WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 25, 2023 – 06:57 AM EDT

PDB ID	:	5VO8
Title	:	X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter
Authors	:	Murakami, K.S.; Shin, Y.; Turnbough Jr, C.L.; Molodtsov, V.
Deposited on	:	2017-05-02
Resolution	:	3.30 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	:	2.35.1
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

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 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
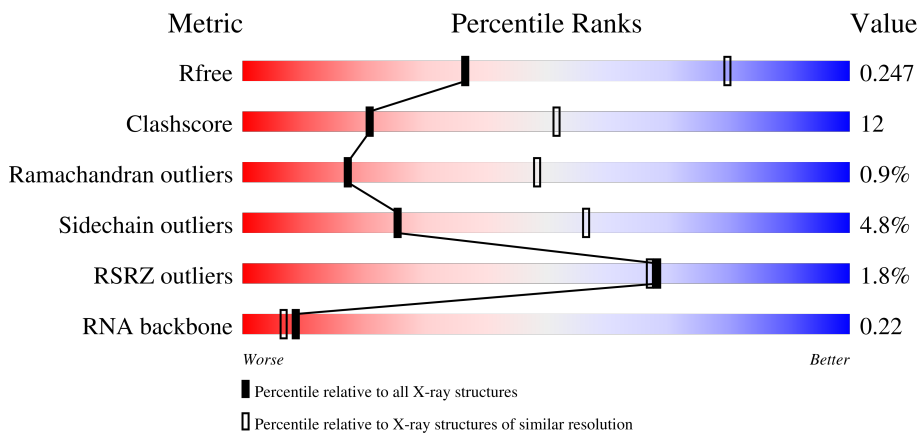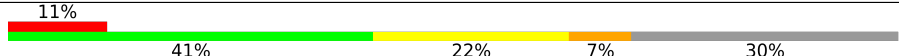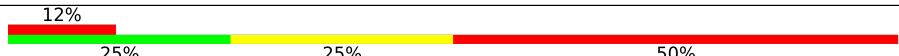
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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	A	315	51% 19% • 28%
1	B	315	51% 19% • 29%
2	C	1119	% 69% 28% ••
3	D	1524	% 68% 27% • •

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Mol	Chain	Length	Quality of chain
4	E	99	71% 22% • 5%
5	F	423	6% 56% 24% • 18%
6	G	22	9% 32% 23% 32% 14%
7	H	27	11% 41% 22% 7% 30%
8	I	8	12% 25% 25% 50%

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
9	MG	B	1001	-	-	-	X

2   Entry composition ⓘ

There are 11 unique types of molecules in this entry. The entry contains 28534 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 protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total 1782	C 1138	N 310	O 332	S 2	0	0	0
1	B	224	Total 1767	C 1129	N 307	O 329	S 2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1107	Total 8726	C 5523	N 1551	O 1628	S 24	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1484	Total 11722	C 7431	N 2065	O 2191	S 35	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total 761	C 486	N 132	O 139	S 4	0	0	0

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total 2790	C 1760	N 508	O 518	S 4	0	0	0

- Molecule 6 is a DNA chain called DNA (5'-D(P*GP*GP*TP*GP*CP*AP*TP*CP*AP*GP *AP*GP*CP*CP*CP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	19	Total 386	C 183	N 75	O 109	P 19	0	0	0

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP* TP*GP*AP*TP*GP*CP*AP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	19	Total 394	C 188	N 76	O 112	P 18	0	0	0

- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*GP*GP*GP*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	8	Total 193	C 80	N 40	O 63	P 10	0	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total 1	Mg 1	0	0
9	D	1	Total 1	Mg 1	0	0

- Molecule 10 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).
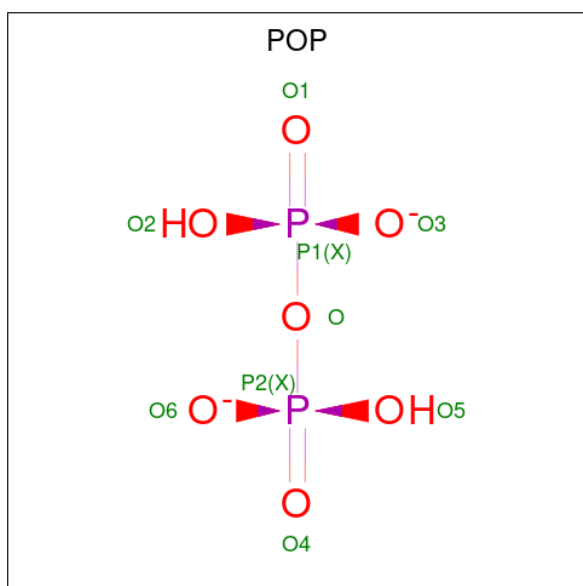
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total 9	O 7	P 2	0	0

• Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total 2	Zn 2	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: DNA-directed RNA polymerase subunit alpha

• Molecule 1: DNA-directed RNA polymerase subunit alpha

• Molecule 2: DNA-directed RNA polymerase subunit beta

• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:

• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:

• Molecule 5: RNA polymerase sigma factor SigA

Chain F:

Y329 I333 L338 P339 A345 L349 E353 L354 E355 K356 A357 L358 S359 K360 L361 S362 E363 R364 E365 A366 M367 V368 L369 K370 K373 G374 L375 I376 D377 G378 R379 E380 H381 T382 L383 E384 E385 V386 G387 A388 F389 F390 G391 V392 T393 R394 E395 R396 I397 R398 Q399 I400 E401 N402

K403 A404 L405 R406 K409 E412 S413 R414 T415 R416 K417 L418 R419 D420 F421 L422 D423

● Molecule 6: DNA (5'-D(P*GP*GP*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*A P*AP*AP*A)-3')

Chain G:

C3 C4 T5 G6 C7 A8 G12 A13 G14 C15 C16 C17 A18 A19 A20 A21 DT DA DC
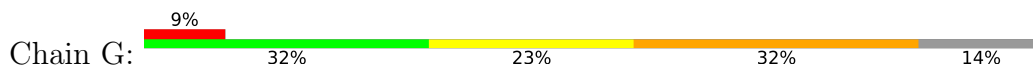
● Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*CP*TP*GP*AP*TP*GP*CP *AP*CP*C)-3')

Chain H:

T1 A2 T3 A4 A5 T6 G7 G8 G9 DA DG DC DT DT DG DG DC DT C16 T17 G18 A23 G24 C25
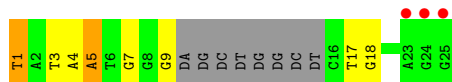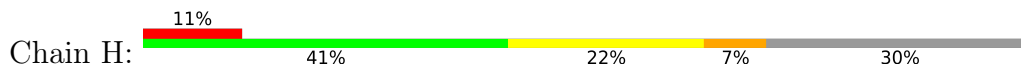
● Molecule 8: RNA (5'-D(*(GTP))-R(P*GP*GP*GP*GP*GP*GP*G)-3')

Chain I:

G1 G2 G3 G4 G5 G8
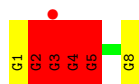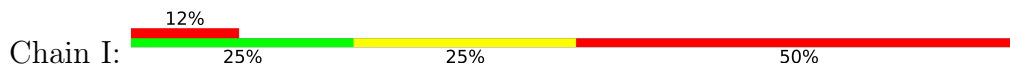
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	186.54Å 101.98Å 296.11Å 90.00° 98.56° 90.00°	Depositor
Resolution (Å)	29.88 – 3.30 29.88 – 3.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (29.88-3.30) 94.2 (29.88-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 3.31Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.185 , 0.246 0.185 , 0.247	Depositor DCC
R_{free} test set	1999 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å^2)	89.9	Xtriage
Anisotropy	0.773	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 69.8	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	28534	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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 $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, POP, GTP

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	0.58	1/1814 (0.1%)	0.82	1/2466 (0.0%)
1	B	0.60	2/1799 (0.1%)	0.90	1/2447 (0.0%)
2	C	0.53	0/8892	0.81	4/12028 (0.0%)
3	D	0.59	0/11928	0.86	13/16127 (0.1%)
4	E	0.50	0/775	0.76	0/1045
5	F	0.50	0/2835	0.81	1/3816 (0.0%)
6	G	1.35	4/433 (0.9%)	1.30	8/664 (1.2%)
7	H	1.03	1/442 (0.2%)	1.03	3/680 (0.4%)
8	I	1.06	0/181	2.00	10/283 (3.5%)
All	All	0.60	8/29099 (0.0%)	0.86	41/39556 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
5	F	0	1
All	All	0	2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	154	GLU	CB-CG	7.78	1.67	1.52
1	B	154	GLU	CG-CD	6.08	1.61	1.51
6	G	19	DA	P-O5'	6.06	1.65	1.59
7	H	1	DT	C1'-N1	5.55	1.56	1.49
6	G	12	DG	C3'-O3'	-5.36	1.36	1.44

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	G	17	DC	O4'-C4'-C3'	-9.24	100.46	106.00
6	G	19	DA	O4'-C4'-C3'	-9.14	100.52	106.00
6	G	16	DC	O5'-P-OP2	-8.29	98.23	105.70
2	C	879	ARG	NE-CZ-NH2	-7.70	116.45	120.30
3	D	1363	LEU	CB-CG-CD2	-7.02	99.06	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	766	GLU	Peptide
5	F	389	PHE	Peptide

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	A	1782	0	1834	44	0
1	B	1767	0	1816	45	0
2	C	8726	0	8814	243	0
3	D	11722	0	11950	309	1
4	E	761	0	778	21	0
5	F	2790	0	2854	79	0
6	G	386	0	212	14	0
7	H	394	0	217	8	0
8	I	193	0	88	8	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	C	9	0	0	0	0
11	D	2	0	0	0	0
All	All	28534	0	28563	694	1

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 12.

The worst 5 of 694 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:D:218:LYS:HG2	3:D:338:GLU:HG2	1.48	0.92
2:C:367:LEU:HA	2:C:371:LYS:HE2	1.49	0.92
2:C:418:LEU:O	2:C:419:THR:OG1	1.88	0.91
5:F:358:LEU:HB3	5:F:366:ALA:HB1	1.49	0.90
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.53	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:985:ASP:N	3:D:1497:GLU:OE1[1_545]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	224/315 (71%)	219 (98%)	5 (2%)	0	100	100
1	B	222/315 (70%)	210 (95%)	11 (5%)	1 (0%)	29	61
2	C	1101/1119 (98%)	1065 (97%)	29 (3%)	7 (1%)	25	57
3	D	1480/1524 (97%)	1439 (97%)	30 (2%)	11 (1%)	22	54
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	14	45
5	F	344/423 (81%)	316 (92%)	18 (5%)	10 (3%)	4	24
All	All	3463/3795 (91%)	3338 (96%)	95 (3%)	30 (1%)	17	48

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	363	SER
2	C	418	LEU
2	C	419	THR
3	D	484	PRO

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Mol	Chain	Res	Type
3	D	486	ARG

5.3.2   Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	199/273 (73%)	188 (94%)	11 (6%)	21	52
1	B	197/273 (72%)	187 (95%)	10 (5%)	24	54
2	C	931/941 (99%)	888 (95%)	43 (5%)	27	58
3	D	1250/1279 (98%)	1182 (95%)	68 (5%)	22	53
4	E	83/88 (94%)	80 (96%)	3 (4%)	35	63
5	F	296/371 (80%)	290 (98%)	6 (2%)	55	76
All	All	2956/3225 (92%)	2815 (95%)	141 (5%)	25	56

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1130	ARG
3	D	1195	GLN
3	D	1493	LYS
2	C	617	ASP
2	C	610	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	640	HIS
3	D	744	GLN
5	F	411	HIS
2	C	683	ASN
2	C	390	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	8/8 (100%)	3 (37%)	3 (37%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	3	G
8	I	4	G
8	I	5	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	I	1	GTP
8	I	2	G
8	I	4	G

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 monosaccharides 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	$\#|Z| > 2$
10	POP	C	1201	2	6,8,8	0.59	0	13,13,13	1.02	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
10	POP	C	1201	2	-	0/6/6/6	-

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.

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6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	226/315 (71%)	-0.36	1 (0%)	92	93	86, 127, 163, 192	0
1	B	224/315 (71%)	-0.42	0	100	100	73, 114, 162, 206	0
2	C	1107/1119 (98%)	-0.24	13 (1%)	79	78	47, 116, 201, 261	0
3	D	1484/1524 (97%)	-0.28	15 (1%)	82	82	46, 105, 183, 273	0
4	E	94/99 (94%)	-0.34	0	100	100	67, 121, 193, 216	0
5	F	346/423 (81%)	0.03	27 (7%)	13	12	82, 136, 247, 282	0
6	G	19/22 (86%)	0.39	2 (10%)	6	6	68, 117, 257, 289	0
7	H	19/27 (70%)	0.11	3 (15%)	2	2	119, 141, 268, 271	0
8	I	7/8 (87%)	0.52	1 (14%)	2	2	88, 104, 219, 238	0
All	All	3526/3852 (91%)	-0.25	62 (1%)	68	67	46, 117, 199, 289	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	375	LEU	5.0
5	F	148	LYS	4.8
2	C	188	LYS	4.8
3	D	1313	VAL	4.0
5	F	391	GLY	3.8

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 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
9	MG	B	1001	1/1	0.53	0.40	80,80,80,80	0
10	POP	C	1201	9/9	0.94	0.11	94,111,146,148	0
11	ZN	D	2002	1/1	0.96	0.09	134,134,134,134	0
9	MG	D	2001	1/1	0.97	0.14	46,46,46,46	0
11	ZN	D	2003	1/1	0.98	0.23	123,123,123,123	0

6.5 Other polymers ⓘ

There are no such residues in this entry.