



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:07 pm GMT

PDB ID : 3IHK  
Title : Crystal Structure of thiamin pyrophosphokinase from S.mutans, Northeast Structural Genomics Consortium Target SmR83  
Authors : Kuzin,A.; Abashidze, M.; Seetharaman,J.; Vorobiev,S.; Mao,M.; Xiao,R.; Ciccocanti,C.; Maglaqui,M.; Foote,E.L.; Zhao,L.; Everett, J.K.; Nair, R.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt,J.F.; Tong,L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2009-07-30  
Resolution : 3.00 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.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

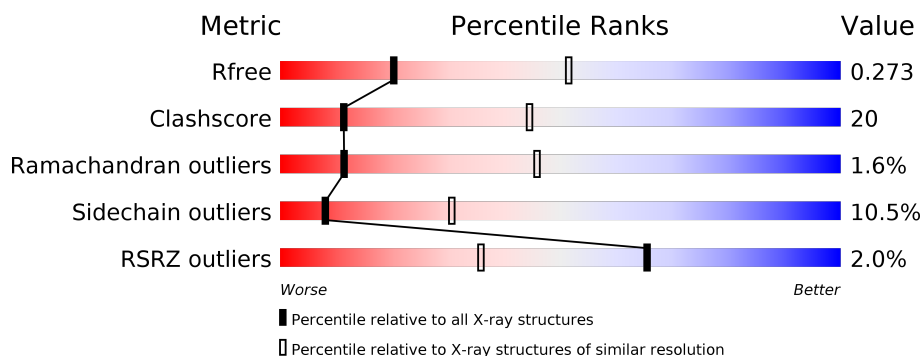
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	218	
1	B	218	
1	C	218	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	220	-	-	-	X
3	MG	B	219	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5108 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 thiamin pyrophosphokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	Se	0	0	0
			1644	1063	261	312	3	5			
1	B	208	Total	C	N	O	S	Se	0	0	0
			1655	1069	265	313	3	5			
1	C	207	Total	C	N	O	S	Se	0	0	0
			1644	1063	261	312	3	5			

There are 24 discrepancies between the modelled and reference sequences:

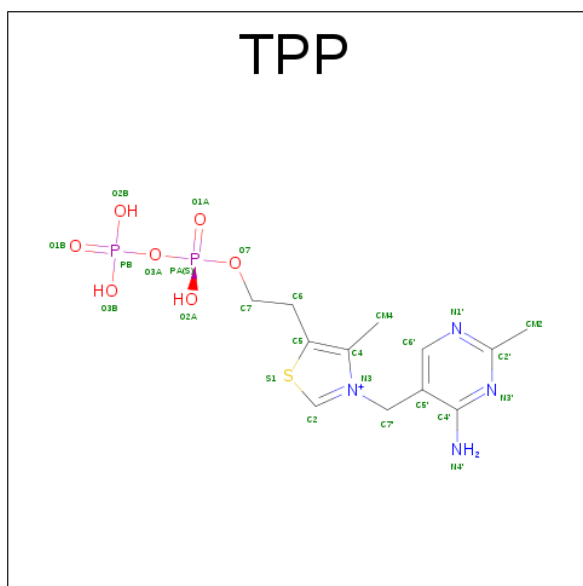
Chain	Residue	Modelled	Actual	Comment	Reference
A	211	LEU	-	expression tag	UNP Q8DVV9
A	212	GLU	-	expression tag	UNP Q8DVV9
A	213	HIS	-	expression tag	UNP Q8DVV9
A	214	HIS	-	expression tag	UNP Q8DVV9
A	215	HIS	-	expression tag	UNP Q8DVV9
A	216	HIS	-	expression tag	UNP Q8DVV9
A	217	HIS	-	expression tag	UNP Q8DVV9
A	218	HIS	-	expression tag	UNP Q8DVV9
B	211	LEU	-	expression tag	UNP Q8DVV9
B	212	GLU	-	expression tag	UNP Q8DVV9
B	213	HIS	-	expression tag	UNP Q8DVV9
B	214	HIS	-	expression tag	UNP Q8DVV9
B	215	HIS	-	expression tag	UNP Q8DVV9
B	216	HIS	-	expression tag	UNP Q8DVV9
B	217	HIS	-	expression tag	UNP Q8DVV9
B	218	HIS	-	expression tag	UNP Q8DVV9
C	211	LEU	-	expression tag	UNP Q8DVV9
C	212	GLU	-	expression tag	UNP Q8DVV9
C	213	HIS	-	expression tag	UNP Q8DVV9
C	214	HIS	-	expression tag	UNP Q8DVV9
C	215	HIS	-	expression tag	UNP Q8DVV9
C	216	HIS	-	expression tag	UNP Q8DVV9
C	217	HIS	-	expression tag	UNP Q8DVV9

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	218	HIS	-	expression tag	UNP Q8DVV9

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula:  $C_{12}H_{19}N_4O_7P_2S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

*Continued on next page...*

*Continued from previous page...*

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

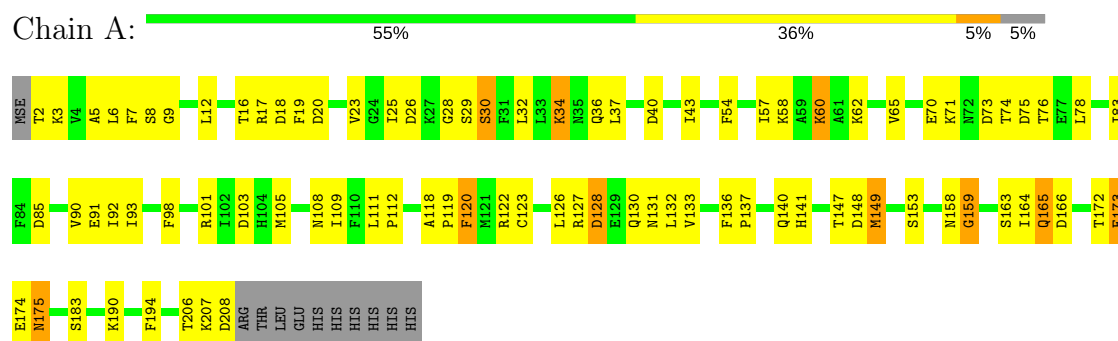
- Molecule 5 is water.

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

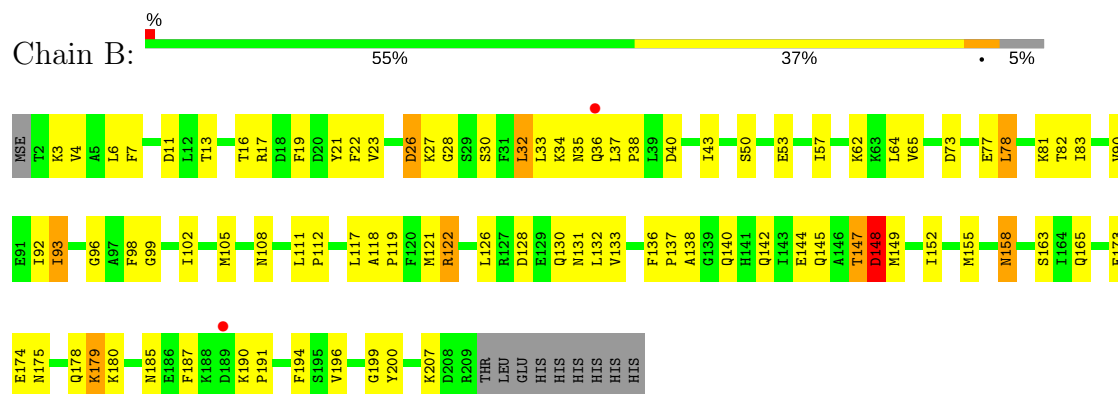
### 3 Residue-property plots [i](#)

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

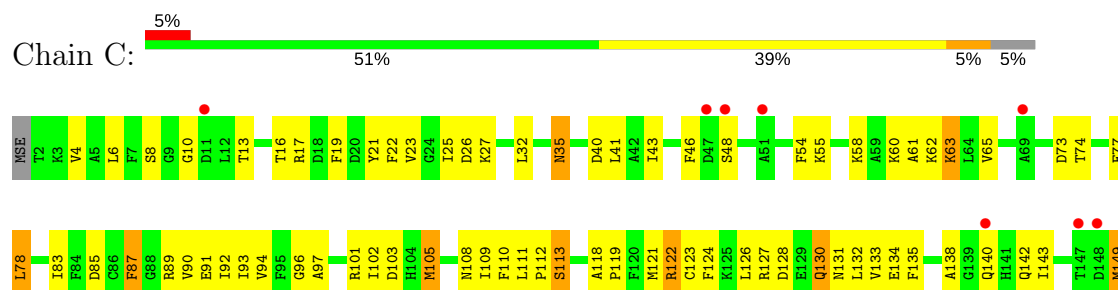
#### • Molecule 1: thiamin pyrophosphokinase



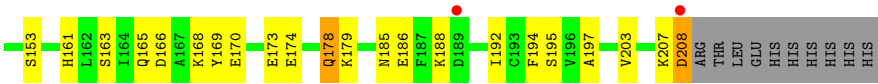
#### • Molecule 1: thiamin pyrophosphokinase



#### • Molecule 1: thiamin pyrophosphokinase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.16Å 105.16Å 121.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	84.3 (20.00-3.00) 99.1 (29.94-3.00)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 3.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.203 , 0.243 0.222 , 0.273	Depositor DCC
$R_{free}$ test set	806 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	5108	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 5.44% 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, 0.333 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: PO4, MG, TPP

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	0.51	0/1675	0.61	1/2249 (0.0%)
1	B	0.45	0/1686	0.60	0/2263
1	C	0.45	0/1675	0.59	0/2249
All	All	0.47	0/5036	0.60	1/6761 (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	159	GLY	N-CA-C	5.04	125.69	113.10

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	1644	0	1614	54	0
1	B	1655	0	1627	77	0
1	C	1644	0	1614	74	0
2	A	26	0	16	0	0
2	C	52	0	32	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2	0	0	0	0
4	A	30	0	0	0	0
4	B	30	0	0	0	0
4	C	20	0	0	0	0
5	A	1	0	0	0	0
All	All	5108	0	4903	198	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 20.

All (198) 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:B:23:VAL:HG21	1:B:83:ILE:HD11	1.34	1.07
1:B:98:PHE:HB3	1:B:105:MSE:HE2	1.47	0.94
1:A:23:VAL:HG21	1:A:83:ILE:HD11	1.48	0.92
1:C:165:GLN:HA	1:C:170:GLU:HG2	1.62	0.82
1:B:131:ASN:ND2	1:C:102:ILE:H	1.84	0.74
1:C:140:GLN:HA	1:C:195:SER:HB3	1.70	0.74
1:B:73:ASP:HB3	1:B:77:GLU:HB3	1.70	0.73
1:B:131:ASN:HD21	1:C:102:ILE:H	1.35	0.73
1:B:102:ILE:H	1:C:131:ASN:HD21	1.35	0.72
1:C:90:VAL:HG22	1:C:91:GLU:H	1.52	0.72
1:C:122:ARG:HA	1:C:122:ARG:HE	1.53	0.72
1:C:22:PHE:HB3	1:C:32:LEU:HD21	1.71	0.71
1:C:126:LEU:HB2	1:C:133:VAL:HB	1.72	0.71
1:A:149:MSE:HE2	1:A:206:THR:HA	1.73	0.70
1:A:147:THR:O	1:A:148:ASP:HB2	1.89	0.70
1:A:23:VAL:HG21	1:A:83:ILE:CD1	2.22	0.70
1:C:19:PHE:HE2	1:C:93:ILE:HD13	1.57	0.69
1:B:158:ASN:HD22	1:B:158:ASN:H	1.41	0.68
1:B:102:ILE:H	1:C:131:ASN:ND2	1.92	0.68
1:C:55:LYS:HA	1:C:58:LYS:HD3	1.76	0.67
1:A:126:LEU:HB2	1:A:133:VAL:HB	1.77	0.67
1:C:105:MSE:O	1:C:109:ILE:HG12	1.94	0.67
1:C:105:MSE:HE3	1:C:109:ILE:HG13	1.76	0.66
1:A:43:ILE:HG13	1:A:65:VAL:HB	1.77	0.65
1:C:149:MSE:HE2	1:C:207:LYS:HG2	1.79	0.65
1:C:97:ALA:HB1	1:C:108:ASN:HD22	1.63	0.64
1:C:163:SER:O	1:C:194:PHE:HA	1.97	0.64
1:C:130:GLN:NE2	1:C:208:ASP:HB2	2.13	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ALA:HB3	1:C:119:PRO:HD3	1.80	0.63
1:B:33:LEU:HD12	1:B:57:ILE:HD13	1.81	0.62
1:A:127:ARG:HD3	1:A:132:LEU:HD23	1.80	0.62
1:B:92:ILE:HG22	1:B:93:ILE:N	2.15	0.62
1:C:173:GLU:H	1:C:173:GLU:CD	2.02	0.62
1:A:108:ASN:HA	1:A:111:LEU:HG	1.80	0.62
1:B:4:VAL:HG11	1:B:83:ILE:HD13	1.82	0.62
1:B:174:GLU:HG2	1:B:175:ASN:H	1.64	0.61
1:B:98:PHE:HA	1:B:105:MSE:HG2	1.83	0.61
1:B:126:LEU:HB2	1:B:133:VAL:HB	1.83	0.60
1:A:98:PHE:HA	1:A:105:MSE:HG2	1.83	0.59
1:B:112:PRO:HB3	1:B:121:MSE:HE2	1.84	0.59
1:C:127:ARG:HD3	1:C:132:LEU:HD23	1.84	0.59
1:B:158:ASN:H	1:B:158:ASN:ND2	2.01	0.59
1:A:7:PHE:O	1:A:28:GLY:HA3	2.03	0.58
1:B:108:ASN:HA	1:B:111:LEU:HG	1.86	0.58
1:B:11:ASP:OD1	1:B:13:THR:HG23	2.03	0.58
1:B:43:ILE:HG13	1:B:65:VAL:HB	1.85	0.58
1:A:118:ALA:HB3	1:A:119:PRO:HD3	1.86	0.58
1:C:74:THR:HB	1:C:77:GLU:HG3	1.86	0.57
1:C:90:VAL:HG22	1:C:91:GLU:N	2.18	0.57
1:A:165:GLN:O	1:A:166:ASP:HB2	2.04	0.57
1:B:30:SER:HB3	1:B:34:LYS:HE3	1.86	0.57
1:B:112:PRO:HB2	1:B:200:TYR:CE2	2.41	0.56
1:B:40:ASP:HA	1:B:62:LYS:HG3	1.88	0.55
1:B:43:ILE:HD11	1:B:78:LEU:HD13	1.88	0.55
1:B:81:LYS:HG3	1:B:117:LEU:HD21	1.88	0.55
1:C:101:ARG:HB3	1:C:103:ASP:OD2	2.06	0.55
1:B:108:ASN:HB3	1:B:126:LEU:HD21	1.89	0.55
1:B:118:ALA:HB3	1:B:119:PRO:HD3	1.89	0.55
1:C:41:LEU:HA	1:C:63:LYS:O	2.06	0.55
1:C:122:ARG:HA	1:C:122:ARG:NE	2.22	0.54
1:C:35:ASN:N	1:C:35:ASN:HD22	2.04	0.54
1:B:145:GLN:HB2	1:B:187:PHE:CD2	2.43	0.54
1:B:163:SER:O	1:B:194:PHE:HA	2.07	0.54
1:A:71:LYS:HE2	1:A:73:ASP:O	2.08	0.53
1:B:144:GLU:OE2	1:B:191:PRO:HG3	2.07	0.53
1:B:148:ASP:HB2	1:B:207:LYS:NZ	2.22	0.53
1:C:108:ASN:HA	1:C:111:LEU:HG	1.90	0.53
1:C:43:ILE:HD11	1:C:78:LEU:HD12	1.90	0.53
1:A:120:PHE:N	1:A:120:PHE:CD1	2.77	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:MSE:HA	1:C:124:PHE:CE2	2.44	0.53
1:C:40:ASP:O	1:C:63:LYS:HB3	2.09	0.53
1:B:81:LYS:HG3	1:B:117:LEU:CD2	2.38	0.52
1:B:16:THR:HG22	1:B:17:ARG:H	1.74	0.52
1:A:90:VAL:O	1:A:123:CYS:HB3	2.08	0.52
1:A:29:SER:HB2	1:A:57:ILE:HD13	1.92	0.52
1:B:158:ASN:HD22	1:B:158:ASN:N	2.01	0.52
1:A:173:GLU:HG2	1:A:174:GLU:OE1	2.09	0.51
1:B:147:THR:O	1:B:149:MSE:N	2.43	0.51
1:C:92:ILE:HD12	1:C:92:ILE:N	2.24	0.51
1:B:30:SER:HB3	1:B:34:LYS:CE	2.41	0.51
1:B:138:ALA:HA	1:B:196:VAL:HG13	1.92	0.50
1:C:16:THR:HG22	1:C:17:ARG:H	1.77	0.50
1:A:16:THR:HG22	1:A:18:ASP:H	1.77	0.50
1:C:143:ILE:HD13	1:C:203:VAL:HG11	1.92	0.50
1:C:4:VAL:HG22	1:C:21:TYR:HB3	1.92	0.50
1:C:165:GLN:O	1:C:166:ASP:HB2	2.11	0.49
1:A:16:THR:HG22	1:A:17:ARG:N	2.26	0.49
1:B:138:ALA:HA	1:B:196:VAL:CG1	2.42	0.49
1:B:174:GLU:HG2	1:B:175:ASN:N	2.27	0.49
1:C:112:PRO:HG2	1:C:135:PHE:CG	2.47	0.49
1:B:30:SER:HB3	1:B:34:LYS:NZ	2.27	0.49
1:C:41:LEU:HD11	1:C:65:VAL:HG23	1.95	0.49
1:A:6:LEU:HD13	1:A:92:ILE:HG23	1.95	0.49
1:C:142:GLN:HA	1:C:192:ILE:O	2.13	0.49
1:A:92:ILE:O	1:A:93:ILE:HD12	2.13	0.48
1:B:102:ILE:HD12	1:C:105:MSE:SE	2.63	0.48
1:A:153:SER:HB3	1:A:183:SER:HA	1.94	0.48
1:B:33:LEU:CD1	1:B:57:ILE:HD13	2.44	0.48
1:C:21:TYR:HA	1:C:40:ASP:OD2	2.14	0.48
1:C:54:PHE:O	1:C:58:LYS:HG3	2.13	0.48
1:A:25:ILE:HG23	1:A:75:ASP:HB3	1.94	0.48
1:B:64:LEU:HD23	1:B:65:VAL:N	2.28	0.48
1:C:46:PHE:C	1:C:48:SER:H	2.17	0.48
1:B:155:MSE:HG3	1:B:180:LYS:O	2.14	0.47
1:B:4:VAL:HG22	1:B:21:TYR:HB3	1.96	0.47
1:C:27:LYS:HE2	1:C:48:SER:HB3	1.95	0.47
1:C:62:LYS:O	1:C:63:LYS:HB2	2.14	0.47
1:A:74:THR:HG22	1:A:76:THR:H	1.80	0.47
1:A:92:ILE:C	1:A:93:ILE:HD12	2.35	0.47
1:A:101:ARG:HB3	1:A:103:ASP:OD2	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:MSE:O	1:A:109:ILE:HG12	2.15	0.47
1:A:3:LYS:NZ	1:A:18:ASP:O	2.47	0.47
1:C:138:ALA:HB1	1:C:197:ALA:O	2.15	0.47
1:C:27:LYS:HG3	1:C:48:SER:HB2	1.96	0.47
1:A:137:PRO:O	1:A:141:HIS:CE1	2.68	0.46
1:C:90:VAL:O	1:C:123:CYS:HB3	2.16	0.46
1:C:83:ILE:O	1:C:87:PHE:HB2	2.16	0.46
1:B:7:PHE:O	1:B:28:GLY:HA3	2.15	0.46
1:B:92:ILE:HG22	1:B:93:ILE:H	1.78	0.46
1:B:98:PHE:HB3	1:B:105:MSE:CE	2.32	0.46
1:B:73:ASP:HA	1:B:77:GLU:OE1	2.16	0.46
1:A:54:PHE:O	1:A:58:LYS:HB2	2.17	0.45
1:A:163:SER:O	1:A:194:PHE:HA	2.16	0.45
1:A:2:THR:N	1:A:20:ASP:OD2	2.50	0.45
1:B:6:LEU:HD11	1:B:83:ILE:HD12	1.97	0.45
1:B:132:LEU:HB2	1:B:149:MSE:HE2	1.99	0.45
1:A:111:LEU:N	1:A:112:PRO:CD	2.80	0.45
1:A:6:LEU:HD13	1:A:92:ILE:CG2	2.47	0.45
1:C:128:ASP:OD1	1:C:131:ASN:HB2	2.17	0.45
1:B:158:ASN:ND2	1:B:158:ASN:N	2.63	0.45
1:B:22:PHE:HB2	1:B:38:PRO:O	2.16	0.45
1:A:149:MSE:HE3	1:A:207:LYS:N	2.32	0.45
1:B:111:LEU:N	1:B:112:PRO:CD	2.80	0.45
1:C:134:GLU:OE1	1:C:143:ILE:HD11	2.17	0.45
1:C:16:THR:HG22	1:C:17:ARG:N	2.32	0.45
1:B:35:ASN:O	1:B:37:LEU:HD13	2.17	0.45
1:C:8:SER:HA	1:C:25:ILE:HB	1.98	0.45
1:B:180:LYS:HG2	1:C:110:PHE:CG	2.52	0.44
1:C:10:GLY:HA3	1:C:96:GLY:O	2.18	0.44
1:C:127:ARG:HG3	1:C:128:ASP:N	2.32	0.44
1:A:174:GLU:N	1:A:174:GLU:OE1	2.51	0.44
1:B:152:ILE:HG23	1:B:185:ASN:HB3	1.99	0.44
1:C:178:GLN:O	1:C:179:LYS:HG2	2.17	0.44
1:B:50:SER:OG	1:B:53:GLU:HB2	2.18	0.44
1:C:149:MSE:HE3	1:C:149:MSE:HA	1.99	0.44
1:C:6:LEU:HG	1:C:25:ILE:HD11	1.99	0.44
1:C:61:ALA:C	1:C:63:LYS:H	2.21	0.44
1:A:190:LYS:HE2	1:A:190:LYS:HB3	1.87	0.44
1:B:17:ARG:HD3	1:B:37:LEU:HD11	2.00	0.44
1:C:130:GLN:NE2	1:C:207:LYS:O	2.51	0.44
1:B:122:ARG:HA	1:B:122:ARG:HE	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ILE:O	1:B:93:ILE:HG13	2.18	0.43
1:B:16:THR:HG22	1:B:17:ARG:N	2.33	0.43
1:B:112:PRO:HB2	1:B:200:TYR:CZ	2.54	0.43
1:C:110:PHE:O	1:C:113:SER:HB2	2.19	0.43
1:C:169:TYR:HB2	1:C:185:ASN:ND2	2.34	0.43
1:C:207:LYS:O	1:C:208:ASP:HB2	2.17	0.43
1:A:90:VAL:HG22	1:A:91:GLU:N	2.34	0.43
1:A:5:ALA:HB2	1:A:19:PHE:CG	2.54	0.43
1:A:153:SER:CB	1:A:183:SER:HA	2.49	0.42
1:B:11:ASP:O	1:B:96:GLY:HA2	2.19	0.42
1:A:175:ASN:O	1:A:175:ASN:ND2	2.53	0.42
1:C:19:PHE:HB2	1:C:22:PHE:CZ	2.55	0.42
1:B:144:GLU:HG2	1:B:191:PRO:HG3	2.01	0.42
1:C:168:LYS:HD3	1:C:169:TYR:CE2	2.54	0.42
1:A:16:THR:CG2	1:A:17:ARG:N	2.82	0.42
1:B:26:ASP:HB3	1:B:27:LYS:H	1.54	0.42
1:A:43:ILE:HD11	1:A:78:LEU:HD12	2.01	0.42
1:B:132:LEU:HB2	1:B:149:MSE:CE	2.50	0.42
1:B:145:GLN:HB2	1:B:187:PHE:CG	2.55	0.42
1:C:21:TYR:HE1	1:C:23:VAL:HG22	1.84	0.42
1:C:46:PHE:C	1:C:48:SER:N	2.73	0.42
1:A:136:PHE:HA	1:A:137:PRO:HD3	1.95	0.41
1:B:130:GLN:HB2	1:B:207:LYS:HG2	2.02	0.41
1:B:92:ILE:CG2	1:B:93:ILE:N	2.83	0.41
1:B:99:GLY:O	1:B:105:MSE:HE3	2.21	0.41
1:A:149:MSE:HE3	1:A:207:LYS:HB3	2.03	0.41
1:A:5:ALA:HB2	1:A:19:PHE:CD2	2.55	0.41
1:B:16:THR:HB	1:B:19:PHE:HE1	1.86	0.41
1:A:34:LYS:NZ	1:A:34:LYS:HB2	2.35	0.41
1:C:6:LEU:HB3	1:C:94:VAL:HG13	2.02	0.41
1:B:6:LEU:HD11	1:B:83:ILE:CD1	2.50	0.41
1:A:128:ASP:OD1	1:A:131:ASN:HB2	2.21	0.41
1:B:32:LEU:HA	1:B:32:LEU:HD12	1.87	0.41
1:B:78:LEU:HD22	1:B:82:THR:HG1	1.85	0.41
1:C:6:LEU:HD12	1:C:23:VAL:HB	2.03	0.41
1:A:172:THR:HB	1:A:174:GLU:OE1	2.21	0.41
1:C:168:LYS:HA	1:C:188:LYS:HD2	2.03	0.41
1:A:163:SER:C	1:A:164:ILE:HG13	2.41	0.41
1:A:30:SER:O	1:A:34:LYS:NZ	2.54	0.41
1:A:6:LEU:HD11	1:A:83:ILE:CD1	2.51	0.41
1:B:179:LYS:HE3	1:C:77:GLU:OE1	2.21	0.41

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:MSE:HB3	1:A:105:MSE:HE2	1.86	0.40
1:A:8:SER:OG	1:A:9:GLY:N	2.54	0.40
1:B:136:PHE:HA	1:B:137:PRO:HD3	1.92	0.40
1:C:111:LEU:N	1:C:112:PRO:CD	2.83	0.40
1:C:43:ILE:HG13	1:C:65:VAL:HB	2.04	0.40
1:B:138:ALA:HB2	1:B:199:GLY:O	2.22	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	205/218 (94%)	187 (91%)	16 (8%)	2 (1%)	18	59
1	B	206/218 (94%)	184 (89%)	17 (8%)	5 (2%)	7	34
1	C	205/218 (94%)	182 (89%)	20 (10%)	3 (2%)	12	48
All	All	616/654 (94%)	553 (90%)	53 (9%)	10 (2%)	11	46

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLY
1	B	148	ASP
1	C	87	PHE
1	A	60	LYS
1	B	147	THR
1	C	63	LYS
1	C	89	ARG
1	B	179	LYS
1	B	90	VAL
1	B	93	ILE

### 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	178/183 (97%)	155 (87%)	23 (13%)	5	22
1	B	179/183 (98%)	164 (92%)	15 (8%)	13	43
1	C	178/183 (97%)	160 (90%)	18 (10%)	9	33
All	All	535/549 (97%)	479 (90%)	56 (10%)	8	30

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	26	ASP
1	A	30	SER
1	A	32	LEU
1	A	34	LYS
1	A	36	GLN
1	A	37	LEU
1	A	40	ASP
1	A	60	LYS
1	A	62	LYS
1	A	70	GLU
1	A	85	ASP
1	A	120	PHE
1	A	122	ARG
1	A	128	ASP
1	A	130	GLN
1	A	140	GLN
1	A	149	MSE
1	A	158	ASN
1	A	165	GLN
1	A	173	GLU
1	A	175	ASN
1	A	208	ASP
1	B	3	LYS
1	B	26	ASP
1	B	32	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	36	GLN
1	B	78	LEU
1	B	122	ARG
1	B	128	ASP
1	B	140	GLN
1	B	142	GLN
1	B	148	ASP
1	B	158	ASN
1	B	165	GLN
1	B	173	GLU
1	B	178	GLN
1	B	190	LYS
1	C	13	THR
1	C	26	ASP
1	C	35	ASN
1	C	60	LYS
1	C	73	ASP
1	C	78	LEU
1	C	85	ASP
1	C	105	MSE
1	C	113	SER
1	C	122	ARG
1	C	130	GLN
1	C	149	MSE
1	C	153	SER
1	C	161	HIS
1	C	174	GLU
1	C	178	GLN
1	C	186	GLU
1	C	208	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	130	GLN
1	A	140	GLN
1	A	141	HIS
1	A	142	GLN
1	A	165	GLN
1	B	35	ASN
1	B	36	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	131	ASN
1	B	140	GLN
1	B	141	HIS
1	B	142	GLN
1	B	158	ASN
1	B	165	GLN
1	C	35	ASN
1	C	72	ASN
1	C	108	ASN
1	C	130	GLN
1	C	131	ASN
1	C	140	GLN
1	C	142	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 25 ligands modelled in this entry, 6 are monoatomic - leaving 19 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	PO4	A	221	-	4,4,4	1.23	0	6,6,6	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	PO4	A	222	-	4,4,4	1.25	0	6,6,6	0.41	0
4	PO4	A	223	-	4,4,4	1.34	0	6,6,6	0.37	0
4	PO4	A	224	-	4,4,4	1.26	0	6,6,6	0.40	0
4	PO4	A	225	-	4,4,4	1.29	0	6,6,6	0.37	0
4	PO4	A	226	-	4,4,4	1.26	0	6,6,6	0.39	0
2	TPP	A	902	3	21,27,27	2.99	4 (19%)	25,40,40	3.14	11 (44%)
4	PO4	B	221	-	4,4,4	1.25	0	6,6,6	0.38	0
4	PO4	B	222	-	4,4,4	1.28	0	6,6,6	0.39	0
4	PO4	B	223	-	4,4,4	1.24	0	6,6,6	0.40	0
4	PO4	B	224	-	4,4,4	1.30	0	6,6,6	0.38	0
4	PO4	B	225	-	4,4,4	1.24	0	6,6,6	0.38	0
4	PO4	B	226	-	4,4,4	1.20	0	6,6,6	0.38	0
2	TPP	C	219	-	21,27,27	2.95	3 (14%)	25,40,40	3.16	11 (44%)
4	PO4	C	222	-	4,4,4	1.20	0	6,6,6	0.40	0
4	PO4	C	223	-	4,4,4	1.22	0	6,6,6	0.40	0
4	PO4	C	224	-	4,4,4	1.21	0	6,6,6	0.40	0
4	PO4	C	225	-	4,4,4	1.29	0	6,6,6	0.40	0
2	TPP	C	902	-	21,27,27	2.94	3 (14%)	25,40,40	3.21	8 (32%)

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	PO4	A	221	-	-	0/0/0/0	0/0/0/0
4	PO4	A	222	-	-	0/0/0/0	0/0/0/0
4	PO4	A	223	-	-	0/0/0/0	0/0/0/0
4	PO4	A	224	-	-	0/0/0/0	0/0/0/0
4	PO4	A	225	-	-	0/0/0/0	0/0/0/0
4	PO4	A	226	-	-	0/0/0/0	0/0/0/0
2	TPP	A	902	3	-	0/16/17/17	0/2/2/2
4	PO4	B	221	-	-	0/0/0/0	0/0/0/0
4	PO4	B	222	-	-	0/0/0/0	0/0/0/0
4	PO4	B	223	-	-	0/0/0/0	0/0/0/0
4	PO4	B	224	-	-	0/0/0/0	0/0/0/0
4	PO4	B	225	-	-	0/0/0/0	0/0/0/0
4	PO4	B	226	-	-	0/0/0/0	0/0/0/0
2	TPP	C	219	-	-	0/16/17/17	0/2/2/2
4	PO4	C	222	-	-	0/0/0/0	0/0/0/0
4	PO4	C	223	-	-	0/0/0/0	0/0/0/0
4	PO4	C	224	-	-	0/0/0/0	0/0/0/0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PO4	C	225	-	-	0/0/0/0	0/0/0/0
2	TPP	C	902	-	-	0/16/17/17	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	902	TPP	C4-N3	-7.67	1.33	1.39
2	C	902	TPP	C4-N3	-7.01	1.33	1.39
2	C	219	TPP	C4-N3	-6.99	1.33	1.39
2	A	902	TPP	CM4-C4	2.02	1.54	1.49
2	C	219	TPP	C2'-N3'	7.20	1.47	1.34
2	A	902	TPP	C2'-N3'	7.20	1.47	1.34
2	C	902	TPP	C2'-N3'	7.21	1.47	1.34
2	A	902	TPP	C2'-N1'	7.37	1.46	1.34
2	C	902	TPP	C2'-N1'	7.74	1.47	1.34
2	C	219	TPP	C2'-N1'	7.87	1.47	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	TPP	N1'-C2'-N3'	-9.54	109.08	125.59
2	C	219	TPP	N1'-C2'-N3'	-9.33	109.44	125.59
2	C	902	TPP	CM2-C2'-N1'	-7.75	108.29	117.06
2	C	219	TPP	CM2-C2'-N1'	-7.62	108.44	117.06
2	A	902	TPP	N1'-C2'-N3'	-7.58	112.47	125.59
2	A	902	TPP	CM2-C2'-N1'	-6.78	109.39	117.06
2	A	902	TPP	CM2-C2'-N3'	-6.61	106.37	117.20
2	A	902	TPP	C2'-N3'-C4'	-6.02	107.77	118.16
2	C	219	TPP	CM2-C2'-N3'	-4.58	109.71	117.20
2	C	902	TPP	CM2-C2'-N3'	-4.23	110.28	117.20
2	C	902	TPP	C6'-N1'-C2'	-4.16	108.69	115.88
2	A	902	TPP	C5'-C4'-N4'	-4.11	116.24	122.22
2	C	902	TPP	C2'-N3'-C4'	-3.86	111.49	118.16
2	C	219	TPP	C2'-N3'-C4'	-3.73	111.72	118.16
2	C	219	TPP	C6'-N1'-C2'	-3.23	110.30	115.88
2	C	902	TPP	CM4-C4-C5	-3.13	121.23	127.29
2	C	219	TPP	CM4-C4-C5	-2.72	122.02	127.29
2	A	902	TPP	CM4-C4-C5	-2.28	122.88	127.29
2	C	219	TPP	C5'-C7'-N3	-2.19	109.67	113.33
2	C	219	TPP	C5'-C6'-N1'	-2.11	120.31	123.87
2	A	902	TPP	C6'-N1'-C2'	-2.10	112.25	115.88
2	A	902	TPP	C7'-C5'-C6'	-2.09	116.69	120.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	219	TPP	N4'-C4'-N3'	2.04	120.02	117.00
2	C	902	TPP	C6'-C5'-C4'	2.31	118.76	115.68
2	A	902	TPP	C7'-C5'-C4'	2.69	129.76	121.83
2	C	219	TPP	C6'-C5'-C4'	2.78	119.37	115.68
2	A	902	TPP	C5'-C4'-N3'	2.84	125.77	121.20
2	A	902	TPP	C5-C4-N3	2.95	113.47	107.57
2	C	219	TPP	C5-C4-N3	4.32	116.22	107.57
2	C	902	TPP	C5-C4-N3	4.44	116.46	107.57

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	202/218 (92%)	-0.23	0 <span>100</span> <span>100</span>	22, 37, 50, 56	0
1	B	203/218 (93%)	-0.18	2 (0%) <span>82</span> <span>58</span>	23, 38, 53, 58	0
1	C	202/218 (92%)	0.05	10 (4%) <span>30</span> <span>12</span>	31, 47, 65, 70	1 (0%)
All	All	607/654 (92%)	-0.12	12 (1%) <span>65</span> <span>36</span>	22, 41, 57, 70	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	189	ASP	3.8
1	B	36	GLN	3.7
1	C	48	SER	3.2
1	C	148	ASP	3.0
1	C	47	ASP	2.6
1	C	51	ALA	2.5
1	C	140	GLN	2.5
1	C	11	ASP	2.5
1	B	189	ASP	2.5
1	C	147	THR	2.5
1	C	69	ALA	2.4
1	C	208	ASP	2.4

### 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
3	MG	A	220	1/1	0.95	0.40	10.44	22,22,22,22	0
3	MG	B	219	1/1	0.97	0.24	3.36	2,2,2,2	0
4	PO4	B	221	5/5	0.82	0.29	0.83	76,77,77,78	0
4	PO4	C	223	5/5	0.79	0.29	0.73	74,74,75,75	0
2	TPP	C	219	26/26	0.85	0.23	0.08	42,52,78,78	0
2	TPP	A	902	26/26	0.93	0.20	-0.08	31,35,64,66	0
4	PO4	C	225	5/5	0.89	0.21	-0.49	93,93,93,94	0
4	PO4	A	226	5/5	0.93	0.17	-0.76	77,77,78,78	0
2	TPP	C	902	26/26	0.94	0.14	-1.29	35,38,54,54	0
4	PO4	A	221	5/5	0.86	0.21	-	72,74,74,74	0
4	PO4	B	222	5/5	0.93	0.29	-	71,71,72,73	0
3	MG	C	221	1/1	0.75	0.14	-	40,40,40,40	0
3	MG	B	220	1/1	0.67	0.14	-	18,18,18,18	0
4	PO4	B	225	5/5	0.85	0.39	-	76,76,77,77	0
4	PO4	B	224	5/5	0.76	0.33	-	72,73,74,74	0
4	PO4	A	222	5/5	0.92	0.23	-	54,55,56,57	0
4	PO4	C	224	5/5	0.89	0.45	-	78,79,80,80	0
3	MG	A	219	1/1	0.95	0.23	-	19,19,19,19	0
4	PO4	A	224	5/5	0.78	0.36	-	81,81,82,82	0
4	PO4	A	225	5/5	0.83	0.44	-	83,83,84,85	0
4	PO4	B	223	5/5	0.93	0.24	-	80,81,81,82	0
3	MG	C	220	1/1	0.85	0.21	-	48,48,48,48	0
4	PO4	C	222	5/5	0.89	0.25	-	77,78,78,79	0
4	PO4	B	226	5/5	0.83	0.47	-	86,86,87,88	0
4	PO4	A	223	5/5	0.90	0.39	-	67,67,68,69	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.