



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 14, 2014 – 05:46 PM EDT

PDB ID : 4OQB
Title : Structure of Human PARP-1 bound to a DNA double strand break in complex with (2Z)-2-{4-[2-(morpholin-4-yl)ethoxy]benzylidene}-3-oxo-2,3-dihydro-1-benzofuran-7-carboxamide
Authors : Pascal, J.M.; Steffen, J.D.
Deposited on : 2014-02-07
Resolution : 3.36 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>

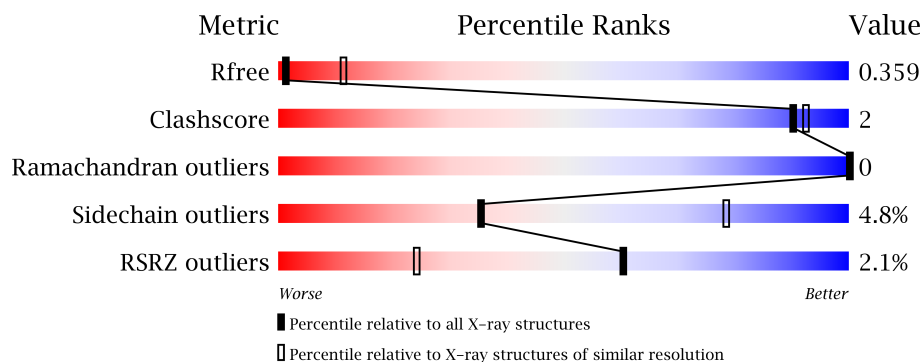
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
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) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 3.36 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	1141 (3.50-3.22)
Clashscore	79885	1030 (3.48-3.24)
Ramachandran outliers	78287	1008 (3.48-3.24)
Sidechain outliers	78261	1007 (3.48-3.24)
RSRZ outliers	66119	1141 (3.50-3.22)

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	A	267	
1	D	267	
2	C	505	
2	F	505	
3	M	26	
3	N	26	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11775 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 protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	1	0
			1755	1110	305	327	13			
1	D	222	Total	C	N	O	S	0	1	0
			1755	1110	305	327	13			

- Molecule 2 is a protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	456	Total	C	N	O	S	0	0	0
			3586	2296	605	672	13			
2	F	456	Total	C	N	O	S	0	0	0
			3586	2296	605	672	13			

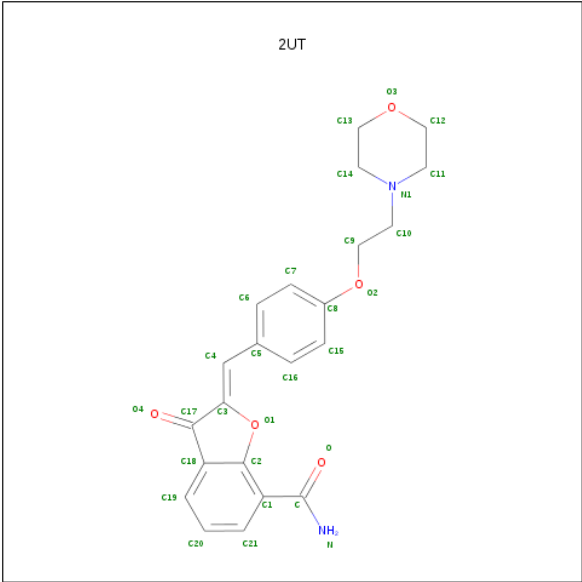
- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	26	Total	C	N	O	P	0	0	0
			530	251	100	154	25			
3	N	26	Total	C	N	O	P	0	0	0
			530	251	100	154	25			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		

- Molecule 5 is (2Z)-2-{4-[2-(MORPHOLIN-4-YL)ETHOXY]BENZYLIDENE}-3-OXO-2,3-DIHYDRO-1-BENZOFURAN-7-CARBOXAMIDE (three-letter code: 2UT) (formula: C₂₂H₂₂N₂O₅).



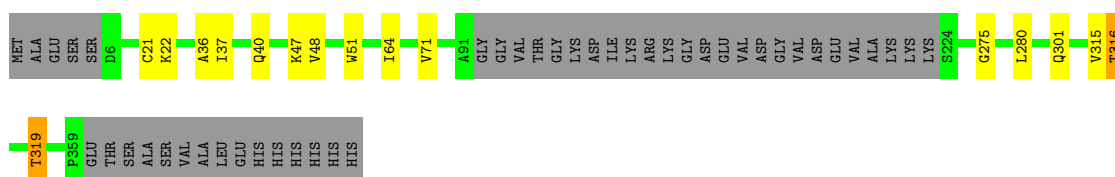
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			29	22	2	5		

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.

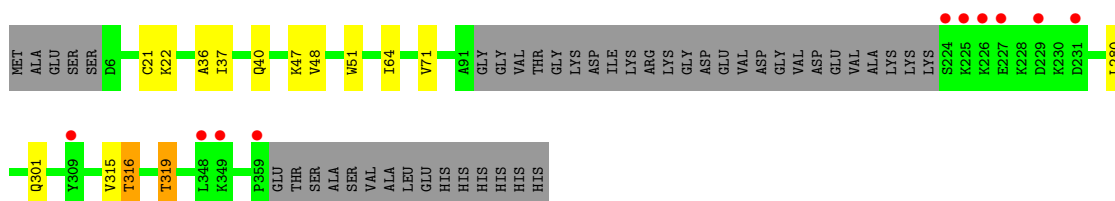
- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



- Molecule 1: Poly [ADP-ribose] polymerase 1

Chain D:



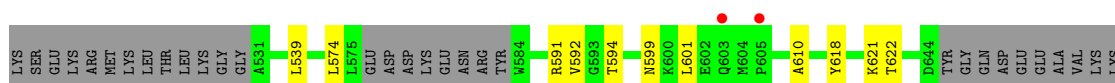
- Molecule 2: Poly [ADP-ribose] polymerase 1

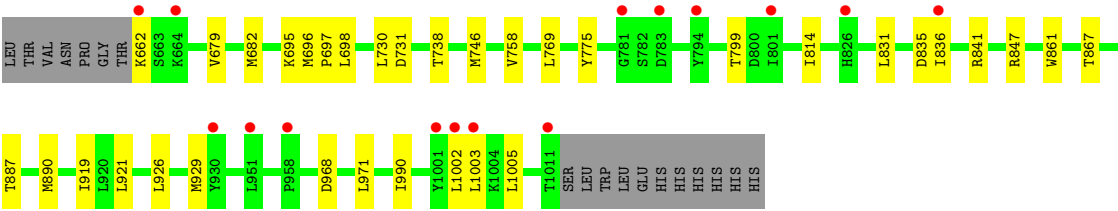
Chain C:



- Molecule 2: Poly [ADP-ribose] polymerase 1

Chain F:





• Molecule 3: DNA (26-MER)

Chain M:



• Molecule 3: DNA (26-MER)

Chain N:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.10Å 113.08Å 296.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.36 49.37 – 3.36	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.36) 98.9 (49.37-3.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.322 , 0.349 0.330 , 0.359	Depositor DCC
R_{free} test set	1625 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	136.5	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 109.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 31745 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11775	wwPDB-VP
Average B, all atoms (Å ²)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.91% 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: ZN, 2UT

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	0.26	0/1795	0.40	0/2416
1	D	0.26	0/1795	0.40	0/2416
2	C	0.26	0/3660	0.42	0/4940
2	F	0.26	0/3660	0.43	0/4940
3	M	0.27	0/594	0.80	0/915
3	N	0.24	0/594	0.78	2/915 (0.2%)
All	All	0.26	0/12098	0.47	2/16542 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1	DG	C5'-C4'-O4'	5.23	119.23	109.30
3	N	1	DG	C5'-C4'-C3'	5.08	123.25	114.10

There are no chirality outliers.

There are no planarity outliers.

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	A	1755	0	1712	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1755	0	1712	6	0
2	C	3586	0	3604	20	0
2	F	3586	0	3604	18	0
3	M	530	0	292	1	0
3	N	530	0	292	1	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	C	29	0	0	2	0
All	All	11775	0	11216	48	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 2.

All (48) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:574:LEU:HD11	2:F:610:ALA:HB1	1.69	0.73
2:C:574:LEU:HD11	2:C:610:ALA:HB1	1.70	0.72
1:A:36:ALA:HB2	1:A:51:TRP:CE3	2.39	0.57
1:D:36:ALA:HB2	1:D:51:TRP:CE3	2.39	0.57
2:C:831:LEU:HD12	2:C:1005:LEU:HD23	1.88	0.54
2:F:831:LEU:HD12	2:F:1005:LEU:HD23	1.88	0.54
2:F:814:ILE:HG21	2:F:836:ILE:HD12	1.92	0.52
2:C:814:ILE:HG21	2:C:836:ILE:HD12	1.92	0.51
2:F:679:VAL:HG11	2:F:775:TYR:CZ	2.46	0.50
2:C:679:VAL:HG11	2:C:775:TYR:CZ	2.47	0.50
2:F:919:ILE:HG22	2:F:1005:LEU:HD11	1.94	0.49
2:C:919:ILE:HG22	2:C:1005:LEU:HD11	1.94	0.49
2:F:696:MET:N	2:F:697:PRO:HD2	2.28	0.49
2:C:696:MET:N	2:C:697:PRO:HD2	2.28	0.48
1:D:315:VAL:HG13	1:D:316:THR:HG22	1.95	0.48
1:A:315:VAL:HG13	1:A:316:THR:HG22	1.96	0.47
2:C:861:TRP:CD2	2:C:921:LEU:HD21	2.49	0.47
3:M:22:DT:H2''	3:M:23:DA:C8	2.50	0.47
1:D:319:THR:HG21	2:F:731:ASP:HA	1.96	0.47
2:C:862:HIS:ND1	5:C:1101:2UT:O	2.48	0.46
2:F:861:TRP:CD2	2:F:921:LEU:HD21	2.49	0.46
2:C:863:GLY:O	5:C:1101:2UT:N	2.50	0.45
2:F:926:LEU:HD13	2:F:929:MET:HE3	1.98	0.44
2:C:926:LEU:HD13	2:C:929:MET:HE3	1.99	0.44
1:A:275:GLY:HA2	3:N:23:DA:H3'	1.99	0.44
2:F:799:THR:HG22	2:F:841:ARG:HA	2.00	0.43
2:C:539:LEU:HD11	2:C:601:LEU:HD21	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:319:THR:CG2	2:F:731:ASP:HA	2.48	0.42
1:D:64:ILE:HD13	1:D:71:VAL:CG2	2.50	0.42
2:C:814:ILE:CG2	2:C:1003:LEU:HD21	2.50	0.42
1:A:64:ILE:HD13	1:A:71:VAL:CG2	2.50	0.42
2:C:799:THR:HG22	2:C:841:ARG:HA	2.00	0.42
2:F:539:LEU:HD11	2:F:601:LEU:HD21	2.00	0.41
2:C:734:ASN:O	2:C:738:THR:OG1	2.38	0.41
2:C:682:MET:HG2	2:C:867:THR:HG22	2.02	0.41
2:F:682:MET:HG2	2:F:867:THR:HG22	2.03	0.41
2:F:696:MET:N	2:F:697:PRO:CD	2.83	0.41
2:C:990:ILE:HD12	2:C:990:ILE:N	2.36	0.41
1:A:319:THR:HG22	2:C:734:ASN:HD22	1.86	0.41
2:C:618:TYR:CE2	2:C:622:THR:HG21	2.56	0.41
2:C:696:MET:N	2:C:697:PRO:CD	2.83	0.41
2:F:591:ARG:HD3	2:F:746:MET:HE1	2.03	0.41
2:F:814:ILE:CG2	2:F:1003:LEU:HD21	2.50	0.41
1:D:36:ALA:HB2	1:D:51:TRP:CZ3	2.56	0.41
2:F:990:ILE:HD12	2:F:990:ILE:N	2.36	0.41
2:C:618:TYR:O	2:C:622:THR:HG22	2.21	0.40
1:A:36:ALA:HB2	1:A:51:TRP:CZ3	2.56	0.40
2:F:618:TYR:O	2:F:622:THR:HG22	2.21	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	
1	A	219/267 (82%)	212 (97%)	7 (3%)	0	100	100
1	D	219/267 (82%)	212 (97%)	7 (3%)	0	100	100
2	C	450/505 (89%)	423 (94%)	27 (6%)	0	100	100
2	F	450/505 (89%)	422 (94%)	28 (6%)	0	100	100
All	All	1338/1544 (87%)	1269 (95%)	69 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	189/237 (80%)	179 (95%)	10 (5%)	32	75
1	D	189/237 (80%)	179 (95%)	10 (5%)	32	75
2	C	391/443 (88%)	373 (95%)	18 (5%)	37	80
2	F	391/443 (88%)	373 (95%)	18 (5%)	37	80
All	All	1160/1360 (85%)	1104 (95%)	56 (5%)	35	78

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	CYS
1	A	22	LYS
1	A	37	ILE
1	A	40	GLN
1	A	47	LYS
1	A	48	VAL
1	A	280	LEU
1	A	301	GLN
1	A	316	THR
1	A	319	THR
2	C	592	VAL
2	C	594	THR
2	C	599	ASN
2	C	621	LYS
2	C	662	LYS
2	C	695	LYS
2	C	698	LEU
2	C	730	LEU
2	C	738	THR
2	C	758	VAL
2	C	769	LEU
2	C	835	ASP
2	C	847	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	887	THR
2	C	890	MET
2	C	968	ASP
2	C	971	LEU
2	C	1002	LEU
1	D	21	CYS
1	D	22	LYS
1	D	37	ILE
1	D	40	GLN
1	D	47	LYS
1	D	48	VAL
1	D	280	LEU
1	D	301	GLN
1	D	316	THR
1	D	319	THR
2	F	592	VAL
2	F	594	THR
2	F	599	ASN
2	F	621	LYS
2	F	662	LYS
2	F	695	LYS
2	F	698	LEU
2	F	730	LEU
2	F	738	THR
2	F	758	VAL
2	F	769	LEU
2	F	835	ASP
2	F	847	ARG
2	F	887	THR
2	F	890	MET
2	F	968	ASP
2	F	971	LEU
2	F	1002	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	573	GLN
2	C	599	ASN
2	C	613	HIS
2	C	820	ASN
2	C	856	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	906	ASN
2	C	961	ASN
2	F	573	GLN
2	F	599	ASN
2	F	613	HIS
2	F	820	ASN
2	F	856	ASN
2	F	906	ASN
2	F	961	ASN

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 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	$\# Z > 2$
5	2UT	C	1101	-	32,32,32	0.23	0	44,44,44	2.32	9 (20%)

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
5	2UT	C	1101	-	-	0/13/34/34	0/4/4/4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1101	2UT	C4-C3-C17	7.32	135.37	126.82
5	C	1101	2UT	O1-C3-C4	-7.02	112.75	123.94
5	C	1101	2UT	C2-C18-C17	5.95	109.63	107.06
5	C	1101	2UT	O4-C17-C3	5.71	132.27	126.48
5	C	1101	2UT	C18-C17-C3	-5.31	100.75	104.17
5	C	1101	2UT	C2-O1-C3	3.23	107.18	105.19
5	C	1101	2UT	O1-C3-C17	2.71	111.79	109.50
5	C	1101	2UT	C18-C2-C1	-2.68	121.65	124.92
5	C	1101	2UT	C2-C1-C	-2.49	121.86	125.82

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	A	222/267 (83%)	-0.06	0 100 100	136, 174, 261, 285	0
1	D	222/267 (83%)	0.18	10 (4%) 32 11	176, 243, 321, 342	0
2	C	456/505 (90%)	0.23	3 (0%) 84 50	135, 195, 248, 286	0
2	F	456/505 (90%)	0.32	17 (3%) 39 14	169, 241, 300, 331	0
3	M	26/26 (100%)	-0.68	0 100 100	161, 187, 226, 228	0
3	N	26/26 (100%)	-0.69	0 100 100	157, 203, 226, 230	0
All	All	1408/1596 (88%)	0.17	30 (2%) 60 24	135, 214, 293, 342	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	349	LYS	5.6
1	D	225	LYS	5.2
1	D	348	LEU	4.9
2	F	1001	TYR	3.3
2	F	603	GLN	3.1
1	D	359	PRO	3.1
1	D	224	SER	3.0
2	C	934	HIS	3.0
2	C	943	LYS	3.0
2	F	1003	LEU	2.8
2	F	783	ASP	2.8
2	F	951	LEU	2.8
2	F	605	PRO	2.7
1	D	227	GLU	2.7
2	F	1011	THR	2.7
2	F	958	PRO	2.7
2	F	794	TYR	2.5
2	C	937	HIS	2.5
2	F	801	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	226	LYS	2.3
2	F	836	ILE	2.3
2	F	662	LYS	2.3
1	D	229	ASP	2.3
2	F	1002	LEU	2.2
2	F	930	TYR	2.2
2	F	826	HIS	2.1
2	F	781	GLY	2.1
1	D	309	TYR	2.1
2	F	664	LYS	2.0
1	D	231	ASP	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	2UT	C	1101	29/29	0.22	-0.85	121,127,140,140	0
4	ZN	D	402	1/1	0.03	-1.63	132,132,132,132	0
4	ZN	D	401	1/1	0.05	-3.16	118,118,118,118	0
4	ZN	A	402	1/1	0.04	-3.27	62,62,62,62	0
4	ZN	A	401	1/1	0.04	-4.95	78,78,78,78	0

6.5 Other polymers ⓘ

There are no such residues in this entry.