



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:57 AM GMT

PDB ID : 3NM3
Title : The Crystal Structure of Candida glabrata THI6, a Bifunctional Enzyme involved in Thiamin Biosynthesis of Eukaryotes
Authors : Paul, D.; Chatterjee, A.; Begley, T.P.; Ealick, S.E.
Deposited on : 2010-06-21
Resolution : 3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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 (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

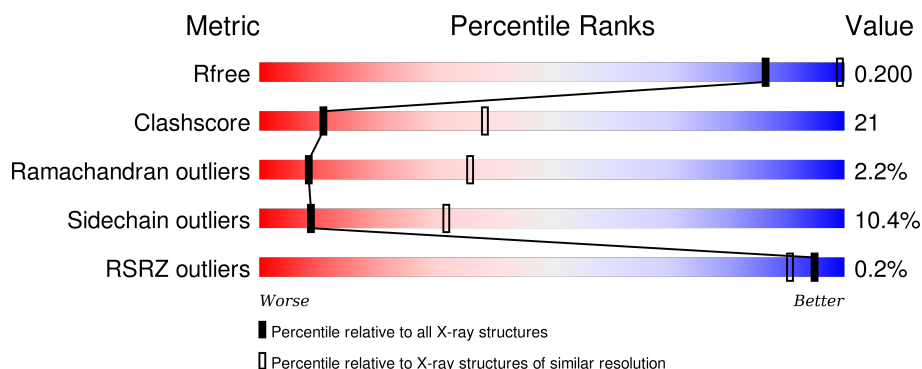
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 ≥ 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	540	<div> <div>57%</div> <div>32%</div> <div>5%</div> <div>6%</div> </div>
1	B	540	<div> <div>55%</div> <div>32%</div> <div>7%</div> <div>6%</div> </div>
1	C	540	<div> <div>57%</div> <div>31%</div> <div>6%</div> <div>6%</div> </div>
1	D	540	<div> <div>57%</div> <div>34%</div> <div>•</div> <div>5%</div> </div>
1	E	540	<div> <div>56%</div> <div>32%</div> <div>5%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	540	

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	3002	-	-	-	X
4	POP	C	4003	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 22991 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.

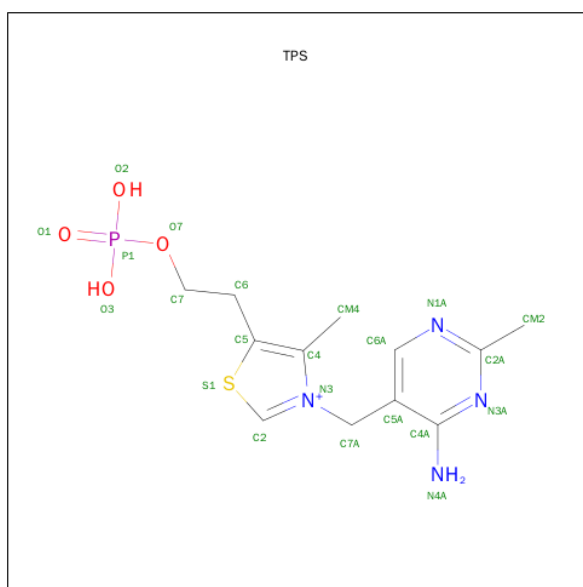
- Molecule 1 is a protein called Thiamine biosynthetic bifunctional enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			3809	2408	643	736	22			
1	B	508	Total	C	N	O	S	0	0	0
			3799	2402	641	734	22			
1	C	510	Total	C	N	O	S	0	0	0
			3803	2403	642	736	22			
1	D	511	Total	C	N	O	S	0	0	0
			3812	2409	644	737	22			
1	E	507	Total	C	N	O	S	0	0	0
			3792	2397	640	733	22			
1	F	507	Total	C	N	O	S	0	0	0
			3784	2391	638	733	22			

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

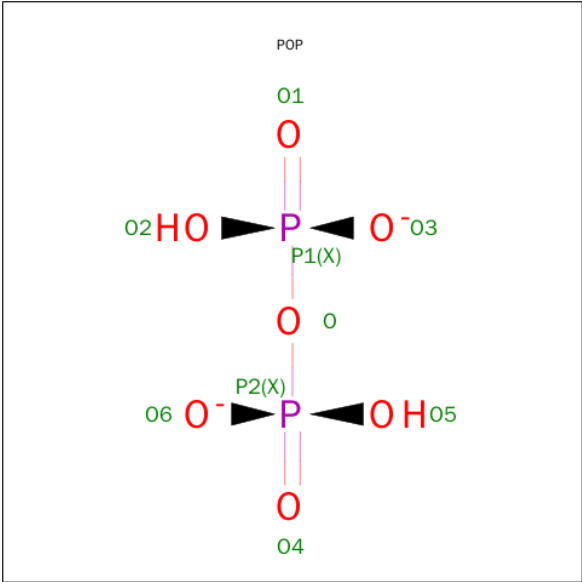
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THIAMIN PHOSPHATE (three-letter code: TPS) (formula: C₁₂H₁₈N₄O₄PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0
3	B	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0
3	C	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0
3	D	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0
3	E	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0
3	F	1	Total 22	C 12	N 4	O 4	P 1	S 1	0	0

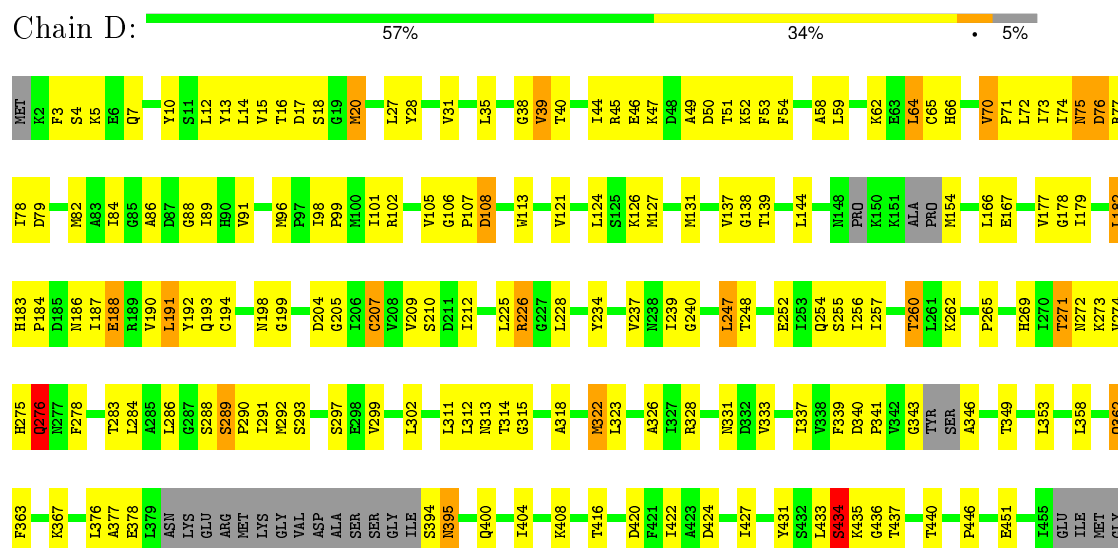
- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).

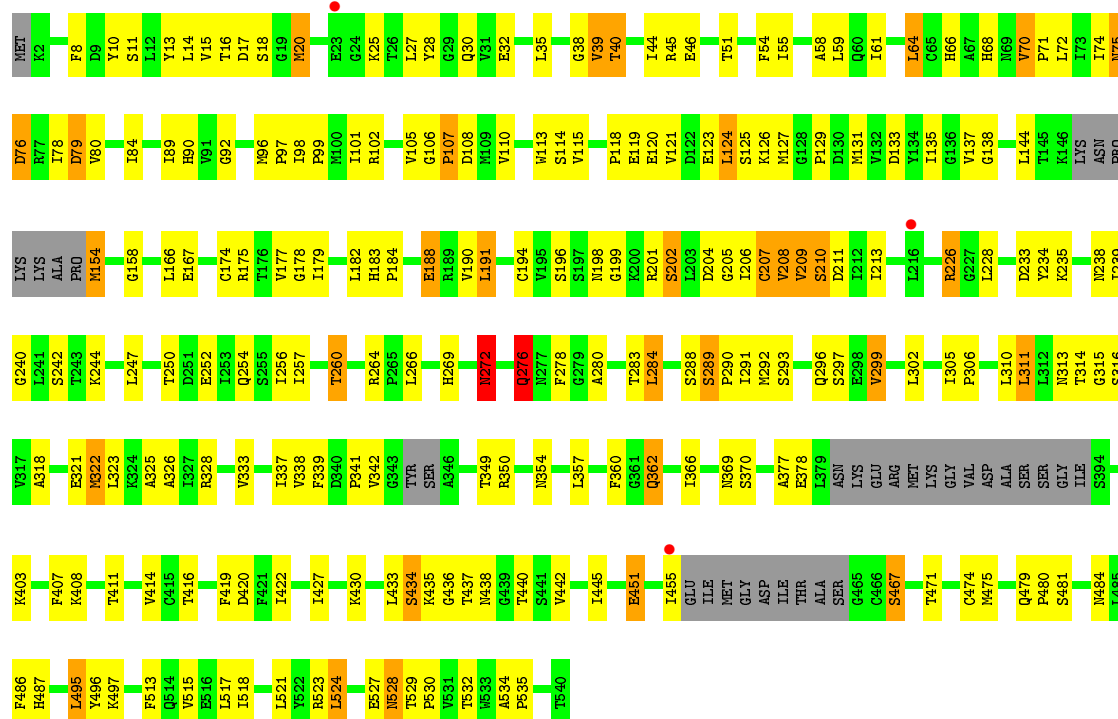


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		
4	C	1	Total	O	P	1	0
			9	7	2		
4	D	1	Total	O	P	0	0
			9	7	2		
4	E	1	Total	O	P	1	0
			9	7	2		
4	F	1	Total	O	P	0	0
			9	7	2		

- Molecule 1: Thiamine biosynthetic bifunctional enzyme

- Molecule 1: Thiamine biosynthetic bifunctional enzyme





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.19Å 154.60Å 148.65Å 90.00° 102.10° 90.00°	Depositor
Resolution (Å)	46.00 – 3.10 47.87 – 3.10	Depositor EDS
% Data completeness (in resolution range)	80.6 (46.00-3.10) 59.4 (47.87-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.197 , 0.251 0.199 , 0.200	Depositor DCC
R_{free} test set	2678 reflections (5.65%)	DCC
Wilson B-factor (Å ²)	69.9	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 52482 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22991	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.93% 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, 0.375 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, TPS, POP

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	0.37	0/3869	0.57	1/5246 (0.0%)
1	B	0.37	0/3859	0.57	1/5232 (0.0%)
1	C	0.37	0/3861	0.55	0/5235
1	D	0.38	0/3870	0.56	0/5246
1	E	0.37	0/3851	0.55	0/5221
1	F	0.36	0/3843	0.57	0/5213
All	All	0.37	0/23153	0.56	2/31393 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	153	PRO	CA-N-CD	-8.58	99.49	111.50
1	B	153	PRO	CA-N-CD	-8.57	99.51	111.50

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	3809	0	3814	163	0
1	B	3799	0	3810	166	0
1	C	3803	0	3796	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3812	0	3809	156	0
1	E	3792	0	3802	162	0
1	F	3784	0	3780	173	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	22	0	16	4	0
3	B	22	0	16	3	0
3	C	22	0	16	0	0
3	D	22	0	16	1	0
3	E	22	0	16	4	0
3	F	22	0	16	4	0
4	A	9	0	0	2	0
4	B	9	0	0	1	0
4	C	9	0	0	2	0
4	D	9	0	0	1	0
4	E	9	0	0	0	0
4	F	9	0	0	1	0
All	All	22991	0	22907	962	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 21.

The worst 5 of 962 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:F:209:VAL:HG11	1:F:213:ILE:HG12	1.27	1.13
1:A:167:GLU:HG2	1:A:198:ASN:HD21	1.14	1.12
1:F:208:VAL:HB	1:F:209:VAL:HA	1.30	1.08
1:C:266:LEU:HD11	1:C:291:ILE:HG13	1.43	1.01
1:B:78:ILE:HG13	1:B:89:ILE:HD12	1.45	0.96

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	500/540 (93%)	438 (88%)	53 (11%)	9 (2%)	11	42
1	B	498/540 (92%)	446 (90%)	39 (8%)	13 (3%)	7	32
1	C	499/540 (92%)	446 (89%)	44 (9%)	9 (2%)	11	42
1	D	499/540 (92%)	448 (90%)	41 (8%)	10 (2%)	9	38
1	E	497/540 (92%)	440 (88%)	47 (10%)	10 (2%)	9	38
1	F	497/540 (92%)	427 (86%)	55 (11%)	15 (3%)	5	28
All	All	2990/3240 (92%)	2645 (88%)	279 (9%)	66 (2%)	8	36

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	138	GLY
1	B	20	MET
1	B	434	SER
1	D	39	VAL

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	413/449 (92%)	374 (91%)	39 (9%)	11	39
1	B	413/449 (92%)	368 (89%)	45 (11%)	8	30
1	C	411/449 (92%)	371 (90%)	40 (10%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	412/449 (92%)	369 (90%)	43 (10%)	9	32
1	E	412/449 (92%)	371 (90%)	41 (10%)	9	34
1	F	410/449 (91%)	362 (88%)	48 (12%)	7	26
All	All	2471/2694 (92%)	2215 (90%)	256 (10%)	9	32

5 of 256 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	362	GLN
1	D	255	SER
1	F	296	GLN
1	C	467	SER
1	D	70	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	276	GLN
1	D	66	HIS
1	F	275	HIS
1	C	281	ASN
1	C	479	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	TPS	A	2001	-	18,23,23	6.16	10 (55%)	25,33,33	2.39	12 (48%)
4	POP	A	4001	2	8,8,8	0.50	0	13,13,13	1.79	1 (7%)
3	TPS	B	2002	-	18,23,23	5.86	9 (50%)	25,33,33	1.76	7 (28%)
4	POP	B	4002	2	8,8,8	0.48	0	13,13,13	1.75	1 (7%)
3	TPS	C	2003	-	18,23,23	6.78	9 (50%)	25,33,33	2.26	13 (52%)
4	POP	C	4003	2	8,8,8	0.64	0	13,13,13	1.94	1 (7%)
3	TPS	D	2004	-	18,23,23	6.21	9 (50%)	25,33,33	2.28	9 (36%)
4	POP	D	4004	2	8,8,8	0.52	0	13,13,13	1.61	1 (7%)
3	TPS	E	2005	-	18,23,23	6.13	9 (50%)	25,33,33	1.99	9 (36%)
4	POP	E	4005	2	8,8,8	0.73	0	13,13,13	1.78	1 (7%)
3	TPS	F	2006	-	18,23,23	6.37	9 (50%)	25,33,33	2.00	7 (28%)
4	POP	F	4006	2	8,8,8	0.44	0	13,13,13	1.90	3 (23%)

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	TPS	A	2001	-	-	0/10/11/11	0/2/2/2
4	POP	A	4001	2	-	0/6/6/6	0/0/0/0
3	TPS	B	2002	-	-	0/10/11/11	0/2/2/2
4	POP	B	4002	2	-	0/6/6/6	0/0/0/0
3	TPS	C	2003	-	-	0/10/11/11	0/2/2/2
4	POP	C	4003	2	-	0/6/6/6	0/0/0/0
3	TPS	D	2004	-	-	0/10/11/11	0/2/2/2
4	POP	D	4004	2	-	0/6/6/6	0/0/0/0
3	TPS	E	2005	-	-	0/10/11/11	0/2/2/2
4	POP	E	4005	2	-	0/6/6/6	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPS	F	2006	-	-	0/10/11/11	0/2/2/2
4	POP	F	4006	2	-	0/6/6/6	0/0/0/0

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2006	TPS	P1-O3	-2.97	1.44	1.54
3	A	2001	TPS	C7A-N3	-2.91	1.43	1.48
3	B	2002	TPS	P1-O3	-2.72	1.44	1.54
3	A	2001	TPS	P1-O3	-2.65	1.45	1.54
3	C	2003	TPS	P1-O3	-2.61	1.45	1.54

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	4003	POP	P2-O-P1	-6.27	115.12	132.73
4	A	4001	POP	P2-O-P1	-5.74	116.62	132.73
4	E	4005	POP	P2-O-P1	-5.49	117.32	132.73
4	F	4006	POP	P2-O-P1	-5.48	117.34	132.73
4	B	4002	POP	P2-O-P1	-5.41	117.54	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	TPS	4	0
4	A	4001	POP	2	0
3	B	2002	TPS	3	0
4	B	4002	POP	1	0
4	C	4003	POP	2	0
3	D	2004	TPS	1	0
4	D	4004	POP	1	0
3	E	2005	TPS	4	0
3	F	2006	TPS	4	0
4	F	4006	POP	1	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, 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	510/540 (94%)	-0.50	0 100 100	26, 86, 109, 133	0
1	B	508/540 (94%)	-0.56	1 (0%) 95 91	26, 80, 103, 129	0
1	C	510/540 (94%)	-0.41	3 (0%) 90 80	42, 87, 113, 135	0
1	D	511/540 (94%)	-0.55	0 100 100	40, 79, 107, 134	0
1	E	507/540 (93%)	-0.50	0 100 100	40, 80, 105, 129	0
1	F	507/540 (93%)	-0.41	3 (0%) 90 80	43, 87, 113, 131	0
All	All	3053/3240 (94%)	-0.49	7 (0%) 95 91	26, 83, 109, 135	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	465	GLY	2.8
1	B	455	ILE	2.2
1	F	216	LEU	2.2
1	C	247	LEU	2.2
1	F	455	ILE	2.1

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	MG	B	3002	1/1	0.91	0.28	6.05	61,61,61,61	0
4	POP	C	4003	9/9	0.98	0.22	3.29	55,68,75,82	3
4	POP	B	4002	9/9	0.97	0.19	1.94	48,57,67,70	2
2	MG	D	3004	1/1	0.97	0.23	1.51	61,61,61,61	0
3	TPS	D	2004	22/22	0.98	0.20	1.50	57,63,69,74	6
3	TPS	C	2003	22/22	0.97	0.21	1.13	66,73,76,79	7
3	TPS	F	2006	22/22	0.97	0.20	0.97	68,73,77,83	8
3	TPS	B	2002	22/22	0.98	0.18	0.66	55,62,70,73	8
2	MG	E	3005	1/1	0.98	0.20	0.65	48,48,48,48	0
3	TPS	E	2005	22/22	0.97	0.19	0.51	54,60,66,68	8
3	TPS	A	2001	22/22	0.98	0.18	0.39	60,69,76,77	7
4	POP	D	4004	9/9	0.97	0.17	0.24	53,60,65,68	5
4	POP	F	4006	9/9	0.98	0.15	0.22	55,63,69,69	4
4	POP	A	4001	9/9	0.98	0.17	-0.15	56,67,80,80	3
2	MG	A	3001	1/1	0.96	0.16	-0.49	70,70,70,70	0
4	POP	E	4005	9/9	0.98	0.15	-0.51	57,61,63,64	6
2	MG	C	3003	1/1	0.98	0.27	-	55,55,55,55	0
2	MG	F	3006	1/1	0.97	0.28	-	63,63,63,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.