Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:32 AM GMT

PDB ID	:	3B6P
Title	:	Structure of TREX1 in complex with a nucleotide and inhibitor ions (sodium and zinc)
Authors	:	Brucet, M.; Querol-Audi, J.; Fita, I.; Celada, A.
Deposited on	:	2007-10-29
Resolution	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

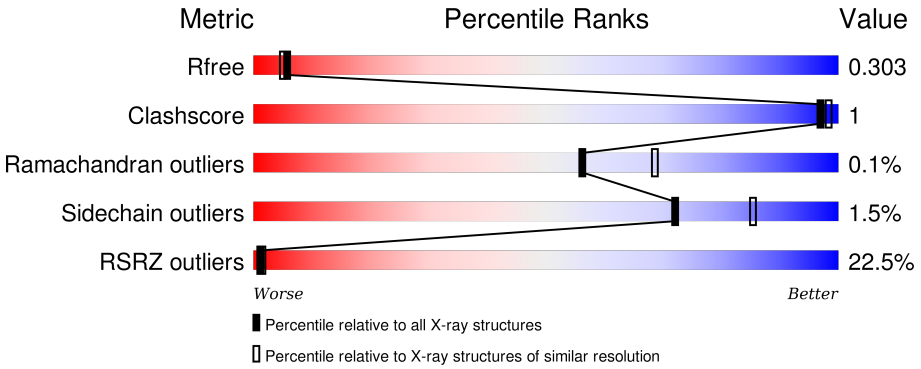
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	247	19% 82% 6% 12%
1	B	247	21% 84% · 12%
1	C	247	22% 85% · 12%
1	D	247	17% 82% 6% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7299 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 Three prime repair exonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	1	0
			1684	1066	295	313	10			
1	B	217	Total	C	N	O	S	0	1	0
			1684	1066	295	313	10			
1	C	217	Total	C	N	O	S	0	1	0
			1684	1066	295	313	10			
1	D	217	Total	C	N	O	S	0	1	0
			1684	1066	295	313	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP Q91XB0
A	0	LYS	-	EXPRESSION TAG	UNP Q91XB0
A	1	HIS	-	EXPRESSION TAG	UNP Q91XB0
A	2	HIS	-	EXPRESSION TAG	UNP Q91XB0
A	3	HIS	-	EXPRESSION TAG	UNP Q91XB0
A	4	HIS	-	EXPRESSION TAG	UNP Q91XB0
A	5	HIS	-	EXPRESSION TAG	UNP Q91XB0
A	6	HIS	-	EXPRESSION TAG	UNP Q91XB0
A	7	PRO	-	EXPRESSION TAG	UNP Q91XB0
A	8	MET	-	EXPRESSION TAG	UNP Q91XB0
B	-1	MET	-	EXPRESSION TAG	UNP Q91XB0
B	0	LYS	-	EXPRESSION TAG	UNP Q91XB0
B	1	HIS	-	EXPRESSION TAG	UNP Q91XB0
B	2	HIS	-	EXPRESSION TAG	UNP Q91XB0
B	3	HIS	-	EXPRESSION TAG	UNP Q91XB0
B	4	HIS	-	EXPRESSION TAG	UNP Q91XB0
B	5	HIS	-	EXPRESSION TAG	UNP Q91XB0
B	6	HIS	-	EXPRESSION TAG	UNP Q91XB0
B	7	PRO	-	EXPRESSION TAG	UNP Q91XB0
B	8	MET	-	EXPRESSION TAG	UNP Q91XB0
C	-1	MET	-	EXPRESSION TAG	UNP Q91XB0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	LYS	-	EXPRESSION TAG	UNP Q91XB0
C	1	HIS	-	EXPRESSION TAG	UNP Q91XB0
C	2	HIS	-	EXPRESSION TAG	UNP Q91XB0
C	3	HIS	-	EXPRESSION TAG	UNP Q91XB0
C	4	HIS	-	EXPRESSION TAG	UNP Q91XB0
C	5	HIS	-	EXPRESSION TAG	UNP Q91XB0
C	6	HIS	-	EXPRESSION TAG	UNP Q91XB0
C	7	PRO	-	EXPRESSION TAG	UNP Q91XB0
C	8	MET	-	EXPRESSION TAG	UNP Q91XB0
D	-1	MET	-	EXPRESSION TAG	UNP Q91XB0
D	0	LYS	-	EXPRESSION TAG	UNP Q91XB0
D	1	HIS	-	EXPRESSION TAG	UNP Q91XB0
D	2	HIS	-	EXPRESSION TAG	UNP Q91XB0
D	3	HIS	-	EXPRESSION TAG	UNP Q91XB0
D	4	HIS	-	EXPRESSION TAG	UNP Q91XB0
D	5	HIS	-	EXPRESSION TAG	UNP Q91XB0
D	6	HIS	-	EXPRESSION TAG	UNP Q91XB0
D	7	PRO	-	EXPRESSION TAG	UNP Q91XB0
D	8	MET	-	EXPRESSION TAG	UNP Q91XB0

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

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0

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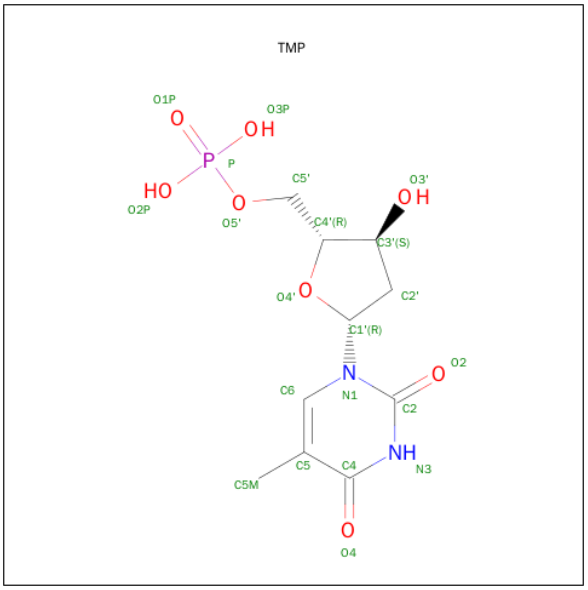
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Na 1 1	0	0

- Molecule 4 is THYMIDINE-5'-PHOSPHATE (three-letter code: TMP) (formula: $C_{10}H_{15}N_2O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 21 10 2 8 1	0	0
4	B	1	Total C N O P 21 10 2 8 1	0	0
4	C	1	Total C N O P 21 10 2 8 1	0	0
4	D	1	Total C N O P 21 10 2 8 1	0	0

- Molecule 5 is water.

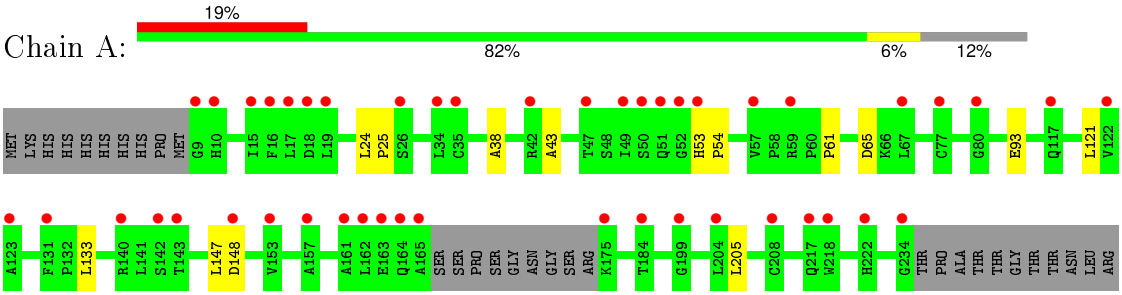
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	125	Total O 125 125	0	0
5	B	103	Total O 103 103	0	0
5	C	105	Total O 105 105	0	0
5	D	138	Total O 138 138	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

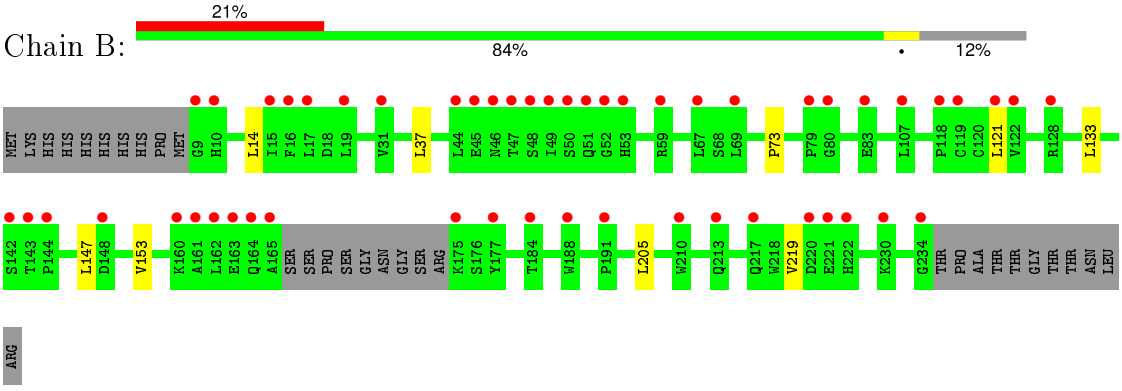
- Molecule 1: Three prime repair exonuclease 1

Chain A:



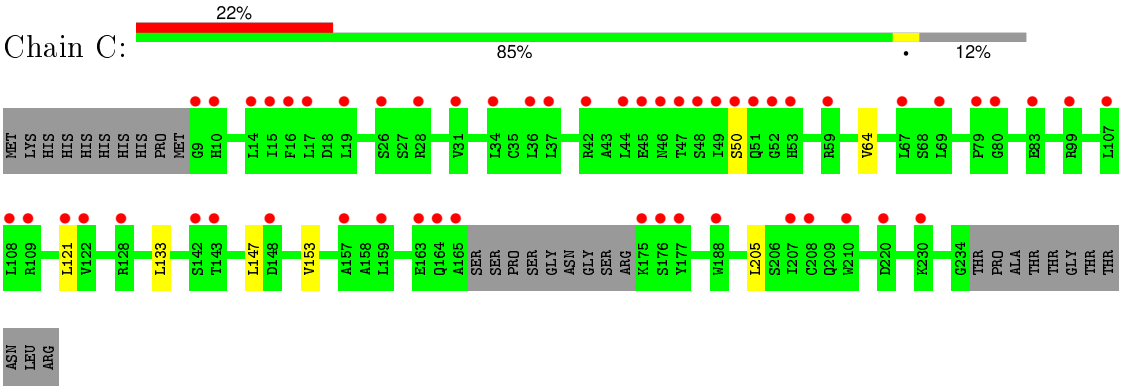
- Molecule 1: Three prime repair exonuclease 1

Chain B:



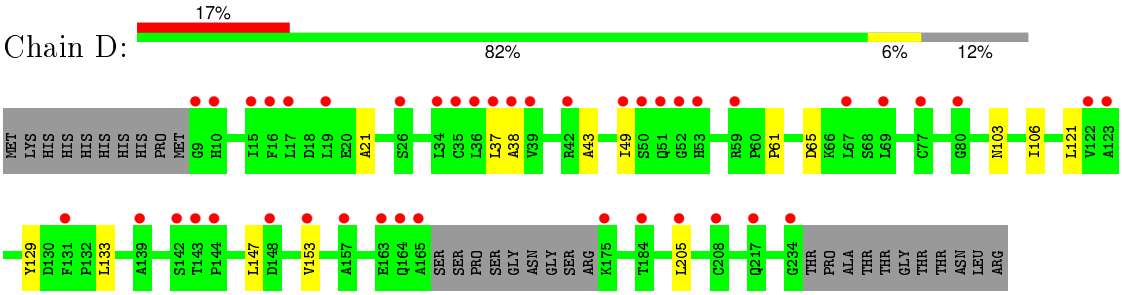
- Molecule 1: Three prime repair exonuclease 1

Chain C:



- Molecule 1: Three prime repair exonuclease 1

Chain D:


17%
82%
6%
12%
MET LYS HIS HIS HIS HIS HIS PRO MET G9 H10 I15 F16 L17 D18 L19 E20 A21 S26 I34 C35 L36 L37 A38 V39 R42 A43 I49 S50 Q51 G52 H53 R59 P60 P61 D65 K66 L67 S68 L69 C77 G80 N103 I106 L121 V122 A123
Y129 D130 F131 P132 L133 A139 S142 T143 P144 L147 D148 V153 A157 E163 Q164 A165 SER SER PRO SER GLY ASN GLY SER ARG K175 T184 L205 C208 Q217 G234 THR PRO ALA THR THR GLY THR THR ASN LEU ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.77Å 81.50Å 92.54Å 90.00° 103.11° 90.00°	Depositor
Resolution (Å)	24.18 – 2.30 24.18 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.18-2.30) 98.2 (24.18-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.246 , 0.285 0.264 , 0.303	Depositor DCC
R_{free} test set	2155 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 48249 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7299	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.06 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.1256e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: TMP, NA, ZN

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	0.30	0/1724	0.49	0/2350
1	B	0.30	0/1724	0.48	0/2350
1	C	0.30	0/1724	0.49	0/2350
1	D	0.30	0/1724	0.50	0/2350
All	All	0.30	0/6896	0.49	0/9400

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	1684	0	1686	6	0
1	B	1684	0	1686	4	0
1	C	1684	0	1686	1	0
1	D	1684	0	1686	7	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
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	21	0	13	0	0
4	B	21	0	13	0	0
4	C	21	0	13	0	0
4	D	21	0	13	0	0
5	A	125	0	0	0	0
5	B	103	0	0	1	0
5	C	105	0	0	0	0
5	D	138	0	0	0	0
All	All	7299	0	6796	17	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 1.

All (17) 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:38:ALA:HB3	1:A:65:ASP:HB2	1.91	0.51
1:B:37:LEU:HD21	1:B:205:LEU:HD22	1.94	0.49
1:D:38:ALA:HB3	1:D:65:ASP:HB2	1.96	0.48
1:B:121:LEU:HD11	1:B:147:LEU:HD22	1.95	0.47
1:D:121:LEU:HD11	1:D:147:LEU:HD22	1.97	0.46
1:A:121:LEU:HD11	1:A:147:LEU:HD22	1.99	0.45
1:C:121:LEU:HD11	1:C:147:LEU:HD22	1.98	0.45
1:A:43:ALA:HB1	1:A:61:PRO:HB3	2.00	0.43
1:B:73:PRO:HD2	5:B:1081:HOH:O	2.18	0.43
1:B:14:LEU:HD21	1:B:219:VAL:HG11	2.00	0.43
1:A:93:GLU:HB3	1:D:49:ILE:HD12	2.01	0.42
1:A:53:HIS:HA	1:A:54:PRO:HA	1.90	0.42
1:A:24:LEU:HB3	1:A:25:PRO:HD2	2.01	0.42
1:D:21:ALA:HB3	1:D:129:TYR:OH	2.20	0.41
1:D:37:LEU:HD21	1:D:205:LEU:HD22	2.03	0.41
1:D:103:ASN:HA	1:D:106:ILE:HD12	2.01	0.41
1:D:43:ALA:HB1	1:D:61:PRO:HB3	2.02	0.41

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	214/247 (87%)	210 (98%)	4 (2%)	0	100 100
1	B	214/247 (87%)	207 (97%)	7 (3%)	0	100 100
1	C	214/247 (87%)	207 (97%)	6 (3%)	1 (0%)	34 41
1	D	214/247 (87%)	210 (98%)	4 (2%)	0	100 100
All	All	856/988 (87%)	834 (97%)	21 (2%)	1 (0%)	56 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	50	SER

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	187/212 (88%)	184 (98%)	3 (2%)	70 84
1	B	187/212 (88%)	185 (99%)	2 (1%)	80 90
1	C	187/212 (88%)	183 (98%)	4 (2%)	61 78
1	D	187/212 (88%)	185 (99%)	2 (1%)	80 90
All	All	748/848 (88%)	737 (98%)	11 (2%)	72 85

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LEU
1	A	148	ASP
1	A	205	LEU
1	B	133	LEU
1	B	153	VAL
1	C	64	VAL
1	C	133	LEU
1	C	153	VAL
1	C	205	LEU
1	D	133	LEU
1	D	153	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	125	ASN
1	A	217	GLN
1	B	125	ASN
1	B	189	GLN
1	B	217	GLN
1	C	46	ASN
1	C	125	ASN
1	C	189	GLN
1	C	217	GLN
1	D	125	ASN
1	D	217	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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	TMP	A	1000	3,2	17,22,22	0.60	0	22,33,33	2.11	5 (22%)
4	TMP	B	1000	3,2	17,22,22	0.61	0	22,33,33	2.14	5 (22%)
4	TMP	C	1000	3,2	17,22,22	0.60	0	22,33,33	2.14	5 (22%)
4	TMP	D	1000	3,2	17,22,22	0.59	0	22,33,33	2.11	5 (22%)

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	TMP	A	1000	3,2	-	0/6/22/22	0/2/2/2
4	TMP	B	1000	3,2	-	0/6/22/22	0/2/2/2
4	TMP	C	1000	3,2	-	0/6/22/22	0/2/2/2
4	TMP	D	1000	3,2	-	0/6/22/22	0/2/2/2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1000	TMP	C5-C4-N3	-5.54	118.97	125.14
4	B	1000	TMP	C5-C4-N3	-5.48	119.03	125.14
4	A	1000	TMP	C5-C4-N3	-5.48	119.04	125.14
4	D	1000	TMP	C5-C4-N3	-5.42	119.10	125.14
4	B	1000	TMP	C2'-C1'-N1	-2.30	108.56	114.16
4	C	1000	TMP	C2'-C1'-N1	-2.23	108.74	114.16
4	D	1000	TMP	C2'-C1'-N1	-2.20	108.81	114.16
4	A	1000	TMP	C2'-C1'-N1	-2.12	109.00	114.16
4	A	1000	TMP	O2P-P-O1P	2.13	117.42	110.58
4	D	1000	TMP	O2P-P-O1P	2.25	117.82	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1000	TMP	O2P-P-O1P	2.33	118.08	110.58
4	C	1000	TMP	O2P-P-O1P	2.35	118.13	110.58
4	C	1000	TMP	O4'-C1'-N1	2.50	112.04	107.72
4	B	1000	TMP	O4'-C1'-N1	2.50	112.05	107.72
4	D	1000	TMP	O4'-C1'-N1	2.57	112.17	107.72
4	A	1000	TMP	O4'-C1'-N1	2.64	112.28	107.72
4	D	1000	TMP	C4-N3-C2	6.78	121.11	115.25
4	B	1000	TMP	C4-N3-C2	6.79	121.11	115.25
4	A	1000	TMP	C4-N3-C2	6.79	121.12	115.25
4	C	1000	TMP	C4-N3-C2	6.90	121.21	115.25

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	217/247 (87%)	1.35	46 (21%)	1	2	25, 28, 33, 39	0
1	B	217/247 (87%)	1.40	52 (23%)	1	1	25, 28, 34, 37	0
1	C	217/247 (87%)	1.35	54 (24%)	1	1	26, 28, 36, 39	0
1	D	217/247 (87%)	1.21	43 (19%)	1	2	25, 28, 34, 39	0
All	All	868/988 (87%)	1.33	195 (22%)	1	1	25, 28, 34, 39	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	49	ILE	10.8
1	B	165	ALA	9.3
1	C	48	SER	9.1
1	A	165	ALA	9.0
1	B	49	ILE	8.5
1	C	47	THR	7.4
1	D	165	ALA	7.3
1	B	48	SER	6.7
1	B	50	SER	6.7
1	B	46	ASN	6.7
1	B	148	ASP	6.3
1	C	50	SER	6.3
1	A	50	SER	6.1
1	C	53	HIS	6.1
1	D	164	GLN	6.0
1	A	164	GLN	6.0
1	D	10	HIS	5.6
1	A	10	HIS	5.5
1	A	49	ILE	5.5
1	B	9	GLY	5.5
1	D	51	GLN	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	163	GLU	5.2
1	A	59	ARG	5.2
1	B	234	GLY	5.1
1	B	47	THR	5.1
1	B	164	GLN	5.1
1	C	46	ASN	5.0
1	B	10	HIS	5.0
1	C	10	HIS	4.9
1	B	163	GLU	4.9
1	A	51	GLN	4.8
1	B	161	ALA	4.8
1	D	59	ARG	4.7
1	D	49	ILE	4.7
1	B	162	LEU	4.6
1	C	9	GLY	4.5
1	B	53	HIS	4.3
1	D	52	GLY	4.3
1	A	122	VAL	4.1
1	C	177	TYR	4.1
1	C	26	SER	4.1
1	B	175	LYS	4.1
1	A	26	SER	4.0
1	C	51	GLN	4.0
1	C	80	GLY	4.0
1	B	121	LEU	4.0
1	D	234	GLY	3.9
1	C	163	GLU	3.8
1	B	217	GLN	3.8
1	B	51	GLN	3.8
1	D	122	VAL	3.7
1	A	19	LEU	3.7
1	A	52	GLY	3.7
1	B	80	GLY	3.7
1	A	148	ASP	3.6
1	C	164	GLN	3.6
1	C	17	LEU	3.6
1	D	163	GLU	3.6
1	A	53	HIS	3.6
1	B	59	ARG	3.5
1	D	142	SER	3.5
1	D	148	ASP	3.5
1	C	44	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	128	ARG	3.4
1	A	42	ARG	3.4
1	D	53	HIS	3.4
1	C	121	LEU	3.4
1	C	42	ARG	3.3
1	A	175	LYS	3.3
1	A	16	PHE	3.3
1	A	234	GLY	3.3
1	A	17	LEU	3.3
1	C	122	VAL	3.2
1	C	99	ARG	3.2
1	B	142	SER	3.2
1	C	188	TRP	3.2
1	B	122	VAL	3.2
1	C	16	PHE	3.2
1	B	177	TYR	3.1
1	C	15	ILE	3.1
1	B	128	ARG	3.1
1	B	44	LEU	3.1
1	D	19	LEU	3.1
1	A	9	GLY	3.1
1	B	160	LYS	3.1
1	B	15	ILE	3.0
1	B	188	TRP	3.1
1	A	143	THR	3.0
1	D	15	ILE	3.0
1	C	148	ASP	3.0
1	B	17	LEU	3.0
1	D	34	LEU	3.0
1	A	142	SER	3.0
1	C	79	PRO	2.9
1	A	157	ALA	2.9
1	A	131	PHE	2.9
1	A	184	THR	2.9
1	D	42	ARG	2.9
1	D	50	SER	2.9
1	B	16	PHE	2.8
1	C	230	LYS	2.8
1	D	16	PHE	2.8
1	C	175	LYS	2.8
1	B	67	LEU	2.8
1	B	79	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	142	SER	2.8
1	C	36	LEU	2.8
1	A	15	ILE	2.7
1	D	175	LYS	2.7
1	D	9	GLY	2.7
1	A	123	ALA	2.7
1	B	19	LEU	2.7
1	B	69	LEU	2.7
1	C	157	ALA	2.7
1	C	143	THR	2.7
1	A	80	GLY	2.7
1	B	230	LYS	2.7
1	A	34	LEU	2.6
1	B	210	TRP	2.6
1	A	208	CYS	2.6
1	B	222	HIS	2.5
1	D	36	LEU	2.5
1	C	165	ALA	2.5
1	B	184	THR	2.5
1	D	26	SER	2.5
1	D	80	GLY	2.5
1	D	35	CYS	2.5
1	D	208	CYS	2.5
1	C	14	LEU	2.5
1	D	67	LEU	2.5
1	D	17	LEU	2.5
1	D	37	LEU	2.4
1	B	220	ASP	2.4
1	C	52	GLY	2.4
1	A	162	LEU	2.4
1	C	19	LEU	2.4
1	D	77	CYS	2.4
1	B	52	GLY	2.4
1	D	157	ALA	2.4
1	D	184	THR	2.4
1	A	140	ARG	2.3
1	B	83	GLU	2.3
1	A	217	GLN	2.3
1	A	35	CYS	2.3
1	A	204	LEU	2.3
1	C	28	ARG	2.3
1	C	220	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	39	VAL	2.3
1	A	218	TRP	2.3
1	C	108	LEU	2.3
1	B	118	PRO	2.3
1	A	77	CYS	2.3
1	B	119[A]	CYS	2.3
1	A	57	VAL	2.3
1	C	67	LEU	2.3
1	C	69	LEU	2.3
1	C	59	ARG	2.3
1	D	144	PRO	2.2
1	C	109	ARG	2.2
1	B	107	LEU	2.2
1	B	191	PRO	2.2
1	C	45	GLU	2.2
1	A	47	THR	2.2
1	A	161	ALA	2.2
1	A	117	GLN	2.2
1	A	153	VAL	2.2
1	D	153	VAL	2.2
1	D	69	LEU	2.2
1	C	176	SER	2.2
1	D	139	ALA	2.2
1	B	31	VAL	2.2
1	C	31	VAL	2.2
1	A	18	ASP	2.2
1	B	213	GLN	2.2
1	D	123	ALA	2.2
1	A	67	LEU	2.2
1	C	208	CYS	2.1
1	C	207	ILE	2.1
1	C	83	GLU	2.1
1	C	210	TRP	2.1
1	B	143	THR	2.1
1	C	37	LEU	2.1
1	D	38	ALA	2.1
1	D	143	THR	2.1
1	B	221	GLU	2.1
1	C	34	LEU	2.1
1	D	205	LEU	2.1
1	C	159	LEU	2.0
1	A	222	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	45	GLU	2.0
1	D	131	PHE	2.0
1	D	217	GLN	2.0
1	C	107	LEU	2.0
1	A	199	GLY	2.0
1	B	144	PRO	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^{th} 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
4	TMP	B	1000	21/21	0.89	0.17	-0.38	23,24,24,24	0
4	TMP	D	1000	21/21	0.90	0.15	-0.67	25,25,26,27	0
4	TMP	C	1000	21/21	0.90	0.16	-0.84	26,27,27,27	0
4	TMP	A	1000	21/21	0.89	0.15	-0.87	22,23,24,24	0
2	ZN	A	800	1/1	1.00	0.05	-2.22	28,28,28,28	0
2	ZN	B	800	1/1	0.99	0.04	-3.04	25,25,25,25	0
2	ZN	D	800	1/1	0.99	0.04	-3.11	28,28,28,28	0
2	ZN	C	800	1/1	0.98	0.03	-4.07	27,27,27,27	0
3	NA	C	801	1/1	0.74	0.20	-	31,31,31,31	0
3	NA	D	801	1/1	0.92	0.25	-	25,25,25,25	0
3	NA	A	801	1/1	0.82	0.24	-	22,22,22,22	0
3	NA	B	801	1/1	0.88	0.17	-	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.