



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:15 AM GMT

PDB ID : 3DYH  
Title : T. Brucei Farnesyl Diphosphate Synthase Complexed with Bisphosphonate BPH-721  
Authors : Cao, R.; Gao, Y.; Robinson, H.; Goddard, A.; Oldfield, E.  
Deposited on : 2008-07-27  
Resolution : 1.94 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

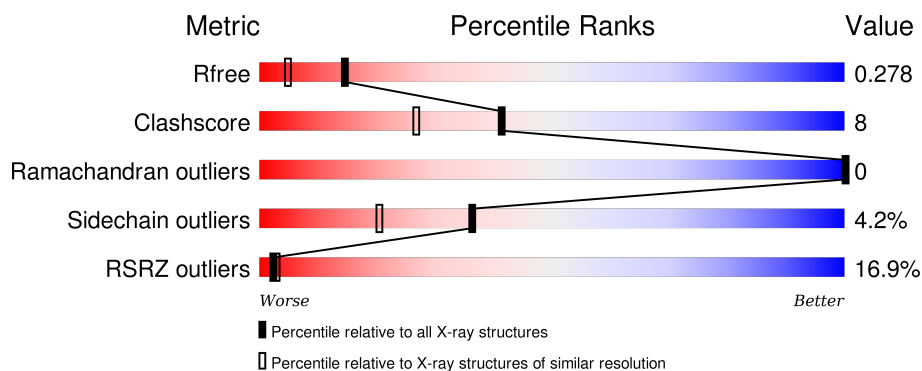
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.94 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))
$R_{free}$	91344	2910 (1.96-1.92)
Clashscore	102246	3095 (1.96-1.92)
Ramachandran outliers	100387	3062 (1.96-1.92)
Sidechain outliers	100360	3062 (1.96-1.92)
RSRZ outliers	91569	2915 (1.96-1.92)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	390	<div> <div>15%</div> <div>73%</div> <div>17%</div> <div>8%</div> </div>
1	B	390	<div> <div>16%</div> <div>77%</div> <div>14%</div> <div>8%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6133 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	358	Total	C	N	O	S	0	0	0
			2864	1826	472	538	28			
1	B	359	Total	C	N	O	S	0	0	0
			2872	1830	474	540	28			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q86C09
A	-21	GLY	-	EXPRESSION TAG	UNP Q86C09
A	-20	SER	-	EXPRESSION TAG	UNP Q86C09
A	-19	SER	-	EXPRESSION TAG	UNP Q86C09
A	-18	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-17	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-16	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-15	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-14	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-13	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-12	SER	-	EXPRESSION TAG	UNP Q86C09
A	-11	SER	-	EXPRESSION TAG	UNP Q86C09
A	-10	GLY	-	EXPRESSION TAG	UNP Q86C09
A	-9	LEU	-	EXPRESSION TAG	UNP Q86C09
A	-8	VAL	-	EXPRESSION TAG	UNP Q86C09
A	-7	PRO	-	EXPRESSION TAG	UNP Q86C09
A	-6	ARG	-	EXPRESSION TAG	UNP Q86C09
A	-5	GLY	-	EXPRESSION TAG	UNP Q86C09
A	-4	SER	-	EXPRESSION TAG	UNP Q86C09
A	-3	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-2	MET	-	EXPRESSION TAG	UNP Q86C09
A	-1	ALA	-	EXPRESSION TAG	UNP Q86C09
A	0	SER	-	EXPRESSION TAG	UNP Q86C09
B	-22	MET	-	EXPRESSION TAG	UNP Q86C09
B	-21	GLY	-	EXPRESSION TAG	UNP Q86C09

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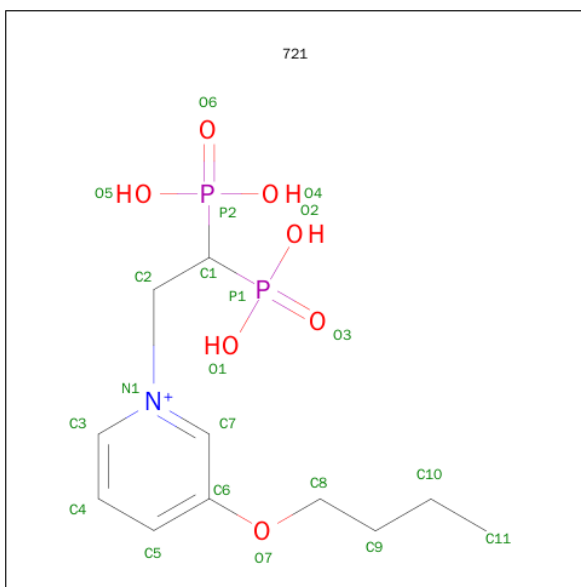
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	EXPRESSION TAG	UNP Q86C09
B	-19	SER	-	EXPRESSION TAG	UNP Q86C09
B	-18	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-17	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-16	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-15	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-14	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-13	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-12	SER	-	EXPRESSION TAG	UNP Q86C09
B	-11	SER	-	EXPRESSION TAG	UNP Q86C09
B	-10	GLY	-	EXPRESSION TAG	UNP Q86C09
B	-9	LEU	-	EXPRESSION TAG	UNP Q86C09
B	-8	VAL	-	EXPRESSION TAG	UNP Q86C09
B	-7	PRO	-	EXPRESSION TAG	UNP Q86C09
B	-6	ARG	-	EXPRESSION TAG	UNP Q86C09
B	-5	GLY	-	EXPRESSION TAG	UNP Q86C09
B	-4	SER	-	EXPRESSION TAG	UNP Q86C09
B	-3	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-2	MET	-	EXPRESSION TAG	UNP Q86C09
B	-1	ALA	-	EXPRESSION TAG	UNP Q86C09
B	0	SER	-	EXPRESSION TAG	UNP Q86C09

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	3	Total Mg 3 3	0	0

- Molecule 3 is 3-BUTOXY-1-(2,2-DIPHOSPHONOETHYL)PYRIDINIUM (three-letter code: 721) (formula: C<sub>11</sub>H<sub>20</sub>NO<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			21	11	1	7	2		
3	B	1	Total	C	N	O	P	0	0
			21	11	1	7	2		

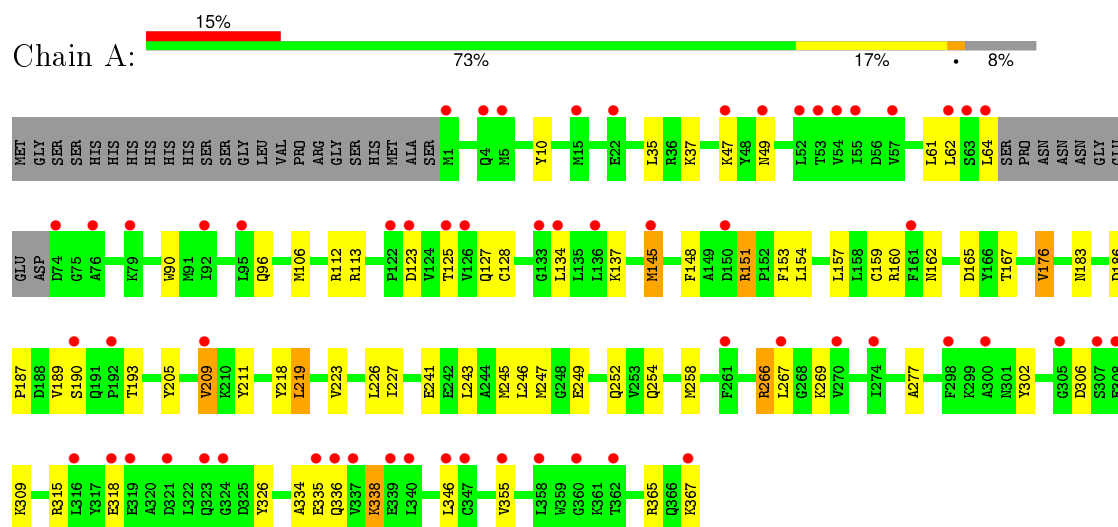
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		
4	B	176	Total	O	0	0
			176	176		

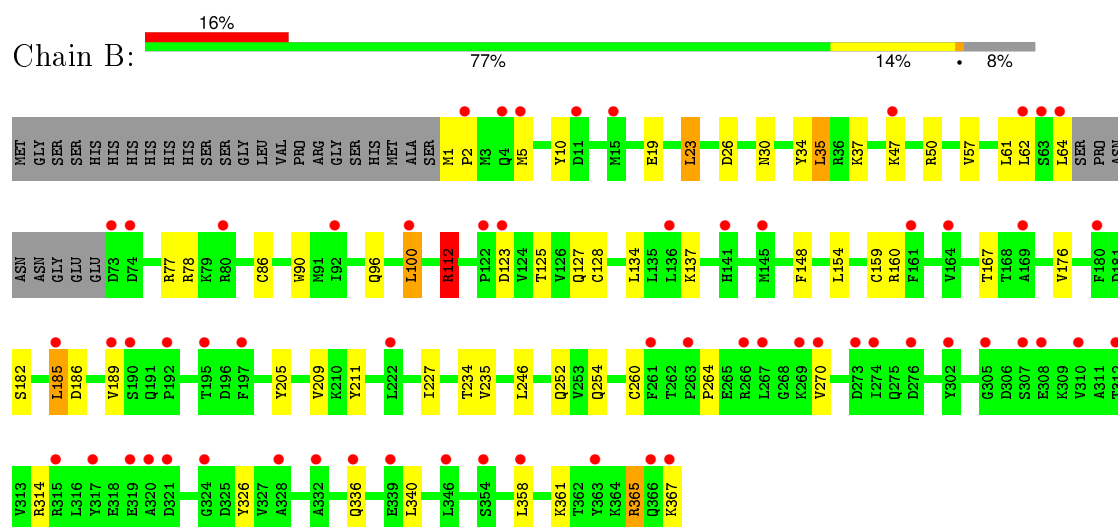
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



#### • Molecule 1: Farnesyl pyrophosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.91Å 118.73Å 63.04Å 90.00° 112.29° 90.00°	Depositor
Resolution (Å)	28.83 – 1.94 28.83 – 1.94	Depositor EDS
% Data completeness (in resolution range)	98.1 (28.83-1.94) 98.1 (28.83-1.94)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.01 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.240 , 0.282 0.238 , 0.278	Depositor DCC
$R_{free}$ test set	3331 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.6	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 42.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65858 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6133	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.53% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, 721

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	0.53	0/2923	0.63	0/3952
1	B	0.55	0/2931	0.64	1/3963 (0.0%)
All	All	0.54	0/5854	0.64	1/7915 (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	B	112	ARG	NE-CZ-NH2	-6.55	117.02	120.30

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	2864	0	2824	61	0
1	B	2872	0	2830	44	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	21	0	16	0	0
3	B	21	0	16	1	0
4	A	173	0	0	9	0
4	B	176	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6133	0	5686	97	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 8.

All (97) 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:47:LYS:HD3	1:A:367:LYS:HD2	1.32	1.11
1:A:123:ASP:CB	1:B:186:ASP:O	2.03	1.07
1:B:112:ARG:NH2	3:B:4001:721:O2	2.01	0.94
1:A:137:LYS:HE2	1:A:165:ASP:OD2	1.69	0.92
1:A:134:LEU:HD21	4:B:4084:HOH:O	1.68	0.92
1:A:159:CYS:HB2	4:A:3176:HOH:O	1.69	0.91
1:A:186:ASP:O	1:B:123:ASP:CB	2.19	0.90
1:B:159:CYS:SG	4:B:4167:HOH:O	2.33	0.86
1:A:96:GLN:HG3	4:A:3171:HOH:O	1.75	0.85
1:B:134:LEU:HD21	4:B:4084:HOH:O	1.75	0.85
1:A:106:MET:O	4:A:3177:HOH:O	1.97	0.81
1:A:334:ALA:O	1:A:338:LYS:HE3	1.82	0.80
1:A:47:LYS:CD	1:A:367:LYS:HD2	2.12	0.79
1:A:218:TYR:CE2	1:A:247:MET:HE2	2.17	0.78
1:A:151:ARG:HG2	1:A:153:PHE:CZ	2.19	0.78
1:A:315:ARG:HA	1:A:318:GLU:HG2	1.68	0.75
1:A:209:VAL:HG22	1:A:252:GLN:HG2	1.71	0.73
1:A:266:ARG:HB2	1:A:266:ARG:NH1	2.05	0.72
1:A:162:ASN:ND2	4:A:3113:HOH:O	2.24	0.70
1:B:125:THR:HG23	4:B:4102:HOH:O	1.93	0.68
1:A:151:ARG:HG2	1:A:153:PHE:CE2	2.29	0.67
4:A:3177:HOH:O	1:B:127:GLN:HG3	2.01	0.60
1:A:209:VAL:HG22	1:A:252:GLN:CG	2.32	0.60
1:A:49:ASN:HD21	1:A:367:LYS:NZ	1.99	0.60
1:B:270:VAL:HA	4:B:4058:HOH:O	2.01	0.58
1:B:361:LYS:HE3	4:B:4118:HOH:O	2.03	0.58
1:B:50:ARG:NH1	1:B:96:GLN:OE1	2.37	0.57
1:B:160:ARG:HD2	1:B:227:ILE:HD11	1.85	0.56
1:A:189:VAL:O	1:B:123:ASP:CB	2.54	0.56
1:A:160:ARG:HD2	1:A:227:ILE:HD11	1.89	0.54
1:B:209:VAL:HG11	1:B:252:GLN:HB3	1.89	0.54
1:A:267:LEU:HD23	1:A:269:LYS:HG2	1.90	0.54
1:A:243:LEU:HD13	1:A:355:VAL:HG11	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD21	1:B:336:GLN:HB2	1.90	0.53
1:A:123:ASP:CB	1:B:189:VAL:O	2.56	0.53
1:A:176:VAL:CG2	1:B:127:GLN:HG3	2.38	0.53
1:B:19:GLU:O	1:B:23:LEU:HD23	2.09	0.53
1:B:96:GLN:NE2	4:B:4054:HOH:O	2.42	0.53
1:A:365:ARG:HB2	1:A:367:LYS:HG2	1.91	0.52
1:A:183:ASN:HD22	1:B:30:ASN:HD21	1.57	0.52
1:B:260:CYS:SG	1:B:314:ARG:HG2	2.50	0.51
1:A:125:THR:HB	1:A:127:GLN:OE1	2.11	0.50
1:A:61:LEU:HD11	1:A:226:LEU:HD23	1.94	0.50
1:B:100:LEU:HG	1:B:112:ARG:CZ	2.41	0.50
1:A:167:THR:HG23	1:A:211:TYR:HD1	1.77	0.49
1:B:264:PRO:HA	4:B:4058:HOH:O	2.12	0.49
1:B:254:GLN:HG2	1:B:326:TYR:OH	2.11	0.49
1:A:49:ASN:ND2	1:A:367:LYS:NZ	2.60	0.49
1:A:266:ARG:HB2	1:A:266:ARG:CZ	2.42	0.49
1:A:219:LEU:HD22	1:A:223:VAL:HG23	1.93	0.49
1:A:258:MET:HB3	1:A:267:LEU:HD11	1.94	0.49
1:A:61:LEU:CD1	1:A:226:LEU:HD23	2.43	0.48
1:A:246:LEU:HD21	1:A:336:GLN:HB2	1.95	0.48
1:B:64:LEU:HD13	1:B:234:THR:HG21	1.94	0.48
1:A:37:LYS:HG3	4:A:3107:HOH:O	2.12	0.48
1:B:167:THR:HG23	1:B:211:TYR:HD1	1.79	0.48
1:A:254:GLN:HG2	1:A:326:TYR:OH	2.14	0.47
1:B:148:PHE:HB2	1:B:154:LEU:HD13	1.96	0.47
1:A:10:TYR:HB2	1:A:90:TRP:CZ2	2.50	0.47
1:A:266:ARG:HB2	1:A:266:ARG:HH11	1.79	0.47
1:A:112:ARG:HG3	1:A:113:ARG:HG3	1.96	0.47
1:A:218:TYR:HE2	1:A:247:MET:HE2	1.73	0.46
1:B:361:LYS:NZ	4:B:4109:HOH:O	2.42	0.46
1:B:182:SER:O	1:B:185:LEU:HB2	2.15	0.46
1:B:125:THR:HB	1:B:127:GLN:OE1	2.16	0.46
4:A:3065:HOH:O	1:B:26:ASP:HB2	2.16	0.46
1:B:57:VAL:O	1:B:61:LEU:HD23	2.16	0.46
1:B:209:VAL:CG1	1:B:252:GLN:HB3	2.45	0.45
1:B:127:GLN:HG2	1:B:128:CYS:N	2.32	0.45
1:A:49:ASN:HD21	1:A:367:LYS:HZ3	1.64	0.45
1:A:148:PHE:HB2	1:A:154:LEU:HD13	1.98	0.45
1:B:62:LEU:HD21	1:B:78:ARG:HG3	1.99	0.44
1:A:145:MET:HE2	1:B:159:CYS:HA	1.98	0.44
1:B:10:TYR:HB2	1:B:90:TRP:CZ2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ARG:HH11	1:A:367:LYS:HG3	1.83	0.44
1:B:47:LYS:HE3	4:B:4071:HOH:O	2.17	0.44
1:A:151:ARG:CG	1:A:153:PHE:CE2	3.00	0.44
1:A:365:ARG:HD2	1:A:367:LYS:HG2	2.00	0.43
1:A:205:TYR:CZ	1:A:209:VAL:HG21	2.53	0.43
1:B:205:TYR:CZ	1:B:209:VAL:HG21	2.54	0.43
1:B:1:MET:HB3	1:B:2:PRO:HD3	2.01	0.43
1:A:96:GLN:CG	4:A:3171:HOH:O	2.50	0.43
1:A:96:GLN:NE2	4:A:3171:HOH:O	2.52	0.42
1:A:306:ASP:HB3	1:A:309:LYS:HD2	2.01	0.42
1:B:34:TYR:HD1	1:B:35:LEU:HD13	1.85	0.42
1:A:367:LYS:HA	1:A:367:LYS:HD3	1.82	0.42
1:B:96:GLN:HG3	4:B:4054:HOH:O	2.19	0.41
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.86	0.41
1:A:49:ASN:ND2	1:A:367:LYS:HZ3	2.17	0.41
1:A:258:MET:HB3	1:A:267:LEU:CD1	2.50	0.41
1:B:365:ARG:HH21	1:B:367:LYS:HG3	1.85	0.41
1:A:241:GLU:O	1:A:245:MET:HG2	2.20	0.41
1:A:127:GLN:HG2	1:A:128:CYS:N	2.35	0.41
1:A:209:VAL:CG1	1:A:249:GLU:HA	2.51	0.40
1:B:5:MET:HG2	1:B:86:CYS:SG	2.61	0.40
1:A:187:PRO:HG2	1:B:37:LYS:HG2	2.02	0.40
1:A:277:ALA:HA	1:A:302:TYR:CE2	2.57	0.40

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	354/390 (91%)	346 (98%)	8 (2%)	0	100	100
1	B	355/390 (91%)	350 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	709/780 (91%)	696 (98%)	13 (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	311/340 (92%)	297 (96%)	14 (4%)	34	18
1	B	312/340 (92%)	300 (96%)	12 (4%)	40	24
All	All	623/680 (92%)	597 (96%)	26 (4%)	36	20

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	64	LEU
1	A	145	MET
1	A	151	ARG
1	A	157	LEU
1	A	176	VAL
1	A	190	SER
1	A	193	THR
1	A	209	VAL
1	A	219	LEU
1	A	266	ARG
1	A	335	GLU
1	A	338	LYS
1	A	346	LEU
1	B	23	LEU
1	B	35	LEU
1	B	77	ARG
1	B	100	LEU
1	B	112	ARG
1	B	137	LYS

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Mol	Chain	Res	Type
1	B	176	VAL
1	B	185	LEU
1	B	235	VAL
1	B	340	LEU
1	B	358	LEU
1	B	365	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	49	ASN
1	A	121	HIS
1	A	183	ASN
1	B	155	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	721	A	3001	2	20,21,21	1.02	0	23,30,30	1.79	2 (8%)
3	721	B	4001	2	20,21,21	1.13	2 (10%)	23,30,30	1.20	2 (8%)

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
3	721	A	3001	2	-	0/19/21/21	0/1/1/1
3	721	B	4001	2	-	0/19/21/21	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4001	721	P1-O2	-2.71	1.50	1.54
3	B	4001	721	P1-O1	-2.26	1.51	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3001	721	C2-N1-C7	-5.68	115.88	119.64
3	B	4001	721	C2-N1-C7	-2.92	117.71	119.64
3	B	4001	721	C2-N1-C3	3.73	122.22	119.66
3	A	3001	721	C2-N1-C3	5.70	123.56	119.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4001	721	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	358/390 (91%)	1.16	60 (16%) 2 3	25, 42, 58, 68	0
1	B	359/390 (92%)	1.14	61 (16%) 2 3	26, 40, 58, 71	0
All	All	717/780 (91%)	1.15	121 (16%) 2 3	25, 41, 58, 71	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	LEU	6.7
1	B	367	LYS	6.2
1	B	73	ASP	5.7
1	A	190	SER	4.6
1	B	308	GLU	4.6
1	B	74	ASP	4.4
1	A	267	LEU	4.3
1	A	79	LYS	4.2
1	B	64	LEU	4.2
1	B	145	MET	4.0
1	A	323	GLN	3.9
1	A	62	LEU	3.9
1	B	270	VAL	3.7
1	A	336	GLN	3.7
1	A	63	SER	3.7
1	A	55	ILE	3.5
1	A	57	VAL	3.5
1	B	63	SER	3.5
1	B	307	SER	3.5
1	A	4	GLN	3.5
1	A	122	PRO	3.5
1	A	358	LEU	3.5
1	A	307	SER	3.4
1	B	328	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	270	VAL	3.4
1	A	145	MET	3.3
1	A	15	MET	3.3
1	B	317	TYR	3.2
1	A	367	LYS	3.2
1	B	321	ASP	3.2
1	A	321	ASP	3.2
1	A	316	LEU	3.2
1	B	189	VAL	3.1
1	A	5	MET	3.1
1	B	305	GLY	3.1
1	A	360	GLY	3.1
1	B	320	ALA	3.1
1	A	319	GLU	3.0
1	B	4	GLN	3.0
1	A	95	LEU	3.0
1	B	263	PRO	3.0
1	A	192	PRO	3.0
1	B	195	THR	2.9
1	A	76	ALA	2.9
1	A	74	ASP	2.9
1	A	125	THR	2.9
1	B	5	MET	2.7
1	B	80	ARG	2.7
1	A	339	GLU	2.7
1	B	267	LEU	2.7
1	B	185	LEU	2.7
1	B	2	PRO	2.7
1	B	269	LYS	2.7
1	A	47	LYS	2.7
1	A	347	CYS	2.6
1	B	92	ILE	2.6
1	A	150	ASP	2.6
1	A	308	GLU	2.6
1	B	319	GLU	2.6
1	B	197	PHE	2.6
1	A	92	ILE	2.6
1	B	346	LEU	2.6
1	B	192	PRO	2.6
1	B	274	ILE	2.6
1	B	366	GLN	2.6
1	A	123	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	276	ASP	2.5
1	A	362	THR	2.5
1	B	315	ARG	2.5
1	A	346	LEU	2.5
1	B	180	PHE	2.5
1	A	54	VAL	2.5
1	B	190	SER	2.5
1	B	62	LEU	2.5
1	B	123	ASP	2.5
1	A	133	GLY	2.5
1	A	1	MET	2.4
1	A	136	LEU	2.4
1	A	53	THR	2.4
1	A	52	LEU	2.4
1	B	266	ARG	2.4
1	B	122	PRO	2.4
1	B	324	GLY	2.4
1	A	161	PHE	2.4
1	B	336	GLN	2.3
1	A	324	GLY	2.3
1	B	332	ALA	2.3
1	B	354	SER	2.3
1	A	300	ALA	2.3
1	B	310	VAL	2.3
1	A	134	LEU	2.2
1	B	164	VAL	2.2
1	B	312	THR	2.2
1	A	335	GLU	2.2
1	B	302	TYR	2.2
1	A	261	PHE	2.2
1	B	15	MET	2.2
1	A	22	GLU	2.2
1	B	169	ALA	2.2
1	B	261	PHE	2.2
1	B	222	LEU	2.2
1	A	318	GLU	2.2
1	A	337	VAL	2.2
1	A	298	PHE	2.2
1	B	136	LEU	2.2
1	A	305	GLY	2.1
1	B	141	HIS	2.1
1	A	209	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	355	VAL	2.1
1	A	49	ASN	2.1
1	B	11	ASP	2.1
1	B	273	ASP	2.1
1	B	161	PHE	2.1
1	A	340	LEU	2.1
1	B	358	LEU	2.1
1	B	100	LEU	2.1
1	B	339	GLU	2.1
1	A	126	VAL	2.1
1	A	274	ILE	2.0
1	B	363	TYR	2.0
1	B	47	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	3004	1/1	0.98	0.20	0.86	30,30,30,30	0
2	MG	B	4004	1/1	0.95	0.15	-0.25	29,29,29,29	0
3	721	B	4001	21/21	0.94	0.14	-0.36	25,32,34,36	0
3	721	A	3001	21/21	0.94	0.14	-0.68	24,28,32,35	0
2	MG	B	4003	1/1	0.85	0.08	-1.29	34,34,34,34	0
2	MG	A	3003	1/1	0.89	0.09	-2.15	33,33,33,33	0
2	MG	A	3002	1/1	0.76	0.17	-	29,29,29,29	0
2	MG	B	4002	1/1	0.96	0.19	-	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.