



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:57 PM UTC

PDB ID : 7DNF / pdb_00007dnf
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

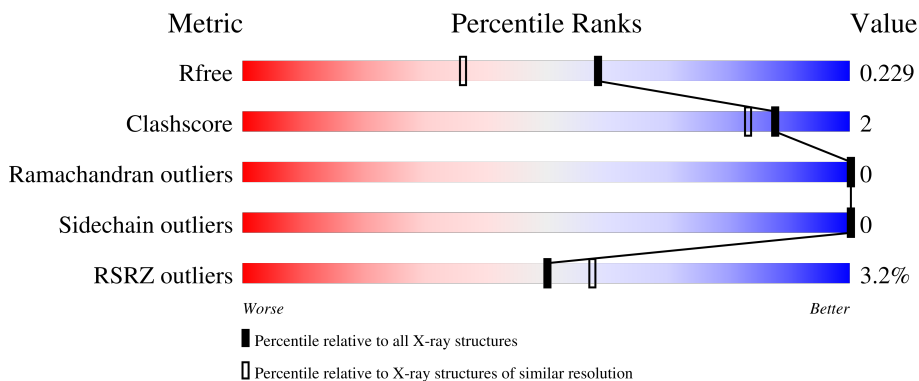
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



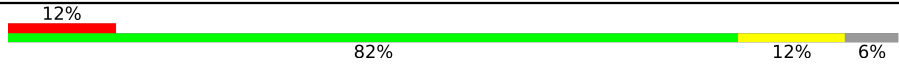
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	169	 4% 88% 5% 7%
1	C	169	 2% 89% 5% 7%
1	D	169	 4% 89% 5% 9%
1	F	169	 % 89% 5% 8%
2	B	17	 82% 12% 6%

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Mol	Chain	Length	Quality of chain
2	E	17	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '12%', a large green segment labeled '82%', a yellow segment labeled '12%', and a small grey segment on the far right labeled '6%'.</p>

2 Entry composition

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

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

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is water.

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

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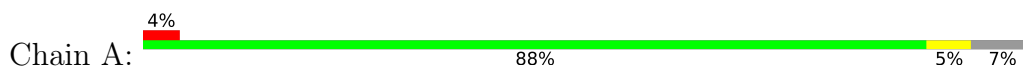
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	14	Total O 14 14	0	0
4	F	174	Total O 174 174	0	0

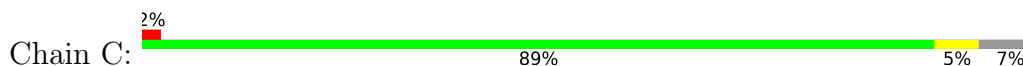
3 Residue-property plots [i](#)

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.

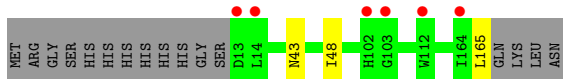
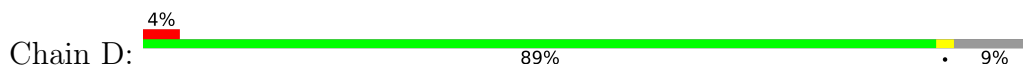
- Molecule 1: DARPin 63_B7



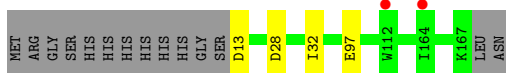
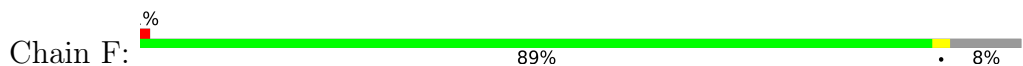
- Molecule 1: DARPin 63_B7



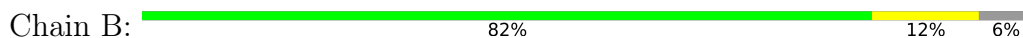
- Molecule 1: DARPin 63_B7



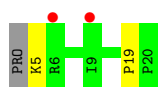
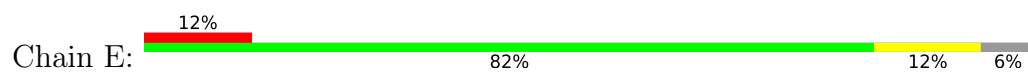
- Molecule 1: DARPin 63_B7



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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.78Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.187 , 0.225 0.190 , 0.229	Depositor DCC
R_{free} test set	1486 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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: 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	0.17	0/1221	0.33	0/1660
1	C	0.17	0/1252	0.31	0/1699
1	D	0.16	0/1180	0.31	0/1605
1	F	0.16	0/1198	0.31	0/1628
2	B	0.18	0/124	0.77	2/164 (1.2%)
2	E	0.20	0/135	1.00	1/178 (0.6%)
All	All	0.17	0/5110	0.37	3/6934 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	LYS	O-C-N	-11.98	103.83	123.00
2	B	5	LYS	CA-C-N	-6.31	110.35	121.70
2	B	5	LYS	C-N-CA	-6.31	110.35	121.70

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	1200	1162	1161	8	0
1	C	1221	1208	1212	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	122	HIS

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	B	19	2	6,7,8	0.59	0	7,8,10	1.42	1 (14%)
2	DPR	E	19	2	6,7,8	0.55	0	7,8,10	1.38	2 (28%)

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	B	19	2	-	0/0/9/11	0/1/1/1
2	DPR	E	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(°)	Ideal(°)
2	B	19	DPR	O-C-CA	-2.39	118.63	124.77
2	E	19	DPR	O-C-CA	-2.24	119.02	124.77
2	E	19	DPR	CB-CA-C	-2.01	109.90	112.66

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 oligosaccharides 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	E	101	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	F	203	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	B	101	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	E	102	-	4,4,4	0.26	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	201	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	C	201	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	F	201	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	F	202	-	4,4,4	0.27	0	6,6,6	0.11	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, 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	158/169 (93%)	0.30	7 (4%) 39 44	22, 32, 64, 104	0
1	C	158/169 (93%)	0.21	4 (2%) 58 66	19, 31, 49, 94	4 (2%)
1	D	153/169 (90%)	0.33	6 (3%) 43 49	21, 33, 56, 83	0
1	F	155/169 (91%)	0.21	2 (1%) 75 81	24, 32, 52, 92	0
2	B	15/17 (88%)	0.24	0 100 100	24, 32, 50, 66	0
2	E	15/17 (88%)	0.56	2 (13%) 7 7	24, 30, 52, 55	1 (6%)
All	All	654/710 (92%)	0.27	21 (3%) 50 57	19, 32, 56, 104	5 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	GLY	3.6
1	A	112	TRP	3.6
1	D	112	TRP	3.4
1	C	12	SER	3.1
1	D	102	HIS	3.0
1	C	112	TRP	2.9
2	E	6[A]	ARG	2.8
1	D	14	LEU	2.7
1	C	168	LEU	2.7
1	F	164	ILE	2.6
1	A	165	LEU	2.5
1	A	9	HIS	2.5
1	A	10	HIS	2.5
1	F	112	TRP	2.4
1	A	11	GLY	2.3
2	E	9	ILE	2.3
1	D	103	GLY	2.2
1	D	13	ASP	2.1
1	D	164	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	166	GLN	2.0
1	A	131	VAL	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, 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(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	0.95	0.06	34,42,51,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
3	SO4	C	201	5/5	0.74	0.13	70,71,76,82	0
3	SO4	E	101	5/5	0.77	0.12	78,81,83,86	0
3	SO4	B	101	5/5	0.83	0.11	69,71,75,85	0
3	SO4	E	102	5/5	0.84	0.12	50,53,60,69	0
3	SO4	F	201	5/5	0.84	0.12	52,57,66,74	0
3	SO4	A	201	5/5	0.87	0.10	54,57,62,71	0
3	SO4	F	203	5/5	0.88	0.10	43,44,47,53	0
3	SO4	F	202	5/5	0.93	0.09	35,40,43,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.