



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:01 AM UTC

PDB ID : 5JKQ / pdb_00005jkq
Title : Crystal structure of Plasmodium falciparum Pf3D7_0606800 (PfVFT1)
Authors : Parker, M.L.; Boulanger, M.J.
Deposited on : 2016-04-26
Resolution : 2.35 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

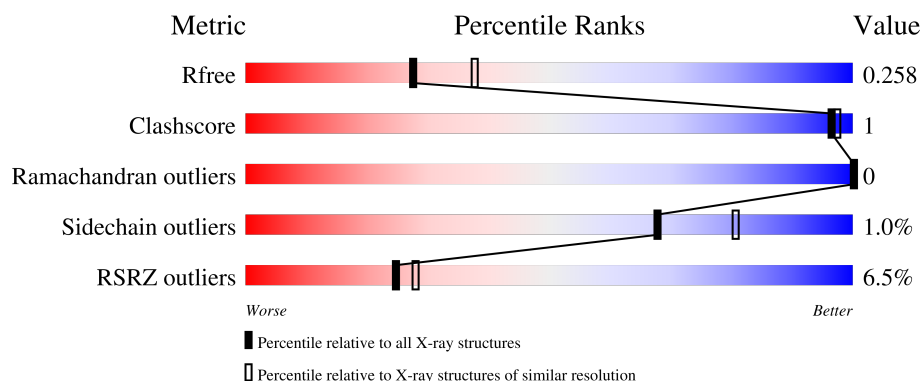
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	284	2% 96% ..
1	B	284	12% 94% 6% .
1	C	284	2% 94% ..
1	D	284	8% 89% . 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9125 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 PfVFT1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	Se	0	0	0
			2260	1452	368	435	2	3			
1	B	282	Total	C	N	O	S	Se	0	0	0
			2265	1455	368	436	2	4			
1	D	263	Total	C	N	O	S	Se	0	0	0
			2126	1375	342	404	2	3			
1	C	273	Total	C	N	O	S	Se	0	0	0
			2201	1418	356	422	2	3			

There are 40 discrepancies between the modelled and reference sequences:

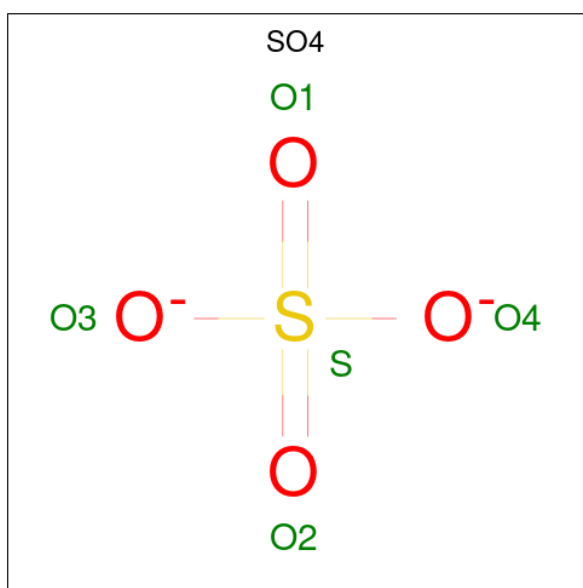
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP C6KSR6
A	20	SER	-	expression tag	UNP C6KSR6
A	21	MSE	-	expression tag	UNP C6KSR6
A	22	GLY	-	expression tag	UNP C6KSR6
A	31	ALA	SER	engineered mutation	UNP C6KSR6
A	75	ALA	SER	engineered mutation	UNP C6KSR6
A	146	ALA	THR	engineered mutation	UNP C6KSR6
A	300	ALA	-	expression tag	UNP C6KSR6
A	301	ALA	-	expression tag	UNP C6KSR6
A	302	ALA	-	expression tag	UNP C6KSR6
B	19	GLY	-	expression tag	UNP C6KSR6
B	20	SER	-	expression tag	UNP C6KSR6
B	21	MSE	-	expression tag	UNP C6KSR6
B	22	GLY	-	expression tag	UNP C6KSR6
B	31	ALA	SER	engineered mutation	UNP C6KSR6
B	75	ALA	SER	engineered mutation	UNP C6KSR6
B	146	ALA	THR	engineered mutation	UNP C6KSR6
B	300	ALA	-	expression tag	UNP C6KSR6
B	301	ALA	-	expression tag	UNP C6KSR6
B	302	ALA	-	expression tag	UNP C6KSR6
D	19	GLY	-	expression tag	UNP C6KSR6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	20	SER	-	expression tag	UNP C6KSR6
D	21	MSE	-	expression tag	UNP C6KSR6
D	22	GLY	-	expression tag	UNP C6KSR6
D	31	ALA	SER	engineered mutation	UNP C6KSR6
D	75	ALA	SER	engineered mutation	UNP C6KSR6
D	146	ALA	THR	engineered mutation	UNP C6KSR6
D	300	ALA	-	expression tag	UNP C6KSR6
D	301	ALA	-	expression tag	UNP C6KSR6
D	302	ALA	-	expression tag	UNP C6KSR6
C	19	GLY	-	expression tag	UNP C6KSR6
C	20	SER	-	expression tag	UNP C6KSR6
C	21	MSE	-	expression tag	UNP C6KSR6
C	22	GLY	-	expression tag	UNP C6KSR6
C	31	ALA	SER	engineered mutation	UNP C6KSR6
C	75	ALA	SER	engineered mutation	UNP C6KSR6
C	146	ALA	THR	engineered mutation	UNP C6KSR6
C	300	ALA	-	expression tag	UNP C6KSR6
C	301	ALA	-	expression tag	UNP C6KSR6
C	302	ALA	-	expression tag	UNP C6KSR6

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

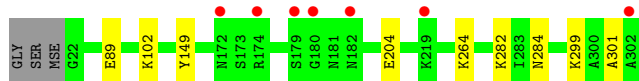
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	64	Total	O	0	0
			64	64		
3	B	48	Total	O	0	0
			48	48		
3	D	54	Total	O	0	0
			54	54		
3	C	77	Total	O	0	0
			77	77		

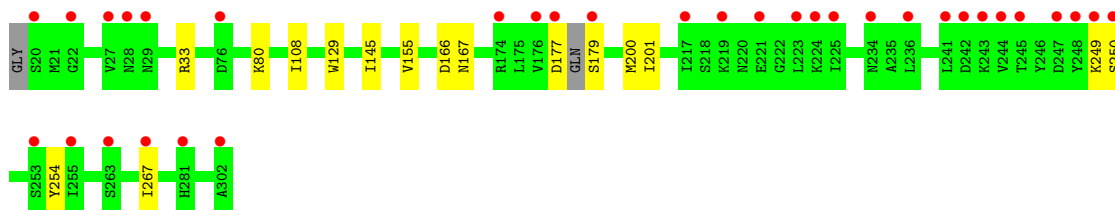
3 Residue-property plots [i](#)

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.

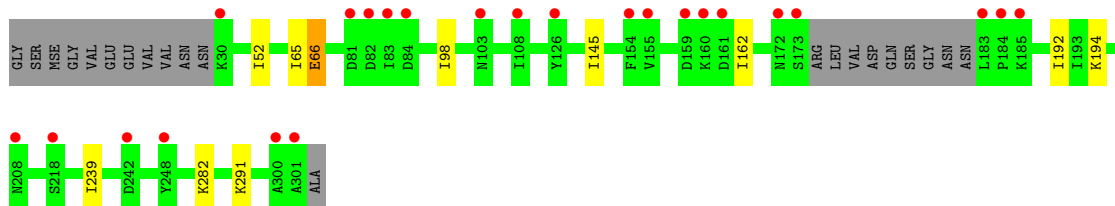
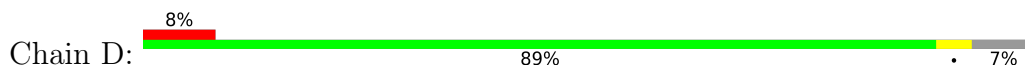
- Molecule 1: PfVFT1



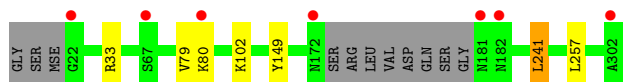
- Molecule 1: PfVFT1



- Molecule 1: PfVFT1



- Molecule 1: PfVFT1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	84.77Å 201.43Å 77.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.45 – 2.35 61.45 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (61.45-2.35) 94.2 (61.45-2.35)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.204 , 0.261 0.214 , 0.258	Depositor DCC
R_{free} test set	2705 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9125	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: 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	0.28	0/2302	0.60	0/3111
1	B	0.29	0/2305	0.62	0/3111
1	C	0.29	0/2242	0.61	1/3029 (0.0%)
1	D	0.29	0/2167	0.63	1/2927 (0.0%)
All	All	0.29	0/9016	0.61	2/12178 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	LEU	CB-CA-C	-5.33	110.44	116.63
1	D	162	ILE	N-CA-C	-5.20	100.88	108.99

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	2260	0	2250	4	0
1	B	2265	0	2255	8	0
1	C	2201	0	2191	2	0
1	D	2126	0	2125	4	0
2	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	64	0	0	1	0
3	B	48	0	0	0	0
3	C	77	0	0	0	0
3	D	54	0	0	0	0
All	All	9125	0	8821	18	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 1.

All (18) 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:299:LYS:NZ	1:A:301:ALA:O	2.31	0.63
1:A:204:GLU:OE2	1:A:264:LYS:NZ	2.33	0.55
1:C:33:ARG:NH2	1:C:80:LYS:O	2.41	0.54
1:B:33:ARG:NH2	1:B:80:LYS:O	2.43	0.50
1:C:102:LYS:HG3	1:C:149:TYR:HB3	1.96	0.48
1:B:177:ASP:C	1:B:179:SER:HA	2.40	0.47
1:B:249:LYS:O	1:B:250:SER:OG	2.18	0.46
1:A:102:LYS:HB3	1:A:149:TYR:HB3	1.97	0.46
1:D:98:ILE:HD13	1:D:145:ILE:HG23	1.98	0.46
1:B:201:ILE:HD13	1:B:267:ILE:O	2.17	0.45
1:B:166:ASP:OD1	1:B:167:ASN:N	2.49	0.45
1:B:129:TRP:HB2	1:B:145:ILE:HD11	1.99	0.44
1:D:66:GLU:OE1	1:D:194:LYS:NZ	2.51	0.43
1:B:200:MSE:HE1	1:B:254:TYR:HB2	2.02	0.42
1:A:89:GLU:OE1	3:A:501:HOH:O	2.22	0.42
1:D:194:LYS:HB3	1:D:291:LYS:HB3	2.03	0.41
1:B:155:VAL:CG2	1:B:177:ASP:HB2	2.51	0.41
1:D:65:ILE:HB	1:D:192:ILE:HA	2.02	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	279/284 (98%)	275 (99%)	4 (1%)	0	100	100
1	B	278/284 (98%)	271 (98%)	7 (2%)	0	100	100
1	C	269/284 (95%)	265 (98%)	4 (2%)	0	100	100
1	D	259/284 (91%)	253 (98%)	6 (2%)	0	100	100
All	All	1085/1136 (96%)	1064 (98%)	21 (2%)	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	255/253 (101%)	253 (99%)	2 (1%)	73	84
1	B	256/253 (101%)	255 (100%)	1 (0%)	84	91
1	C	248/253 (98%)	245 (99%)	3 (1%)	63	77
1	D	240/253 (95%)	236 (98%)	4 (2%)	53	68
All	All	999/1012 (99%)	989 (99%)	10 (1%)	68	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	LYS
1	A	284	ASN

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Mol	Chain	Res	Type
1	B	108	ILE
1	D	52	ILE
1	D	66	GLU
1	D	239	ILE
1	D	282	LYS
1	C	79	VAL
1	C	241	LEU
1	C	257	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	208	ASN
1	A	220	ASN
1	B	47	GLN
1	B	59	ASN
1	B	148	ASN
1	B	152	ASN
1	D	135	HIS
1	C	148	ASN
1	C	158	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	$\# Z > 2$
2	SO4	D	402	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	D	401	-	4,4,4	0.23	0	6,6,6	0.05	0
2	SO4	C	401	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	401	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	401	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	C	402	-	4,4,4	0.24	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	278/284 (97%)	0.22	7 (2%) 58 64	13, 24, 39, 58	0
1	B	278/284 (97%)	0.60	33 (11%) 9 10	13, 27, 50, 64	0
1	C	270/284 (95%)	0.16	7 (2%) 57 63	11, 22, 39, 57	0
1	D	260/284 (91%)	0.45	24 (9%) 14 17	12, 24, 49, 78	0
All	All	1086/1136 (95%)	0.36	71 (6%) 25 28	11, 24, 46, 78	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	184	PRO	6.6
1	D	301	ALA	5.9
1	D	30	LYS	4.3
1	D	161	ASP	4.2
1	B	255	ILE	4.1
1	B	223	LEU	3.9
1	D	173	SER	3.7
1	B	176	VAL	3.6
1	B	177	ASP	3.5
1	D	172	ASN	3.5
1	B	27	VAL	3.4
1	B	242	ASP	3.4
1	D	103	ASN	3.4
1	D	160	LYS	3.3
1	D	242	ASP	3.3
1	B	248	TYR	3.3
1	B	244	VAL	3.2
1	C	172	ASN	3.2
1	C	22	GLY	3.2
1	B	174	ARG	3.1
1	B	20	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	182	ASN	2.9
1	B	241	LEU	2.8
1	C	67	SER	2.7
1	B	219	LYS	2.7
1	B	247	ASP	2.7
1	B	281	HIS	2.7
1	B	179	SER	2.7
1	B	236	LEU	2.7
1	A	180	GLY	2.7
1	C	181	ASN	2.6
1	A	302	ALA	2.6
1	B	28	ASN	2.6
1	D	154	PHE	2.5
1	B	217	ILE	2.5
1	B	302	ALA	2.5
1	B	22	GLY	2.5
1	D	185	LYS	2.5
1	B	245	THR	2.5
1	B	250	SER	2.5
1	D	159	ASP	2.5
1	B	234	ASN	2.4
1	A	174	ARG	2.4
1	D	126	TYR	2.4
1	D	248	TYR	2.4
1	B	29	ASN	2.4
1	A	172	ASN	2.3
1	C	302	ALA	2.3
1	A	179	SER	2.3
1	D	208	ASN	2.3
1	D	183	LEU	2.3
1	B	221	GLU	2.2
1	B	249	LYS	2.2
1	B	253	SER	2.2
1	D	218	SER	2.2
1	D	155	VAL	2.2
1	C	182	ASN	2.1
1	B	243	LYS	2.1
1	B	267	ILE	2.1
1	D	83	ILE	2.1
1	B	76	ASP	2.1
1	D	81	ASP	2.1
1	B	225	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	82	ASP	2.1
1	A	219	LYS	2.1
1	D	300	ALA	2.1
1	B	263	SER	2.0
1	D	108	ILE	2.0
1	D	84	ASP	2.0
1	B	224	LYS	2.0
1	C	80	LYS	2.0

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 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($\text{\AA}^2$)	Q<0.9
2	SO4	A	401	5/5	0.86	0.16	35,41,47,52	0
2	SO4	D	402	5/5	0.90	0.15	39,40,46,49	0
2	SO4	D	401	5/5	0.93	0.11	35,41,42,47	0
2	SO4	C	402	5/5	0.93	0.14	32,41,47,49	0
2	SO4	C	401	5/5	0.98	0.07	24,26,35,36	0
2	SO4	B	401	5/5	0.99	0.07	25,26,31,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.