09	0.52
1:J:10:DA:H2''	1:J:11:DC:C5'	2.40	0.52
4:E:462:VAL:HB	4:E:474:LEU:HB2	1.92	0.52
4:A:474:LEU:HD22	4:A:490:ASP:OD2	2.10	0.52
4:E:385:GLU:CG	4:E:485:ARG:HH12	2.23	0.52
4:I:265:LYS:HD3	4:I:336:GLU:CD	2.30	0.52
4:E:568:ARG:HG2	4:E:572:GLU:HB2	1.91	0.52
4:I:332:VAL:HB	4:I:333:PRO:HD3	1.92	0.52
4:E:266:ALA:O	4:E:270:GLN:HG3	2.11	0.51
4:E:415:CYS:HA	4:E:419:ARG:HB2	1.91	0.51
4:E:431:LEU:HD23	4:E:503:LEU:CD2	2.41	0.51
2:O:5:DG:H4'	4:M:342:TRP:CZ2	2.45	0.51
4:M:252:HIS:HB3	4:M:292:PRO:HD3	1.91	0.51
3:P:2:DC:H2'	3:P:3:DC:C6	2.45	0.51
4:E:385:GLU:CG	4:E:485:ARG:NH1	2.74	0.51
4:I:519:LEU:HD22	4:I:563:LEU:HD22	1.93	0.51
4:M:467:ASN:ND2	4:M:529:GLU:OE2	2.39	0.51
4:M:332:VAL:HB	4:M:333:PRO:HD3	1.92	0.51
4:E:361:GLU:CD	4:E:361:GLU:H	2.13	0.51
4:I:308:ARG:NH1	4:I:308:ARG:HG3	2.25	0.51
4:A:251:ASN:ND2	4:A:254:LEU:HA	2.26	0.50
4:E:275:ARG:HB2	4:E:275:ARG:HH11	1.76	0.50
4:E:363:ILE:HG23	4:E:367:ALA:HB3	1.93	0.50
2:K:5:DG:H4'	4:I:342:TRP:CZ2	2.46	0.50
4:A:387:MET:HE1	4:A:392:ALA:HA	1.93	0.50
4:M:387:MET:HE2	4:M:391:GLU:HB3	1.94	0.50
4:I:334:VAL:HG21	4:I:353:TYR:CE2	2.47	0.50
4:I:519:LEU:HD11	4:I:565:LEU:HD21	1.93	0.50
1:J:10:DA:C2'	1:J:11:DC:H5''	2.42	0.50
4:I:511:HIS:ND1	4:I:514:ARG:NH2	2.60	0.50
1:J:10:DA:H2''	1:J:11:DC:H5''	1.94	0.50
4:E:536:VAL:HG12	4:E:537:VAL:N	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:519:LEU:CD1	4:I:565:LEU:HD21	2.41	0.49
1:J:1:DC:H2"	1:J:2:DG:C8	2.47	0.49
3:H:3:DC:H2"	3:H:4:DG:C8	2.47	0.49
4:I:370:THR:OG1	4:I:373:GLN:HG3	2.12	0.49
4:I:549:ARG:HG2	4:I:549:ARG:HH11	1.78	0.49
4:A:474:LEU:HD22	4:A:490:ASP:CG	2.33	0.49
1:B:9:DC:H2"	1:B:10:DA:C8	2.48	0.49
4:E:431:LEU:HD23	4:E:503:LEU:HD23	1.94	0.49
4:E:429:ASP:OD1	4:E:490:ASP:HB2	2.13	0.49
4:M:540:THR:C	4:M:542:GLY:H	2.16	0.49
4:E:256:ILE:HD13	4:E:313:ILE:HG23	1.94	0.48
4:I:465:GLU:OE1	4:I:472:LYS:HE2	2.12	0.48
4:E:352:TRP:CD2	4:E:363:ILE:HD12	2.48	0.48
4:E:549:ARG:NH1	4:E:549:ARG:HG2	2.28	0.48
4:E:277:LEU:C	4:E:277:LEU:HD23	2.34	0.47
4:E:364:ARG:CB	4:E:377:LEU:HD21	2.43	0.47
4:M:538:ARG:HB2	4:M:543:CYS:H	1.79	0.47
4:M:538:ARG:HD3	4:M:542:GLY:HA2	1.95	0.47
4:I:449:ASP:O	4:I:453:GLN:HG3	2.14	0.47
4:A:473:TYR:O	4:A:474:LEU:HD23	2.14	0.47
4:E:363:ILE:HA	4:E:367:ALA:CB	2.45	0.47
4:M:538:ARG:HD3	4:M:542:GLY:CA	2.45	0.46
4:A:272:ASP:OD2	4:A:275:ARG:NH1	2.49	0.46
4:E:361:GLU:CD	4:E:361:GLU:N	2.69	0.46
4:E:271:GLY:HA2	4:E:346:THR:HG21	1.97	0.46
4:E:357:PHE:CE1	4:E:367:ALA:HB2	2.51	0.46
4:A:501:CYS:SG	4:A:531:ALA:HA	2.56	0.46
4:E:269:VAL:HG21	4:E:332:VAL:HG13	1.98	0.46
4:A:387:MET:HE2	4:A:392:ALA:N	2.31	0.45
4:I:570:PRO:HA	4:I:573:ARG:HD2	1.98	0.45
4:A:534:THR:O	4:A:548:GLY:HA3	2.17	0.45
4:I:395:ILE:HG23	4:I:456:PHE:HZ	1.82	0.45
4:I:415:CYS:HA	4:I:419:ARG:HB2	1.98	0.45
4:M:549:ARG:HG2	4:M:549:ARG:NH1	2.31	0.45
1:F:10:DA:H1'	1:F:11:DC:H5"	1.99	0.45
4:I:431:LEU:HD23	4:I:503:LEU:HD23	1.99	0.45
4:M:387:MET:HE2	4:M:392:ALA:N	2.32	0.45
4:A:255:HIS:NE2	4:A:259:LYS:HE2	2.31	0.45
4:E:277:LEU:HD21	4:E:281:LYS:CE	2.47	0.45
4:I:296:TYR:CA	4:I:314:ILE:HD11	2.47	0.45
4:A:536:VAL:CG2	4:A:538:ARG:NH1	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:499:PHE:CE2	4:E:503:LEU:HD11	2.52	0.44
4:I:364:ARG:HG2	4:I:364:ARG:HH11	1.83	0.44
4:E:257:THR:O	4:E:261:GLU:HG3	2.18	0.44
3:P:2:DC:OP1	4:M:309:MET:HB2	2.18	0.44
4:I:305:ILE:HG23	4:I:309:MET:HB3	2.00	0.44
3:D:3:DC:H2''	3:D:4:DG:C8	2.52	0.43
1:F:4:DC:H6	1:F:4:DC:H2'	1.72	0.43
4:I:570:PRO:HA	4:I:573:ARG:CD	2.48	0.43
4:M:519:LEU:C	4:M:519:LEU:HD23	2.38	0.43
2:C:5:DG:H4'	4:A:342:TRP:CZ2	2.53	0.43
3:H:1:DG:H5''	4:E:279:TYR:HE1	1.82	0.43
4:A:290:HIS:CE1	4:A:291:LYS:HG2	2.54	0.43
3:D:1:DG:H2''	3:D:2:DC:C6	2.53	0.43
4:I:275:ARG:NH1	4:I:275:ARG:HB2	2.34	0.43
4:M:536:VAL:HG13	4:M:546:GLY:O	2.19	0.43
4:A:472:LYS:HD2	4:A:474:LEU:HD21	2.00	0.43
4:I:453:GLN:C	4:I:455:GLY:H	2.21	0.43
7:J:780:HOH:O	4:I:372:GLN:HG3	2.17	0.43
4:A:427:ASP:OD1	4:A:427:ASP:C	2.57	0.43
4:E:462:VAL:HG21	4:E:474:LEU:HD12	2.00	0.43
4:E:274:TRP:HA	4:E:274:TRP:CE3	2.54	0.43
4:E:277:LEU:HD21	4:E:281:LYS:NZ	2.34	0.42
4:I:557:LYS:HG2	4:I:567:TYR:CG	2.53	0.42
4:M:265:LYS:HD3	4:M:336:GLU:OE2	2.19	0.42
4:E:389:ARG:HB2	4:E:423:ALA:O	2.19	0.42
4:E:499:PHE:CZ	4:E:503:LEU:HD11	2.54	0.42
4:E:534:THR:O	4:E:548:GLY:HA3	2.20	0.42
4:E:275:ARG:CB	4:E:275:ARG:HH11	2.32	0.42
4:E:357:PHE:CD1	4:E:363:ILE:HD13	2.54	0.42
4:M:315:GLU:OE2	4:M:323:ARG:HD3	2.19	0.42
3:L:2:DC:OP1	4:I:309:MET:HB2	2.19	0.42
4:E:434:HIS:HA	4:E:435:PRO:HD3	1.78	0.42
4:I:525:MET:HE3	4:I:563:LEU:HD23	2.02	0.42
4:A:494:VAL:HB	4:A:495:PRO:HD2	2.02	0.42
4:A:256:ILE:HG13	7:A:2286:HOH:O	2.20	0.41
4:E:267:TYR:CZ	4:E:275:ARG:HD3	2.55	0.41
4:E:410:LEU:HD21	4:E:443:ILE:HD13	2.01	0.41
4:E:363:ILE:HA	4:E:367:ALA:HB3	2.00	0.41
4:A:536:VAL:CG2	4:A:538:ARG:HH12	2.33	0.41
4:M:291:LYS:HB2	4:M:292:PRO:HD2	2.03	0.41
4:A:384:LEU:HD12	4:A:384:LEU:HA	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:549:ARG:HG2	4:I:549:ARG:NH1	2.34	0.41
3:H:1:DG:H2"	3:H:2:DC:C6	2.56	0.41
4:I:257:THR:O	4:I:261:GLU:HG3	2.19	0.41
1:N:9:DC:H2"	1:N:10:DA:C8	2.55	0.41
4:E:387:MET:HE1	4:E:395:ILE:HD12	2.03	0.41
4:I:505:TYR:CD2	4:I:529:GLU:HB3	2.56	0.41
1:N:7:DC:H2"	1:N:8:DG:C8	2.55	0.41
4:E:434:HIS:CD2	4:E:439:SER:HB2	2.55	0.41
4:E:263:LEU:HD13	4:E:325:LEU:HD23	2.03	0.41
4:I:385:GLU:HG2	4:I:386:ARG:N	2.36	0.41
4:I:465:GLU:HB3	4:I:472:LYS:HB3	2.02	0.41
4:E:444:PHE:CE2	4:E:464:GLN:HG3	2.56	0.41
4:E:505:TYR:CD2	4:E:529:GLU:HB3	2.56	0.40
1:B:4:DC:H6	1:B:4:DC:H2'	1.80	0.40
4:E:551:LEU:O	4:E:553:THR:HG23	2.20	0.40
4:I:398:THR:HG21	4:I:456:PHE:CD1	2.56	0.40
4:I:474:LEU:HD22	4:I:490:ASP:OD2	2.22	0.40
4:A:359:SER:O	4:A:363:ILE:HG12	2.21	0.40
4:A:259:LYS:HE3	4:A:320:GLY:O	2.21	0.40
1:J:6:DA:H2"	1:J:7:DC:OP2	2.22	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	
4	A	326/331 (98%)	318 (98%)	7 (2%)	1 (0%)	44	44
4	E	324/331 (98%)	306 (94%)	18 (6%)	0	100	100
4	I	324/331 (98%)	307 (95%)	15 (5%)	2 (1%)	28	24
4	M	325/331 (98%)	314 (97%)	9 (3%)	2 (1%)	28	24
All	All	1299/1324 (98%)	1245 (96%)	49 (4%)	5 (0%)	38	35

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	539	ASN
4	I	323	ARG
4	A	540	THR
4	M	544	LYS
4	M	250	THR

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	
4	A	271/278 (98%)	269 (99%)	2 (1%)	87	91
4	E	268/278 (96%)	263 (98%)	5 (2%)	62	68
4	I	264/278 (95%)	260 (98%)	4 (2%)	70	76
4	M	271/278 (98%)	267 (98%)	4 (2%)	70	76
All	All	1074/1112 (97%)	1059 (99%)	15 (1%)	71	78

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	454	GLU
4	A	569	GLU
4	E	291	LYS
4	E	317	LEU
4	E	384	LEU
4	E	404	GLN
4	E	569	GLU
4	I	291	LYS
4	I	321	HIS
4	I	361	GLU
4	I	549	ARG
4	M	286	LEU
4	M	317	LEU
4	M	449	ASP
4	M	569	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	321	HIS
4	A	354	GLN
4	E	284	ASN
4	E	290	HIS
4	E	297	GLN
4	E	400	GLN
4	I	397	GLN
4	I	400	GLN
4	I	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 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	$\# Z > 2$
6	EDO	M	2801	-	3,3,3	2.04	2 (66%)	2,2,2	0.49	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
6	EDO	M	2801	-	-	0/1/1/1	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	2801	EDO	O1-C1	2.12	1.53	1.42
6	M	2801	EDO	O2-C2	2.69	1.56	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	B	11/11 (100%)	-0.56	0 100 100	23, 31, 37, 40	0
1	F	11/11 (100%)	0.24	1 (9%) 10 13	38, 45, 54, 56	0
1	J	11/11 (100%)	-0.08	0 100 100	31, 42, 53, 57	0
1	N	11/11 (100%)	-0.56	0 100 100	22, 28, 38, 41	0
2	C	5/5 (100%)	-0.36	0 100 100	21, 23, 44, 50	0
2	G	5/5 (100%)	0.48	0 100 100	39, 43, 63, 68	0
2	K	5/5 (100%)	0.43	0 100 100	33, 35, 52, 55	0
2	O	5/5 (100%)	-0.36	0 100 100	20, 22, 38, 39	0
3	D	4/4 (100%)	-0.31	0 100 100	33, 33, 37, 38	0
3	H	4/4 (100%)	0.10	0 100 100	41, 43, 50, 52	0
3	L	4/4 (100%)	0.14	0 100 100	47, 47, 50, 53	0
3	P	4/4 (100%)	-0.10	0 100 100	30, 32, 40, 42	0
4	A	327/331 (98%)	0.21	11 (3%) 46 53	15, 28, 52, 80	0
4	E	326/331 (98%)	0.76	39 (11%) 5 6	27, 46, 68, 86	0
4	I	326/331 (98%)	0.71	42 (12%) 4 5	29, 46, 74, 88	0
4	M	327/331 (98%)	0.21	20 (6%) 22 27	15, 27, 51, 81	0
All	All	1386/1404 (98%)	0.44	113 (8%) 12 16	15, 37, 67, 88	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	540	THR	7.9
4	I	540	THR	7.6
4	I	541	HIS	7.2
4	M	249	ALA	6.9
4	E	535	ALA	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	E	543	CYS	5.8
4	I	537	VAL	5.8
4	E	539	ASN	5.7
4	I	539	ASN	5.7
4	E	546	GLY	5.4
4	I	482	PRO	5.3
4	I	543	CYS	5.3
4	E	537	VAL	5.1
4	E	453	GLN	5.1
4	E	545	VAL	5.0
4	I	290	HIS	4.9
4	I	542	GLY	4.8
4	M	540	THR	4.7
4	E	483	GLY	4.7
4	I	538	ARG	4.7
4	E	538	ARG	4.6
4	E	542	GLY	4.5
4	A	542	GLY	4.5
4	E	482	PRO	4.5
4	I	321	HIS	4.3
4	M	541	HIS	4.2
4	M	537	VAL	4.1
4	I	483	GLY	4.1
4	A	543	CYS	4.1
4	E	541	HIS	4.1
4	I	575	TRP	4.0
4	A	540	THR	4.0
4	I	546	GLY	3.9
4	M	543	CYS	3.9
4	E	481	GLY	3.8
4	M	542	GLY	3.8
4	E	250	THR	3.7
4	I	481	GLY	3.7
4	I	423	ALA	3.7
4	A	537	VAL	3.6
4	M	431	LEU	3.5
4	E	290	HIS	3.3
4	E	575	TRP	3.3
4	I	252	HIS	3.3
4	A	321	HIS	3.3
4	M	539	ASN	3.3
4	I	547	PRO	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	E	480	PRO	3.2
4	E	321	HIS	3.2
4	I	405	ALA	3.2
4	E	408	SER	3.2
4	I	316	ILE	3.2
4	E	364	ARG	3.2
4	I	430	VAL	3.1
4	I	319	SER	3.1
4	M	546	GLY	2.9
4	I	294	THR	2.9
4	E	361	GLU	2.9
4	E	362	ASP	2.9
4	E	350	GLN	2.9
4	I	327	HIS	2.9
4	M	494	VAL	2.8
4	E	363	ILE	2.8
4	A	538	ARG	2.8
4	I	535	ALA	2.8
4	I	313	ILE	2.8
4	E	367	ALA	2.8
4	I	326	ASP	2.7
4	M	492	ILE	2.7
4	I	384	LEU	2.6
4	I	320	GLY	2.6
4	I	569	GLU	2.6
4	E	492	ILE	2.6
4	E	289	PHE	2.6
4	A	541	HIS	2.6
4	E	252	HIS	2.6
4	I	254	LEU	2.6
4	I	545	VAL	2.5
4	I	295	SER	2.5
4	A	303	PRO	2.5
4	I	536	VAL	2.5
4	E	251	ASN	2.5
4	E	354	GLN	2.4
4	A	546	GLY	2.4
4	I	428	VAL	2.3
4	I	435	PRO	2.3
4	M	545	VAL	2.3
4	M	493	VAL	2.3
4	A	250	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	M	317	LEU	2.2
4	M	504	LEU	2.2
4	M	536	VAL	2.2
4	E	572	GLU	2.2
4	M	430	VAL	2.2
4	I	250	THR	2.2
4	I	317	LEU	2.2
4	E	327	HIS	2.2
4	E	332	VAL	2.2
4	I	364	ARG	2.2
4	M	502	ALA	2.2
4	M	503	LEU	2.1
4	E	390	GLU	2.1
4	A	539	ASN	2.1
4	E	254	LEU	2.1
4	E	357	PHE	2.1
4	M	501	CYS	2.1
4	E	491	ILE	2.1
1	F	1	DC	2.1
4	E	329	SER	2.1
4	I	449	ASP	2.1
4	I	485	ARG	2.1
4	I	305	ILE	2.0
4	I	314	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NA	A	2008	1/1	0.34	0.54	22.75	72,72,72,72	0
6	EDO	M	2801	4/4	0.62	0.22	2.95	49,50,51,54	0
5	NA	A	2001	1/1	0.98	0.17	2.94	26,26,26,26	0
5	NA	M	2005	1/1	0.94	0.14	0.95	20,20,20,20	0
5	NA	J	2011	1/1	0.32	0.19	0.76	57,57,57,57	0
5	NA	M	2006	1/1	0.89	0.08	-1.45	34,34,34,34	0
5	NA	I	2003	1/1	0.98	0.07	-2.15	29,29,29,29	0
5	NA	E	2002	1/1	0.91	0.08	-2.92	47,47,47,47	0
5	NA	F	2007	1/1	0.90	0.23	-	64,64,64,64	0
5	NA	J	2010	1/1	0.45	0.20	-	74,74,74,74	0
5	NA	B	2009	1/1	0.63	0.15	-	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.