



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5QTD / pdb_00005qtd
Title : Unliganded T. brucei FPPS
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Resolution : 1.64 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

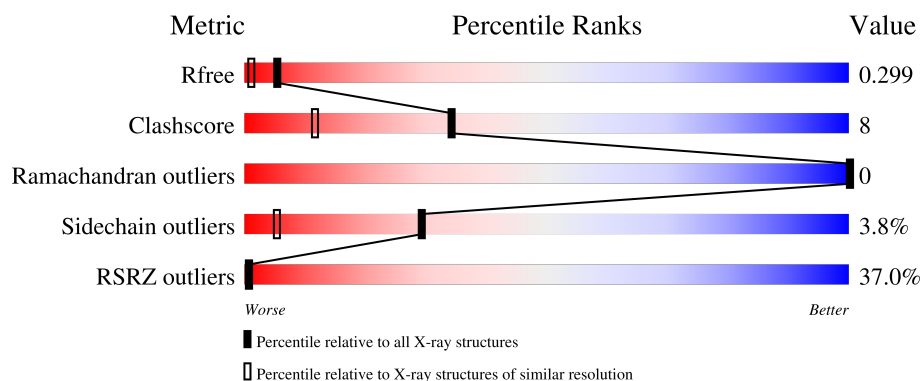
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	369	33% 72% 16% 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2764 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
			Total	C	N	O	S			
1	A	330	2629	1678	426	498	27	0	0	0

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 PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

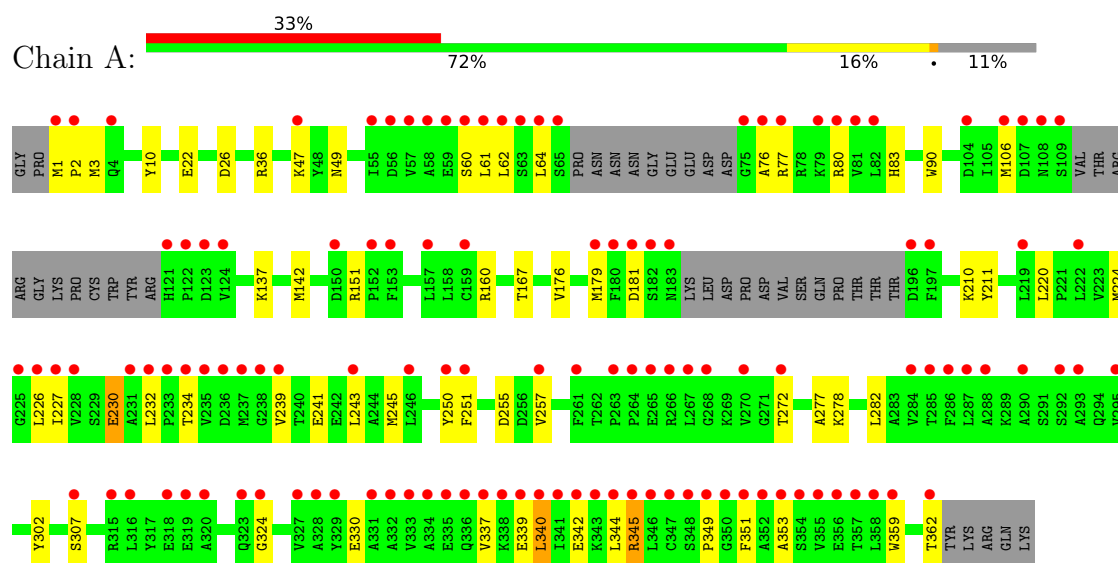
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	118	Total	O	0	0
			118	118		

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	60.45Å 60.45Å 340.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.68 – 1.64 56.68 – 1.64	Depositor EDS
% Data completeness (in resolution range)	58.6 (56.68-1.64) 58.6 (56.68-1.64)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 1.64Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.250 , 0.298 0.252 , 0.299	Depositor DCC
R_{free} test set	1379 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2764	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.11% 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

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	0.32	0/2679	0.50	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	40	0
2	A	10	0	0	0	0
3	A	1	0	0	0	0
4	A	6	0	8	0	0
5	A	118	0	0	17	3
All	All	2764	0	2592	40	3

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 8.

All (40) 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:60:SER:OG	5:A:502:HOH:O	1.86	0.92
1:A:230:GLU:OE1	5:A:501:HOH:O	1.85	0.92
1:A:22:GLU:O	5:A:503:HOH:O	1.91	0.89
1:A:151:ARG:O	5:A:504:HOH:O	1.91	0.86
1:A:137:LYS:HG2	5:A:602:HOH:O	1.78	0.83
1:A:36:ARG:HD2	5:A:521:HOH:O	1.87	0.73
1:A:83:HIS:ND1	5:A:512:HOH:O	2.22	0.72
1:A:353:ALA:O	5:A:505:HOH:O	2.06	0.72
1:A:77:ARG:HG2	1:A:80:ARG:HH21	1.53	0.71
1:A:324:GLY:O	5:A:506:HOH:O	2.08	0.70
1:A:234:THR:OG1	5:A:507:HOH:O	2.14	0.66
1:A:339:GLU:O	5:A:508:HOH:O	2.15	0.65
1:A:241:GLU:O	1:A:245:MET:HG2	1.99	0.62
1:A:47:LYS:HD3	1:A:49:ASN:HD21	1.65	0.62
1:A:239:VAL:HG13	1:A:340:LEU:HD22	1.82	0.61
1:A:160:ARG:HD2	1:A:227:ILE:HD11	1.82	0.61
1:A:337:VAL:HG11	1:A:359:TRP:CD2	2.37	0.58
1:A:26:ASP:O	5:A:509:HOH:O	2.17	0.56
1:A:167:THR:HG23	1:A:211:TYR:HD1	1.71	0.56
1:A:61:LEU:HD21	1:A:226:LEU:HD23	1.88	0.55
1:A:106:MET:O	5:A:510:HOH:O	2.18	0.52
1:A:257:VAL:HG22	1:A:282:LEU:HD21	1.93	0.50
1:A:167:THR:HG23	1:A:211:TYR:CD1	2.46	0.49
1:A:64:LEU:HD23	1:A:349:PRO:HG2	1.94	0.49
1:A:77:ARG:HG2	1:A:80:ARG:NH2	2.26	0.49
1:A:272:THR:HG23	5:A:543:HOH:O	2.14	0.48
1:A:1:MET:N	1:A:2:PRO:HD2	2.31	0.46
1:A:278:LYS:HA	1:A:278:LYS:HD2	1.75	0.46
1:A:342:GLU:OE2	1:A:345:ARG:NH2	2.45	0.45
1:A:10:TYR:HB2	1:A:90:TRP:CZ2	2.53	0.44
1:A:251:PHE:HB2	1:A:362:THR:HG23	2.00	0.43
1:A:220:LEU:O	1:A:224:MET:HG3	2.19	0.43
1:A:36:ARG:NH1	5:A:521:HOH:O	2.35	0.42
1:A:344:LEU:HD21	1:A:351:PHE:CD2	2.55	0.42
1:A:277:ALA:HA	1:A:302:TYR:CE2	2.54	0.42
1:A:76:ALA:O	5:A:511:HOH:O	2.22	0.42
1:A:210:LYS:HG3	1:A:245:MET:SD	2.59	0.42
1:A:3:MET:HE2	1:A:3:MET:HB2	1.98	0.41
1:A:142:MET:HE3	5:A:547:HOH:O	2.21	0.40
1:A:250:TYR:CE2	1:A:330:GLU:HB3	2.55	0.40

All (3) 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)
5:A:539:HOH:O	5:A:577:HOH:O[10_554]	1.91	0.29
5:A:551:HOH:O	5:A:551:HOH:O[10_554]	2.16	0.04
5:A:596:HOH:O	5:A:602:HOH:O[8_555]	2.17	0.03

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%)	316 (98%)	6 (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%)	275 (96%)	11 (4%)	29	5

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	176	VAL
1	A	179	MET
1	A	181	ASP
1	A	230	GLU
1	A	232	LEU

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Mol	Chain	Res	Type
1	A	243	LEU
1	A	255	ASP
1	A	307	SER
1	A	340	LEU
1	A	345	ARG

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 ⓘ

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 ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
4	GOL	A	404	-	5,5,5	0.89	0	5,5,5	1.31	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	401	-	4,4,4	0.95	0	6,6,6	0.41	0
2	PO4	A	403	-	4,4,4	0.91	0	6,6,6	0.42	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
4	GOL	A	404	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	404	GOL	C3-C2-C1	-2.11	104.06	111.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	GOL	C1-C2-C3-O3
4	A	404	GOL	O2-C2-C3-O3

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%)	1.60	122 (36%) ⓘ ⓘ	14, 43, 71, 81	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	LEU	6.4
1	A	346	LEU	5.1
1	A	341	ILE	5.1
1	A	232	LEU	5.1
1	A	76	ALA	4.7
1	A	344	LEU	4.6
1	A	75	GLY	4.6
1	A	355	VAL	4.6
1	A	61	LEU	4.5
1	A	349	PRO	4.4
1	A	359	TRP	4.3
1	A	353	ALA	4.1
1	A	235	VAL	4.1
1	A	350	GLY	4.0
1	A	233	PRO	3.9
1	A	182	SER	3.8
1	A	122	PRO	3.8
1	A	231	ALA	3.7
1	A	288	ALA	3.7
1	A	351	PHE	3.7
1	A	57	VAL	3.7
1	A	243	LEU	3.7
1	A	287	LEU	3.6
1	A	293	ALA	3.6
1	A	183	ASN	3.6
1	A	327	VAL	3.6
1	A	181	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	352	ALA	3.5
1	A	354	SER	3.5
1	A	1	MET	3.5
1	A	290	ALA	3.5
1	A	226	LEU	3.5
1	A	345	ARG	3.4
1	A	340	LEU	3.4
1	A	337	VAL	3.4
1	A	109	SER	3.4
1	A	328	ALA	3.3
1	A	333	VAL	3.3
1	A	307	SER	3.3
1	A	225	GLY	3.3
1	A	106	MET	3.3
1	A	251	PHE	3.3
1	A	81	VAL	3.3
1	A	257	VAL	3.3
1	A	121	HIS	3.2
1	A	331	ALA	3.2
1	A	107	ASP	3.2
1	A	334	ALA	3.2
1	A	357	THR	3.1
1	A	108	ASN	3.1
1	A	270	VAL	3.1
1	A	77	ARG	3.1
1	A	59	GLU	3.1
1	A	222	LEU	3.1
1	A	60	SER	3.1
1	A	272	THR	3.0
1	A	153	PHE	3.0
1	A	180	PHE	3.0
1	A	358	LEU	3.0
1	A	58	ALA	2.9
1	A	295	VAL	2.9
1	A	62	LEU	2.9
1	A	228	VAL	2.8
1	A	347	CYS	2.8
1	A	234	THR	2.8
1	A	324	GLY	2.8
1	A	316	LEU	2.8
1	A	362	THR	2.8
1	A	47	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	65	SER	2.7
1	A	82	LEU	2.6
1	A	179	MET	2.6
1	A	339	GLU	2.6
1	A	338	LYS	2.6
1	A	238	GLY	2.6
1	A	239	VAL	2.6
1	A	343	LYS	2.6
1	A	265	GLU	2.6
1	A	286	PHE	2.5
1	A	152	PRO	2.5
1	A	332	ALA	2.5
1	A	56	ASP	2.5
1	A	196	ASP	2.5
1	A	320	ALA	2.5
1	A	123	ASP	2.5
1	A	236	ASP	2.5
1	A	246	LEU	2.5
1	A	63	SER	2.5
1	A	336	GLN	2.4
1	A	329	TYR	2.4
1	A	124	VAL	2.4
1	A	266	ARG	2.4
1	A	318	GLU	2.4
1	A	79	LYS	2.4
1	A	80	ARG	2.4
1	A	227	ILE	2.4
1	A	284	VAL	2.4
1	A	342	GLU	2.3
1	A	55	ILE	2.3
1	A	348	SER	2.3
1	A	150	ASP	2.3
1	A	250	TYR	2.3
1	A	264	PRO	2.2
1	A	285	THR	2.2
1	A	335	GLU	2.2
1	A	292	SER	2.2
1	A	268	GLY	2.2
1	A	237	MET	2.2
1	A	261	PHE	2.2
1	A	263	PRO	2.2
1	A	157	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	104	ASP	2.1
1	A	2	PRO	2.1
1	A	4	GLN	2.1
1	A	315	ARG	2.1
1	A	197	PHE	2.1
1	A	319	GLU	2.0
1	A	356	GLU	2.0
1	A	323	GLN	2.0
1	A	159	CYS	2.0
1	A	219	LEU	2.0
1	A	267	LEU	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	PO4	A	403	5/5	0.68	0.22	70,76,80,80	0
2	PO4	A	401	5/5	0.73	0.18	76,82,88,89	0
4	GOL	A	404	6/6	0.75	0.18	41,50,51,68	0
3	NA	A	402	1/1	0.94	0.10	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.