WORLDWIDE wwPDB

PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2023 – 09:56 PM EDT

PDB ID	:	1NZB
Title	:	Crystal structure of wild type Cre recombinase-loxP synapse
Authors	:	Ennifar, E.; Meyer, J.E.W.; Buchholz, F.; Stewart, A.F.; Suck, D.
Deposited on	:	2003-02-17
Resolution	:	3.10 Å(reported)

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

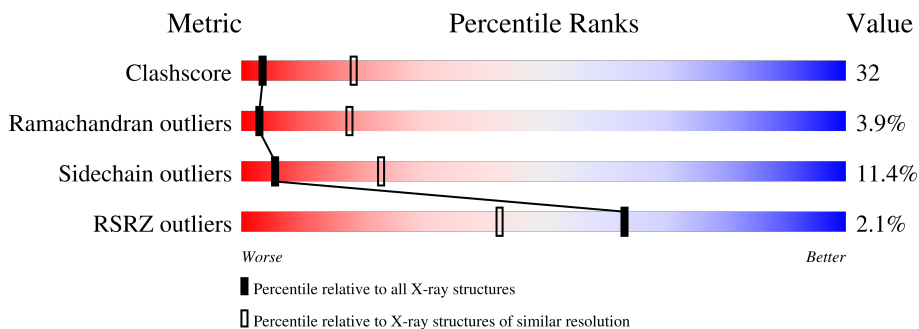|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	Percentile Ranks	Value
Clashscore		32
Ramachandran outliers		3.9%
Sidechain outliers		11.4%
RSRZ outliers		2.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	C	37	41% / 57% / •
1	G	37	46% / 49% / 5%
2	D	37	3% 27% / 73%
2	H	37	38% / 59% / •
3	A	343	2% 50% / 37% / 9% ••
3	B	343	% 44% / 42% / 7% • 6%
3	E	343	4% 38% / 45% / 10% • 6%

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Mol	Chain	Length	Quality of chain
3	F	343	

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
4	MG	F	5307	-	-	-	X

2   Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13299 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 loxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	37	Total	C	N	O	P	0	0	0
			754	363	134	221	36			
1	G	37	Total	C	N	O	P	0	0	0
			754	363	134	221	36			

- Molecule 2 is a DNA chain called loxP DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	37	Total	C	N	O	P	0	0	0
			756	364	137	219	36			
2	H	37	Total	C	N	O	P	0	0	0
			756	364	137	219	36			

- Molecule 3 is a protein called Cre recombinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	332	Total	C	N	O	S	0	0	0
			2620	1629	497	479	15			
3	B	322	Total	C	N	O	S	0	0	0
			2550	1584	486	465	15			
3	E	321	Total	C	N	O	S	0	0	0
			2544	1581	485	463	15			
3	F	322	Total	C	N	O	S	0	0	0
			2550	1584	486	465	15			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		
4	D	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Mg 1	0	0
4	A	3	Total 3	Mg 3	0	0
4	F	2	Total 2	Mg 2	0	0

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	I 1	0	0
5	F	1	Total 1	I 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	O 2	0	0
6	F	1	Total 1	O 1	0	0

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: loxP DNA

Chain C:
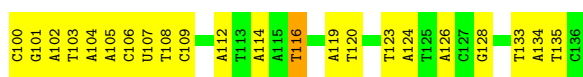
- Molecule 1: loxP DNA
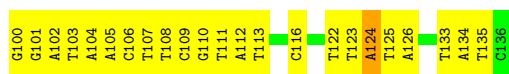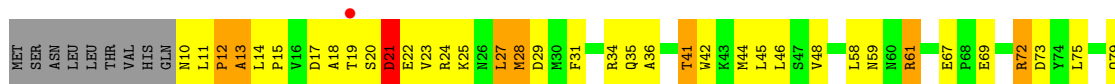
Chain G:

- Molecule 2: loxP DNA
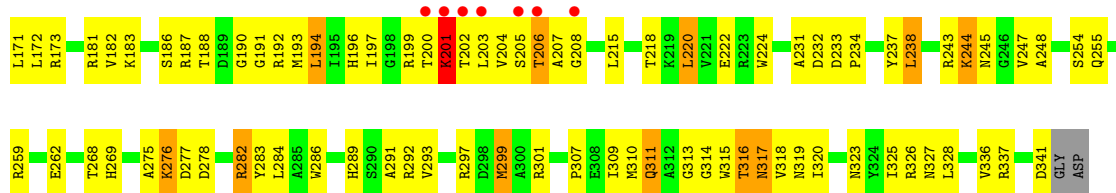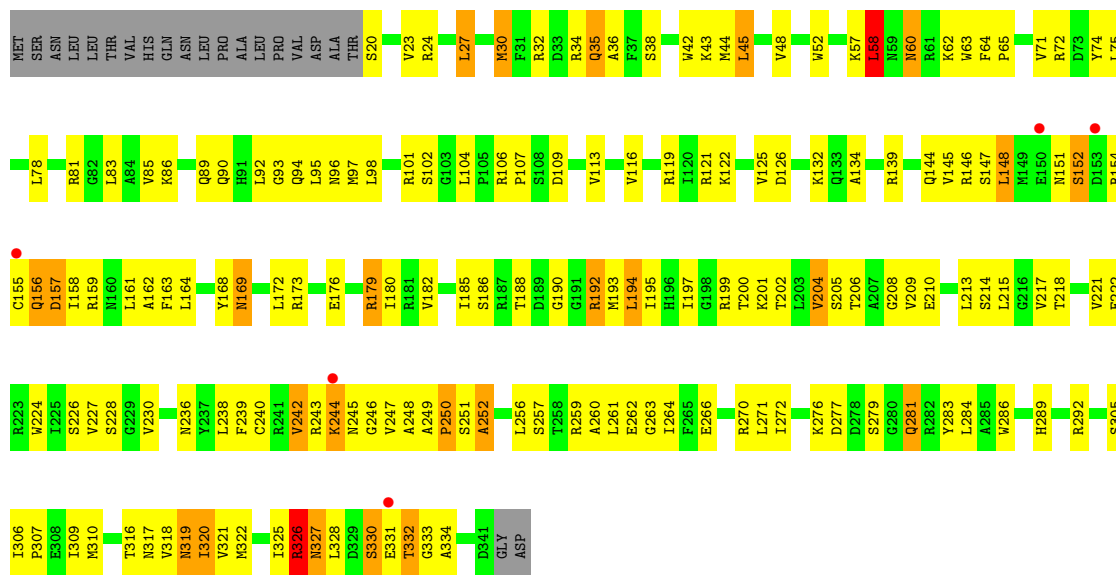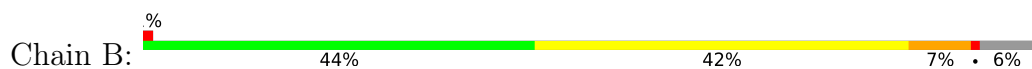
Chain D:

- Molecule 2: loxP DNA
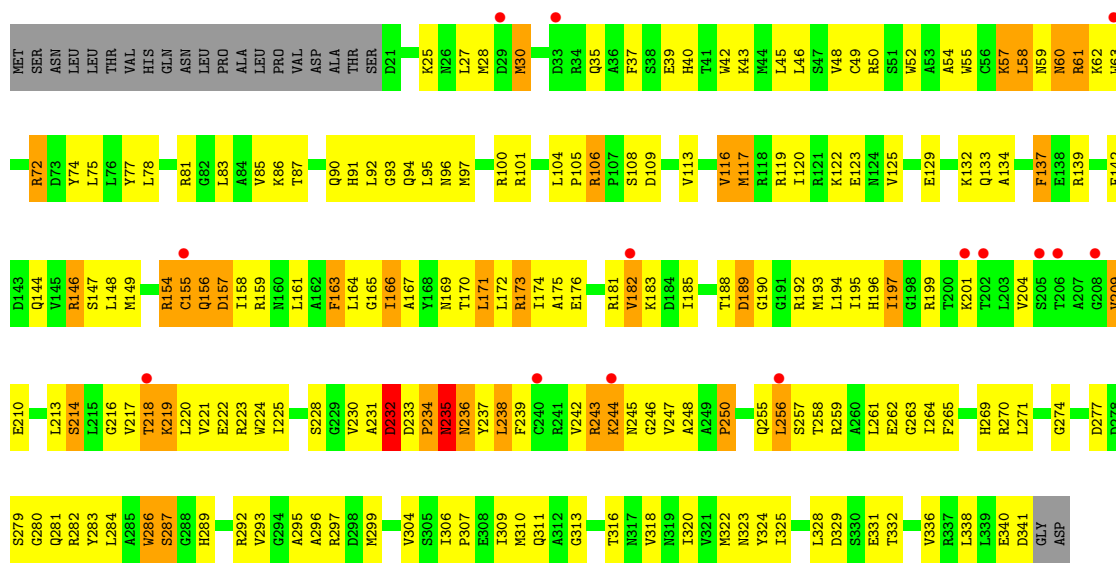
Chain H:

- Molecule 3: Cre recombinase

Chain A:

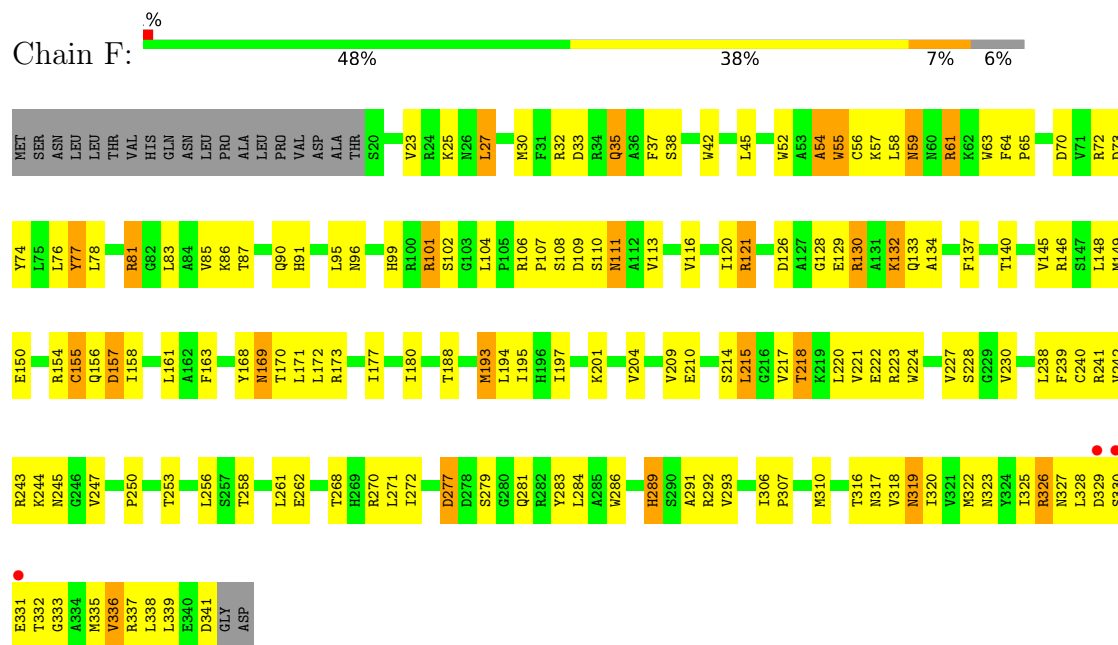• Molecule 3: Cre recombinase

Chain B:

• Molecule 3: Cre recombinase

Chain E:

• Molecule 3: Cre recombinase

Chain F:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.89Å 163.53Å 195.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10 49.95 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.6 (8.00-3.10) 98.3 (49.95-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 3.12Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.257 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	75.8	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 77.7	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13299	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, UMP, MG

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	C	0.50	0/823	0.81	0/1266
1	G	0.45	0/823	0.77	0/1266
2	D	0.51	0/848	0.81	0/1307
2	H	0.41	0/848	0.76	0/1307
3	A	0.45	0/2663	0.69	0/3595
3	B	0.37	0/2591	0.64	2/3493 (0.1%)
3	E	0.37	0/2585	0.63	0/3485
3	F	0.38	0/2591	0.63	1/3493 (0.0%)
All	All	0.42	0/13772	0.69	3/19212 (0.0%)

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	C	0	1
1	G	0	2
2	H	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	137	PHE	N-CA-C	-5.68	95.66	111.00
3	B	326	ARG	N-CA-C	-5.41	96.38	111.00
3	B	58	LEU	CA-CB-CG	5.19	127.24	115.30

There are no chirality outliers.

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All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	116	DT	Sidechain
1	G	106	DC	Sidechain
1	G	115	DA	Sidechain
2	H	124	DA	Sidechain

5.2   Too-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 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	C	754	0	420	32	0
1	G	754	0	420	22	0
2	D	756	0	421	56	0
2	H	756	0	421	39	0
3	A	2620	0	2643	164	0
3	B	2550	0	2571	181	0
3	E	2544	0	2566	258	0
3	F	2550	0	2571	165	0
4	A	3	0	0	0	0
4	C	1	0	0	0	0
4	D	3	0	0	0	0
4	F	2	0	0	0	0
4	G	1	0	0	0	0
5	B	1	0	0	1	0
5	F	1	0	0	0	0
6	A	2	0	0	0	0
6	F	1	0	0	0	0
All	All	13299	0	12033	812	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 32.

The worst 5 of 812 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)
3:E:166:ILE:HD13	3:E:213:LEU:HD11	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:332:THR:HG22	3:B:333:GLY:H	1.17	1.04
3:E:188:THR:HB	3:E:192:ARG:H	1.21	1.04
3:A:72:ARG:HG3	3:A:116:VAL:HG21	1.37	1.03
3:A:276:LYS:HG2	3:A:277:ASP:H	1.18	1.02

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	
3	A	330/343 (96%)	286 (87%)	34 (10%)	10 (3%)	4	23
3	B	320/343 (93%)	256 (80%)	48 (15%)	16 (5%)	2	13
3	E	319/343 (93%)	253 (79%)	50 (16%)	16 (5%)	2	13
3	F	320/343 (93%)	269 (84%)	43 (13%)	8 (2%)	5	27
All	All	1289/1372 (94%)	1064 (82%)	175 (14%)	50 (4%)	3	18

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	13	ALA
3	A	182	VAL
3	B	327	ASN
3	B	332	THR
3	E	280	GLY

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	
3	A	277/287 (96%)	237 (86%)	40 (14%)	3	14
3	B	269/287 (94%)	250 (93%)	19 (7%)	14	44
3	E	268/287 (93%)	234 (87%)	34 (13%)	4	18
3	F	269/287 (94%)	239 (89%)	30 (11%)	6	24
All	All	1083/1148 (94%)	960 (89%)	123 (11%)	5	23

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	281	GLN
3	F	133	GLN
3	E	146	ARG
3	F	132	LYS
3	F	241	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	35	GLN
3	F	281	GLN
3	F	90	GLN
3	F	133	GLN
3	F	319	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\#|Z| > 2$
1	UMP	C	107	1,2	17,20,21	0.42	0	24,28,31	0.40	0
1	UMP	G	107	1,2	17,20,21	0.51	0	24,28,31	0.45	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
1	UMP	C	107	1,2	-	0/7/21/22	0/2/2/2
1	UMP	G	107	1,2	-	0/7/21/22	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	107	UMP	2	0
1	G	107	UMP	1	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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	C	36/37 (97%)	-0.17	0	100	100	32, 53, 86, 95	0
1	G	36/37 (97%)	-0.14	0	100	100	39, 69, 96, 147	0
2	D	37/37 (100%)	-0.14	1 (2%)	54	31	33, 50, 85, 93	0
2	H	37/37 (100%)	-0.01	0	100	100	39, 72, 96, 114	0
3	A	332/343 (96%)	-0.09	8 (2%)	59	37	17, 48, 94, 149	0
3	B	322/343 (93%)	-0.03	5 (1%)	72	51	27, 62, 98, 142	0
3	E	321/343 (93%)	0.15	14 (4%)	34	17	38, 71, 109, 156	0
3	F	322/343 (93%)	-0.15	3 (0%)	84	69	31, 57, 95, 138	0
All	All	1443/1520 (94%)	-0.04	31 (2%)	63	43	17, 60, 99, 156	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	202	THR	5.8
3	E	208	GLY	4.8
3	F	331	GLU	4.6
3	A	201	LYS	4.3
3	F	330	SER	4.2

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. 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	B-factors(Å^2)	Q<0.9
1	UMP	C	107	19/20	0.95	0.14	43,57,72,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	UMP	G	107	19/20	0.97	0.20	54,58,65,71	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	MG	D	5310	1/1	0.60	0.36	65,65,65,65	0
4	MG	F	5307	1/1	0.66	1.07	62,62,62,62	1
4	MG	C	5308	1/1	0.78	0.35	49,49,49,49	0
4	MG	F	5309	1/1	0.84	0.63	44,44,44,44	1
4	MG	G	5306	1/1	0.85	0.37	69,69,69,69	0
4	MG	A	5301	1/1	0.86	0.49	70,70,70,70	0
4	MG	D	5305	1/1	0.87	0.40	42,42,42,42	0
4	MG	D	5304	1/1	0.87	0.36	53,53,53,53	0
4	MG	A	5302	1/1	0.94	0.28	44,44,44,44	0
4	MG	A	5303	1/1	0.95	0.54	44,44,44,44	0
5	IOD	B	344	1/1	0.97	0.17	69,69,69,69	1
5	IOD	F	344	1/1	0.98	0.11	64,64,64,64	1

6.5 Other polymers ⓘ

There are no such residues in this entry.