



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:26 am GMT

PDB ID : 3DYF  
Title : T. Brucei Farnesyl Diphosphate Synthase Complexed with Bisphosphonate BPH-461 and Isopentyl Diphosphate  
Authors : Cao, R.; Gao, Y.; Robinson, H.; Goddard, A.; Oldfield, E.  
Deposited on : 2008-07-27  
Resolution : 2.65 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 : 1.7.2 (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

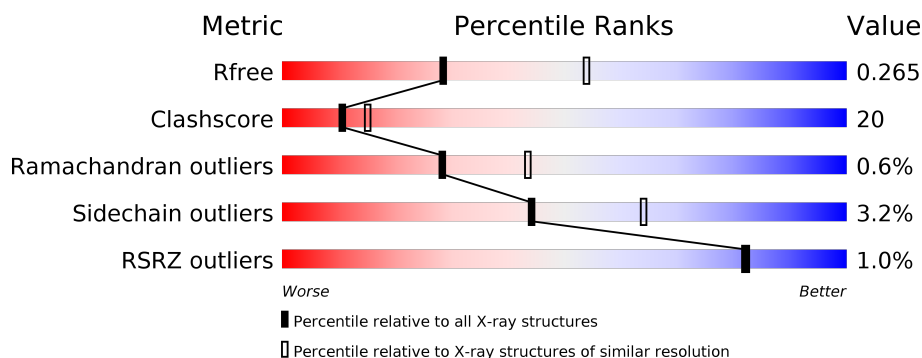
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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>%</div> <div> <div></div> <div>59%</div> <div>31%</div> <div>8%</div> </div> </div>
1	B	390	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>31%</div> <div>8%</div> </div> </div>

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
2	MG	B	4004	-	-	-	X
4	NI9	B	4001	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6117 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	357	Total	C	N	O	S	0	0	0
			2862	1823	472	539	28			
1	B	358	Total	C	N	O	S	0	0	0
			2871	1829	473	541	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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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).

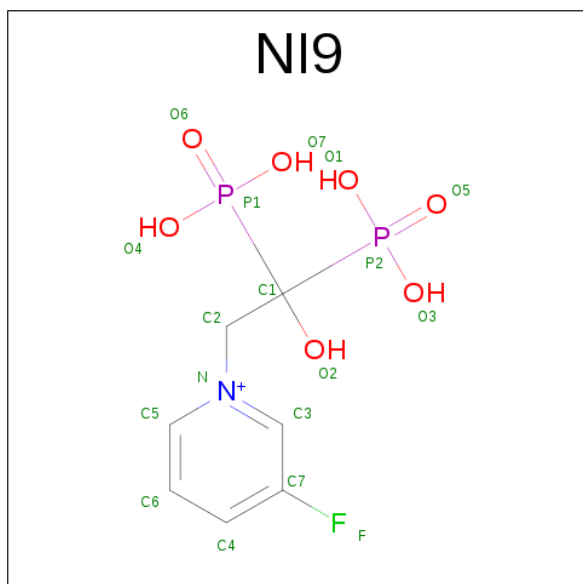
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	3	Total Mg 3 3	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



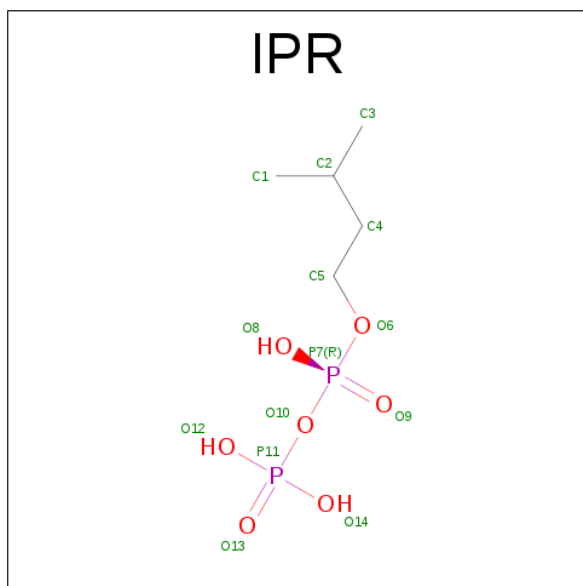
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 3-FLUORO-1-(2-HYDROXY-2,2-DIPHOSPHONOETHYL)PYRIDINIUM (three-letter code: NI9) (formula:  $C_7H_{11}FNO_7P_2$ ).



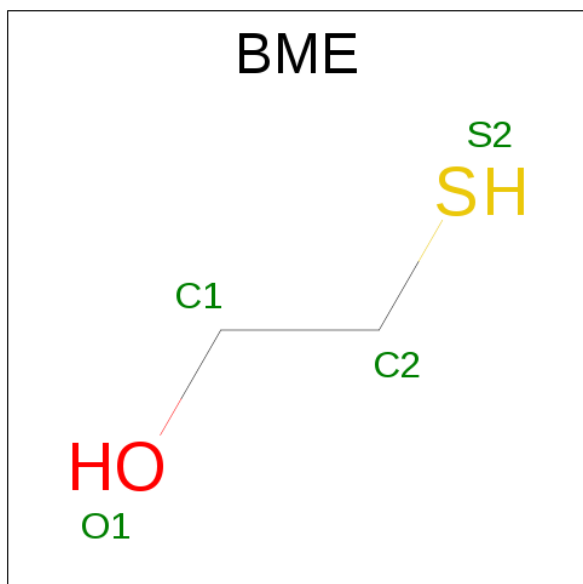
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	P	0	0
			18	7	1	1	7	2		
4	B	1	Total	C	F	N	O	P	0	0
			18	7	1	1	7	2		

- Molecule 5 is ISOPENTYL PYROPHOSPHATE (three-letter code: IPR) (formula:  $C_5H_{14}O_7P_2$ ).



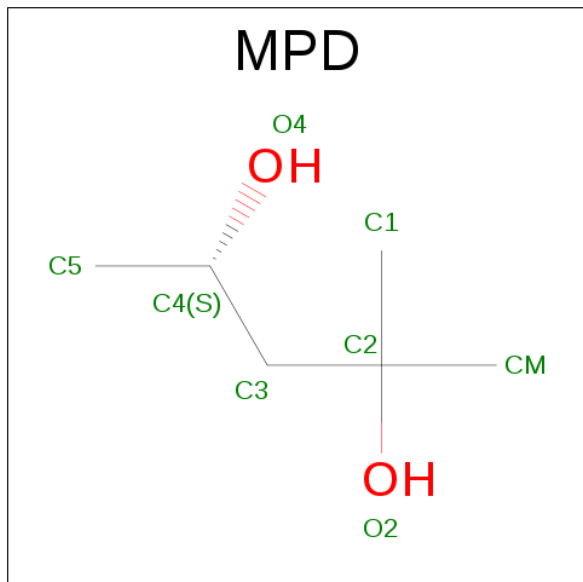
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			14	5	7	2		
5	B	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 6 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	143	Total	O	0	0
			143	143		
8	B	155	Total	O	0	0
			155	155		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.94Å 117.90Å 63.27Å 90.00° 111.27° 90.00°	Depositor
Resolution (Å)	29.48 – 2.65 29.48 – 2.64	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.48-2.65) 94.8 (29.48-2.64)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.89 (at 2.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.201 , 0.268 0.197 , 0.265	Depositor DCC
$R_{free}$ test set	1244 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.2	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6117	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 6.73% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BME, MPD, IPR, NI9, ACT

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	0.33	0/2921	0.53	0/3950
1	B	0.33	0/2930	0.53	0/3961
All	All	0.33	0/5851	0.53	0/7911

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	2862	0	2821	127	0
1	B	2871	0	2832	130	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	3	0	0
4	A	18	0	7	1	0
4	B	18	0	7	1	0
5	A	14	0	10	1	0
5	B	14	0	10	1	0
6	B	4	0	6	2	0
7	A	8	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	143	0	0	13	0
8	B	155	0	0	19	0
All	All	6117	0	5710	236	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 (236) 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:365:ARG:HB2	1:A:367:LYS:HE2	1.42	0.99
1:B:127:GLN:H	1:B:127:GLN:HE21	0.96	0.96
1:A:367:LYS:HZ2	1:A:367:LYS:HA	1.32	0.92
1:B:127:GLN:N	1:B:127:GLN:HE21	1.75	0.84
1:B:127:GLN:H	1:B:127:GLN:NE2	1.75	0.83
1:B:191:GLN:HG3	1:B:192:PRO:HD2	1.63	0.81
1:A:1:MET:O	1:A:4:GLN:HG2	1.81	0.81
1:A:123:ASP:HB2	1:B:186:ASP:O	1.82	0.79
1:A:37:LYS:HD2	1:B:187:PRO:HD2	1.63	0.78
1:A:47:LYS:HE3	1:A:367:LYS:HE3	1.65	0.77
1:A:367:LYS:NZ	1:A:367:LYS:HA	1.99	0.77
1:A:127:GLN:H	1:A:127:GLN:NE2	1.84	0.75
1:A:301:ASN:ND2	1:A:312:THR:HG21	2.02	0.75
1:A:187:PRO:HG3	1:B:37:LYS:HG2	1.66	0.75
1:A:230:GLU:HA	8:A:5246:HOH:O	1.87	0.73
1:A:1:MET:N	1:A:2:PRO:HD2	2.02	0.73
1:A:189:VAL:O	1:B:123:ASP:HB2	1.88	0.73
1:A:167:THR:HG22	1:B:25:PHE:CE1	2.24	0.72
1:A:306:ASP:OD1	1:A:308:GLU:HG2	1.88	0.72
1:A:297:GLU:HG2	1:A:316:LEU:HD11	1.71	0.71
1:B:115:LYS:HB3	1:B:116:PRO:HD2	1.73	0.71
1:B:176:VAL:HG13	1:B:177:THR:HG23	1.72	0.70
1:A:25:PHE:HE1	1:B:167:THR:HG22	1.56	0.70
1:A:15:MET:O	1:A:19:GLU:HG3	1.92	0.69
1:B:163:ARG:O	1:B:167:THR:HG23	1.92	0.69
1:A:127:GLN:H	1:A:127:GLN:HE21	1.40	0.69
8:A:5068:HOH:O	1:B:106:MET:HE1	1.92	0.68
1:B:156:ASP:O	1:B:160:ARG:HG3	1.92	0.68
1:B:159:CYS:HG	6:B:9001:BME:HS2	0.70	0.68
1:A:122:PRO:HB3	1:B:190:SER:HB3	1.76	0.67
1:B:10:TYR:HB2	1:B:90:TRP:CZ2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASP:O	1:B:32:VAL:HG23	1.96	0.66
1:A:167:THR:HG22	1:B:25:PHE:HE1	1.60	0.66
1:A:232:LEU:HB3	1:A:233:PRO:HD3	1.77	0.65
1:A:187:PRO:CG	1:B:37:LYS:HG2	2.26	0.65
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.61	0.65
1:B:125:THR:HB	1:B:127:GLN:HE22	1.62	0.65
1:B:83:HIS:HD2	8:B:5163:HOH:O	1.80	0.64
1:B:220:LEU:HB3	1:B:221:PRO:HD3	1.78	0.64
1:A:186:ASP:O	1:B:123:ASP:HB2	1.96	0.64
1:A:12:GLU:OE1	1:A:83:HIS:HE1	1.81	0.63
1:A:157:LEU:HD21	1:A:224:MET:HE2	1.79	0.63
1:A:10:TYR:HB2	1:A:90:TRP:CZ2	2.33	0.63
1:A:209:VAL:HG22	1:A:252:GLN:HG2	1.82	0.62
1:B:267:LEU:HG	1:B:269:LYS:HG2	1.81	0.61
1:A:338:LYS:HE2	8:A:5279:HOH:O	1.99	0.61
1:A:366:GLN:O	1:A:367:LYS:HB2	2.00	0.61
1:B:266:ARG:HD3	8:B:5292:HOH:O	2.00	0.61
1:A:163:ARG:O	1:A:167:THR:HG23	2.00	0.61
1:B:254:GLN:O	1:B:258:MET:HG3	2.00	0.61
1:B:332:ALA:O	1:B:335:GLU:HB3	2.01	0.61
1:B:117:CYS:HB2	1:B:120:ARG:HG3	1.81	0.61
1:A:367:LYS:HD2	1:A:367:LYS:N	2.15	0.61
1:A:187:PRO:HA	1:B:123:ASP:HB3	1.83	0.60
1:A:243:LEU:HD21	1:A:340:LEU:HB2	1.84	0.59
1:A:317:TYR:O	1:A:322:LEU:HD23	2.02	0.59
1:B:52:LEU:HD12	8:B:5295:HOH:O	2.03	0.59
1:B:186:ASP:HA	8:B:5286:HOH:O	2.01	0.59
1:A:50:ARG:HD3	1:A:217:THR:HA	1.84	0.59
1:B:209:VAL:HG11	1:B:249:GLU:HA	1.85	0.58
1:A:176:VAL:HG21	1:B:127:GLN:HG2	1.85	0.58
1:A:106:MET:HA	1:B:127:GLN:HB2	1.84	0.58
1:B:323:GLN:O	1:B:327:VAL:HG23	2.03	0.58
1:A:22:GLU:CG	1:A:32:VAL:HG21	2.34	0.58
1:B:62:LEU:HD23	1:B:78:ARG:NH1	2.19	0.58
1:A:25:PHE:CE1	1:B:167:THR:HG22	2.37	0.58
1:B:102:GLU:C	1:B:106:MET:HE2	2.24	0.58
1:A:37:LYS:HE3	8:B:5286:HOH:O	2.02	0.57
1:B:145:MET:HE3	8:B:5058:HOH:O	2.05	0.57
1:A:167:THR:HG21	7:A:7001:MPD:H12	1.86	0.57
1:A:166:TYR:OH	1:B:21:LEU:HD21	2.05	0.57
1:B:50:ARG:HH21	5:B:6002:IPR:HC12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:HB3	8:B:5175:HOH:O	2.04	0.56
1:A:242:GLU:HB3	8:A:5272:HOH:O	2.06	0.55
1:B:98:HIS:HD2	1:B:133:GLY:O	1.88	0.55
1:A:1:MET:H2	1:A:2:PRO:HD2	1.69	0.55
1:A:200:PHE:CE2	1:A:279:CYS:HA	2.40	0.55
1:B:49:ASN:HB2	8:B:5275:HOH:O	2.05	0.55
1:B:304:SER:OG	1:B:309:LYS:HD2	2.06	0.55
1:B:4:GLN:HG3	8:B:5191:HOH:O	2.06	0.55
1:A:209:VAL:HG11	1:A:249:GLU:HA	1.88	0.55
1:B:160:ARG:HD3	1:B:227:ILE:HD11	1.87	0.55
1:A:365:ARG:HD2	1:A:367:LYS:CE	2.36	0.55
1:B:62:LEU:O	1:B:63:SER:HB3	2.06	0.54
1:A:315:ARG:HD3	1:A:319:GLU:OE2	2.07	0.54
1:B:339:GLU:HG3	8:B:5204:HOH:O	2.08	0.54
1:A:115:LYS:HG2	1:A:116:PRO:HD2	1.91	0.53
1:A:314:ARG:HD2	8:A:5257:HOH:O	2.08	0.53
1:A:126:VAL:O	1:A:130:ILE:HG13	2.08	0.53
1:A:1:MET:N	1:A:2:PRO:CD	2.72	0.53
1:A:117:CYS:O	1:A:120:ARG:HB2	2.09	0.52
1:A:1:MET:H3	1:A:2:PRO:HD2	1.74	0.52
1:A:259:ASP:OD1	1:A:271:GLY:HA2	2.09	0.52
1:B:277:ALA:HA	1:B:302:TYR:CE2	2.44	0.52
1:A:182:SER:HA	1:A:185:LEU:HB2	1.92	0.52
1:A:186:ASP:O	1:B:123:ASP:CB	2.58	0.52
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.24	0.51
1:B:184:LYS:HG2	1:B:191:GLN:OE1	2.10	0.51
1:A:209:VAL:CG1	1:A:249:GLU:HA	2.41	0.51
1:A:236:ASP:CG	1:A:239:VAL:HG23	2.31	0.51
1:B:59:GLU:HG3	1:B:82:LEU:HD21	1.92	0.51
1:B:242:GLU:HG2	8:B:5145:HOH:O	2.11	0.51
1:B:351:PHE:O	1:B:355:VAL:HG23	2.11	0.51
1:A:78:ARG:HD2	8:A:5269:HOH:O	2.10	0.51
1:B:261:PHE:HE1	1:B:314:ARG:HG3	1.75	0.51
1:B:159:CYS:SG	6:B:9001:BME:S2	2.72	0.51
1:A:266:ARG:HH11	1:A:266:ARG:HG2	1.77	0.50
1:B:283:ALA:O	1:B:287:LEU:HG	2.10	0.50
1:B:103:ASP:HA	1:B:106:MET:HE3	1.94	0.50
1:B:125:THR:HB	1:B:127:GLN:NE2	2.25	0.50
1:B:133:GLY:HA2	1:B:136:LEU:HD12	1.93	0.50
1:B:62:LEU:O	1:B:63:SER:CB	2.60	0.50
1:B:295:VAL:O	1:B:298:PHE:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:THR:HG21	7:A:7001:MPD:C1	2.42	0.50
1:B:9:VAL:HG21	1:B:86:CYS:CB	2.41	0.50
1:B:126:VAL:HG12	8:B:5090:HOH:O	2.10	0.50
1:B:317:TYR:HB3	1:B:322:LEU:HD12	1.94	0.50
8:A:5070:HOH:O	1:B:26:ASP:HB2	2.11	0.50
1:A:206:LYS:HG2	1:A:249:GLU:OE2	2.12	0.49
1:A:236:ASP:OD1	1:A:239:VAL:HG23	2.12	0.49
1:A:238:GLY:O	1:A:242:GLU:HG3	2.13	0.49
1:A:365:ARG:NH1	1:A:367:LYS:HD3	2.27	0.49
1:A:96:GLN:O	1:A:100:LEU:HG	2.12	0.49
1:B:208:ILE:O	1:B:212:LYS:HG2	2.13	0.49
1:A:366:GLN:C	1:A:367:LYS:HD2	2.33	0.49
1:B:241:GLU:O	1:B:245:MET:HG2	2.12	0.49
1:A:365:ARG:CB	1:A:367:LYS:HE2	2.30	0.49
1:B:102:GLU:O	1:B:106:MET:HE2	2.13	0.49
1:B:358:LEU:O	1:B:358:LEU:HD22	2.12	0.49
1:A:9:VAL:O	1:A:13:ILE:HG13	2.13	0.49
1:B:209:VAL:HG13	1:B:252:GLN:CB	2.42	0.49
1:A:289:LYS:HB3	8:A:5176:HOH:O	2.13	0.49
1:A:337:VAL:O	1:A:341:ILE:HG13	2.13	0.48
1:A:83:HIS:HD2	8:A:5071:HOH:O	1.96	0.48
1:B:209:VAL:CG1	1:B:249:GLU:HA	2.42	0.48
1:B:61:LEU:O	1:B:63:SER:N	2.47	0.48
1:A:220:LEU:HB3	1:A:221:PRO:HD3	1.94	0.48
1:B:286:PHE:HZ	1:B:294:GLN:HB3	1.78	0.48
1:B:57:VAL:O	1:B:61:LEU:HD23	2.13	0.48
1:B:254:GLN:OE1	1:B:365:ARG:HD3	2.14	0.48
1:B:258:MET:CE	1:B:367:LYS:HA	2.44	0.48
1:A:57:VAL:O	1:A:61:LEU:HD13	2.14	0.48
1:B:295:VAL:HG12	1:B:299:LYS:HE3	1.96	0.47
1:A:123:ASP:CB	1:B:189:VAL:O	2.63	0.47
1:A:323:GLN:O	1:A:327:VAL:HG23	2.14	0.47
1:A:365:ARG:HD2	1:A:367:LYS:HE2	1.96	0.47
1:B:230:GLU:HA	8:B:5062:HOH:O	2.14	0.47
1:B:53:THR:O	1:B:57:VAL:HG23	2.14	0.47
1:A:226:LEU:HB3	1:A:232:LEU:HA	1.96	0.47
1:B:62:LEU:HD23	1:B:78:ARG:HG3	1.96	0.47
1:A:266:ARG:HG2	1:A:266:ARG:NH1	2.28	0.47
1:B:98:HIS:CD2	1:B:137:LYS:HB2	2.49	0.47
1:B:58:ALA:HA	1:B:229:SER:OG	2.15	0.47
1:A:102:GLU:O	1:A:106:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:SER:HB3	8:A:5106:HOH:O	2.15	0.47
1:A:164:VAL:HG13	1:A:215:TYR:HB3	1.97	0.47
1:B:126:VAL:O	1:B:130:ILE:HG13	2.15	0.46
1:A:367:LYS:NZ	1:A:367:LYS:CA	2.76	0.46
1:A:98:HIS:HD2	1:A:133:GLY:O	1.98	0.46
1:B:36:ARG:HG2	1:B:36:ARG:HH11	1.80	0.46
1:B:98:HIS:O	1:B:102:GLU:HG2	2.16	0.46
1:A:160:ARG:HD2	1:A:227:ILE:HD11	1.97	0.46
1:A:102:GLU:OE2	1:A:133:GLY:HA3	2.16	0.46
1:B:260:CYS:SG	1:B:314:ARG:HD3	2.56	0.46
1:A:12:GLU:OE1	1:A:83:HIS:CE1	2.65	0.46
1:B:59:GLU:O	1:B:62:LEU:N	2.49	0.46
1:A:47:LYS:HB2	8:A:5022:HOH:O	2.15	0.45
1:B:275:GLN:NE2	8:B:5179:HOH:O	2.44	0.45
1:A:113:ARG:HA	8:A:5244:HOH:O	2.16	0.45
1:A:153:PHE:CD1	1:A:153:PHE:C	2.90	0.45
1:A:123:ASP:HB2	1:B:189:VAL:O	2.17	0.45
1:B:62:LEU:CD2	1:B:78:ARG:HG3	2.47	0.45
1:A:187:PRO:CA	1:B:123:ASP:HB3	2.47	0.45
1:A:123:ASP:CB	1:B:186:ASP:O	2.60	0.45
1:A:98:HIS:CD2	1:A:137:LYS:HB2	2.53	0.44
1:A:160:ARG:CD	1:A:227:ILE:HD11	2.48	0.44
1:A:74:ASP:CG	1:A:75:GLY:N	2.70	0.44
1:B:218:TYR:CD2	1:B:358:LEU:HD11	2.51	0.44
1:A:137:LYS:O	1:A:140:THR:OG1	2.33	0.44
1:B:235:VAL:HG23	8:B:5194:HOH:O	2.17	0.44
1:B:235:VAL:HG22	1:B:236:ASP:N	2.32	0.44
1:B:21:LEU:HA	1:B:25:PHE:HB2	1.99	0.44
1:A:9:VAL:O	1:A:12:GLU:HB3	2.17	0.44
1:A:162:ASN:HD22	1:B:141:HIS:CG	2.35	0.44
1:B:323:GLN:HG2	8:B:5250:HOH:O	2.18	0.44
1:B:160:ARG:CD	1:B:227:ILE:HD11	2.48	0.43
1:B:229:SER:O	1:B:230:GLU:HB2	2.18	0.43
1:B:9:VAL:HG21	1:B:86:CYS:HB3	1.99	0.43
1:A:96:GLN:HG3	1:A:216:TYR:HE2	1.83	0.43
4:A:3001:NI9:H21	5:A:6001:IPR:HC42	2.00	0.43
1:B:246:LEU:HD11	1:B:333:VAL:HG13	2.00	0.43
1:B:145:MET:HB2	1:B:145:MET:HE3	1.81	0.43
1:B:110:VAL:HA	1:B:120:ARG:HD3	2.00	0.43
1:B:261:PHE:CE1	1:B:314:ARG:HG3	2.54	0.43
1:A:14:GLN:HG3	1:A:39:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PHE:CD1	1:B:153:PHE:C	2.92	0.43
1:A:179:MET:CE	1:A:278:LYS:HD3	2.48	0.43
1:A:1:MET:HG3	1:A:2:PRO:CD	2.49	0.43
1:B:258:MET:HE2	1:B:367:LYS:HA	2.01	0.42
1:A:181:ASP:OD1	1:A:183:ASN:HB2	2.20	0.42
1:A:28:ASP:OD1	1:A:30:ASN:HB2	2.19	0.42
1:A:346:LEU:HA	1:A:346:LEU:HD12	1.88	0.42
1:B:137:LYS:HE3	8:B:5267:HOH:O	2.19	0.42
1:B:92:ILE:HD11	1:B:224:MET:SD	2.59	0.42
1:A:1:MET:HG3	1:A:2:PRO:HD3	2.02	0.42
1:A:262:THR:HA	1:A:263:PRO:HD2	1.91	0.42
1:A:96:GLN:HE21	1:A:96:GLN:HB3	1.55	0.42
1:B:345:ARG:NH1	8:B:5092:HOH:O	2.44	0.42
1:B:112:ARG:NH2	4:B:4001:NI9:O1	2.42	0.42
1:A:98:HIS:CE1	1:A:137:LYS:HE3	2.54	0.42
1:B:141:HIS:HB3	8:B:5058:HOH:O	2.19	0.42
1:B:286:PHE:CZ	1:B:294:GLN:HB3	2.55	0.42
1:A:209:VAL:HG22	1:A:252:GLN:CG	2.48	0.42
1:A:123:ASP:OD2	1:B:189:VAL:O	2.37	0.42
1:A:10:TYR:HB2	1:A:90:TRP:CE2	2.55	0.41
1:B:297:GLU:HG2	1:B:316:LEU:HD11	2.01	0.41
1:A:327:VAL:HG13	8:A:5049:HOH:O	2.20	0.41
1:B:132:ASP:HA	1:B:135:LEU:HD12	2.01	0.41
1:B:251:PHE:CE1	1:B:365:ARG:CZ	3.03	0.41
1:A:176:VAL:O	1:A:176:VAL:HG22	2.21	0.41
1:A:263:PRO:HA	1:A:264:PRO:HD2	1.91	0.41
1:A:277:ALA:HA	1:A:302:TYR:CE2	2.55	0.41
1:B:344:LEU:O	1:B:345:ARG:C	2.59	0.41
1:A:205:TYR:CZ	1:A:209:VAL:HG21	2.55	0.41
1:B:156:ASP:OD1	1:B:160:ARG:NH1	2.53	0.41
1:A:111:THR:OG1	1:A:269:LYS:HA	2.22	0.40
1:B:133:GLY:O	1:B:136:LEU:HB2	2.21	0.40
1:B:18:LEU:HD11	1:B:36:ARG:HB2	2.03	0.40
1:B:337:VAL:O	1:B:341:ILE:HG13	2.22	0.40
1:A:239:VAL:HG13	1:A:340:LEU:HD22	2.04	0.40
1:B:204:ASN:O	1:B:208:ILE:HG13	2.22	0.40
1:B:218:TYR:O	1:B:222:LEU:HG	2.22	0.40
1:A:251:PHE:HA	1:A:254:GLN:OE1	2.21	0.40
1:B:276:ASP:HB3	1:B:278:LYS:HE2	2.04	0.40
1:A:50:ARG:NH1	1:A:216:TYR:CE2	2.89	0.40
1:B:167:THR:O	1:B:170:VAL:HB	2.20	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	353/390 (90%)	334 (95%)	17 (5%)	2 (1%)	28	43
1	B	354/390 (91%)	330 (93%)	22 (6%)	2 (1%)	28	43
All	All	707/780 (91%)	664 (94%)	39 (6%)	4 (1%)	28	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	SER
1	A	185	LEU
1	B	62	LEU
1	A	198	ALA

### 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	312/340 (92%)	300 (96%)	12 (4%)	38	57
1	B	313/340 (92%)	305 (97%)	8 (3%)	51	72
All	All	625/680 (92%)	605 (97%)	20 (3%)	44	64

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	123	ASP
1	A	127	GLN
1	A	153	PHE
1	A	185	LEU
1	A	188	ASP
1	A	265	GLU
1	A	325	ASP
1	A	335	GLU
1	A	338	LYS
1	A	346	LEU
1	A	367	LYS
1	B	62	LEU
1	B	77	ARG
1	B	100	LEU
1	B	115	LYS
1	B	127	GLN
1	B	191	GLN
1	B	275	GLN
1	B	358	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	49	ASN
1	A	83	HIS
1	A	96	GLN
1	A	98	HIS
1	A	127	GLN
1	A	141	HIS
1	A	146	HIS
1	A	162	ASN
1	A	172	GLN
1	A	183	ASN
1	A	204	ASN
1	A	252	GLN
1	A	301	ASN
1	A	323	GLN
1	A	336	GLN
1	B	30	ASN
1	B	49	ASN
1	B	83	HIS

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Mol	Chain	Res	Type
1	B	98	HIS
1	B	127	GLN
1	B	204	ASN
1	B	275	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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	NI9	A	3001	2	17,18,18	1.44	3 (17%)	25,29,29	1.44	4 (16%)
5	IPR	A	6001	-	12,13,13	1.15	1 (8%)	13,19,19	1.82	5 (38%)
7	MPD	A	7001	-	7,7,7	0.52	0	9,10,10	0.39	0
3	ACT	A	8001	-	1,3,3	1.69	0	0,3,3	0.00	-
4	NI9	B	4001	2	17,18,18	1.30	2 (11%)	25,29,29	1.64	5 (20%)
5	IPR	B	6002	-	12,13,13	1.18	1 (8%)	13,19,19	1.81	5 (38%)
6	BME	B	9001	-	3,3,3	0.47	0	2,2,2	0.49	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	NI9	A	3001	2	-	0/23/23/23	0/1/1/1
5	IPR	A	6001	-	-	0/13/13/13	0/0/0/0
7	MPD	A	7001	-	-	0/5/5/5	0/0/0/0
3	ACT	A	8001	-	-	0/0/0/0	0/0/0/0
4	NI9	B	4001	2	-	0/23/23/23	0/1/1/1
5	IPR	B	6002	-	-	0/13/13/13	0/0/0/0
6	BME	B	9001	-	-	0/1/1/1	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	6002	IPR	C3-C2	-2.54	1.37	1.51
5	A	6001	IPR	C3-C2	-2.52	1.37	1.51
4	A	3001	NI9	P2-O5	-2.00	1.47	1.50
4	B	4001	NI9	C5-N	2.09	1.39	1.34
4	A	3001	NI9	C5-N	2.14	1.39	1.34
4	B	4001	NI9	P2-C1	2.76	1.87	1.85
4	A	3001	NI9	P2-C1	4.15	1.88	1.85

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4001	NI9	C2-N-C3	-5.36	115.20	119.54
4	A	3001	NI9	C2-N-C3	-4.49	115.90	119.54
4	B	4001	NI9	P1-C1-P2	-2.73	107.64	112.70
5	B	6002	IPR	O6-C5-C4	-2.54	100.17	109.11
5	A	6001	IPR	O6-C5-C4	-2.41	100.59	109.11
4	A	3001	NI9	P1-C1-P2	-2.20	108.64	112.70
4	A	3001	NI9	C7-C3-N	-2.03	117.59	121.03
4	B	4001	NI9	C5-N-C3	2.01	123.06	121.18
4	A	3001	NI9	P1-C1-O2	2.04	112.05	107.24
5	A	6001	IPR	O12-P11-O13	2.10	118.70	110.50
5	B	6002	IPR	O12-P11-O13	2.11	118.74	110.50
5	B	6002	IPR	C3-C2-C4	2.23	125.87	111.50
4	B	4001	NI9	P1-C1-O2	2.23	112.50	107.24
5	A	6001	IPR	C3-C2-C4	2.25	126.05	111.50
4	B	4001	NI9	C2-N-C5	2.66	121.75	119.62
5	A	6001	IPR	O12-P11-O14	3.15	120.32	107.61
5	B	6002	IPR	O12-P11-O14	3.19	120.48	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	6002	IPR	C3-C2-C1	3.23	125.76	110.50
5	A	6001	IPR	C3-C2-C1	3.24	125.83	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	NI9	1	0
5	A	6001	IPR	1	0
7	A	7001	MPD	2	0
4	B	4001	NI9	1	0
5	B	6002	IPR	1	0
6	B	9001	BME	2	0

## 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	357/390 (91%)	-0.05	3 (0%) 86 86	20, 41, 60, 73	0
1	B	358/390 (91%)	-0.18	4 (1%) 80 80	21, 40, 57, 75	0
All	All	715/780 (91%)	-0.11	7 (0%) 82 82	20, 41, 58, 75	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	308	GLU	2.8
1	B	123	ASP	2.8
1	A	123	ASP	2.6
1	A	4	GLN	2.3
1	B	63	SER	2.2
1	B	74	ASP	2.1
1	A	308	GLU	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( $\text{\AA}^2$ )	Q<0.9
2	MG	B	4004	1/1	0.91	0.46	6.53	27,27,27,27	0
4	NI9	B	4001	18/18	0.96	0.25	2.06	36,50,58,67	0
2	MG	A	3004	1/1	0.89	0.24	1.25	41,41,41,41	0
2	MG	A	3002	1/1	0.96	0.18	1.14	42,42,42,42	0
7	MPD	A	7001	8/8	0.81	0.25	1.12	33,53,57,57	0
4	NI9	A	3001	18/18	0.97	0.20	0.93	21,43,52,62	0
5	IPR	B	6002	14/14	0.97	0.15	-0.39	24,37,52,54	0
5	IPR	A	6001	14/14	0.97	0.15	-0.54	15,33,43,43	0
2	MG	B	4003	1/1	0.79	0.12	-1.86	23,23,23,23	0
3	ACT	A	8001	4/4	0.95	0.26	-	49,49,56,63	0
2	MG	B	4002	1/1	0.91	0.30	-	36,36,36,36	0
2	MG	A	3003	1/1	0.77	0.19	-	21,21,21,21	0
6	BME	B	9001	4/4	0.88	0.23	-	44,47,56,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.