



Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 03:55 pm BST

PDB ID : 8TLI
Title : THERMOLYSIN (100% ISOPROPANOL SOAKED CRYSTALS)
Authors : English, A.C.; Done, S.H.; Groom, C.R.; Hubbard, R.E.
Deposited on : 1998-10-30
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

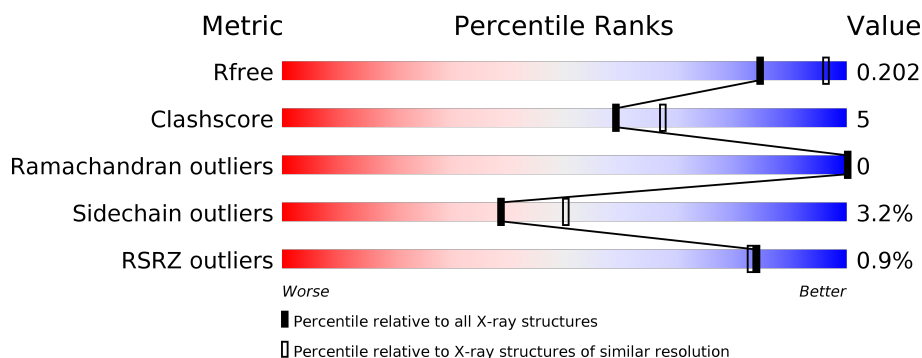
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	<div> <div></div> <div>75%</div> <div>23%</div> <div></div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2613 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 PROTEIN (THERMOLYSIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	6	0
			2461	1544	418	497	2			

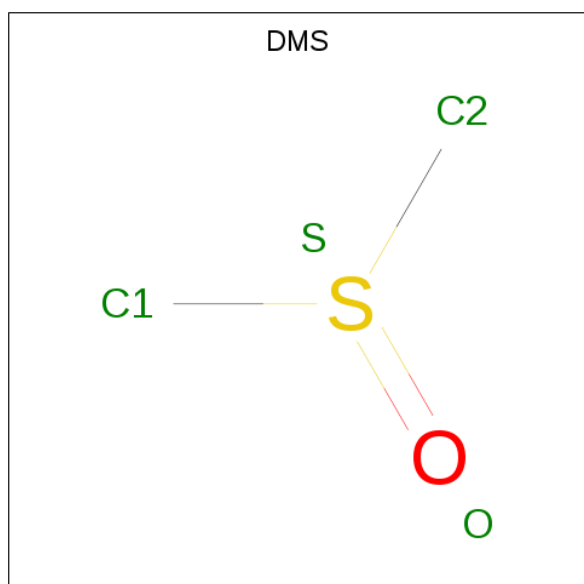
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

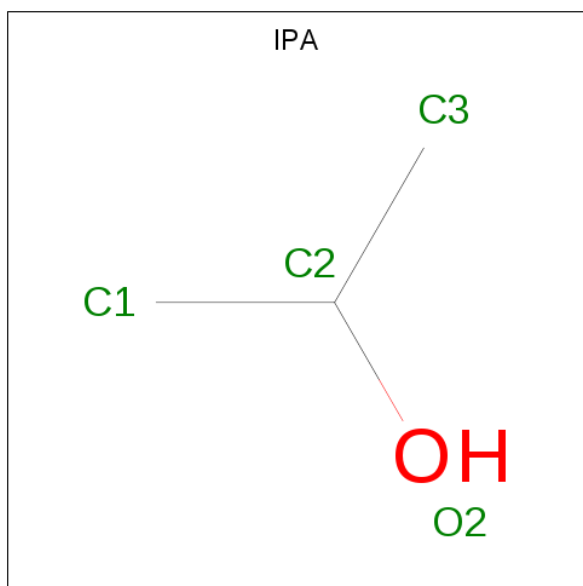
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Ca	0	0
			4	4		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



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

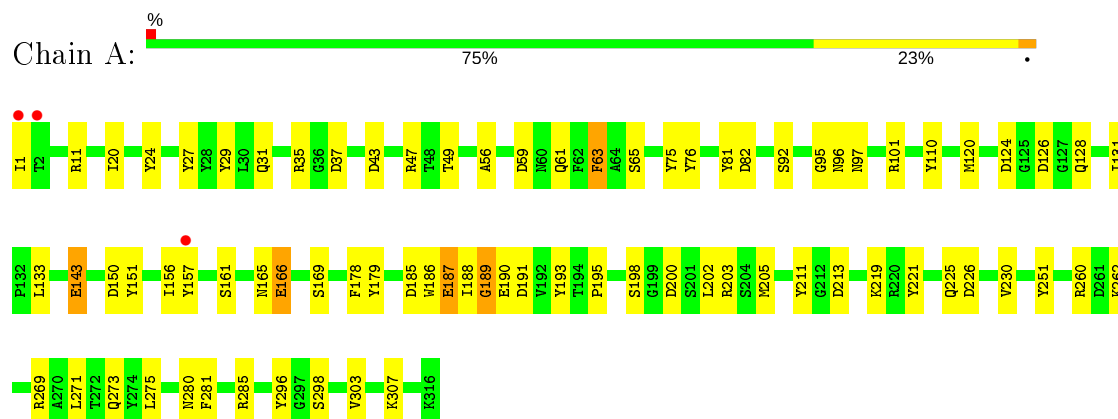
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total	O	0	0
			99	99		

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: PROTEIN (THERMOLYSIN)



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	93.04Å 93.04Å 130.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.66 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-2.20) 96.2 (29.66-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.07 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.223 0.163 , 0.202	Depositor DCC
R_{free} test set	853 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2613	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DMS, IPA, CA

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	0.83	1/2551 (0.0%)	1.83	62/3470 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	TRP	NE1-CE2	8.73	1.48	1.37

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	GLU	OE1-CD-OE2	-17.41	102.40	123.30
1	A	190	GLU	OE1-CD-OE2	-17.32	102.51	123.30
1	A	59	ASP	CB-CG-OD2	13.92	130.82	118.30
1	A	166	GLU	CG-CD-OE1	11.98	142.26	118.30
1	A	101[A]	ARG	NE-CZ-NH1	11.35	125.97	120.30
1	A	101[B]	ARG	NE-CZ-NH1	11.35	125.97	120.30
1	A	269	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	A	63	PHE	CB-CG-CD1	-10.08	113.75	120.80
1	A	191	ASP	CB-CG-OD2	-9.94	109.35	118.30
1	A	150	ASP	CB-CG-OD2	-9.79	109.49	118.30
1	A	185	ASP	CB-CG-OD1	8.89	126.31	118.30
1	A	63	PHE	CB-CG-CD2	8.72	126.91	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ASP	CB-CG-OD2	8.63	126.07	118.30
1	A	179	TYR	CB-CG-CD1	7.89	125.74	121.00
1	A	37	ASP	CB-CG-OD1	-7.88	111.21	118.30
1	A	27	TYR	CB-CG-CD2	7.82	125.69	121.00
1	A	37	ASP	CB-CG-OD2	7.75	125.28	118.30
1	A	27	TYR	CB-CG-CD1	-7.40	116.56	121.00
1	A	59	ASP	CB-CG-OD1	-7.26	111.77	118.30
1	A	110	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	A	179	TYR	CB-CG-CD2	-7.01	116.79	121.00
1	A	126	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	221	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	187	GLU	O-C-N	-6.75	111.89	122.70
1	A	200	ASP	CB-CG-OD1	-6.73	112.24	118.30
1	A	203	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	A	82	ASP	CB-CG-OD2	-6.57	112.38	118.30
1	A	213	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	191	ASP	OD1-CG-OD2	6.44	135.53	123.30
1	A	75	TYR	CG-CD1-CE1	-6.29	116.27	121.30
1	A	221	TYR	CB-CG-CD1	6.28	124.77	121.00
1	A	190	GLU	O-C-N	-6.21	112.77	122.70
1	A	49	THR	OG1-CB-CG2	-6.07	96.04	110.00
1	A	35	ARG	CD-NE-CZ	6.07	132.09	123.60
1	A	280	ASN	CB-CG-OD1	6.05	133.71	121.60
1	A	101[A]	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
1	A	101[B]	ARG	NH1-CZ-NH2	-5.81	113.01	119.40
1	A	178	PHE	CB-CG-CD1	-5.81	116.73	120.80
1	A	43	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	205	MET	CA-CB-CG	-5.78	103.47	113.30
1	A	61	GLN	CA-C-N	5.78	129.91	117.20
1	A	24	TYR	O-C-N	5.76	131.91	122.70
1	A	185	ASP	OD1-CG-OD2	-5.68	112.51	123.30
1	A	190	GLU	CA-C-N	5.66	129.66	117.20
1	A	49	THR	CA-CB-CG2	5.60	120.24	112.40
1	A	285	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	185	ASP	CA-CB-CG	-5.56	101.17	113.40
1	A	124	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	190	GLU	CG-CD-OE2	5.49	129.28	118.30
1	A	273	GLN	CA-C-O	-5.48	108.59	120.10
1	A	150	ASP	OD1-CG-OD2	5.40	133.56	123.30
1	A	143	GLU	CG-CD-OE1	5.35	129.00	118.30
1	A	75	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	A	95	GLY	O-C-N	-5.27	114.27	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	GLN	CA-C-N	5.27	128.79	117.20
1	A	81	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	269	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	A	189	GLY	O-C-N	-5.18	114.41	122.70
1	A	151	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	203	ARG	NH1-CZ-NH2	-5.05	113.85	119.40
1	A	260[A]	ARG	CD-NE-CZ	5.03	130.64	123.60
1	A	260[B]	ARG	CD-NE-CZ	5.03	130.64	123.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	GLY	Mainchain
1	A	193	TYR	Mainchain
1	A	219	LYS	Mainchain
1	A	226	ASP	Mainchain
1	A	230	VAL	Mainchain
1	A	251	TYR	Mainchain
1	A	281	PHE	Mainchain
1	A	47	ARG	Mainchain
1	A	76	TYR	Mainchain
1	A	96	ASN	Mainchain

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	2461	0	2303	20	0
2	A	1	0	0	0	0
3	A	4	0	0	0	0
4	A	4	0	6	0	0
5	A	44	0	88	5	0
6	A	99	0	0	1	0
All	All	2613	0	2397	23	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 5.

All (23) 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:1:ILE:HB	1:A:31:GLN:HE22	1.33	0.93
1:A:1:ILE:HB	1:A:31:GLN:NE2	1.96	0.79
5:A:2001:IPA:C3	5:A:2008:IPA:H12	2.13	0.77
5:A:2001:IPA:H33	6:A:1067:HOH:O	1.92	0.68
1:A:157[B]:TYR:CE2	1:A:165:ASN:ND2	2.62	0.68
1:A:11[A]:ARG:HG3	1:A:63:PHE:HD1	1.63	0.64
1:A:157[A]:TYR:OH	1:A:166:GLU:OE2	2.16	0.63
1:A:11[A]:ARG:HG3	1:A:63:PHE:CD1	2.34	0.61
1:A:211:TYR:O	5:A:2003:IPA:H12	2.00	0.61
1:A:120:MET:SD	1:A:143:GLU:HB3	2.41	0.61
1:A:157[B]:TYR:CZ	1:A:165:ASN:ND2	2.70	0.58
5:A:2001:IPA:H32	5:A:2008:IPA:H12	1.88	0.53
1:A:128:GLN:O	1:A:195:PRO:HD2	2.07	0.53
1:A:92:SER:HA	5:A:2002:IPA:O2	2.09	0.52
1:A:187:GLU:O	1:A:188:ILE:HD13	2.12	0.49
1:A:131:ILE:HG23	1:A:195:PRO:HG3	1.97	0.47
1:A:271:LEU:HA	1:A:275:LEU:HD12	1.96	0.46
1:A:262:LYS:HG2	1:A:296:TYR:OH	2.14	0.46
1:A:303:VAL:CG1	1:A:307:LYS:HE2	2.49	0.42
1:A:92:SER:HB2	1:A:97:ASN:HA	2.01	0.41
1:A:29:TYR:CE1	1:A:56:ALA:HB2	2.55	0.41
1:A:156:ILE:HG13	1:A:161[A]:SER:OG	2.21	0.41
1:A:303:VAL:HG12	1:A:307:LYS:HE2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	320/316 (101%)	306 (96%)	14 (4%)	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	258/252 (102%)	250 (97%)	8 (3%)	40	51

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	65	SER
1	A	133	LEU
1	A	169	SER
1	A	198	SER
1	A	202	LEU
1	A	225	GLN
1	A	298	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	33	ASN
1	A	97	ASN
1	A	227	ASN
1	A	290	GLN
1	A	301	GLN

5.3.3 RNA ⓘ

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 17 ligands modelled in this entry, 5 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	$\# Z > 2$
5	IPA	A	2011	-	3,3,3	0.59	0	3,3,3	0.87	0
5	IPA	A	2001	-	3,3,3	0.57	0	3,3,3	0.48	0
4	DMS	A	2000	-	3,3,3	0.70	0	3,3,3	0.70	0
5	IPA	A	2002	-	3,3,3	0.50	0	3,3,3	0.11	0
5	IPA	A	2005	-	3,3,3	0.58	0	3,3,3	0.37	0
5	IPA	A	2010	-	3,3,3	0.58	0	3,3,3	0.43	0
5	IPA	A	2006	-	3,3,3	0.64	0	3,3,3	0.66	0
5	IPA	A	2008	-	3,3,3	0.62	0	3,3,3	0.81	0
5	IPA	A	2003	-	3,3,3	0.40	0	3,3,3	0.74	0
5	IPA	A	2007	-	3,3,3	0.53	0	3,3,3	1.01	0
5	IPA	A	2004	-	3,3,3	0.60	0	3,3,3	0.68	0
5	IPA	A	2009	-	3,3,3	0.63	0	3,3,3	0.67	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2001	IPA	3	0
5	A	2002	IPA	1	0
5	A	2008	IPA	2	0
5	A	2003	IPA	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	316/316 (100%)	-0.92	3 (0%) 84 83	19, 29, 48, 86	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	4.4
1	A	1	ILE	3.3
1	A	157[A]	TYR	2.3

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	IPA	A	2011	4/4	0.69	0.23	59,61,64,67	0
5	IPA	A	2008	4/4	0.72	0.23	65,70,70,71	0
5	IPA	A	2001	4/4	0.76	0.39	50,59,62,62	0
5	IPA	A	2003	4/4	0.80	0.24	51,52,56,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	IPA	A	2009	4/4	0.82	0.25	60,61,61,61	0
4	DMS	A	2000	4/4	0.84	0.26	53,57,60,62	4
5	IPA	A	2007	4/4	0.88	0.22	54,59,61,63	0
5	IPA	A	2005	4/4	0.92	0.15	57,58,59,59	0
5	IPA	A	2010	4/4	0.93	0.21	60,62,63,64	0
5	IPA	A	2004	4/4	0.93	0.12	50,57,59,60	0
5	IPA	A	2006	4/4	0.93	0.19	60,62,63,66	0
5	IPA	A	2002	4/4	0.94	0.15	43,43,44,45	0
3	CA	A	405	1/1	0.94	0.06	35,35,35,35	0
3	CA	A	404	1/1	0.98	0.09	35,35,35,35	0
3	CA	A	403	1/1	0.99	0.11	31,31,31,31	0
3	CA	A	402	1/1	0.99	0.15	27,27,27,27	0
2	ZN	A	401	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.