



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:10 PM EDT

PDB ID : 5QTF / pdb_00005qtf
Title : T. brucei FPPS in complex with CID 144539
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Deposited on : 2019-08-09
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)
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

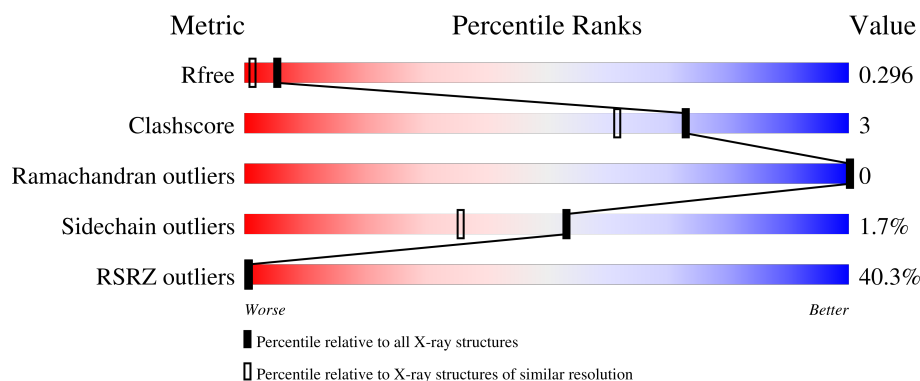
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	369	36% 80% 9% 11%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2754 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.

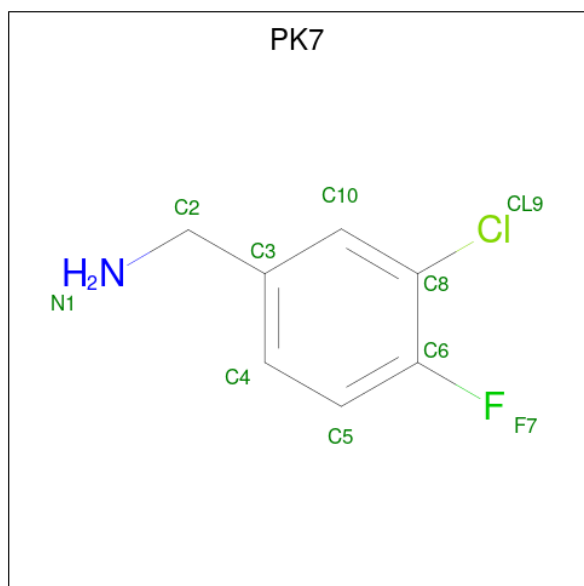
- Molecule 1 is a protein called Farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	0	0
			2629	1678	426	498	27			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q86C09
A	0	PRO	-	expression tag	UNP Q86C09

- Molecule 2 is 1-(3-chloro-4-fluorophenyl)methanamine (CCD ID: PK7) (formula: C_7H_7ClFN).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	0	0
			10	7	1	1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).

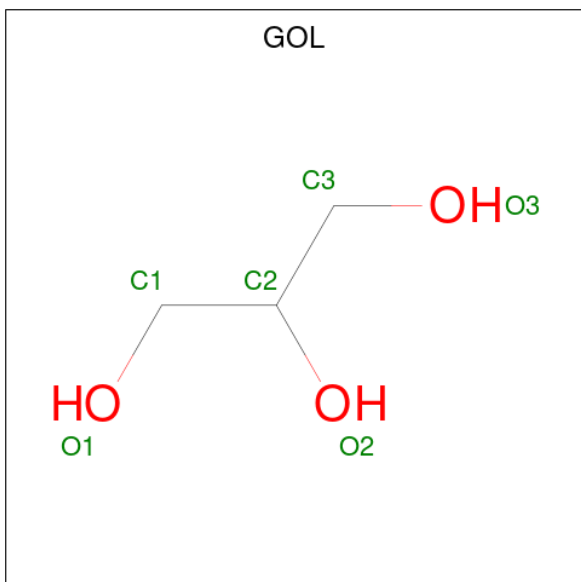


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

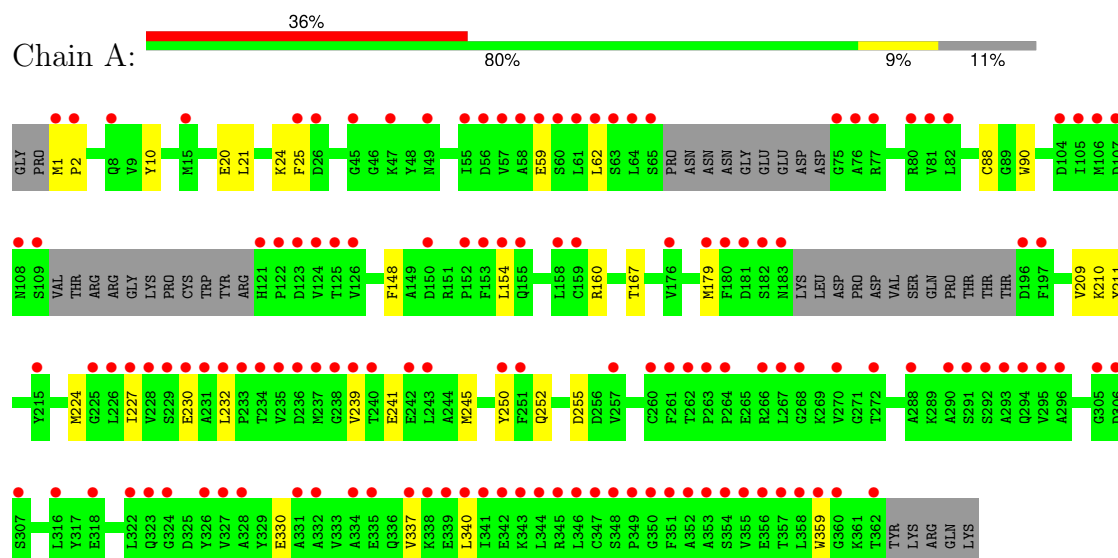
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	98	Total	O	0	0
			98	98		

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: Farnesyl pyrophosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	60.62Å 60.62Å 341.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.89 – 1.78 56.89 – 1.78	Depositor EDS
% Data completeness (in resolution range)	65.0 (56.89-1.78) 65.0 (56.89-1.78)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.250 , 0.293 0.254 , 0.296	Depositor DCC
R_{free} test set	1192 reflections (3.16%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2754	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, GOL, NA, PK7

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	0.12	0/2679	0.30	0/3619

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	2629	0	2584	17	0
2	A	10	0	0	0	0
3	A	10	0	0	0	0
4	A	1	0	0	0	0
5	A	6	0	8	0	0
6	A	98	0	0	0	0
All	All	2754	0	2592	17	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 3.

All (17) 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:241:GLU:O	1:A:245:MET:HG2	2.03	0.59
1:A:20:GLU:HG3	1:A:24:LYS:HD2	1.91	0.53
1:A:239:VAL:HG13	1:A:340:LEU:HD22	1.92	0.51
1:A:148:PHE:HB2	1:A:154:LEU:HD13	1.94	0.49
1:A:167:THR:HG23	1:A:211:TYR:CD1	2.48	0.49
1:A:10:TYR:HB2	1:A:90:TRP:CZ2	2.49	0.47
1:A:209:VAL:HG22	1:A:252:GLN:HG2	1.97	0.46
1:A:210:LYS:HG3	1:A:245:MET:SD	2.56	0.45
1:A:167:THR:HG23	1:A:211:TYR:HD1	1.83	0.44
1:A:337:VAL:HG11	1:A:359:TRP:CD2	2.53	0.44
1:A:10:TYR:HB2	1:A:90:TRP:CE2	2.52	0.44
1:A:227:ILE:HG12	1:A:232:LEU:HD22	2.01	0.43
1:A:21:LEU:HA	1:A:25:PHE:HB2	2.00	0.43
1:A:88:CYS:SG	1:A:224:MET:HE2	2.59	0.42
1:A:160:ARG:HD2	1:A:227:ILE:HD11	2.02	0.42
1:A:250:TYR:CE2	1:A:330:GLU:HB3	2.55	0.41
1:A:1:MET:N	1:A:2:PRO:HD2	2.36	0.41

There are no symmetry-related clashes.

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	322/369 (87%)	315 (98%)	7 (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	286/322 (89%)	281 (98%)	5 (2%)	53 36

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	A	62	LEU
1	A	179	MET
1	A	230	GLU
1	A	255	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	131	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z > 2$
3	PO4	A	402	-	4,4,4	0.97	0	6,6,6	0.46	0
2	PK7	A	401	-	10,10,10	0.80	0	13,13,13	0.74	0
3	PO4	A	404	-	4,4,4	0.93	0	6,6,6	0.49	0
5	GOL	A	405	-	5,5,5	0.89	0	5,5,5	1.11	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	PK7	A	401	-	-	0/2/2/2	0/1/1/1
5	GOL	A	405	-	-	0/4/4/4	-

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	330/369 (89%)	1.85	133 (40%) 0 1	19, 50, 93, 110	3 (0%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	PHE	10.8
1	A	344	LEU	8.9
1	A	318	GLU	8.0
1	A	323	GLN	7.7
1	A	232	LEU	7.3
1	A	64	LEU	6.2
1	A	346	LEU	6.2
1	A	61	LEU	5.9
1	A	81	VAL	5.8
1	A	351	PHE	5.8
1	A	75	GLY	5.6
1	A	231	ALA	5.4
1	A	350	GLY	5.1
1	A	359	TRP	5.0
1	A	341	ILE	4.9
1	A	180	PHE	4.9
1	A	235	VAL	4.9
1	A	122	PRO	4.9
1	A	353	ALA	4.6
1	A	76	ALA	4.5
1	A	62	LEU	4.5
1	A	349	PRO	4.3
1	A	340	LEU	4.3
1	A	324	GLY	4.2
1	A	1	MET	4.1
1	A	233	PRO	4.1
1	A	106	MET	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	182	SER	4.1
1	A	181	ASP	4.1
1	A	234	THR	4.0
1	A	347	CYS	4.0
1	A	82	LEU	4.0
1	A	226	LEU	3.9
1	A	153	PHE	3.9
1	A	236	ASP	3.9
1	A	293	ALA	3.8
1	A	251	PHE	3.8
1	A	228	VAL	3.8
1	A	60	SER	3.8
1	A	124	VAL	3.8
1	A	345	ARG	3.8
1	A	327	VAL	3.6
1	A	183	ASN	3.6
1	A	348	SER	3.6
1	A	58	ALA	3.6
1	A	337	VAL	3.5
1	A	355	VAL	3.5
1	A	123	ASP	3.5
1	A	109	SER	3.5
1	A	65	SER	3.4
1	A	292	SER	3.4
1	A	338	LYS	3.4
1	A	352	ALA	3.4
1	A	362	THR	3.3
1	A	358	LEU	3.3
1	A	326	TYR	3.2
1	A	63	SER	3.2
1	A	270	VAL	3.2
1	A	2	PRO	3.1
1	A	343	LYS	3.1
1	A	290	ALA	3.1
1	A	121	HIS	3.1
1	A	356	GLU	3.1
1	A	15	MET	3.0
1	A	225	GLY	3.0
1	A	227	ILE	3.0
1	A	56	ASP	3.0
1	A	342	GLU	3.0
1	A	328	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	307	SER	2.9
1	A	237	MET	2.9
1	A	268	GLY	2.9
1	A	230	GLU	2.9
1	A	158	LEU	2.9
1	A	229	SER	2.9
1	A	159	CYS	2.8
1	A	77	ARG	2.8
1	A	357	THR	2.8
1	A	331	ALA	2.8
1	A	354	SER	2.8
1	A	152	PRO	2.8
1	A	267	LEU	2.8
1	A	238	GLY	2.8
1	A	59	GLU	2.8
1	A	55	ILE	2.8
1	A	105	ILE	2.8
1	A	150	ASP	2.7
1	A	176	VAL	2.7
1	A	47	LYS	2.7
1	A	260	CYS	2.7
1	A	240	THR	2.6
1	A	57	VAL	2.6
1	A	266	ARG	2.6
1	A	332	ALA	2.6
1	A	263	PRO	2.6
1	A	107	ASP	2.6
1	A	154	LEU	2.6
1	A	250	TYR	2.6
1	A	179	MET	2.6
1	A	197	PHE	2.6
1	A	316	LEU	2.6
1	A	296	ALA	2.5
1	A	196	ASP	2.5
1	A	242	GLU	2.5
1	A	25	PHE	2.5
1	A	272	THR	2.5
1	A	291	SER	2.4
1	A	80	ARG	2.4
1	A	104	ASP	2.4
1	A	125	THR	2.4
1	A	335	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	262	THR	2.3
1	A	305	GLY	2.3
1	A	339	GLU	2.3
1	A	295	VAL	2.3
1	A	360	GLY	2.3
1	A	126	VAL	2.3
1	A	239	VAL	2.3
1	A	257	VAL	2.3
1	A	288	ALA	2.2
1	A	294	GLN	2.2
1	A	334	ALA	2.2
1	A	45	GLY	2.2
1	A	155	GLN	2.2
1	A	49	ASN	2.1
1	A	264	PRO	2.1
1	A	243	LEU	2.1
1	A	322	LEU	2.1
1	A	306	ASP	2.1
1	A	215	TYR	2.1
1	A	26	ASP	2.1
1	A	108	ASN	2.0
1	A	8	GLN	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
3	PO4	A	404	5/5	0.67	0.23	99,100,102,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PO4	A	402	5/5	0.75	0.17	99,101,105,106	0
2	PK7	A	401	10/10	0.76	0.40	72,75,78,79	10
5	GOL	A	405	6/6	0.80	0.18	63,64,65,67	0
4	NA	A	403	1/1	0.94	0.09	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.