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 23, 2023 – 03:04 PM EDT

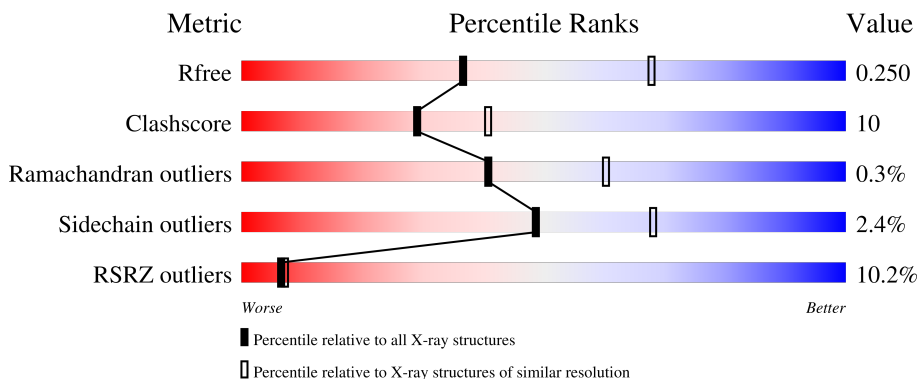|		
PDB ID	:	3F7P
Title	:	Crystal structure of a complex between integrin beta4 and plectin
Authors	:	de Pereda, J.M.
Deposited on	:	2008-11-10
Resolution	:	2.75 Å(reported)

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 2.75 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		0.250
Clashscore		10
Ramachandran outliers		0.3%
Sidechain outliers		2.4%
RSRZ outliers		10.2%

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	296	% 65% 12% • 22%
1	B	296	5% 64% 13% • 22%
2	C	248	13% 59% 21% • 19%
2	D	248	11% 54% 24% 21%
2	E	248	13% 63% 22% 15%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 8564 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 Plectin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total 1897	C 1195	N 346	O 350	S 6	0	0	0
1	B	230	Total 1892	C 1192	N 345	O 349	S 6	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q15149
A	-1	SER	-	expression tag	UNP Q15149
A	0	HIS	-	expression tag	UNP Q15149
B	-2	GLY	-	expression tag	UNP Q15149
B	-1	SER	-	expression tag	UNP Q15149
B	0	HIS	-	expression tag	UNP Q15149

- Molecule 2 is a protein called Integrin beta-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	200	Total 1556	C 982	N 270	O 296	S 8	0	0	0
2	D	196	Total 1529	C 964	N 265	O 292	S 8	0	0	0
2	E	212	Total 1654	C 1041	N 283	O 321	S 9	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1123	GLY	-	expression tag	UNP P16144
C	1124	SER	-	expression tag	UNP P16144
C	1125	HIS	-	expression tag	UNP P16144
D	1123	GLY	-	expression tag	UNP P16144

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1124	SER	-	expression tag	UNP P16144
D	1125	HIS	-	expression tag	UNP P16144
E	1123	GLY	-	expression tag	UNP P16144
E	1124	SER	-	expression tag	UNP P16144
E	1125	HIS	-	expression tag	UNP P16144

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 7	C 4	O 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	Ca 1	0	0

- Molecule 6 is water.

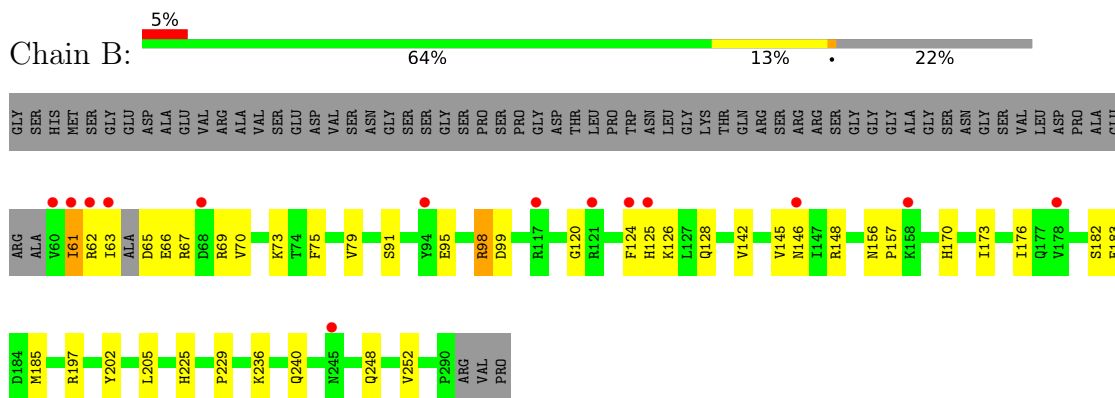| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total 8	O 8	0	0
6	B	3	Total 3	O 3	0	0
6	C	3	Total 3	O 3	0	0
6	D	3	Total 3	O 3	0	0
6	E	3	Total 3	O 3	0	0

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.
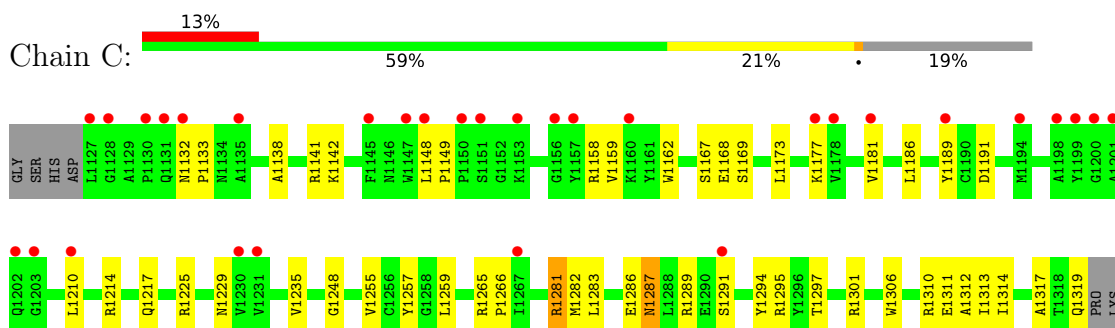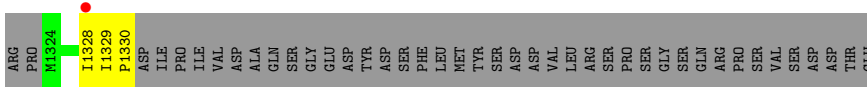
- Molecule 1: Plectin-1
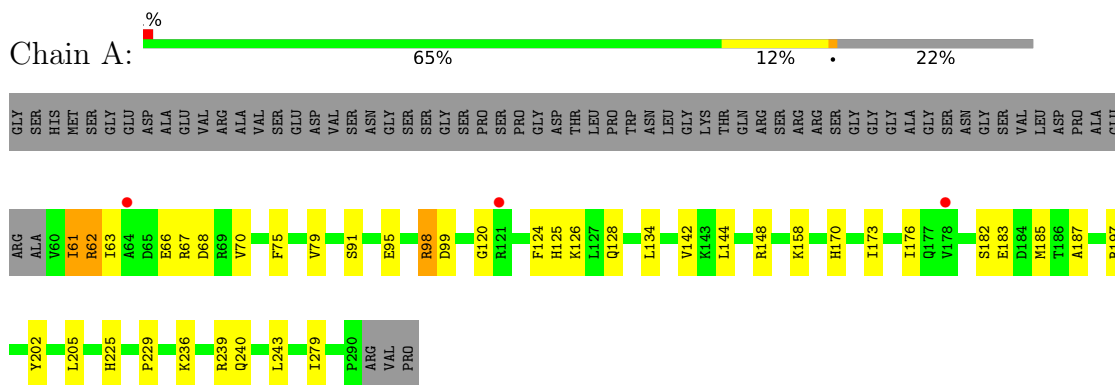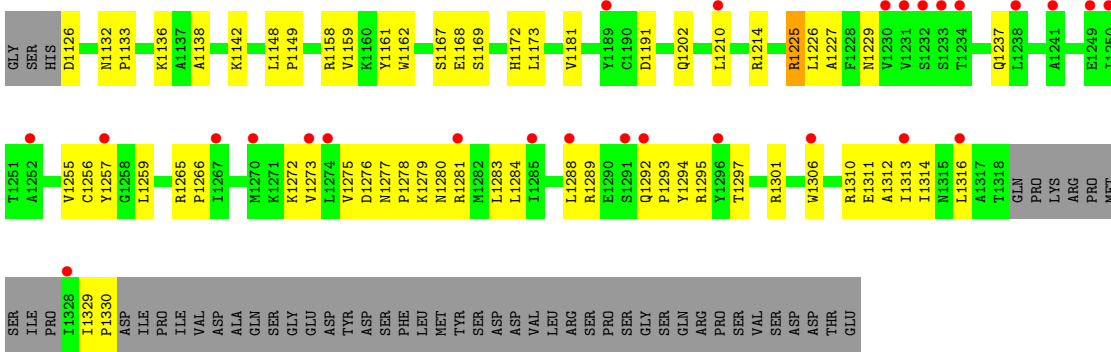
Chain A:

- Molecule 1: Plectin-1

Chain B:

- Molecule 2: Integrin beta-4

Chain C:

• Molecule 2: Integrin beta-4

Chain D:

• Molecule 2: Integrin beta-4

Chain E:
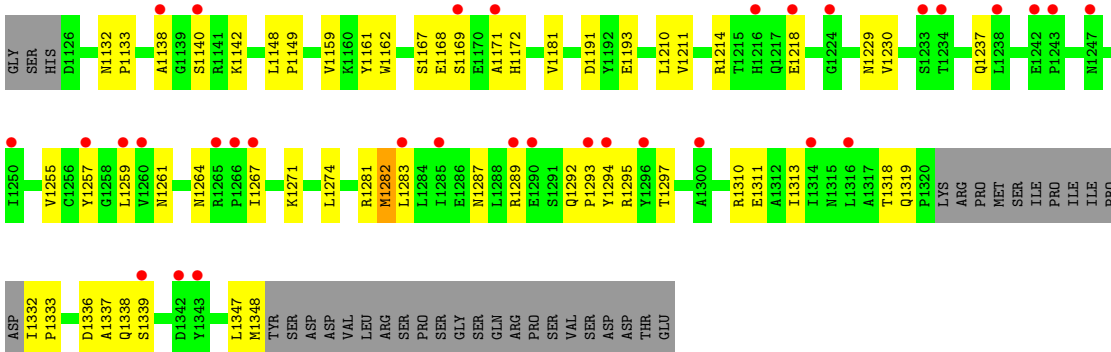
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	107.25Å 107.25Å 203.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.53 – 2.75 84.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (84.53-2.75) 99.8 (84.53-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.204 , 0.257 0.197 , 0.250	Depositor DCC
R_{free} test set	1897 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	63.0	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8564	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: PEG, EDO, CA

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	0.33	0/1931	0.60	3/2608 (0.1%)
1	B	0.31	0/1925	0.59	3/2598 (0.1%)
2	C	0.33	0/1596	0.83	6/2174 (0.3%)
2	D	0.31	0/1568	0.55	2/2135 (0.1%)
2	E	0.32	0/1696	0.70	5/2309 (0.2%)
All	All	0.32	0/8716	0.66	19/11824 (0.2%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1289	ARG	NE-CZ-NH1	-16.30	112.15	120.30
2	C	1289	ARG	NE-CZ-NH2	15.20	127.90	120.30
2	C	1281	ARG	NE-CZ-NH1	-14.06	113.27	120.30
1	B	148	ARG	NE-CZ-NH2	-13.26	113.67	120.30
2	C	1281	ARG	NE-CZ-NH2	12.78	126.69	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1897	0	1915	28	0

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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1892	0	1909	34	0
2	C	1556	0	1520	36	0
2	D	1529	0	1491	50	0
2	E	1654	0	1597	36	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	B	7	0	10	1	0
5	D	1	0	0	0	0
6	A	8	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	D	3	0	0	0	0
6	E	3	0	0	0	0
All	All	8564	0	8454	163	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 163 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:B:61:ILE:HD13	2:D:1273:VAL:HG21	1.54	0.89
2:C:1177:LYS:NZ	2:D:1272:LYS:HE3	1.91	0.86
1:B:61:ILE:HD11	2:D:1283:LEU:HD21	1.57	0.84
1:B:95:GLU:O	1:B:98:ARG:HG3	1.82	0.80
1:A:95:GLU:O	1:A:98:ARG:HG3	1.81	0.79

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	229/296 (77%)	221 (96%)	8 (4%)	0	100	100
1	B	226/296 (76%)	219 (97%)	7 (3%)	0	100	100
2	C	196/248 (79%)	191 (97%)	4 (2%)	1 (0%)	29	47
2	D	192/248 (77%)	187 (97%)	4 (2%)	1 (0%)	29	47
2	E	208/248 (84%)	199 (96%)	8 (4%)	1 (0%)	29	47
All	All	1051/1336 (79%)	1017 (97%)	31 (3%)	3 (0%)	41	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	1168	GLU
2	E	1168	GLU
2	C	1168	GLU

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	212/261 (81%)	204 (96%)	8 (4%)	33	53
1	B	212/261 (81%)	205 (97%)	7 (3%)	38	58
2	C	169/214 (79%)	166 (98%)	3 (2%)	59	75
2	D	166/214 (78%)	164 (99%)	2 (1%)	71	82
2	E	180/214 (84%)	177 (98%)	3 (2%)	60	76
All	All	939/1164 (81%)	916 (98%)	23 (2%)	49	68

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	GLU
2	C	1287	ASN
2	C	1282	MET
2	D	1225	ARG
1	A	128	GLN

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

Mol	Chain	Res	Type
1	B	170	HIS
2	C	1237	GLN
2	D	1229	ASN
1	A	170	HIS
1	A	101	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#|Z| > 2$
4	PEG	B	295	-	6,6,6	0.77	0	5,5,5	0.94	0
3	EDO	B	294	-	3,3,3	0.53	0	2,2,2	0.45	0
3	EDO	A	294	-	3,3,3	0.57	0	2,2,2	0.53	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
4	PEG	B	295	-	-	1/4/4/4	-
3	EDO	B	294	-	-	0/1/1/1	-
3	EDO	A	294	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	295	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	295	PEG	1	0

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 (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(Å²)	Q<0.9
1	A	231/296 (78%)	0.44	3 (1%)	77	84	35, 59, 121, 171	0
1	B	230/296 (77%)	0.65	14 (6%)	21	26	45, 76, 128, 153	0
2	C	200/248 (80%)	0.94	32 (16%)	1	2	43, 88, 148, 171	0
2	D	196/248 (79%)	0.98	27 (13%)	2	3	43, 85, 130, 147	0
2	E	212/248 (85%)	1.02	33 (15%)	2	2	46, 82, 137, 165	0
All	All	1069/1336 (80%)	0.79	109 (10%)	6	7	35, 77, 133, 171	0

The worst 5 of 109 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	1127	LEU	6.4
2	C	1147	TRP	6.4
2	C	1181	VAL	5.6
2	E	1234	THR	5.6
2	E	1289	ARG	5.5

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(Å²)	Q<0.9
3	EDO	A	294	4/4	0.81	0.33	46,57,63,91	0
3	EDO	B	294	4/4	0.87	0.17	60,69,78,80	0
4	PEG	B	295	7/7	0.92	0.15	53,74,87,89	0
5	CA	D	101	1/1	0.98	0.27	43,43,43,43	1

6.5 Other polymers ⓘ

There are no such residues in this entry.