



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 20, 2024 – 10:23 pm BST

PDB ID : 4AV1
Title : Crystal structure of the human PARP-1 DNA binding domain in complex with DNA
Authors : Ali, A.A.E.; Timinszky, G.; Arribas-Bosacoma, R.; Kozlowski, M.; Hassa, P.O.; Hassler, M.; Ladurner, A.G.; Pearl, L.H.; Oliver, A.W.
Deposited on : 2012-05-23
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

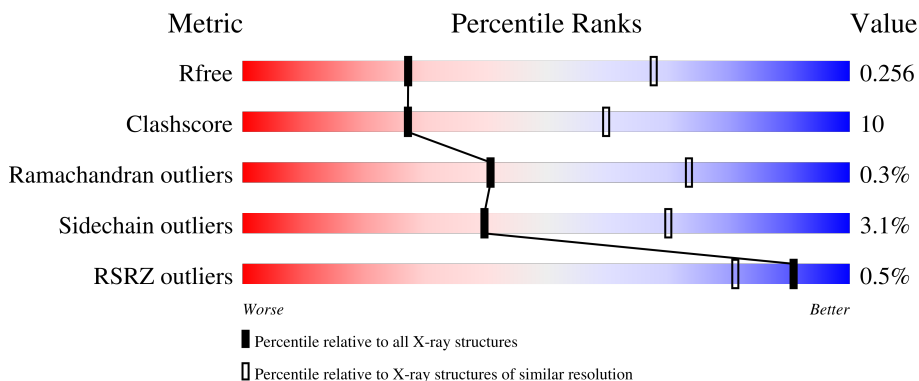
1 Overall quality at a glance

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.



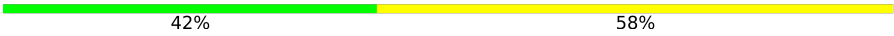
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	223	 29% 9% 61%
1	B	223	 32% 10% 57%
1	C	223	 29% 9% 62%
1	D	223	 33% 9% 57%
2	X	12	 67% 25% 8%

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Mol	Chain	Length	Quality of chain
3	Y	12	 42% 58%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3344 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 POLY [ADP-RIBOSE] POLYMERASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	86	Total 656	C 417	N 111	O 122	S 6	0	0	0
1	B	96	Total 766	C 484	N 136	O 140	S 6	0	1	0
1	C	85	Total 642	C 407	N 111	O 118	S 6	0	0	0
1	D	95	Total 746	C 472	N 131	O 137	S 6	0	0	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P09874
A	-19	ALA	-	expression tag	UNP P09874
A	-18	SER	-	expression tag	UNP P09874
A	-17	TRP	-	expression tag	UNP P09874
A	-16	SER	-	expression tag	UNP P09874
A	-15	HIS	-	expression tag	UNP P09874
A	-14	PRO	-	expression tag	UNP P09874
A	-13	GLN	-	expression tag	UNP P09874
A	-12	PHE	-	expression tag	UNP P09874
A	-11	GLU	-	expression tag	UNP P09874
A	-10	LYS	-	expression tag	UNP P09874
A	-9	GLY	-	expression tag	UNP P09874
A	-8	ALA	-	expression tag	UNP P09874
A	-7	LEU	-	expression tag	UNP P09874
A	-6	GLU	-	expression tag	UNP P09874
A	-5	VAL	-	expression tag	UNP P09874
A	-4	LEU	-	expression tag	UNP P09874
A	-3	PHE	-	expression tag	UNP P09874
A	-2	GLN	-	expression tag	UNP P09874
A	-1	GLY	-	expression tag	UNP P09874
A	0	PRO	-	expression tag	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1	LEU	-	expression tag	UNP P09874
A	2	GLY	-	expression tag	UNP P09874
A	3	SER	-	expression tag	UNP P09874
A	4	HIS	-	expression tag	UNP P09874
B	-20	MET	-	expression tag	UNP P09874
B	-19	ALA	-	expression tag	UNP P09874
B	-18	SER	-	expression tag	UNP P09874
B	-17	TRP	-	expression tag	UNP P09874
B	-16	SER	-	expression tag	UNP P09874
B	-15	HIS	-	expression tag	UNP P09874
B	-14	PRO	-	expression tag	UNP P09874
B	-13	GLN	-	expression tag	UNP P09874
B	-12	PHE	-	expression tag	UNP P09874
B	-11	GLU	-	expression tag	UNP P09874
B	-10	LYS	-	expression tag	UNP P09874
B	-9	GLY	-	expression tag	UNP P09874
B	-8	ALA	-	expression tag	UNP P09874
B	-7	LEU	-	expression tag	UNP P09874
B	-6	GLU	-	expression tag	UNP P09874
B	-5	VAL	-	expression tag	UNP P09874
B	-4	LEU	-	expression tag	UNP P09874
B	-3	PHE	-	expression tag	UNP P09874
B	-2	GLN	-	expression tag	UNP P09874
B	-1	GLY	-	expression tag	UNP P09874
B	0	PRO	-	expression tag	UNP P09874
B	1	LEU	-	expression tag	UNP P09874
B	2	GLY	-	expression tag	UNP P09874
B	3	SER	-	expression tag	UNP P09874
B	4	HIS	-	expression tag	UNP P09874
C	-20	MET	-	expression tag	UNP P09874
C	-19	ALA	-	expression tag	UNP P09874
C	-18	SER	-	expression tag	UNP P09874
C	-17	TRP	-	expression tag	UNP P09874
C	-16	SER	-	expression tag	UNP P09874
C	-15	HIS	-	expression tag	UNP P09874
C	-14	PRO	-	expression tag	UNP P09874
C	-13	GLN	-	expression tag	UNP P09874
C	-12	PHE	-	expression tag	UNP P09874
C	-11	GLU	-	expression tag	UNP P09874
C	-10	LYS	-	expression tag	UNP P09874
C	-9	GLY	-	expression tag	UNP P09874
C	-8	ALA	-	expression tag	UNP P09874

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	LEU	-	expression tag	UNP P09874
C	-6	GLU	-	expression tag	UNP P09874
C	-5	VAL	-	expression tag	UNP P09874
C	-4	LEU	-	expression tag	UNP P09874
C	-3	PHE	-	expression tag	UNP P09874
C	-2	GLN	-	expression tag	UNP P09874
C	-1	GLY	-	expression tag	UNP P09874
C	0	PRO	-	expression tag	UNP P09874
C	1	LEU	-	expression tag	UNP P09874
C	2	GLY	-	expression tag	UNP P09874
C	3	SER	-	expression tag	UNP P09874
C	4	HIS	-	expression tag	UNP P09874
D	-20	MET	-	expression tag	UNP P09874
D	-19	ALA	-	expression tag	UNP P09874
D	-18	SER	-	expression tag	UNP P09874
D	-17	TRP	-	expression tag	UNP P09874
D	-16	SER	-	expression tag	UNP P09874
D	-15	HIS	-	expression tag	UNP P09874
D	-14	PRO	-	expression tag	UNP P09874
D	-13	GLN	-	expression tag	UNP P09874
D	-12	PHE	-	expression tag	UNP P09874
D	-11	GLU	-	expression tag	UNP P09874
D	-10	LYS	-	expression tag	UNP P09874
D	-9	GLY	-	expression tag	UNP P09874
D	-8	ALA	-	expression tag	UNP P09874
D	-7	LEU	-	expression tag	UNP P09874
D	-6	GLU	-	expression tag	UNP P09874
D	-5	VAL	-	expression tag	UNP P09874
D	-4	LEU	-	expression tag	UNP P09874
D	-3	PHE	-	expression tag	UNP P09874
D	-2	GLN	-	expression tag	UNP P09874
D	-1	GLY	-	expression tag	UNP P09874
D	0	PRO	-	expression tag	UNP P09874
D	1	LEU	-	expression tag	UNP P09874
D	2	GLY	-	expression tag	UNP P09874
D	3	SER	-	expression tag	UNP P09874
D	4	HIS	-	expression tag	UNP P09874

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*GP*TP*GP*TP*TP*GP*CP*AP*TP*T P)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	X	12	245	119	43	72	11	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	Y	12	241	117	45	68	11	0	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Zn 1	0	0
4	B	1	Total 1	Zn 1	0	0
4	C	1	Total 1	Zn 1	0	0
4	D	1	Total 1	Zn 1	0	0

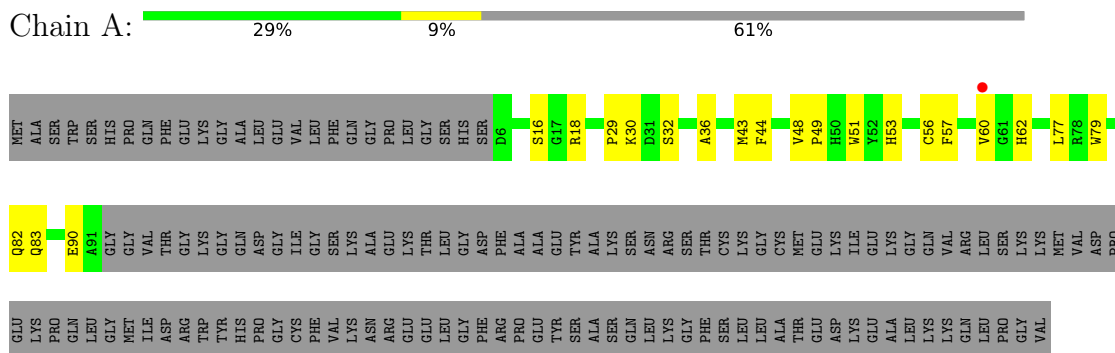
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total 5	O 5	0	0
5	B	17	Total 17	O 17	0	0
5	C	4	Total 4	O 4	0	0
5	D	5	Total 5	O 5	0	0
5	X	8	Total 8	O 8	0	0
5	Y	5	Total 5	O 5	0	0

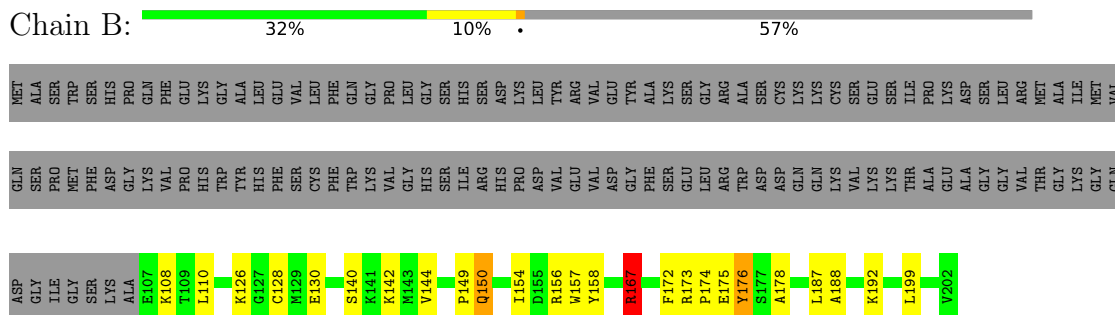
3 Residue-property plots

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.

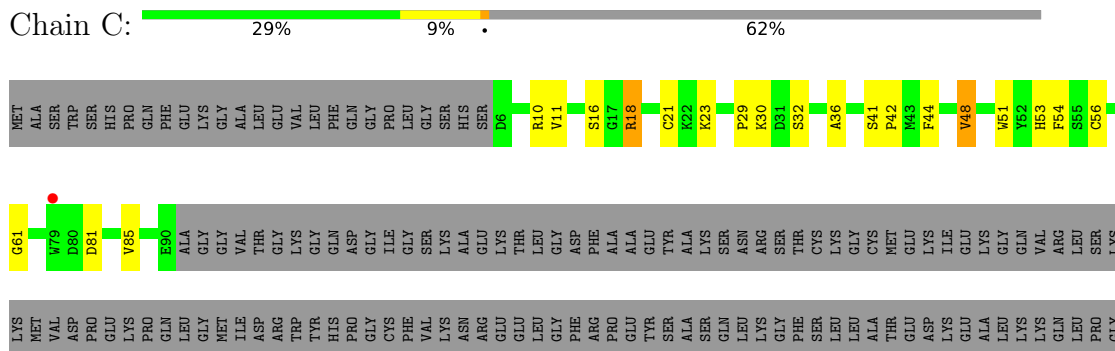
- Molecule 1: POLY [ADP-RIBOSE] POLYMERASE 1



- Molecule 1: POLY [ADP-RIBOSE] POLYMERASE 1



- Molecule 1: POLY [ADP-RIBOSE] POLYMERASE 1



VAL

- Molecule 1: POLY [ADP-RIBOSE] POLYMERASE 1

Chain D:  33% 9% 57%

MET	ALA	SER	TRP	PHE	HIS	PRO	GLN	PHE	GLU	LEU	LYS	GLY	ALA	LEU	GLU	VAL	PHE	LEU	GLY	GLN	GLY	PRO	LEU	HIS	GLY	SER	HIS	SER	ASP	LEU	TYR	ARG	VAL	GLU	TYR	ALA	LYS	SER	GLY	ARG	ALA	SER	CYS	LYS	CYS	SER	GLU	SER	THR	ILE	PRO	LYS	ASP	SER	LEU	VAL	ARG	MET	ALA	ILE	GLN	VAL
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GLN	SER	PRO	MET	PHE	ASP	GLY	LYS	VAL	PRO	HIS	TRP	TYR	HIS	PHE	SER	CYS	PHE	TRP	LYS	VAL	GLY	HIS	SER	ILE	ARG	HIS	ASP	PRO	ASP	LEU	VAL	GLU	ARG	VAL	ASP	GLY	PHE	SER	GLU	LEU	ARG	TRP	ALA	ASP	CYS	GLN	LYS	GLN	LYS	VAL	SER	LYS	LYS	THR	ALA	GLU	ALA	GLY	GLY	VAL	THR	GLY	LYS	GLN	VAL
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ASP	GLY	ILE	GLY	SER	LYS	ALA	GLU	K108	K126	G127	C128	R129	E130	S140	K148	P149	Q150	L151	G152	W157	Y158	R167	R173	P174	E175	Y176	S177	A178	L187	A188	K192	K196	L199	V202
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- Molecule 2: 5'-D(*AP*AP*GP*TP*GP*TP*TP*GP*CP*AP*TP*TP)-3'

Chain X:  67% 25% 8%

A1	A2	G3	T12
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- Molecule 3: 5'-D(*TP*AP*AP*TP*GP*CP*AP*AP*CP*AP*CP*TP)-3'

Chain Y:  42% 58%

T1	A2	A3	T4	G5	C6	A7	T12
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.98Å 59.50Å 61.58Å 90.00° 101.18° 90.00°	Depositor
Resolution (Å)	44.35 – 3.10 44.35 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.7 (44.35-3.10) 92.0 (44.35-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.230 , 0.249 0.231 , 0.256	Depositor DCC
R_{free} test set	460 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtrriage
Anisotropy	0.766	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3344	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.71% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.22	0/676	0.66	3/918 (0.3%)
1	B	0.22	0/783	0.67	3/1044 (0.3%)
1	C	0.21	0/659	0.66	3/891 (0.3%)
1	D	0.22	0/760	0.66	3/1015 (0.3%)
2	X	0.44	0/274	1.07	1/422 (0.2%)
3	Y	0.43	0/270	0.92	0/414
All	All	0.27	0/3422	0.73	13/4704 (0.3%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	167	ARG	NE-CZ-NH2	-11.95	114.33	120.30
1	B	167	ARG	NE-CZ-NH1	11.95	126.27	120.30
1	D	167	ARG	NE-CZ-NH2	-11.85	114.38	120.30
1	A	18	ARG	NE-CZ-NH2	-11.37	114.61	120.30
1	D	167	ARG	NE-CZ-NH1	11.26	125.93	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	656	0	579	12	0
1	B	766	0	778	17	0
1	C	642	0	576	14	0
1	D	746	0	750	15	0
2	X	245	0	139	4	0
3	Y	241	0	137	9	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	0	0	0
5	B	17	0	0	2	0
5	C	4	0	0	0	0
5	D	5	0	0	0	0
5	X	8	0	0	0	0
5	Y	5	0	0	0	0
All	All	3344	0	2959	63	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.

The worst 5 of 63 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:LEU:HB2	1:D:152:GLY:HA2	1.65	0.78
1:C:18:ARG:HH11	3:Y:3:DA:H62	1.34	0.75
3:Y:5:DG:H2''	3:Y:6:DC:H5''	1.70	0.73
1:B:140:SER:HB3	1:B:157:TRP:CE3	2.32	0.65
1:D:148:LYS:HD2	2:X:12:DT:H2''	1.77	0.64

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	84/223 (38%)	73 (87%)	11 (13%)	0	100	100
1	B	95/223 (43%)	88 (93%)	7 (7%)	0	100	100
1	C	83/223 (37%)	72 (87%)	10 (12%)	1 (1%)	13	44
1	D	93/223 (42%)	86 (92%)	7 (8%)	0	100	100
All	All	355/892 (40%)	319 (90%)	35 (10%)	1 (0%)	41	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	61	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	66/188 (35%)	64 (97%)	2 (3%)	41	71
1	B	82/188 (44%)	77 (94%)	5 (6%)	18	49
1	C	64/188 (34%)	63 (98%)	1 (2%)	62	84
1	D	79/188 (42%)	78 (99%)	1 (1%)	69	87
All	All	291/752 (39%)	282 (97%)	9 (3%)	40	70

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	48	VAL
1	D	176	TYR
1	B	110	LEU
1	B	150	GLN
1	B	167	ARG

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

Mol	Chain	Res	Type
1	B	150	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	86/223 (38%)	0.10	1 (1%) 79 61	48, 78, 105, 118	0
1	B	96/223 (43%)	-0.27	0 100 100	36, 57, 82, 99	0
1	C	85/223 (38%)	0.18	1 (1%) 79 61	48, 79, 112, 130	0
1	D	95/223 (42%)	-0.26	0 100 100	36, 59, 85, 93	0
2	X	12/12 (100%)	-0.29	0 100 100	36, 42, 47, 85	0
3	Y	12/12 (100%)	-0.13	0 100 100	32, 38, 55, 89	0
All	All	386/916 (42%)	-0.08	2 (0%) 91 81	32, 66, 105, 130	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	79	TRP	2.5
1	A	60	VAL	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
4	ZN	C	1600	1/1	0.89	0.11	110,110,110,110	0
4	ZN	B	1600	1/1	0.98	0.15	63,63,63,63	0
4	ZN	A	1600	1/1	0.98	0.12	84,84,84,84	0
4	ZN	D	1600	1/1	0.99	0.16	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.