



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:18 PM UTC

PDB ID : 4Q9K / pdb_00004q9k
Title : P-glycoprotein cocrystallised with QZ-Leu
Authors : McGrath, A.P.; Szewczyk, P.; Chang, G.
Deposited on : 2014-05-01
Resolution : 3.80 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)
Xtriage (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

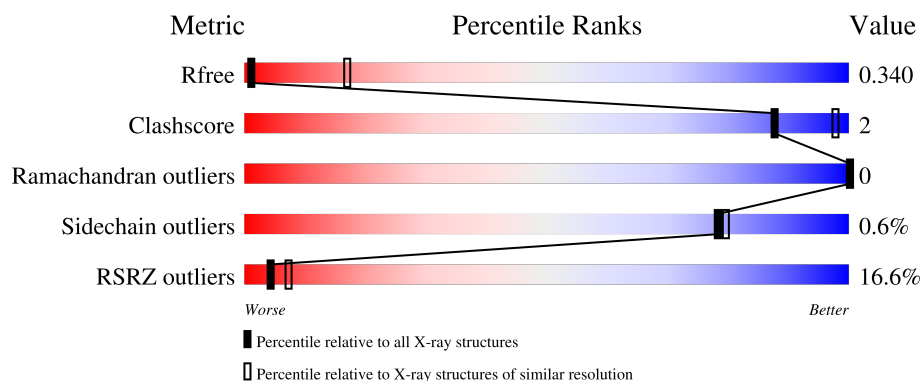
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	1284	15% 86% 6% 8%
2	B	6	33% 50% 50%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9246 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 Multidrug resistance protein 1A.

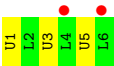
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1187	Total	C	N	O	S	0	0	0
			9207	5919	1562	1688	38			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	conflict	UNP P21447
A	87	GLN	ASN	conflict	UNP P21447
A	90	GLN	ASN	conflict	UNP P21447
A	1277	LEU	-	expression tag	UNP P21447
A	1278	GLU	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
A	1283	HIS	-	expression tag	UNP P21447
A	1284	HIS	-	expression tag	UNP P21447

- Molecule 2 is a protein called (30F)L(30F)L(30F)L Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	Se	0	0	0
			39	27	6	3	3			



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.24Å 138.60Å 195.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.55 – 3.80 49.55 – 3.80	Depositor EDS
% Data completeness (in resolution range)	91.6 (49.55-3.80) 91.1 (49.55-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.292 , 0.321 0.307 , 0.340	Depositor DCC
R_{free} test set	1162 reflections (3.60%)	wwPDB-VP
Wilson B-factor (Å ²)	168.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 115.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	9246	wwPDB-VP
Average B, all atoms (Å ²)	184.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: 30F

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	0.34	0/9376	0.71	1/12671 (0.0%)
2	B	0.66	0/18	0.74	0/21
All	All	0.34	0/9394	0.71	1/12692 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1111	ILE	N-CA-C	5.41	116.38	109.30

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	9207	0	9398	38	0
2	B	39	0	33	0	0
All	All	9246	0	9431	38	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 2.

All (38) 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:A:160:ASP:OD2	1:A:901:ARG:NH2	2.28	0.66
1:A:266:GLN:NE2	1:A:793:LEU:O	2.32	0.62
1:A:1050:GLN:NE2	1:A:1244:ASN:O	2.33	0.61
1:A:1207:GLU:OE1	1:A:1229:ARG:NH2	2.36	0.59
1:A:604:GLU:OE1	1:A:617:ILE:N	2.38	0.57
1:A:922:ILE:HB	1:A:923:PRO:HD3	1.88	0.56
1:A:1173:SER:OG	1:A:1176:GLN:OE1	2.24	0.55
1:A:734:VAL:O	1:A:738:GLY:N	2.40	0.55
1:A:387:ASN:O	1:A:450:ASP:N	2.40	0.54
1:A:1249:GLU:OE1	1:A:1262:ILE:N	2.41	0.53
1:A:1114:GLN:O	1:A:1178:GLN:NE2	2.43	0.52
1:A:477:ALA:O	1:A:478:THR:HG23	2.10	0.51
1:A:93:GLU:OE1	1:A:93:GLU:N	2.44	0.50
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.45	0.50
1:A:801:ASP:OD2	1:A:1083:TYR:OH	2.28	0.49
1:A:694:TRP:O	1:A:697:LEU:N	2.46	0.49
1:A:1036:VAL:O	1:A:1051:GLY:N	2.46	0.49
1:A:938:PHE:O	1:A:941:THR:OG1	2.29	0.48
1:A:694:TRP:CD1	1:A:694:TRP:C	2.94	0.46
1:A:729:SER:O	1:A:733:GLY:N	2.48	0.45
1:A:1165:VAL:HG12	1:A:1166:GLY:N	2.32	0.45
1:A:219:PRO:O	1:A:222:GLY:N	2.49	0.45
1:A:745:ARG:O	1:A:749:ASN:ND2	2.50	0.45
1:A:1122:SER:OG	1:A:1161:TYR:O	2.34	0.45
1:A:963:GLN:HG2	1:A:964:LEU:H	1.83	0.44
1:A:495:GLU:OE1	1:A:495:GLU:N	2.51	0.44
1:A:952:CYS:HB3	1:A:974:PHE:CZ	2.53	0.44
1:A:231:ILE:O	1:A:234:SER:OG	2.36	0.43
1:A:762:SER:HA	1:A:765:THR:HG22	2.00	0.43
1:A:544:ASN:O	1:A:544:ASN:ND2	2.53	0.42
1:A:704:TRP:N	1:A:705:PRO:HD2	2.34	0.42
1:A:851:TRP:C	1:A:853:LEU:H	2.28	0.41
1:A:721:GLN:HB3	1:A:722:PRO:HD3	2.01	0.41
1:A:906:LEU:O	1:A:907:THR:OG1	2.30	0.41
1:A:481:ALA:O	1:A:485:ARG:N	2.54	0.41
1:A:397:TYR:O	1:A:399:SER:N	2.53	0.41
1:A:1132:ASN:C	1:A:1134:ARG:H	2.28	0.41
1:A:893:ALA:HB2	1:A:916:TYR:HE1	1.85	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	1183/1284 (92%)	1127 (95%)	56 (5%)	0	100	100
2	B	2/6 (33%)	2 (100%)	0	0	100	100
All	All	1185/1290 (92%)	1129 (95%)	56 (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	978/1065 (92%)	972 (99%)	6 (1%)	78	79
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	981/1068 (92%)	975 (99%)	6 (1%)	78	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	245	LYS
1	A	753	LEU
1	A	909	GLU
1	A	1090	VAL
1	A	1195	LEU
1	A	1202	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	531	GLN
1	A	544	ASN
1	A	749	ASN
1	A	805	ASN
1	A	932	HIS
1	A	1003	HIS
1	A	1114	GLN
1	A	1149	ASN
1	A	1250	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	30F	B	5	2	2,5,6	3.41	1 (50%)	1,5,7	0.94	0
2	30F	B	3	2	2,5,6	3.21	1 (50%)	1,5,7	0.92	0
2	30F	B	1	2	2,5,6	3.30	1 (50%)	1,5,7	0.47	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
2	30F	B	5	2	-	0/0/4/6	-
2	30F	B	3	2	-	0/0/4/6	-
2	30F	B	1	2	-	0/0/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	30F	C-CA	-4.81	1.37	1.45
2	B	1	30F	C-CA	-4.66	1.37	1.45
2	B	3	30F	C-CA	-4.53	1.37	1.45

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.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	1187/1284 (92%)	0.93	195 (16%) 4 7	95, 172, 293, 445	0
2	B	3/6 (50%)	4.66	2 (66%) 0 0	193, 193, 193, 193	0
All	All	1190/1290 (92%)	0.94	197 (16%) 4 7	95, 172, 293, 445	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	704	TRP	19.0
1	A	708	VAL	14.0
1	A	700	ASN	11.6
1	A	343	GLN	11.5
1	A	705	PRO	10.6
1	A	306	TYR	10.3
1	A	701	SER	10.3
1	A	302	ILE	9.9
1	A	339	PHE	9.5
1	A	1275	ARG	9.4
1	A	221	LEU	9.2
1	A	574	GLU	9.0
1	A	575	GLY	8.8
1	A	272	ARG	8.6
1	A	41	TYR	8.6
1	A	268	LYS	8.5
1	A	299	PHE	8.4
1	A	1278	GLU	8.1
1	A	265	GLY	8.1
1	A	1059	GLY	8.0
1	A	887	GLU	8.0
1	A	365	ILE	7.8
1	A	142	LYS	7.8
1	A	269	GLU	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	707	PHE	7.5
1	A	883	LYS	7.5
1	A	298	ALA	7.3
1	A	146	LYS	7.2
1	A	224	SER	6.9
1	A	304	ALA	6.8
2	B	6	LEU	6.6
1	A	698	LYS	6.5
1	A	254	LEU	6.4
1	A	886	LEU	6.4
1	A	42	ALA	6.3
1	A	702	THR	6.2
1	A	220	VAL	6.2
1	A	253	VAL	6.0
2	B	4	LEU	5.9
1	A	366	ASP	5.9
1	A	266	GLN	5.7
1	A	260	VAL	5.7
1	A	342	GLY	5.6
1	A	264	GLY	5.5
1	A	1120	ASP	5.4
1	A	368	LYS	5.3
1	A	145	GLN	5.3
1	A	252	GLU	5.2
1	A	1276	SER	5.2
1	A	1117	ILE	5.2
1	A	982	MET	5.2
1	A	1071	GLY	5.2
1	A	367	ASN	5.1
1	A	261	ILE	5.1
1	A	424	ASN	5.1
1	A	798	SER	5.0
1	A	882	ASP	4.9
1	A	217	ILE	4.8
1	A	257	ILE	4.8
1	A	332	PHE	4.7
1	A	141	HIS	4.7
1	A	364	ILE	4.6
1	A	576	ARG	4.6
1	A	979	PHE	4.6
1	A	1060	GLN	4.5
1	A	303	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	709	VAL	4.4
1	A	697	LEU	4.4
1	A	149	HIS	4.3
1	A	703	GLU	4.3
1	A	36	LEU	4.3
1	A	90	GLN	4.2
1	A	1119	PHE	4.2
1	A	544	ASN	4.1
1	A	433	VAL	4.1
1	A	1097	ILE	3.9
1	A	258	ARG	3.9
1	A	197	PHE	3.9
1	A	1125	GLU	3.8
1	A	793	LEU	3.7
1	A	1127	ILE	3.7
1	A	262	ALA	3.7
1	A	480	ILE	3.7
1	A	1258	ALA	3.6
1	A	296	GLY	3.6
1	A	800	PHE	3.6
1	A	95	ASP	3.6
1	A	88	SER	3.6
1	A	699	LEU	3.5
1	A	1268	SER	3.5
1	A	1058	LYS	3.5
1	A	468	VAL	3.5
1	A	425	SER	3.5
1	A	722	PRO	3.4
1	A	1183	ALA	3.4
1	A	335	LEU	3.4
1	A	259	THR	3.4
1	A	68	MET	3.4
1	A	301	LEU	3.4
1	A	959	LEU	3.4
1	A	1250	HIS	3.4
1	A	389	GLU	3.3
1	A	694	TRP	3.3
1	A	305	SER	3.3
1	A	714	ALA	3.2
1	A	143	ILE	3.2
1	A	509	ILE	3.2
1	A	1129	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	71	PHE	3.2
1	A	913	GLU	3.2
1	A	200	PHE	3.1
1	A	1103	GLN	3.1
1	A	203	GLY	3.1
1	A	1233	ILE	3.1
1	A	1111	ILE	3.0
1	A	1121	CYS	3.0
1	A	572	ALA	3.0
1	A	797	VAL	2.9
1	A	1187	VAL	2.9
1	A	884	LYS	2.9
1	A	1041	PRO	2.9
1	A	852	GLN	2.9
1	A	551	ASP	2.8
1	A	211	THR	2.8
1	A	267	LYS	2.8
1	A	891	LYS	2.8
1	A	1222	THR	2.8
1	A	776	ALA	2.8
1	A	398	PRO	2.8
1	A	1141	ILE	2.7
1	A	263	PHE	2.7
1	A	175	VAL	2.7
1	A	255	ALA	2.7
1	A	516	PHE	2.7
1	A	1154	ILE	2.6
1	A	300	LEU	2.6
1	A	728	PHE	2.6
1	A	201	ILE	2.6
1	A	176	SER	2.6
1	A	428	GLY	2.6
1	A	1220	GLY	2.6
1	A	40	ARG	2.6
1	A	1057	LYS	2.5
1	A	1277	LEU	2.5
1	A	188	MET	2.5
1	A	963	GLN	2.5
1	A	1148	ALA	2.5
1	A	577	THR	2.5
1	A	899	ASN	2.5
1	A	531	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	476	PHE	2.5
1	A	308	LEU	2.5
1	A	912	PHE	2.4
1	A	1219	GLU	2.4
1	A	331	PHE	2.4
1	A	430	SER	2.4
1	A	113	TYR	2.4
1	A	1272	GLY	2.4
1	A	249	VAL	2.3
1	A	580	VAL	2.3
1	A	1055	GLU	2.3
1	A	711	ILE	2.3
1	A	549	LEU	2.3
1	A	1138	TYR	2.3
1	A	199	GLY	2.3
1	A	960	VAL	2.3
1	A	792	MET	2.3
1	A	390	PHE	2.3
1	A	171	LEU	2.3
1	A	35	VAL	2.3
1	A	76	ASP	2.3
1	A	34	SER	2.2
1	A	228	TRP	2.2
1	A	495	GLU	2.2
1	A	1257	LEU	2.2
1	A	976	ALA	2.2
1	A	493	MET	2.2
1	A	1259	GLN	2.2
1	A	336	ILE	2.2
1	A	491	VAL	2.1
1	A	726	VAL	2.1
1	A	869	VAL	2.1
1	A	432	THR	2.1
1	A	579	ILE	2.1
1	A	706	TYR	2.1
1	A	540	ALA	2.1
1	A	1264	PHE	2.1
1	A	187	GLY	2.1
1	A	1143	ARG	2.1
1	A	986	GLN	2.1
1	A	295	MET	2.1
1	A	282	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	196	PHE	2.1
1	A	1186	LEU	2.1
1	A	427	CYS	2.0
1	A	541	LEU	2.0
1	A	399	SER	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	30F	B	5	6/7	0.68	0.15	193,193,193,193	0
2	30F	B	1	6/7	0.83	0.14	193,193,193,193	0
2	30F	B	3	6/7	0.88	0.14	193,193,193,193	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.