Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 09:36 PM JST

PDB ID	:	7DNF
Title	:	DARPin 63_B7 in complex with V3-IY (MN) crown mimetic
Authors	:	Wu, Y.; Plueckthun, A.
Deposited on	:	2020-12-09
Resolution	:	1.78 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) 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 (1)) were used in the production of this report:

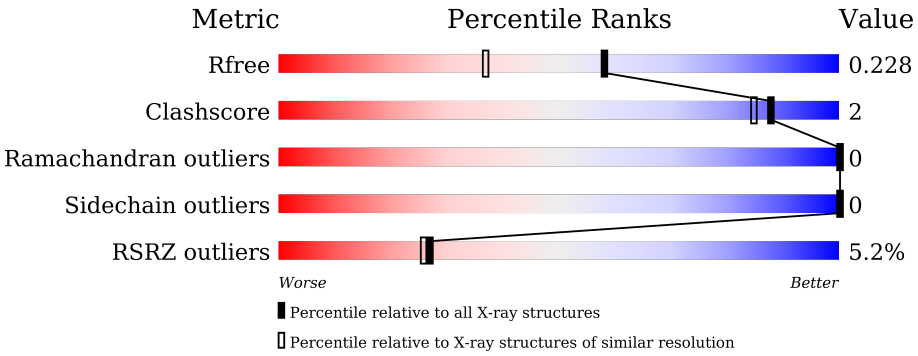
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	169	6% 88% 5% 7%
1	C	169	5% 89% 5% 7%
1	D	169	7% 89% • 9%
1	F	169	2% 89% • 8%
2	B	17	88% 6% 6%
2	E	17	6% 88% 6% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10630 atoms, of which 4926 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.

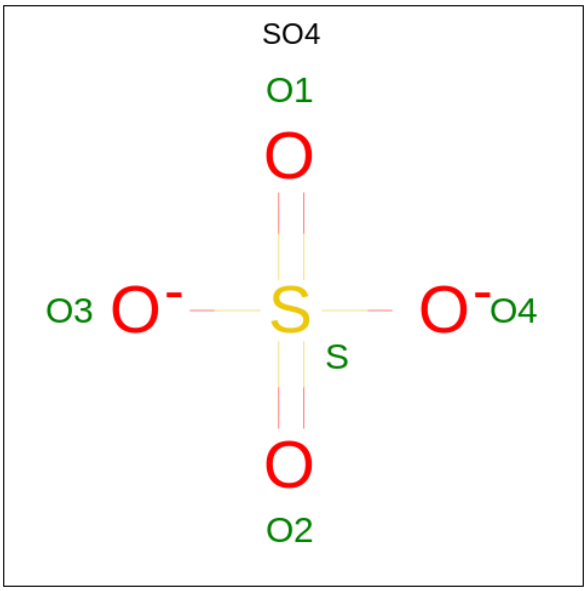
- Molecule 1 is a protein called DARPin 63_B7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	158	Total	C	H	N	O	S	0	0	0
			2362	752	1162	208	238	2			
1	C	158	Total	C	H	N	O	S	0	4	0
			2429	770	1208	209	240	2			
1	D	153	Total	C	H	N	O	S	0	0	0
			2292	730	1131	198	231	2			
1	F	155	Total	C	H	N	O	S	0	0	0
			2331	741	1152	202	234	2			

- Molecule 2 is a protein called V3-IY (MN) crown mimetic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	16	Total	C	H	N	O	0	0	0
			259	84	131	25	19			
2	E	16	Total	C	H	N	O	0	1	0
			278	89	142	28	19			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	146	Total O 146 146	0	0
4	B	13	Total O 13 13	0	0
4	C	153	Total O 153 153	0	0
4	D	139	Total O 139 139	0	0

Continued on next page...

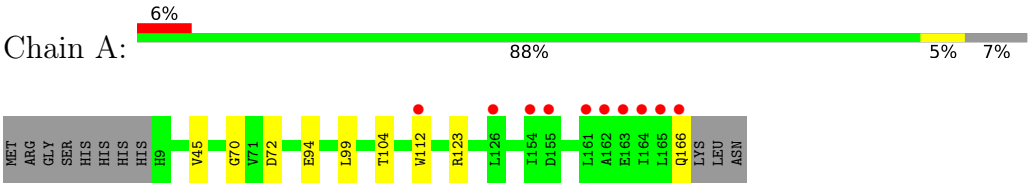
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	14	Total O 14 14	0	0
4	F	174	Total O 174 174	0	0

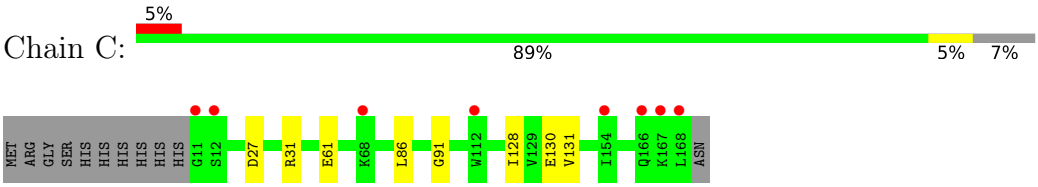
3 Residue-property plots (i)

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.

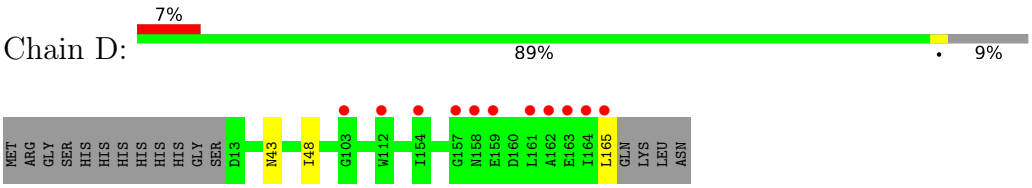
• Molecule 1: DARPin 63_B7



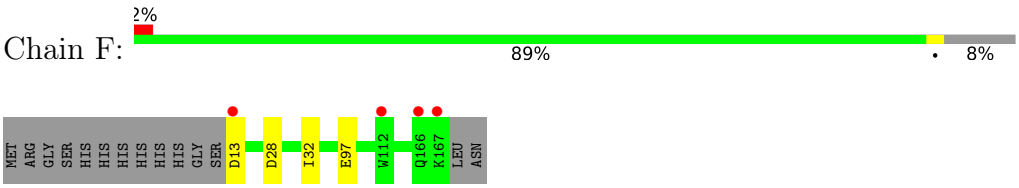
• Molecule 1: DARPin 63_B7



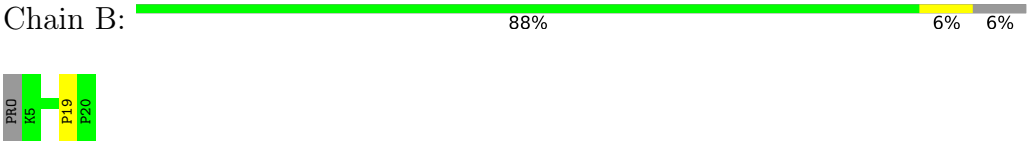
• Molecule 1: DARPin 63_B7



• Molecule 1: DARPin 63_B7

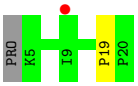


• Molecule 2: V3-IY (MN) crown mimetic peptide



• Molecule 2: V3-IY (MN) crown mimetic peptide

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.35Å 105.98Å 64.02Å 90.00° 93.44° 90.00°	Depositor
Resolution (Å)	48.26 – 1.78 48.26 – 1.78	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.26-1.78) 96.5 (48.26-1.78)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 1.78Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.187 , 0.225 0.188 , 0.228	Depositor DCC
R_{free} test set	1486 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å^2)	26.2	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10630	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: DPR, SO4

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	0.27	0/1221	0.43	0/1660
1	C	0.27	0/1252	0.44	0/1699
1	D	0.26	0/1180	0.43	0/1605
1	F	0.27	0/1198	0.44	0/1628
2	B	0.30	0/124	0.43	0/164
2	E	0.31	0/135	0.48	0/178
All	All	0.27	0/5110	0.44	0/6934

There are no bond length outliers.

There are no bond angle outliers.

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	1200	1162	1161	8	0
1	C	1221	1208	1212	8	0
1	D	1161	1131	1131	2	0
1	F	1179	1152	1152	3	0
2	B	128	131	131	0	0
2	E	136	142	144	0	0
3	A	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	E	10	0	0	0	0
3	F	15	0	0	0	0
4	A	146	0	0	6	0
4	B	13	0	0	0	0
4	C	153	0	0	4	0
4	D	139	0	0	1	1
4	E	14	0	0	0	0
4	F	174	0	0	2	1
All	All	5704	4926	4931	20	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 2.

All (20) 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:C:31[B]:ARG:NH2	4:C:301:HOH:O	2.08	0.85
1:A:94:GLU:OE2	4:A:301:HOH:O	1.96	0.81
1:C:61:GLU:OE2	4:C:301:HOH:O	1.98	0.79
1:F:13:ASP:N	4:F:302:HOH:O	2.19	0.76
1:A:112:TRP:NE1	4:A:304:HOH:O	2.20	0.73
1:D:165:LEU:O	4:D:201:HOH:O	2.11	0.68
1:A:72:ASP:OD1	4:A:302:HOH:O	2.15	0.64
1:A:70:GLY:O	4:A:303:HOH:O	2.17	0.58
1:A:123:ARG:NH2	4:A:309:HOH:O	2.39	0.55
1:C:130[B]:GLU:OE2	4:C:302:HOH:O	2.18	0.54
1:F:97:GLU:OE1	4:F:301:HOH:O	2.18	0.54
1:C:31[A]:ARG:NH1	4:C:306:HOH:O	2.42	0.48
1:A:166:GLN:O	4:A:305:HOH:O	2.20	0.48
1:C:91:GLY:HA2	1:C:128:ILE:CD1	2.45	0.46
1:C:128:ILE:HA	1:C:131:VAL:HG12	1.99	0.45
1:C:27:ASP:OD1	1:C:27:ASP:N	2.52	0.43
1:D:43:ASN:HA	1:D:48:ILE:O	2.19	0.42
1:F:28:ASP:O	1:F:32:ILE:HG12	2.19	0.42
1:A:45:VAL:HG21	1:C:86:LEU:HD22	2.02	0.41
1:A:99:LEU:HB3	1:A:104:THR:HG21	2.02	0.41

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)
4:D:312:HOH:O	4:F:426:HOH:O[1_655]	2.05	0.15

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	156/169 (92%)	151 (97%)	5 (3%)	0	100	100
1	C	160/169 (95%)	159 (99%)	1 (1%)	0	100	100
1	D	151/169 (89%)	149 (99%)	2 (1%)	0	100	100
1	F	153/169 (90%)	152 (99%)	1 (1%)	0	100	100
2	B	13/17 (76%)	12 (92%)	1 (8%)	0	100	100
2	E	14/17 (82%)	13 (93%)	1 (7%)	0	100	100
All	All	647/710 (91%)	636 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	125/135 (93%)	125 (100%)	0	100	100
1	C	129/135 (96%)	129 (100%)	0	100	100
1	D	121/135 (90%)	121 (100%)	0	100	100
1	F	123/135 (91%)	123 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	12/13 (92%)	12 (100%)	0	100	100
2	E	13/13 (100%)	13 (100%)	0	100	100
All	All	523/566 (92%)	523 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	DPR	E	19	2	5,7,8	0.50	0	7,8,10	1.36	2 (28%)
2	DPR	B	19	2	5,7,8	0.52	0	7,8,10	1.40	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	DPR	E	19	2	-	0/0/9/11	0/1/1/1
2	DPR	B	19	2	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	19	DPR	O-C-CA	-2.34	118.63	124.78
2	E	19	DPR	O-C-CA	-2.20	119.02	124.78
2	E	19	DPR	CB-CA-C	-2.03	109.90	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands 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	$\#\|Z\| > 2$
3	SO4	F	202	-	4,4,4	0.16	0	6,6,6	0.17	0
3	SO4	A	201	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	B	101	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	C	201	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	F	201	-	4,4,4	0.15	0	6,6,6	0.12	0
3	SO4	E	102	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	F	203	-	4,4,4	0.14	0	6,6,6	0.12	0
3	SO4	E	101	-	4,4,4	0.13	0	6,6,6	0.08	0

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

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, 95^{th} 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	158/169 (93%)	0.46	10 (6%) 20 19	20, 29, 58, 95	0
1	C	158/169 (93%)	0.26	8 (5%) 28 26	20, 28, 45, 85	0
1	D	153/169 (90%)	0.50	11 (7%) 15 15	19, 30, 53, 78	0
1	F	155/169 (91%)	0.20	4 (2%) 56 55	21, 29, 47, 81	0
2	B	15/17 (88%)	0.27	0 100 100	22, 27, 43, 58	0
2	E	15/17 (88%)	0.62	1 (6%) 17 17	22, 27, 49, 50	0
All	All	654/710 (92%)	0.36	34 (5%) 27 26	19, 29, 52, 95	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	168	LEU	5.1
1	A	165	LEU	4.9
1	C	12	SER	4.7
1	D	154	ILE	4.5
1	A	164	ILE	4.0
1	F	167	LYS	3.9
1	D	159	GLU	3.8
1	C	11	GLY	3.8
1	A	166	GLN	3.8
1	A	112	TRP	3.7
1	F	166	GLN	3.5
1	D	103	GLY	3.4
1	D	165	LEU	3.3
1	D	158	ASN	3.3
2	E	9	ILE	2.9
1	D	112	TRP	2.7
1	D	163	GLU	2.6
1	D	161	LEU	2.5
1	F	13	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	155	ASP	2.4
1	A	162	ALA	2.3
1	A	126	LEU	2.2
1	A	154	ILE	2.2
1	D	162	ALA	2.1
1	F	112	TRP	2.1
1	D	157	GLY	2.1
1	A	161	LEU	2.1
1	D	164	ILE	2.1
1	C	166	GLN	2.1
1	C	112	TRP	2.1
1	C	167[A]	LYS	2.0
1	A	163	GLU	2.0
1	C	154	ILE	2.0
1	C	68	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
2	DPR	B	19	7/8	0.95	0.08	34,43,52,52	0
2	DPR	E	19	7/8	0.97	0.06	34,42,51,51	0

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, 95^{th} 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
3	SO4	C	201	5/5	0.80	0.16	70,71,76,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	E	101	5/5	0.91	0.10	78,81,83,86	0
3	SO4	F	201	5/5	0.91	0.13	52,57,66,74	0
3	SO4	E	102	5/5	0.94	0.19	50,53,60,69	0
3	SO4	B	101	5/5	0.94	0.14	69,71,75,85	0
3	SO4	F	203	5/5	0.94	0.11	43,44,47,53	0
3	SO4	A	201	5/5	0.95	0.14	54,57,62,71	0
3	SO4	F	202	5/5	0.96	0.11	35,40,43,49	0

6.5 Other polymers (i)

There are no such residues in this entry.