W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2024 – 12:24 AM EDT

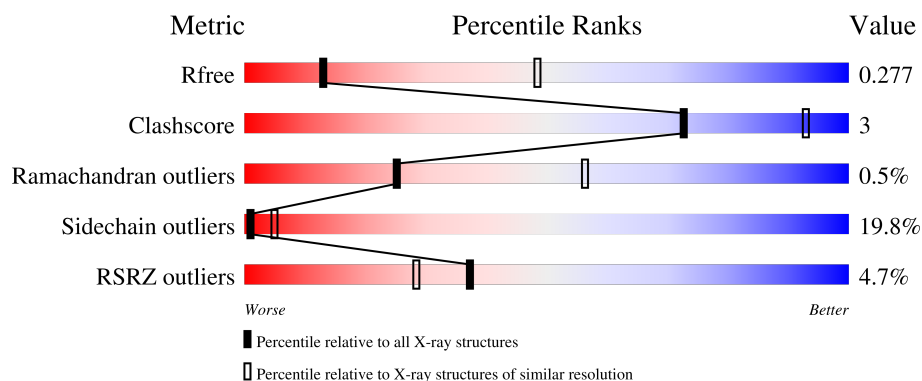|		
PDB ID	:	1T2V
Title	:	Structural basis of phospho-peptide recognition by the BRCT domain of BRCA1, structure with phosphopeptide
Authors	:	Williams, R.S.; Lee, M.S.; Hau, D.D.; Glover, J.N.M.
Deposited on	:	2004-04-22
Resolution	:	3.30 Å(reported)

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.

Metric	Percentile Ranks	Value
Rfree		0.277
Clashscore		3
Ramachandran outliers		0.5%
Sidechain outliers		19.8%
RSRZ outliers		4.7%

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))
R$_{free}$	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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	214	% 72% 23% • •
1	B	214	3% 75% 21% • •
1	C	214	6% 70% 23% • 6%
1	D	214	7% 73% 21% • •
1	E	214	2% 77% 20% • •

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Mol	Chain	Length	Quality of chain
2	F	16	25% 56% 31% 12%
2	G	16	6% 62% 12% 12% 12%
2	H	16	12% 62% 25% 12%
2	I	16	6% 50% 19% 31%
2	J	16	12% 38% 25% 12% 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8380 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 Breast cancer type 1 susceptibility protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1601	1030	264	293	14			
1	B	210	Total	C	N	O	S	0	0	0
			1605	1026	271	295	13			
1	C	202	Total	C	N	O	S	0	0	0
			1532	988	249	282	13			
1	D	205	Total	C	N	O	S	0	0	0
			1523	982	252	276	13			
1	E	211	Total	C	N	O	S	0	0	0
			1620	1041	267	298	14			

- Molecule 2 is a protein called BRCTide-7PS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	14	Total	C	N	O	P	0	0	0
			107	69	15	22	1			
2	G	14	Total	C	N	O	P	0	0	0
			101	63	15	22	1			
2	H	14	Total	C	N	O	P	0	0	0
			107	69	15	22	1			
2	I	11	Total	C	N	O	P	0	0	0
			86	54	12	19	1			
2	J	12	Total	C	N	O	P	0	0	0
			98	64	13	20	1			

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 geometr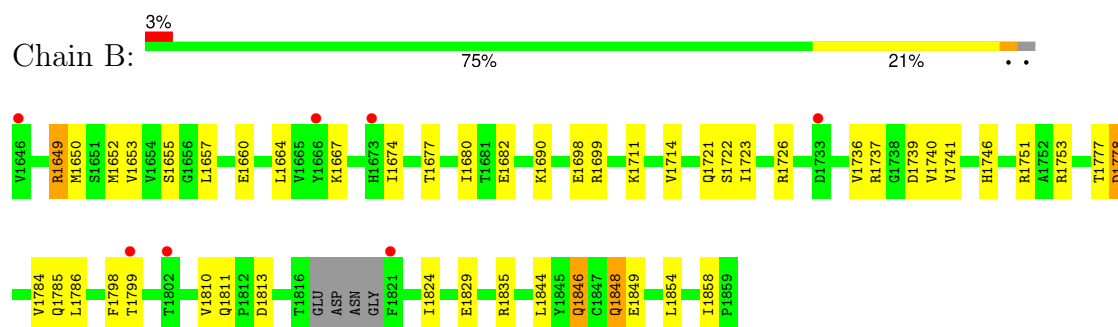ic quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Breast cancer type 1 susceptibility protein
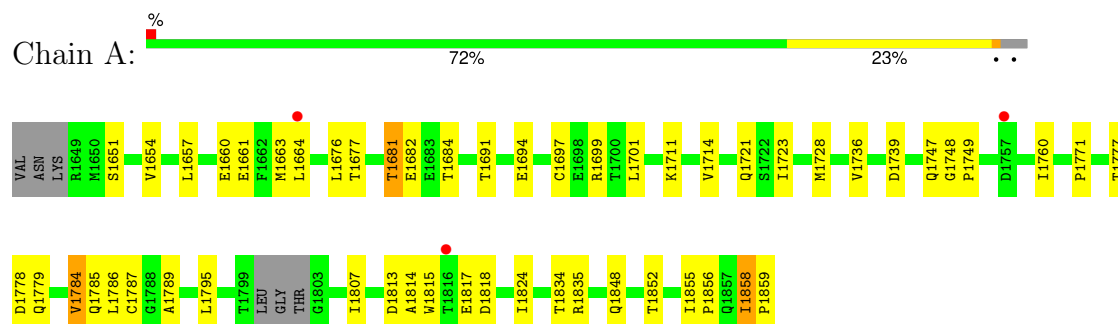
Chain A:

• Molecule 1: Breast cancer type 1 susceptibility protein

Chain B:

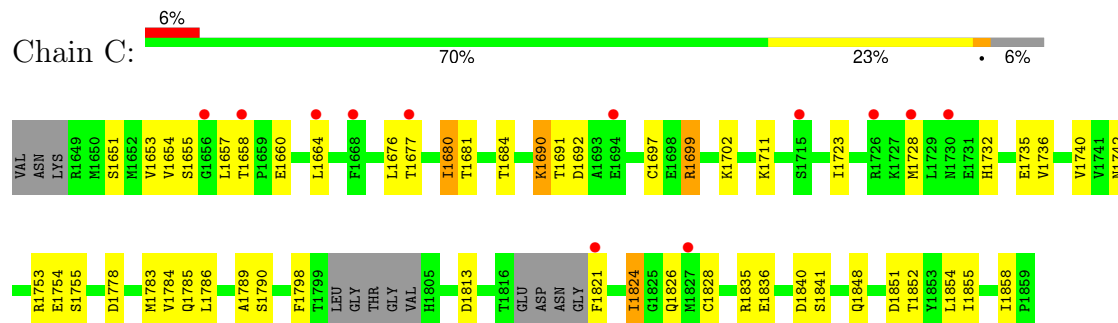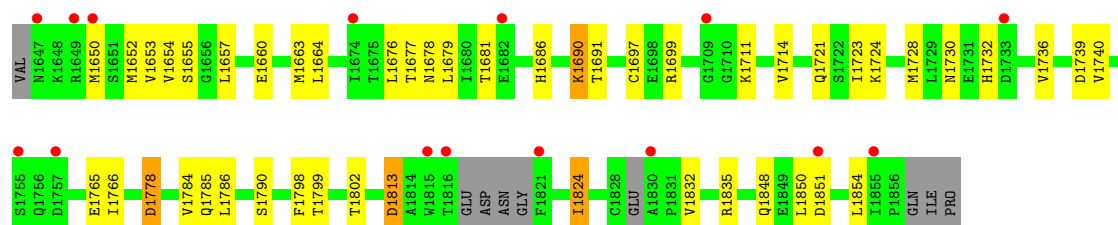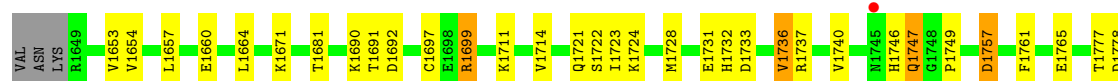• Molecule 1: Breast cancer type 1 susceptibility protein

Chain C:

• Molecule 1: Breast cancer type 1 susceptibility protein

Chain D:

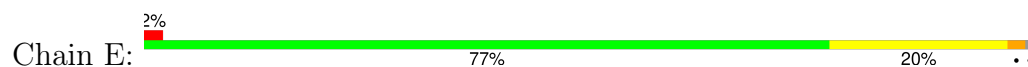• Molecule 1: Breast cancer type 1 susceptibility protein

Chain E:

• Molecule 2: BRCTide-7PS

Chain F:

• Molecule 2: BRCTide-7PS

Chain G:

• Molecule 2: BRCTide-7PS

Chain H:

• Molecule 2: BRCTide-7PS

Chain I:

• Molecule 2: BRCTide-7PS

Chain J:
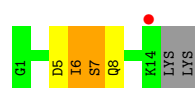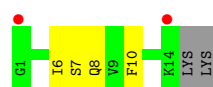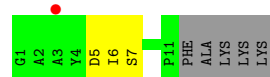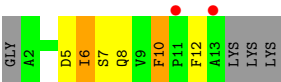
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	97.12Å 138.36Å 198.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-3.30) 99.3 (50.00-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.92 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.258 , 0.301 0.232 , 0.277	Depositor DCC
R_{free} test set	1016 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 87.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	8380	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: SEP

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	0.38	0/1641	0.68	4/2238 (0.2%)
1	B	0.37	0/1642	0.67	3/2238 (0.1%)
1	C	0.39	0/1569	0.67	3/2144 (0.1%)
1	D	0.35	0/1558	0.66	2/2126 (0.1%)
1	E	0.40	0/1661	0.71	5/2266 (0.2%)
2	F	0.52	0/99	0.80	0/133
2	G	0.52	0/92	0.85	1/124 (0.8%)
2	H	0.54	0/99	0.76	0/133
2	I	0.49	0/77	0.79	1/103 (1.0%)
2	J	0.88	0/90	1.65	2/121 (1.7%)
All	All	0.39	0/8528	0.70	21/11626 (0.2%)

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	E	0	1

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	10	PHE	CA-C-N	6.58	135.51	117.10
1	B	1739	ASP	CB-CG-OD2	5.99	123.69	118.30
1	D	1739	ASP	CB-CG-OD2	5.86	123.57	118.30
2	J	5	ASP	CB-CG-OD2	5.84	123.55	118.30
1	A	1818	ASP	CB-CG-OD2	5.76	123.48	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	1817	GLU	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	1601	0	1516	14	0
1	B	1605	0	1520	8	0
1	C	1532	0	1433	11	0
1	D	1523	0	1425	7	0
1	E	1620	0	1536	10	0
2	F	107	0	92	3	0
2	G	101	0	85	3	0
2	H	107	0	92	2	0
2	I	86	0	76	0	0
2	J	98	0	84	2	0
All	All	8380	0	7859	51	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 3.

The worst 5 of 51 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:E:1777:THR:HG21	2:F:3:ALA:HB1	1.47	0.95
1:B:1751:ARG:NH1	1:B:1844:LEU:O	2.20	0.74
1:D:1691:THR:HG22	1:D:1697:CYS:HB3	1.71	0.70
1:A:1691:THR:HG22	1:A:1697:CYS:HB3	1.82	0.61
1:E:1691:THR:HG22	1:E:1697:CYS:HB3	1.84	0.60

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	204/214 (95%)	194 (95%)	9 (4%)	1 (0%)	25	56
1	B	206/214 (96%)	196 (95%)	9 (4%)	1 (0%)	25	56
1	C	196/214 (92%)	187 (95%)	8 (4%)	1 (0%)	25	56
1	D	199/214 (93%)	190 (96%)	8 (4%)	1 (0%)	25	56
1	E	209/214 (98%)	204 (98%)	5 (2%)	0	100	100
2	F	11/16 (69%)	10 (91%)	0	1 (9%)	0	3
2	G	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
2	H	11/16 (69%)	10 (91%)	1 (9%)	0	100	100
2	I	8/16 (50%)	8 (100%)	0	0	100	100
2	J	9/16 (56%)	8 (89%)	1 (11%)	0	100	100
All	All	1064/1150 (92%)	1017 (96%)	42 (4%)	5 (0%)	25	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1851	ASP
2	F	2	ALA
1	D	1802	THR
1	A	1748	GLY
1	B	1726	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	169/191 (88%)	144 (85%)	25 (15%)	2	11
1	B	168/191 (88%)	132 (79%)	36 (21%)	1	4
1	C	159/191 (83%)	124 (78%)	35 (22%)	1	3
1	D	154/191 (81%)	117 (76%)	37 (24%)	0	3
1	E	171/191 (90%)	141 (82%)	30 (18%)	1	7
2	F	8/11 (73%)	7 (88%)	1 (12%)	3	16
2	G	7/11 (64%)	6 (86%)	1 (14%)	2	12
2	H	8/11 (73%)	7 (88%)	1 (12%)	3	16
2	I	7/11 (64%)	6 (86%)	1 (14%)	2	12
2	J	8/11 (73%)	5 (62%)	3 (38%)	0	0
All	All	859/1010 (85%)	689 (80%)	170 (20%)	1	5

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1730	ASN
1	E	1722	SER
1	D	1765	GLU
1	D	1835	ARG
1	E	1737	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1746	HIS
1	E	1747	GLN
2	G	8	GLN
1	E	1785	GLN
1	B	1742	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	#$|Z| > 2$
2	SEP	I	7	2	8,9,10	1.57	1 (12%)	7,12,14	1.48	2 (28%)
2	SEP	F	7	2	8,9,10	1.54	1 (12%)	7,12,14	1.68	1 (14%)
2	SEP	H	7	2	8,9,10	1.61	1 (12%)	7,12,14	2.05	1 (14%)
2	SEP	J	7	2	8,9,10	1.69	1 (12%)	7,12,14	1.64	1 (14%)
2	SEP	G	7	2	8,9,10	1.61	1 (12%)	7,12,14	1.53	1 (14%)

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
2	SEP	I	7	2	-	3/6/8/10	-
2	SEP	F	7	2	-	2/6/8/10	-
2	SEP	H	7	2	-	2/6/8/10	-
2	SEP	J	7	2	-	2/6/8/10	-
2	SEP	G	7	2	-	5/6/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	7	SEP	P-O1P	3.57	1.61	1.50
2	H	7	SEP	P-O1P	3.57	1.61	1.50
2	G	7	SEP	P-O1P	3.53	1.61	1.50
2	I	7	SEP	P-O1P	3.45	1.61	1.50
2	F	7	SEP	P-O1P	3.40	1.61	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7	SEP	OG-CB-CA	5.00	113.01	108.14
2	F	7	SEP	OG-CB-CA	3.76	111.81	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	7	SEP	OG-CB-CA	3.55	111.60	108.14
2	G	7	SEP	OG-CB-CA	3.41	111.47	108.14
2	I	7	SEP	OG-CB-CA	2.87	110.94	108.14

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	7	SEP	N-CA-CB-OG
2	F	7	SEP	C-CA-CB-OG
2	G	7	SEP	N-CA-CB-OG
2	G	7	SEP	C-CA-CB-OG
2	G	7	SEP	CB-OG-P-O1P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	7	SEP	1	0

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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(Å²)	Q<0.9
1	A	208/214 (97%)	0.53	3 (1%)	73	60	69, 69, 69, 69	0
1	B	210/214 (98%)	0.55	7 (3%)	49	36	69, 69, 69, 69	0
1	C	202/214 (94%)	0.80	12 (5%)	29	24	69, 69, 69, 69	0
1	D	205/214 (95%)	0.71	15 (7%)	22	19	69, 69, 69, 69	0
1	E	211/214 (98%)	0.32	4 (1%)	66	51	69, 69, 69, 69	0
2	F	13/16 (81%)	1.86	4 (30%)	1	1	69, 69, 69, 69	0
2	G	13/16 (81%)	1.21	1 (7%)	21	18	69, 69, 69, 69	0
2	H	13/16 (81%)	1.23	2 (15%)	6	6	69, 69, 69, 69	0
2	I	10/16 (62%)	1.32	1 (10%)	14	13	69, 69, 69, 69	0
2	J	11/16 (68%)	1.24	2 (18%)	4	4	69, 69, 69, 69	0
All	All	1096/1150 (95%)	0.62	51 (4%)	37	28	69, 69, 69, 69	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	2	ALA	5.4
1	C	1821	PHE	4.3
1	B	1802	THR	4.3
1	E	1818	ASP	4.0
2	F	1	GLY	3.9

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.

WORLDWIDE
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PROTEIN DATA BANK

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	SEP	H	7	10/11	0.88	0.15	69,69,69,69	0
2	SEP	F	7	10/11	0.89	0.14	69,69,69,69	0
2	SEP	I	7	10/11	0.91	0.11	69,69,69,69	0
2	SEP	J	7	10/11	0.93	0.10	69,69,69,69	0
2	SEP	G	7	10/11	0.95	0.10	69,69,69,69	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.