WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:27 PM GMT

PDB ID : 3ZHQ
Title : Crystal structure of the H747A mutant of the SucA domain of Mycobacterium smegmatis KGD
Authors : Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.
Deposited on : 2012-12-24
Resolution : 2.50 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 (i)) 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 2.50 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.
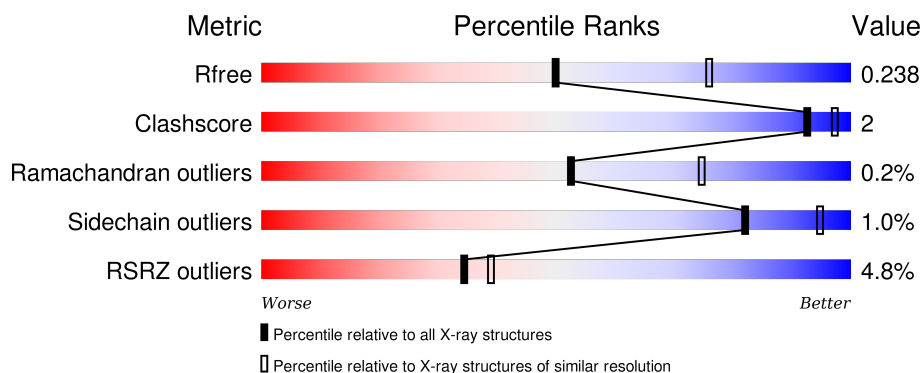
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	868	3% ... 88% ... 5% 7%
1	B	868	5% ... 87% ... 6% 7%
1	C	868	5% ... 88% ... 5% 6%
1	D	868	6% ... 89% ... • 7%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 25781 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 MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	811	Total 6283	C 3959	N 1108	O 1194	S 22	0	1	0
1	B	808	Total 6208	C 3913	N 1103	O 1168	S 24	0	0	0
1	C	812	Total 6301	C 3971	N 1110	O 1197	S 23	0	0	0
1	D	810	Total 6234	C 3933	N 1097	O 1180	S 24	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	EXPRESSION TAG	UNP A0R2B1
A	747	ALA	HIS	ENGINEERED MUTATION	UNP A0R2B1
B	360	GLY	-	EXPRESSION TAG	UNP A0R2B1
B	747	ALA	HIS	ENGINEERED MUTATION	UNP A0R2B1
C	360	GLY	-	EXPRESSION TAG	UNP A0R2B1
C	747	ALA	HIS	ENGINEERED MUTATION	UNP A0R2B1
D	360	GLY	-	EXPRESSION TAG	UNP A0R2B1
D	747	ALA	HIS	ENGINEERED MUTATION	UNP A0R2B1

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).
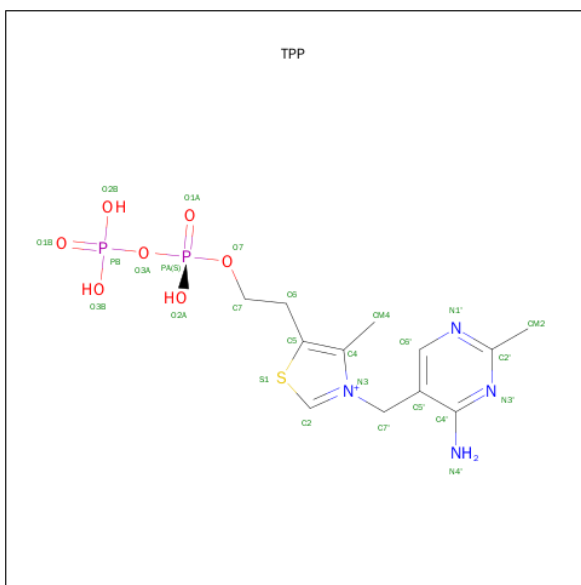
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Ca 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	197	Total 197	O 197	0	0
5	B	154	Total 154	O 154	0	0
5	C	165	Total 165	O 165	0	0
5	D	127	Total 127	O 127	0	0

3 Residue-property plots ⓘ

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.
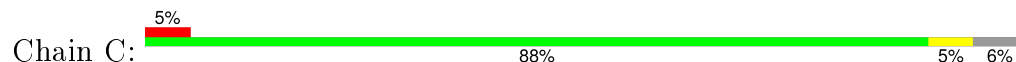
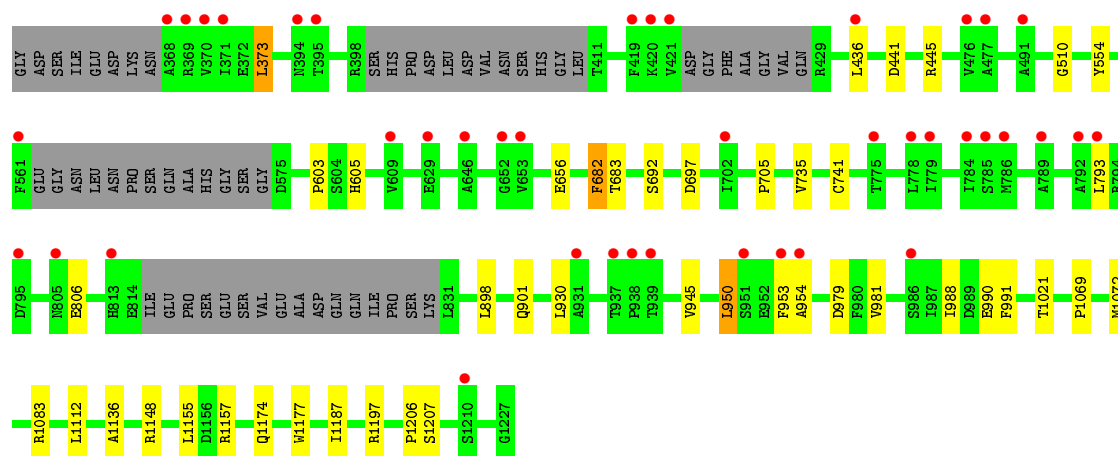- Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME
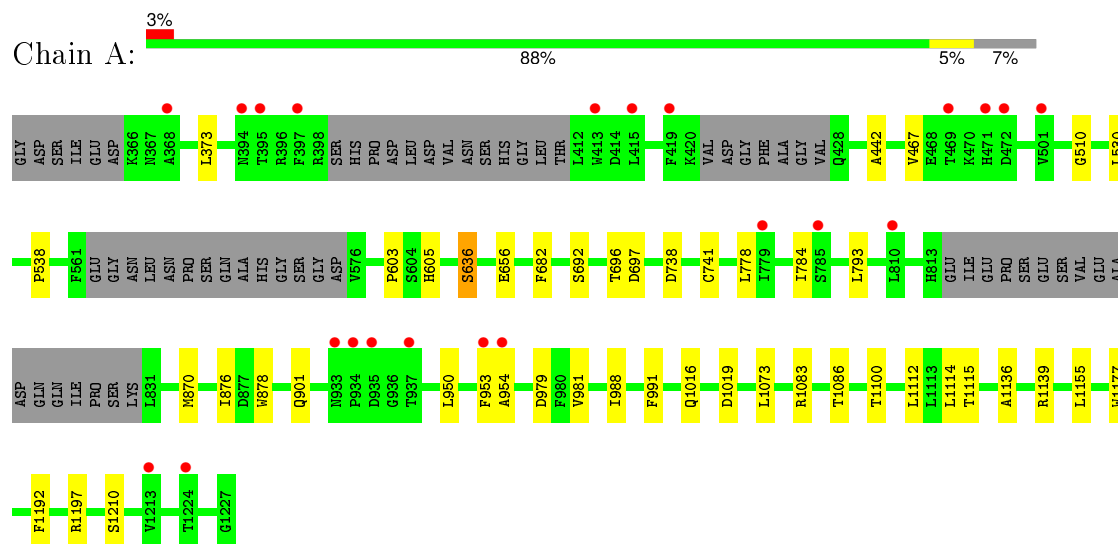
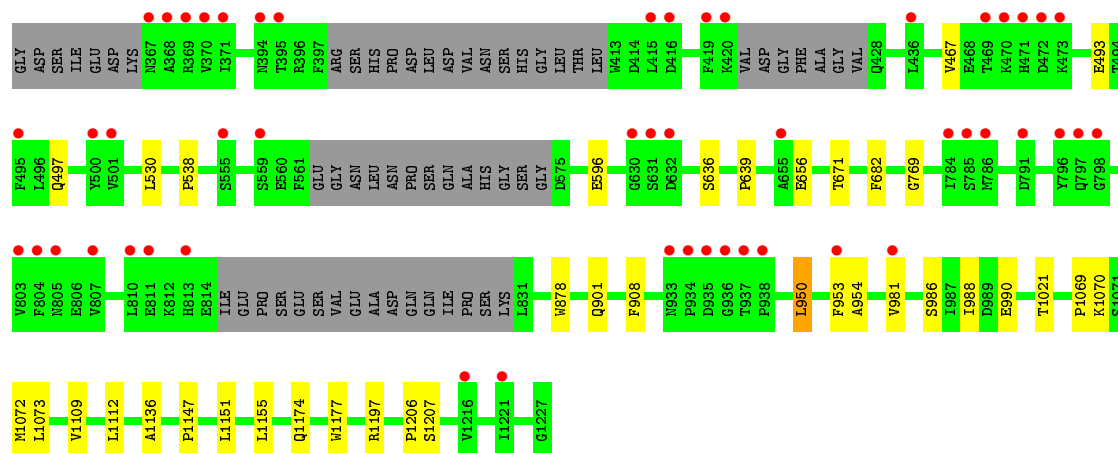- Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

- Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

● Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain D:
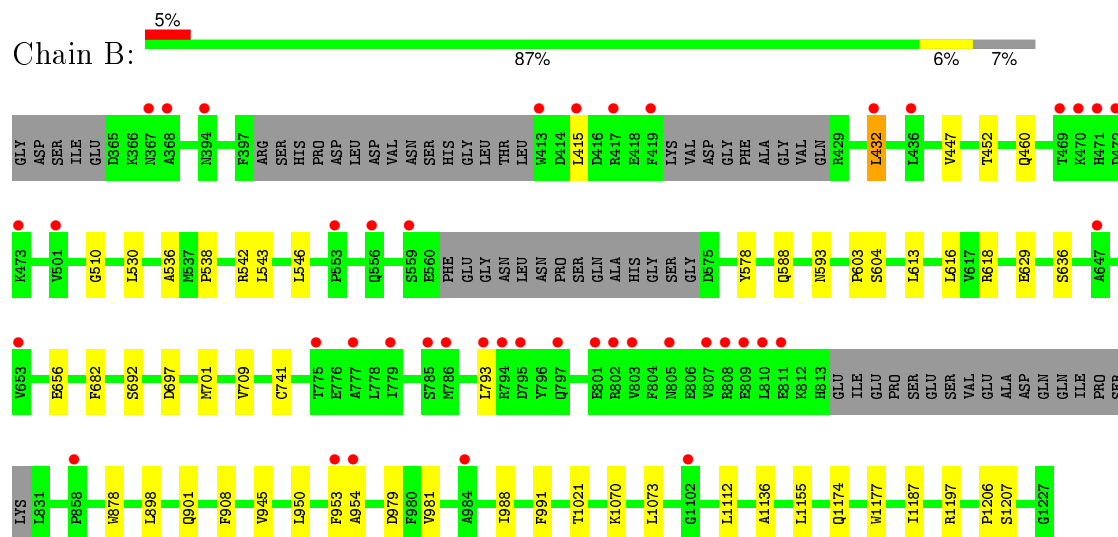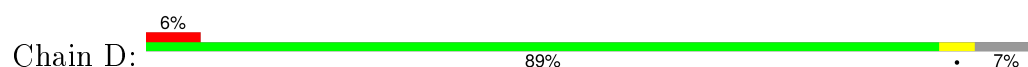
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	80.67Å 83.74Å 159.58Å 99.86° 98.95° 100.44°	Depositor
Resolution (Å)	48.97 – 2.50 48.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.97-2.50) 90.6 (48.97-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.28 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.194 , 0.223 0.203 , 0.238	Depositor DCC
R_{free} test set	6717 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 53.4	EDS
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.48, <L^2> = 0.31$	Xtriage
Outliers	0 of 133092 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25781	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, TPP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.51	0/6411	0.65	0/8699
1	B	0.51	0/6335	0.65	0/8600
1	C	0.50	0/6427	0.65	0/8712
1	D	0.50	0/6359	0.65	0/8625
All	All	0.50	0/25532	0.65	0/34636

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 (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	6283	0	6051	23	0
1	B	6208	0	5963	27	0
1	C	6301	0	6108	27	0
1	D	6234	0	6017	23	0
2	A	26	0	16	2	0
2	B	26	0	16	2	0
2	C	26	0	16	2	0
2	D	26	0	16	2	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	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	197	0	0	2	0
5	B	154	0	0	1	0
5	C	165	0	0	0	0
5	D	127	0	0	4	0
All	All	25781	0	24203	99	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 2.

All (99) 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:C:705:PRO:HG2	1:C:735:VAL:HG13	1.69	0.73
1:C:373:LEU:CD1	1:C:436:LEU:HD21	2.20	0.71
1:C:692:SER:HB2	1:C:697:ASP:OD2	1.93	0.67
1:C:373:LEU:HD11	1:C:436:LEU:CD2	2.27	0.65
1:A:692:SER:HB2	1:A:697:ASP:OD2	1.98	0.63
1:C:373:LEU:HD11	1:C:436:LEU:HD21	1.82	0.62
1:C:373:LEU:CD1	1:C:436:LEU:CD2	2.78	0.61
1:C:373:LEU:HD12	1:C:436:LEU:HD21	1.84	0.57
1:A:530:LEU:HD22	1:A:636:SER:HA	1.88	0.56
1:A:901:GLN:OE1	2:B:2001:TPP:H6'	2.07	0.55
1:D:1174:GLN:OE1	1:D:1206:PRO:HA	2.07	0.55
1:C:1112:LEU:HD12	1:C:1136:ALA:HB3	1.91	0.53
1:B:542:ARG:HD3	1:B:578:TYR:HA	1.90	0.53
1:D:1069:PRO:HB3	1:D:1072:MET:HB3	1.91	0.53
1:A:442:ALA:HB1	1:A:467:VAL:HG12	1.91	0.52
1:B:603:PRO:HD3	1:B:991:PHE:CZ	2.45	0.52
1:C:898:LEU:O	1:C:945:VAL:HA	2.09	0.52
1:A:603:PRO:HD3	1:A:991:PHE:CZ	2.45	0.51
1:D:1112:LEU:HD12	1:D:1136:ALA:HB3	1.93	0.51
1:B:1112:LEU:HD12	1:B:1136:ALA:HB3	1.92	0.51
1:C:901:GLN:OE1	2:D:2001:TPP:H6'	2.11	0.51
1:A:1112:LEU:HD12	1:A:1136:ALA:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:ARG:HH21	1:B:629:GLU:HG2	1.77	0.49
1:D:639:PRO:HB2	1:D:671:THR:HG23	1.94	0.49
1:C:441:ASP:HA	1:C:445:ARG:HG3	1.94	0.49
1:C:1148:ARG:HG3	1:C:1187:ILE:HD12	1.94	0.49
1:B:530:LEU:HD22	1:B:636:SER:HA	1.93	0.49
2:C:2001:TPP:H6'	1:D:901:GLN:OE1	2.12	0.49
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.94	0.49
1:D:538:PRO:HB2	5:D:3019:HOH:O	2.13	0.49
1:D:493:GLU:O	1:D:497:GLN:HG2	2.13	0.48
1:B:536:ALA:HB3	1:B:613:LEU:HD22	1.94	0.48
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.95	0.48
1:A:1086:THR:O	1:C:1157:ARG:NH2	2.41	0.48
1:D:1147:PRO:O	1:D:1151:LEU:HB2	2.13	0.48
1:B:452:THR:HA	1:B:460:GLN:NE2	2.29	0.48
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.96	0.47
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.96	0.47
1:A:878:TRP:HB3	1:A:1073:LEU:HD23	1.95	0.47
1:B:510:GLY:O	1:B:741:CYS:HB2	2.15	0.47
1:C:603:PRO:HD3	1:C:991:PHE:CZ	2.51	0.46
1:A:1112:LEU:HD21	1:A:1155:LEU:HD22	1.98	0.46
1:D:986:SER:O	1:D:990:GLU:HB2	2.16	0.46
1:C:1069:PRO:HB2	1:C:1072:MET:HB3	1.97	0.46
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.51	0.46
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.96	0.46
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.51	0.46
1:A:538:PRO:HD2	5:A:3028:HOH:O	2.15	0.46
1:C:1069:PRO:CB	1:C:1072:MET:HB3	2.47	0.45
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.51	0.45
2:C:2001:TPP:HM41	1:D:950:LEU:HD22	1.98	0.45
1:C:1174:GLN:OE1	1:C:1206:PRO:HA	2.17	0.45
1:B:898:LEU:O	1:B:945:VAL:HA	2.17	0.45
1:C:510:GLY:O	1:C:741:CYS:HB2	2.16	0.45
1:A:692:SER:HB3	1:B:701:MET:O	2.16	0.45
1:A:1083:ARG:HA	1:A:1086:THR:OG1	2.16	0.44
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.52	0.44
1:D:530:LEU:HD22	1:D:636:SER:HA	1.98	0.44
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.53	0.44
1:A:870:MET:HB3	1:A:876:ILE:HG12	2.00	0.44
1:B:538:PRO:HB2	5:B:3018:HOH:O	2.18	0.44
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.53	0.44
1:D:596:GLU:HG3	5:D:3029:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:SER:HB2	1:B:697:ASP:OD2	2.18	0.44
1:D:878:TRP:HB3	1:D:1073:LEU:HD23	2.00	0.44
1:C:554:TYR:HD2	1:C:806:GLU:OE1	2.01	0.43
1:D:1069:PRO:CB	1:D:1072:MET:HB3	2.48	0.43
2:A:2001:TPP:H61	2:A:2001:TPP:HM41	1.93	0.43
1:B:878:TRP:HB3	1:B:1073:LEU:HD23	2.01	0.43
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	2.00	0.43
1:C:682:PHE:HD1	1:C:683:THR:HG23	1.83	0.43
1:B:447:VAL:HG22	1:B:709:VAL:HG23	2.00	0.43
1:D:656:GLU:HB3	1:D:954:ALA:HB2	2.01	0.43
1:A:1016:GLN:NE2	5:A:3143:HOH:O	2.22	0.43
1:B:1174:GLN:OE1	1:B:1206:PRO:HA	2.18	0.42
1:B:656:GLU:HB3	1:B:954:ALA:HB2	2.02	0.42
1:A:656:GLU:HB3	1:A:954:ALA:HB2	2.01	0.42
2:B:2001:TPP:HM41	2:B:2001:TPP:H61	1.93	0.42
2:A:2001:TPP:H6'	1:B:901:GLN:OE1	2.18	0.42
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.01	0.42
1:B:543:LEU:HA	1:B:546:LEU:HD12	2.01	0.42
1:D:1021:THR:HG21	1:D:1207:SER:HB3	2.02	0.41
1:A:778:LEU:HB3	1:A:784:ILE:HG12	2.01	0.41
1:B:536:ALA:CB	1:B:613:LEU:HD22	2.50	0.41
1:A:1155:LEU:HD11	1:A:1192:PHE:CZ	2.55	0.41
1:D:596:GLU:CG	5:D:3029:HOH:O	2.68	0.41
1:C:656:GLU:HB3	1:C:954:ALA:HB2	2.02	0.41
1:B:415:LEU:HA	1:B:432:LEU:HB3	2.02	0.41
1:D:769:GLY:HA3	5:D:3009:HOH:O	2.21	0.41
1:B:1021:THR:HG21	1:B:1207:SER:HB3	2.03	0.41
1:D:1112:LEU:HD21	1:D:1155:LEU:HD22	2.01	0.41
1:B:588:GLN:OE1	1:B:593:ASN:HB2	2.21	0.41
1:A:510:GLY:O	1:A:741:CYS:HB2	2.21	0.41
1:C:603:PRO:HG3	1:C:990:GLU:HB3	2.03	0.40
1:C:1021:THR:HG21	1:C:1207:SER:HB3	2.03	0.40
1:C:950:LEU:HD22	2:D:2001:TPP:HM41	2.02	0.40
1:A:1115:THR:O	1:A:1139:ARG:HA	2.21	0.40
1:D:1109:VAL:HG21	1:D:1136:ALA:HB2	2.03	0.40
1:A:1019:ASP:CB	1:B:604:SER:HB2	2.51	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	802/868 (92%)	779 (97%)	20 (2%)	3 (0%)	39	61
1	B	798/868 (92%)	779 (98%)	18 (2%)	1 (0%)	56	78
1	C	802/868 (92%)	779 (97%)	21 (3%)	2 (0%)	52	75
1	D	800/868 (92%)	777 (97%)	22 (3%)	1 (0%)	56	78
All	All	3202/3472 (92%)	3114 (97%)	81 (2%)	7 (0%)	52	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	605	HIS
1	A	605	HIS
1	A	636	SER
1	A	682	PHE
1	B	682	PHE
1	C	682	PHE
1	D	682	PHE

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	645/725 (89%)	637 (99%)	8 (1%)	78	93
1	B	629/725 (87%)	622 (99%)	7 (1%)	80	94
1	C	651/725 (90%)	644 (99%)	7 (1%)	80	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	637/725 (88%)	634 (100%)	3 (0%)	92	98
All	All	2562/2900 (88%)	2537 (99%)	25 (1%)	82	95

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	373	LEU
1	A	793	LEU
1	A	950	LEU
1	A	953	PHE
1	A	979	ASP
1	A	1100	THR
1	A	1114	LEU
1	A	1210	SER
1	B	432	LEU
1	B	616	LEU
1	B	793	LEU
1	B	950	LEU
1	B	953	PHE
1	B	979	ASP
1	B	1187	ILE
1	C	373	LEU
1	C	793	LEU
1	C	930	LEU
1	C	950	LEU
1	C	953	PHE
1	C	979	ASP
1	C	1083	ARG
1	D	467	VAL
1	D	950	LEU
1	D	953	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	464	GLN
1	D	464	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	#$|Z| > 2$
2	TPP	A	2001	3	20,27,27	1.56	2 (10%)	31,40,40	1.75	9 (29%)
2	TPP	B	2001	3	20,27,27	2.03	2 (10%)	31,40,40	1.72	8 (25%)
2	TPP	C	2001	3	20,27,27	2.01	2 (10%)	31,40,40	1.76	8 (25%)
2	TPP	D	2001	3	20,27,27	2.02	2 (10%)	31,40,40	1.66	7 (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
2	TPP	A	2001	3	-	0/16/17/17	0/2/2/2
2	TPP	B	2001	3	-	0/16/17/17	0/2/2/2
2	TPP	C	2001	3	-	0/16/17/17	0/2/2/2
2	TPP	D	2001	3	-	0/16/17/17	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TPP	C4-N3	-7.49	1.33	1.39
2	C	2001	TPP	C4-N3	-7.38	1.33	1.39
2	B	2001	TPP	C4-N3	-7.34	1.33	1.39
2	A	2001	TPP	C4-N3	-5.16	1.35	1.39
2	A	2001	TPP	PB-O1B	2.44	1.59	1.51
2	C	2001	TPP	PB-O1B	2.77	1.60	1.51
2	D	2001	TPP	PB-O1B	3.33	1.62	1.51
2	B	2001	TPP	PB-O1B	3.40	1.62	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	TPP	CM4-C4-C5	-4.92	117.84	128.90
2	B	2001	TPP	CM4-C4-C5	-4.77	118.19	128.90
2	C	2001	TPP	CM4-C4-C5	-4.59	118.59	128.90
2	D	2001	TPP	CM4-C4-C5	-4.35	119.11	128.90
2	C	2001	TPP	N1'-C2'-N3'	-2.56	120.87	125.60
2	D	2001	TPP	C5'-C6'-N1'	-2.49	119.53	123.86
2	A	2001	TPP	N1'-C2'-N3'	-2.29	121.37	125.60
2	B	2001	TPP	C5'-C6'-N1'	-2.14	120.14	123.86
2	B	2001	TPP	N1'-C2'-N3'	-2.13	121.66	125.60
2	A	2001	TPP	C6-C5-S1	2.00	123.04	120.24
2	C	2001	TPP	O3A-PA-O7	2.19	108.74	102.94
2	A	2001	TPP	O3A-PA-O7	2.19	108.75	102.94
2	C	2001	TPP	CM2-C2'-N1'	2.21	119.68	117.03
2	B	2001	TPP	C6-C5-C4	2.33	129.66	127.56
2	A	2001	TPP	C6-C5-C4	2.49	129.80	127.56
2	D	2001	TPP	O3A-PA-O7	2.50	109.56	102.94
2	A	2001	TPP	CM4-C4-N3	2.51	125.93	122.59
2	A	2001	TPP	C6'-N1'-C2'	2.58	120.27	115.77
2	D	2001	TPP	CM4-C4-N3	2.66	126.14	122.59
2	A	2001	TPP	CM2-C2'-N1'	2.68	120.24	117.03
2	B	2001	TPP	O3A-PA-O7	2.68	110.05	102.94
2	C	2001	TPP	CM4-C4-N3	2.68	126.17	122.59
2	D	2001	TPP	C6-C5-C4	2.71	130.00	127.56
2	B	2001	TPP	CM4-C4-N3	2.97	126.55	122.59
2	C	2001	TPP	C6-C5-C4	3.00	130.25	127.56
2	B	2001	TPP	C6'-N1'-C2'	3.02	121.05	115.77
2	D	2001	TPP	C6'-N1'-C2'	3.11	121.20	115.77
2	D	2001	TPP	C5-C4-N3	3.15	114.62	107.69
2	C	2001	TPP	C6'-N1'-C2'	3.37	121.66	115.77
2	C	2001	TPP	C5-C4-N3	3.37	115.11	107.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	TPP	C5-C4-N3	3.42	115.22	107.69
2	A	2001	TPP	C5-C4-N3	3.81	116.06	107.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	TPP	2	0
2	B	2001	TPP	2	0
2	C	2001	TPP	2	0
2	D	2001	TPP	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, 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(Å²)	Q<0.9
1	A	811/868 (93%)	0.07	22 (2%)	58	62	22, 39, 68, 97	0
1	B	808/868 (93%)	0.17	43 (5%)	30	34	20, 40, 75, 103	0
1	C	812/868 (93%)	0.21	41 (5%)	32	37	22, 42, 74, 98	0
1	D	810/868 (93%)	0.25	50 (6%)	24	27	23, 42, 75, 114	0
All	All	3241/3472 (93%)	0.18	156 (4%)	34	39	20, 41, 73, 114	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	ALA	6.2
1	B	472	ASP	6.0
1	B	810	LEU	5.6
1	C	779	ILE	5.6
1	D	368	ALA	5.4
1	D	472	ASP	5.3
1	B	368	ALA	5.3
1	D	471	HIS	5.0
1	A	394	ASN	4.6
1	D	394	ASN	4.5
1	D	473	LYS	4.2
1	B	471	HIS	4.0
1	A	469	THR	3.9
1	C	939	THR	3.9
1	B	470	LYS	3.8
1	D	937	THR	3.7
1	B	808	ARG	3.7
1	D	810	LEU	3.7
1	B	775	THR	3.6
1	D	367	ASN	3.6
1	B	793	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	501	VAL	3.6
1	D	811	GLU	3.6
1	D	370	VAL	3.5
1	C	792	ALA	3.4
1	B	779	ILE	3.4
1	B	501	VAL	3.4
1	A	415	LEU	3.4
1	A	779	ILE	3.4
1	D	797	GLN	3.4
1	C	394	ASN	3.4
1	C	421	VAL	3.4
1	D	470	LYS	3.3
1	D	813	HIS	3.3
1	D	371	ILE	3.3
1	B	786	MET	3.3
1	B	797	GLN	3.2
1	B	858	PRO	3.2
1	C	785	SER	3.2
1	C	938	PRO	3.2
1	A	471	HIS	3.1
1	B	1102	GLY	3.1
1	B	805	ASN	3.1
1	A	810	LEU	3.1
1	D	934	PRO	3.1
1	B	809	GLU	3.1
1	D	369	ARG	3.1
1	D	786	MET	3.0
1	D	805	ASN	3.0
1	C	937	THR	3.0
1	D	935	ASP	3.0
1	D	784	ILE	3.0
1	B	367	ASN	2.9
1	C	368	ALA	2.9
1	C	786	MET	2.9
1	C	931	ALA	2.9
1	B	473	LYS	2.8
1	D	632	ASP	2.8
1	B	559	SER	2.8
1	D	953	PHE	2.8
1	C	805	ASN	2.8
1	C	652	GLY	2.8
1	D	415	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	472	ASP	2.7
1	A	1224	THR	2.7
1	B	419	PHE	2.7
1	C	561	PHE	2.7
1	D	419	PHE	2.7
1	C	420	LYS	2.7
1	A	413	TRP	2.6
1	D	416	ASP	2.6
1	C	477	ALA	2.6
1	D	938	PRO	2.6
1	B	413	TRP	2.6
1	D	420	LYS	2.6
1	B	647	ALA	2.6
1	C	436	LEU	2.6
1	B	811	GLU	2.5
1	B	803	VAL	2.5
1	D	436	LEU	2.5
1	C	793	LEU	2.5
1	C	371	ILE	2.5
1	B	802	ARG	2.5
1	D	803	VAL	2.4
1	B	556	GLN	2.4
1	B	794	ARG	2.4
1	C	702	ILE	2.4
1	B	801	GLU	2.4
1	B	807	VAL	2.4
1	A	953	PHE	2.4
1	C	953	PHE	2.4
1	C	476	VAL	2.4
1	C	778	LEU	2.4
1	A	395	THR	2.4
1	C	784	ILE	2.3
1	D	804	PHE	2.3
1	B	469	THR	2.3
1	C	775	THR	2.3
1	C	813	HIS	2.3
1	B	394	ASN	2.3
1	B	953	PHE	2.3
1	C	1210	SER	2.3
1	D	500	TYR	2.3
1	C	795	ASP	2.3
1	B	777	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	395	THR	2.3
1	D	796	TYR	2.3
1	C	954	ALA	2.2
1	D	469	THR	2.2
1	B	795	ASP	2.2
1	C	419	PHE	2.2
1	C	491	ALA	2.2
1	A	419	PHE	2.2
1	D	1216	VAL	2.2
1	A	933	ASN	2.2
1	D	791	ASP	2.2
1	B	415	LEU	2.2
1	D	395	THR	2.2
1	D	798	GLY	2.2
1	D	936	GLY	2.2
1	C	369	ARG	2.2
1	B	553	PRO	2.2
1	B	653	VAL	2.1
1	A	785	SER	2.1
1	A	935	ASP	2.1
1	A	1213	VAL	2.1
1	B	785	SER	2.1
1	C	370	VAL	2.1
1	C	789	ALA	2.1
1	C	986	SER	2.1
1	D	807	VAL	2.1
1	A	397	PHE	2.1
1	B	432	LEU	2.1
1	B	436	LEU	2.1
1	A	501	VAL	2.1
1	D	630	GLY	2.1
1	B	984	ALA	2.1
1	D	655	ALA	2.1
1	A	937	THR	2.1
1	B	417	ARG	2.1
1	C	646	ALA	2.1
1	C	653	VAL	2.1
1	D	933	ASN	2.1
1	D	555	SER	2.1
1	C	951	SER	2.1
1	C	629	GLU	2.0
1	D	785	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	495	PHE	2.0
1	D	559	SER	2.0
1	A	954	ALA	2.0
1	B	954	ALA	2.0
1	C	609	VAL	2.0
1	D	981	VAL	2.0
1	A	934	PRO	2.0
1	D	1221	ILE	2.0
1	D	631	SER	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, 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
3	MG	A	2002	1/1	0.96	0.15	0.23	20,20,20,20	0
2	TPP	D	2001	26/26	0.97	0.18	-0.12	23,33,36,38	0
2	TPP	A	2001	26/26	0.97	0.15	-0.50	16,26,33,34	0
2	TPP	B	2001	26/26	0.98	0.16	-0.82	20,31,37,38	0
2	TPP	C	2001	26/26	0.98	0.16	-1.08	23,34,39,40	0
3	MG	D	2002	1/1	0.96	0.12	-1.36	23,23,23,23	0
3	MG	C	2002	1/1	0.99	0.14	-1.58	15,15,15,15	0
4	CA	D	2003	1/1	0.99	0.06	-1.74	40,40,40,40	0
4	CA	A	2003	1/1	0.99	0.10	-1.99	32,32,32,32	0
3	MG	B	2002	1/1	0.99	0.08	-2.70	18,18,18,18	0
4	CA	B	2003	1/1	0.99	0.06	-3.32	38,38,38,38	0
4	CA	C	2003	1/1	0.96	0.03	-5.22	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.