



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 09:46 AM GMT

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 : 2003-12-29
Resolution : 2.10 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>

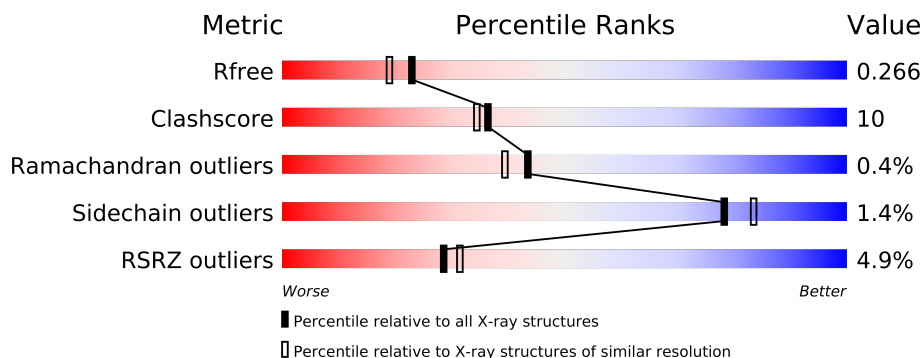
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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. 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	B	11	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	F	11	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	J	11	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
1	N	11	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	C	5	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	G	5	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	K	5	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
2	O	5	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	D	4	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>
3	H	4	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>
3	L	4	<div><div></div><div><div></div><div></div><div></div><div></div></div></div>
3	P	4	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>
4	A	331	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>
4	E	331	<div><div></div><div><div></div><div></div><div></div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	I	331	
4	M	331	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	NA	A	2001	-	X
5	NA	A	2008	-	X
5	NA	F	2007	-	X
5	NA	J	2010	-	X
5	NA	J	2011	-	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 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 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			

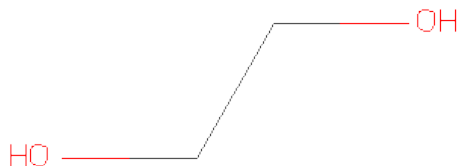
- Molecule 4 is a protein called DNA polymerase lambda.

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	A	289	Total	O	0	0
			289	289		
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	E	109	Total	O	0	0
			109	109		
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	I	134	Total	O	0	0
			134	134		
7	J	20	Total	O	0	0
			20	20		
7	K	11	Total	O	0	0
			11	11		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	6	Total 6	O 6	0	0
7	M	329	Total 329	O 329	0	0
7	N	34	Total 34	O 34	0	0
7	O	16	Total 16	O 16	0	0
7	P	6	Total 6	O 6	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 errors 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: 



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

Chain O:



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

Chain D:



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

Chain H:



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

Chain L:



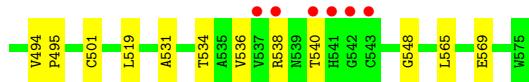
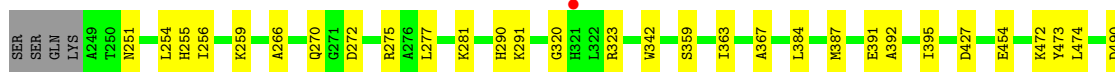
- Molecule 3: 5'-D(P*GP*CP*CP*G)-3'

Chain P:



- Molecule 4: DNA polymerase lambda

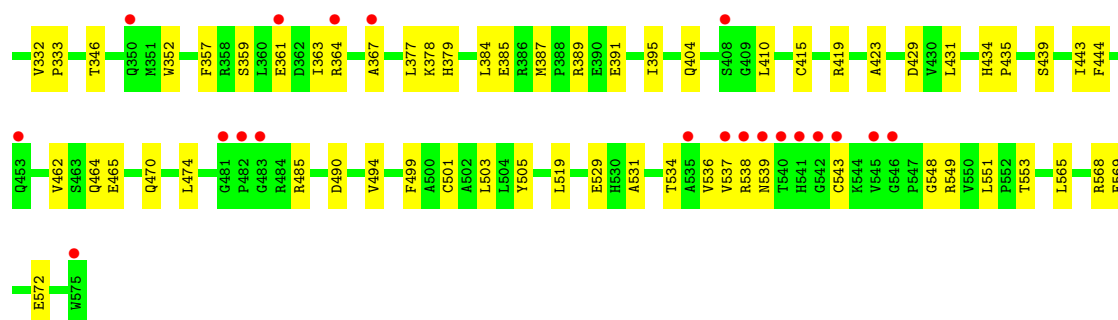
Chain A:



- Molecule 4: DNA polymerase lambda

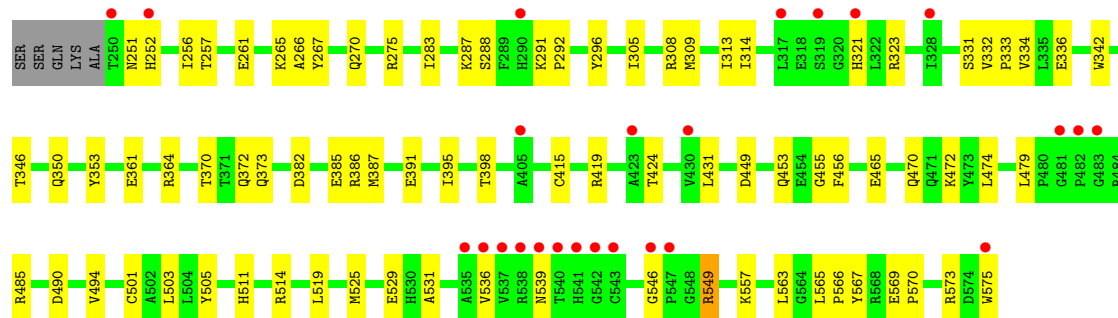
Chain E:





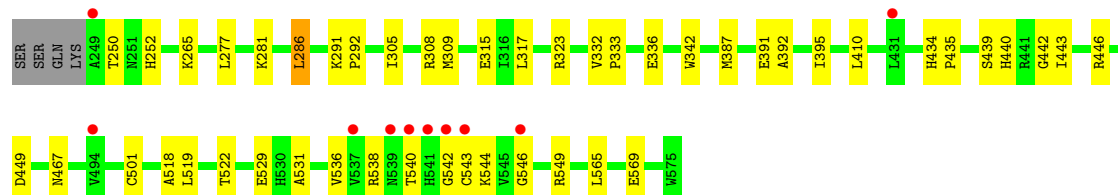
• Molecule 4: DNA polymerase lambda

Chain I:



• Molecule 4: DNA polymerase lambda

Chain M:



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 0.240 , 0.266	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)	0.35 , 39.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 111172 reflections	Xtriage
F_o, F_c correlation	0.93	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.

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 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	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	1	0	0	0	0
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

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 10.

All (236) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HH11	4:M:308:ARG:HG3	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
4:I:251:ASN:OD1	4:I:287:LYS:HA	1.86	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:M:519:LEU:CD1	4:M:565:LEU:HD11	2.18	0.73
4:I:288:SER:HB3	4:I:575:TRP:HZ3	1.52	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:M:308:ARG:HG3	4:M:308:ARG:NH1	2.06	0.68
4:I:346:THR:O	4:I:350:GLN:HB2	1.94	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: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:251:ASN:ND2	4:E:287:LYS:HG2	2.12	0.65
4:E:501:CYS:SG	4:E:531:ALA:HA	2.38	0.64
4:M:387:MET:CE	4:M:395:ILE:HD12	2.29	0.62
4:E:385:GLU:HG3	4:E:485:ARG:NH1	2.14	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
1:B:1:DC:H2''	1:B:2:DG:C8	2.37	0.59
4:A:323:ARG:HG2	4:A:323:ARG:HH11	1.67	0.59
4:M:439:SER:O	4:M:443:ILE:HD11	2.02	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:E:332:VAL:HB	4:E:333:PRO:HD3	1.84	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
1:F:10:DA:H2''	1:F:11:DC:H5'	1.87	0.57
4:E:279:TYR:O	4:E:283:ILE:HG13	2.05	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:I:557:LYS:HG2	4:I:567:TYR:CD2	2.41	0.56
4:A:251:ASN:HD21	4:A:254:LEU:HA	1.70	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:I:261:GLU:CG	4:I:283:ILE:HD13	2.38	0.54
4:E:305:ILE:HG23	4:E:309:MET:HB3	1.90	0.54
1:J:10:DA:H1'	1:J:11:DC:H5''	1.88	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:A:277:LEU:HG	4:A:281:LYS:HE3	1.89	0.54
4:M:434:HIS:ND1	4:M:435:PRO:HD2	2.22	0.53
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:M:286:LEU:HD13	4:M:305:ILE:HD11	1.91	0.53
4:I:382:ASP:OD1	4:I:485:ARG:HD3	2.09	0.53
4:A:281:LYS:HE2	7:A:2133:HOH:O	2.08	0.53
4:I:569:GLU:HG3	4:I:570:PRO:HD2	1.91	0.53
4:A:367:ALA:O	4:I:566:PRO:HB3	2.08	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: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:A:474:LEU:HD22	4:A:490:ASP:OD2	2.10	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:415:CYS:HA	4:E:419:ARG:HB2	1.91	0.51
4:E:266:ALA:O	4:E:270:GLN:HG3	2.11	0.51
2:O:5:DG:H4'	4:M:342:TRP:CZ2	2.45	0.51
4:E:431:LEU:HD23	4:E:503:LEU:CD2	2.41	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:I:519:LEU:HD22	4:I:563:LEU:HD22	1.93	0.51
4:E:385:GLU:CG	4:E:485:ARG:NH1	2.74	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:I:308:ARG:NH1	4:I:308:ARG:HG3	2.25	0.51
4:E:361:GLU:CD	4:E:361:GLU:H	2.13	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
1:J:10:DA:H2''	1:J:11:DC:H5''	1.94	0.50
4:I:511:HIS:ND1	4:I:514:ARG:NH2	2.60	0.50
4:E:536:VAL:HG12	4:E:537:VAL:N	2.27	0.50
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:I:549:ARG:HG2	4:I:549:ARG:HH11	1.78	0.49
1:B:9:DC:H2"	1:B:10:DA:C8	2.48	0.49
4:A:474:LEU:HD22	4:A:490:ASP:CG	2.33	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:I:465:GLU:OE1	4:I:472:LYS:HE2	2.12	0.48
4:E:256:ILE:HD13	4:E:313:ILE:HG23	1.94	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:M:538:ARG:HB2	4:M:543:CYS:H	1.79	0.47
4:E:364:ARG:CB	4:E:377:LEU:HD21	2.43	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:E:361:GLU:CD	4:E:361:GLU:N	2.69	0.46
4:A:272:ASP:OD2	4:A:275:ARG:NH1	2.49	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:E:269:VAL:HG21	4:E:332:VAL:HG13	1.98	0.46
4:A:501:CYS:SG	4:A:531:ALA:HA	2.56	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:I:395:ILE:HG23	4:I:456:PHE:HZ	1.82	0.45
4:M:549:ARG:HG2	4:M:549:ARG:NH1	2.31	0.45
4:I:415:CYS:HA	4:I:419:ARG:HB2	1.98	0.45
4:A:534:THR:O	4:A:548:GLY:HA3	2.17	0.45
1:F:10:DA:H1'	1:F:11:DC:H5"	1.99	0.45
4:M:387:MET:HE2	4:M:392:ALA:N	2.32	0.45
4:I:431:LEU:HD23	4:I:503:LEU:HD23	1.99	0.45
4:I:296:TYR:CA	4:I:314:ILE:HD11	2.47	0.45
4:E:277:LEU:HD21	4:E:281:LYS:CE	2.47	0.45
4:A:255:HIS:NE2	4:A:259:LYS:HE2	2.31	0.45
4:E:499:PHE:CE2	4:E:503:LEU:HD11	2.52	0.44
4:A:536:VAL:CG2	4:A:538:ARG:NH1	2.80	0.44
4:I:364:ARG:HG2	4:I:364:ARG:HH11	1.83	0.44
3:P:2:DC:OP1	4:M:309:MET:HB2	2.18	0.44
4:E:257:THR:O	4:E:261:GLU:HG3	2.18	0.44
4:I:305:ILE:HG23	4:I:309:MET:HB3	2.00	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:M:519:LEU:C	4:M:519:LEU:HD23	2.38	0.43
4:I:570:PRO:HA	4:I:573:ARG:CD	2.48	0.43
1:F:4:DC:H6	1:F:4:DC:H2'	1.72	0.43
3:D:3:DC:H2''	3:D:4:DG:C8	2.52	0.43
3:H:1:DG:H5''	4:E:279:TYR:HE1	1.82	0.43
2:C:5:DG:H4'	4:A:342:TRP:CZ2	2.53	0.43
4:I:275:ARG:NH1	4:I:275:ARG:HB2	2.34	0.43
3:D:1:DG:H2''	3:D:2:DC:C6	2.53	0.43
4:A:290:HIS:CE1	4:A:291:LYS:HG2	2.54	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:E:462:VAL:HG21	4:E:474:LEU:HD12	2.00	0.43
4:A:427:ASP:OD1	4:A:427:ASP:C	2.57	0.43
4:E:274:TRP:HA	4:E:274:TRP:CE3	2.54	0.43
4:I:557:LYS:HG2	4:I:567:TYR:CG	2.53	0.42
4:E:277:LEU:HD21	4:E:281:LYS:NZ	2.34	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:I:525:MET:HE3	4:I:563:LEU:HD23	2.02	0.42
4:E:434:HIS:HA	4:E:435:PRO:HD3	1.78	0.42
4:A:494:VAL:HB	4:A:495:PRO:HD2	2.02	0.42
4:E:410:LEU:HD21	4:E:443:ILE:HD13	2.01	0.41
4:E:267:TYR:CZ	4:E:275:ARG:HD3	2.55	0.41
4:A:256:ILE:HG13	7:A:2286:HOH:O	2.20	0.41
4:E:363:ILE:HA	4:E:367:ALA:HB3	2.00	0.41
4:M:291:LYS:HB2	4:M:292:PRO:HD2	2.03	0.41
4:A:536:VAL:CG2	4:A:538:ARG:HH12	2.33	0.41
4:I:549:ARG:HG2	4:I:549:ARG:NH1	2.34	0.41
4:A:384:LEU:HD12	4:A:384:LEU:HA	1.93	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
3:H:1:DG:H2''	3:H:2:DC:C6	2.56	0.41
4:E:387:MET:HE1	4:E:395:ILE:HD12	2.03	0.41
1:N:7:DC:H2''	1:N:8:DG:C8	2.55	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:I:505:TYR:CD2	4:I:529:GLU:HB3	2.56	0.41
4:E:434:HIS:CD2	4:E:439:SER:HB2	2.55	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:263:LEU:HD13	4:E:325:LEU:HD23	2.03	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: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:E:551:LEU:O	4:E:553:THR:HG23	2.20	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%)	50	49
4	E	324/331 (98%)	306 (94%)	18 (6%)	0	100	100
4	I	324/331 (98%)	307 (95%)	15 (5%)	2 (1%)	33	28
4	M	325/331 (98%)	314 (97%)	9 (3%)	2 (1%)	33	28
All	All	1299/1324 (98%)	1245 (96%)	49 (4%)	5 (0%)	43	39

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

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Mol	Chain	Res	Type
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%)	91	94
4	E	268/278 (96%)	263 (98%)	5 (2%)	69	73
4	I	264/278 (95%)	260 (98%)	4 (2%)	76	81
4	M	271/278 (98%)	267 (98%)	4 (2%)	76	81
All	All	1074/1112 (97%)	1059 (99%)	15 (1%)	78	83

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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.51	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	O2-C2	2.67	1.56	1.42
6	M	2801	EDO	O1-C1	2.10	1.53	1.42

There are no bond angle outliers.

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	B	11/11 (100%)	-0.60	0	100	100	23, 31, 37, 40	0
1	F	11/11 (100%)	-0.13	0	100	100	38, 45, 54, 56	0
1	J	11/11 (100%)	-0.29	0	100	100	31, 42, 53, 57	0
1	N	11/11 (100%)	-0.61	0	100	100	22, 28, 38, 41	0
2	C	5/5 (100%)	-0.46	0	100	100	21, 23, 44, 50	0
2	G	5/5 (100%)	0.23	0	100	100	39, 43, 63, 68	0
2	K	5/5 (100%)	0.13	0	100	100	33, 35, 52, 55	0
2	O	5/5 (100%)	-0.51	0	100	100	20, 22, 38, 39	0
3	D	4/4 (100%)	-0.38	0	100	100	33, 33, 37, 38	0
3	H	4/4 (100%)	-0.13	0	100	100	41, 43, 50, 52	0
3	L	4/4 (100%)	-0.07	0	100	100	47, 47, 50, 53	0
3	P	4/4 (100%)	-0.15	0	100	100	30, 32, 40, 42	0
4	A	327/331 (98%)	0.05	7 (2%)	60	65	15, 28, 52, 80	0
4	E	326/331 (98%)	0.43	25 (7%)	13	15	27, 46, 68, 86	0
4	I	326/331 (98%)	0.39	25 (7%)	13	15	29, 46, 74, 88	0
4	M	327/331 (98%)	0.05	10 (3%)	47	52	15, 27, 51, 81	0
All	All	1386/1404 (98%)	0.20	67 (4%)	28	32	15, 37, 67, 88	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	540	THR	6.9
4	M	249	ALA	6.2
4	I	541	HIS	5.4
4	I	540	THR	5.3
4	I	539	ASN	5.2

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Mol	Chain	Res	Type	RSRZ
4	I	537	VAL	5.2
4	E	543	CYS	5.0
4	E	546	GLY	4.7
4	I	482	PRO	4.7
4	E	483	GLY	4.5
4	E	453	GLN	4.5
4	I	538	ARG	4.4
4	E	539	ASN	4.3
4	E	482	PRO	4.0
4	I	290	HIS	4.0
4	E	535	ALA	3.8
4	A	542	GLY	3.8
4	E	538	ARG	3.8
4	E	537	VAL	3.7
4	A	537	VAL	3.6
4	M	541	HIS	3.6
4	E	541	HIS	3.5
4	E	481	GLY	3.5
4	I	252	HIS	3.4
4	E	542	GLY	3.4
4	E	545	VAL	3.4
4	I	542	GLY	3.3
4	I	483	GLY	3.2
4	I	575	TRP	3.2
4	I	423	ALA	3.2
4	M	540	THR	3.1
4	I	543	CYS	3.1
4	M	537	VAL	3.0
4	A	540	THR	3.0
4	I	546	GLY	2.9
4	E	364	ARG	2.9
4	I	405	ALA	2.9
4	A	541	HIS	2.7
4	E	367	ALA	2.7
4	M	542	GLY	2.7
4	A	543	CYS	2.7
4	I	430	VAL	2.7
4	E	575	TRP	2.7
4	A	321	HIS	2.6
4	I	321	HIS	2.6
4	E	321	HIS	2.6
4	I	481	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
4	M	431	LEU	2.6
4	E	289	PHE	2.5
4	M	539	ASN	2.5
4	M	546	GLY	2.4
4	E	290	HIS	2.4
4	E	408	SER	2.3
4	M	494	VAL	2.3
4	I	547	PRO	2.3
4	E	250	THR	2.3
4	E	254	LEU	2.2
4	I	328	ILE	2.2
4	E	361	GLU	2.2
4	M	543	CYS	2.2
4	I	319	SER	2.2
4	I	317	LEU	2.2
4	I	536	VAL	2.1
4	A	538	ARG	2.1
4	E	350	GLN	2.1
4	I	535	ALA	2.0
4	I	250	THR	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 ⓘ

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(Å ²)	Q<0.9
5	NA	A	2008	1/1	0.47	13.76	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NA	F	2007	1/1	0.26	11.70	64,64,64,64	0
5	NA	J	2010	1/1	0.20	4.75	74,74,74,74	0
5	NA	J	2011	1/1	0.29	4.72	57,57,57,57	0
5	NA	A	2001	1/1	0.14	2.59	26,26,26,26	0
6	EDO	M	2801	4/4	0.19	2.28	49,50,51,54	0
5	NA	B	2009	1/1	0.13	1.32	48,48,48,48	0
5	NA	M	2005	1/1	0.12	0.73	20,20,20,20	0
5	NA	M	2006	1/1	0.08	-1.23	34,34,34,34	0
5	NA	E	2002	1/1	0.06	-2.93	47,47,47,47	0
5	NA	I	2003	1/1	0.06	-4.30	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.