Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:28 PM GMT

PDB ID	:	3ZHS
Title	:	Crystal structure of the SucA domain of Mycobacterium smegmatis KGD, first post-decarboxylation intermediate from alpha-ketoglutarate
Authors	:	Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.
Deposited on	:	2012-12-24
Resolution	:	2.10 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:

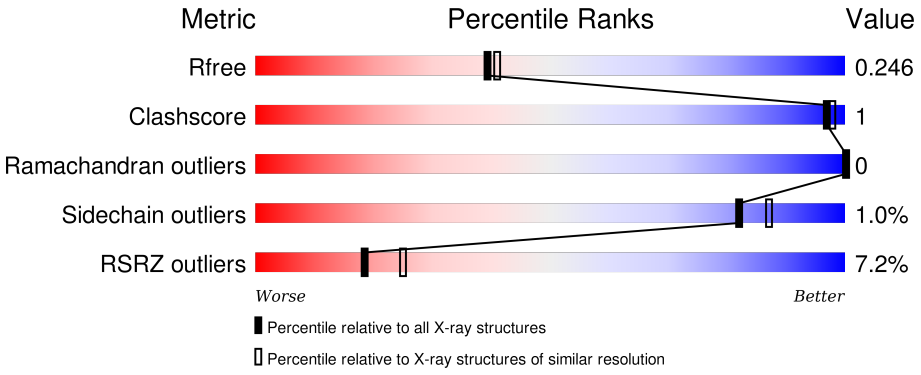
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	7% 89% 5% 6%
1	B	868	6% 90% • 6%
1	C	868	6% 89% • 7%
1	D	868	8% 89% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26258 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.

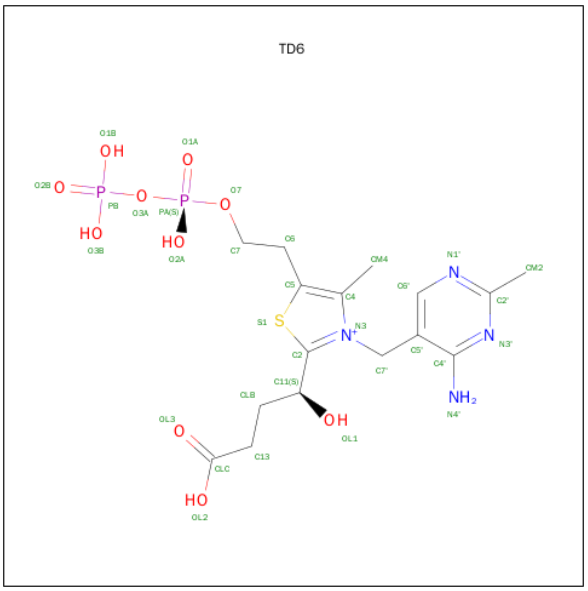
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	817	Total	C	N	O	S	0	0	0
			6319	3983	1114	1200	22			
1	B	813	Total	C	N	O	S	0	0	0
			6254	3946	1106	1179	23			
1	C	808	Total	C	N	O	S	0	0	0
			6280	3962	1108	1187	23			
1	D	810	Total	C	N	O	S	0	0	0
			6225	3926	1102	1173	24			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	360	GLY	-	EXPRESSION TAG	UNP A0R2B1
B	360	GLY	-	EXPRESSION TAG	UNP A0R2B1
C	360	GLY	-	EXPRESSION TAG	UNP A0R2B1
D	360	GLY	-	EXPRESSION TAG	UNP A0R2B1

- Molecule 2 is (4S)-4-{3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-5-(2-{[(S)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3LAMBDA 5 -THIAZOL-2-YL}-4-HYDROXYBUTANOIC ACID (three-letter code: TD6) (formula: $C_{16}H_{25}N_4O_{10}P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			33	16	4	10	2	1		

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

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

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

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

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

- Molecule 5 is water.

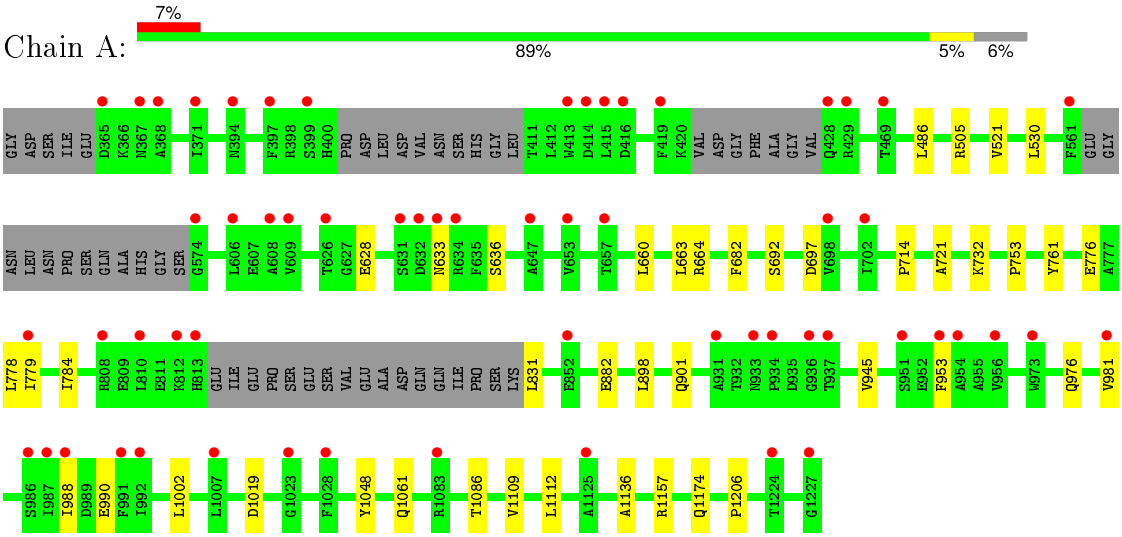
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	316	Total O 316 316	0	0
5	B	241	Total O 241 241	0	0
5	C	272	Total O 272 272	0	0
5	D	211	Total O 211 211	0	0

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.

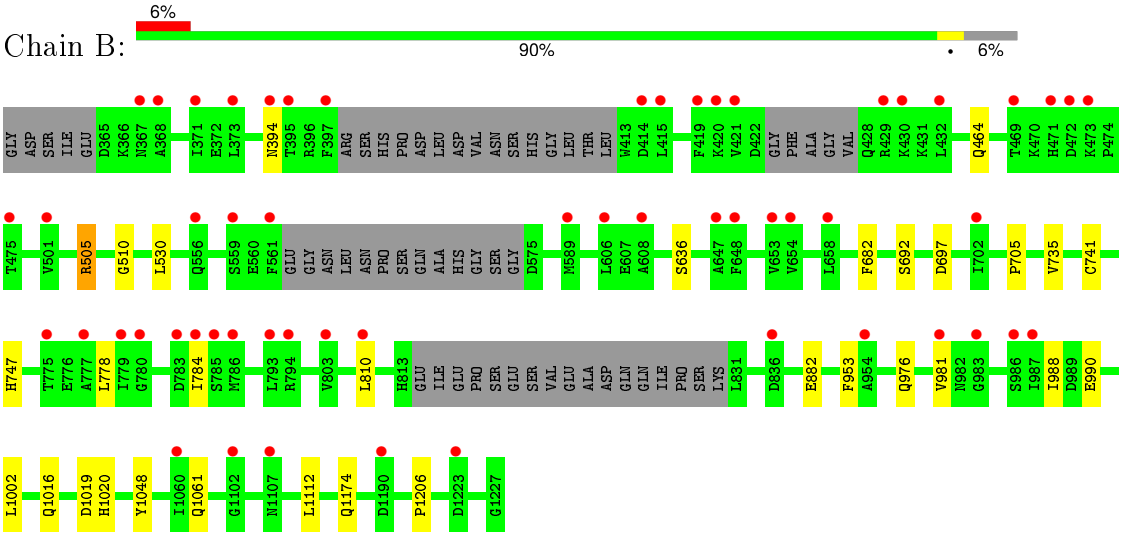
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain A:



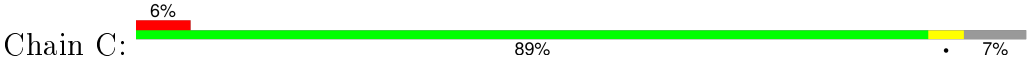
• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

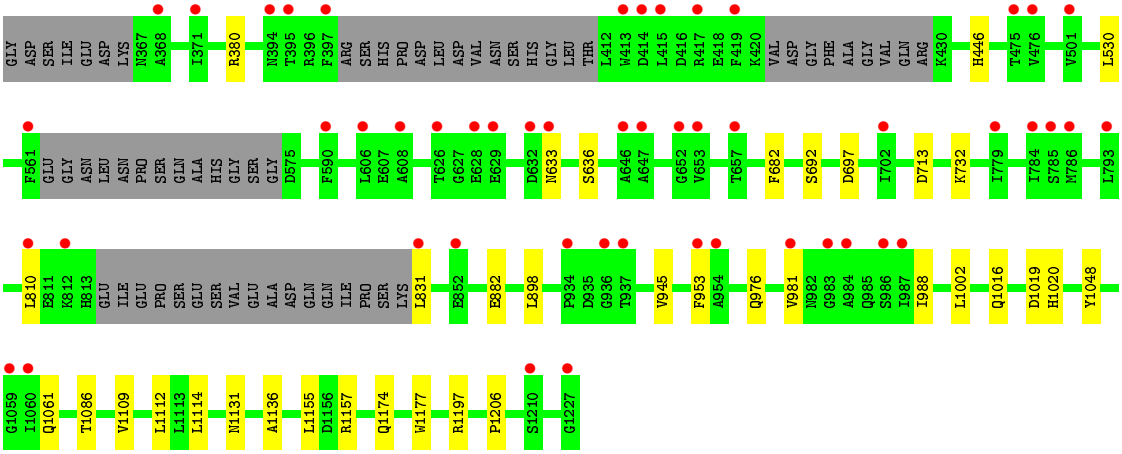
Chain B:



• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

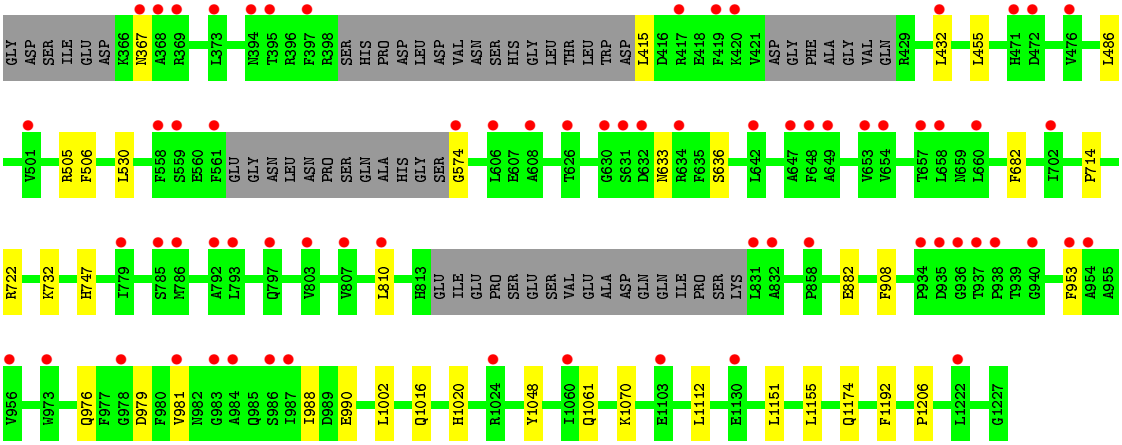
Chain C:





- 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	80.85Å 83.71Å 159.94Å 99.89° 99.03° 100.20°	Depositor
Resolution (Å)	30.75 – 2.10 47.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.75-2.10) 87.9 (47.43-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.200 , 0.228 0.215 , 0.246	Depositor DCC
R_{free} test set	10966 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.3	EDS
Estimated twinning fraction	0.015 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 220123 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	26258	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MG, CA, TD6

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	0/6448	0.62	0/8749
1	B	0.50	0/6381	0.62	0/8661
1	C	0.50	0/6407	0.63	0/8684
1	D	0.50	0/6351	0.62	0/8615
All	All	0.50	0/25587	0.62	0/34709

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	6319	0	6087	22	0
1	B	6254	0	6025	13	0
1	C	6280	0	6099	19	0
1	D	6225	0	6004	17	0
2	A	33	0	21	0	0
2	B	33	0	21	1	0
2	C	33	0	21	0	0
2	D	33	0	21	1	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	316	0	0	1	0
5	B	241	0	0	0	0
5	C	272	0	0	0	0
5	D	211	0	0	1	0
All	All	26258	0	24299	66	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 (66) 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:1112:LEU:HD21	1:C:1155:LEU:HD22	1.77	0.65
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.84	0.59
1:C:1109:VAL:HG21	1:C:1136:ALA:HB2	1.84	0.58
1:A:1157:ARG:NH2	1:C:1086:THR:O	2.33	0.58
1:C:380:ARG:NH1	1:D:455:LEU:O	2.33	0.56
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.89	0.54
1:D:1151:LEU:O	1:D:1155:LEU:HG	2.08	0.52
1:B:505:ARG:HA	1:B:747:HIS:O	2.09	0.52
1:D:415:LEU:HA	1:D:432:LEU:HD12	1.91	0.52
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.91	0.52
1:B:882:GLU:HB2	1:B:1048:TYR:HE2	1.75	0.51
1:A:486:LEU:HD11	1:A:714:PRO:HG3	1.93	0.50
1:A:1086:THR:O	1:C:1157:ARG:NH2	2.40	0.50
1:A:753:PRO:HB2	1:A:761:TYR:CD1	2.46	0.50
1:B:530:LEU:HD22	1:B:636:SER:HA	1.94	0.49
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.94	0.48
1:A:778:LEU:HB3	1:A:784:ILE:HG12	1.96	0.48
1:C:446:HIS:ND1	1:C:713:ASP:OD2	2.47	0.47
1:D:506:PHE:CZ	1:D:574:GLY:HA2	2.50	0.46
1:A:1109:VAL:HG21	1:A:1136:ALA:HB2	1.97	0.46
1:A:628:GLU:HG2	1:A:664:ARG:O	2.16	0.46
1:A:1019:ASP:OD1	1:B:990:GLU:OE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:GLU:HB2	1:D:1048:TYR:HE2	1.81	0.45
1:C:530:LEU:HD22	1:C:636:SER:HA	1.98	0.45
1:D:722:ARG:NH1	5:D:3087:HOH:O	2.50	0.45
1:A:692:SER:HB2	1:A:697:ASP:OD2	2.17	0.45
1:D:633:ASN:O	1:D:732:LYS:HE3	2.17	0.45
1:A:776:GLU:HA	1:A:779:ILE:HD12	1.99	0.44
1:A:882:GLU:HB2	1:A:1048:TYR:HE2	1.82	0.44
1:D:486:LEU:HD11	1:D:714:PRO:HG3	1.99	0.44
1:C:1112:LEU:HD23	1:C:1114:LEU:HD11	2.00	0.44
1:D:530:LEU:HD22	1:D:636:SER:HA	2.00	0.44
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.52	0.44
1:D:1002:LEU:HB3	1:D:1061:GLN:HB2	2.00	0.43
1:A:660:LEU:HA	1:A:663:LEU:HD12	2.01	0.43
1:D:1155:LEU:HD11	1:D:1192:PHE:CZ	2.54	0.43
1:D:505:ARG:HA	1:D:747:HIS:O	2.19	0.43
1:D:1174:GLN:OE1	1:D:1206:PRO:HA	2.19	0.43
1:A:1174:GLN:OE1	1:A:1206:PRO:HA	2.18	0.43
1:B:705:PRO:HG2	1:B:735:VAL:HG13	2.01	0.42
1:C:692:SER:HB2	1:C:697:ASP:OD2	2.20	0.42
1:C:633:ASN:O	1:C:732:LYS:HE2	2.19	0.42
1:B:1016:GLN:HB3	1:B:1020:HIS:HB2	2.01	0.42
1:C:1112:LEU:CD2	1:C:1155:LEU:HD22	2.46	0.42
1:A:990:GLU:OE1	1:B:1019:ASP:OD1	2.38	0.42
1:C:1019:ASP:OD1	1:D:990:GLU:OE1	2.37	0.42
1:C:1016:GLN:HB3	1:C:1020:HIS:HB2	2.02	0.42
1:C:1002:LEU:HB3	1:C:1061:GLN:CB	2.50	0.42
1:D:1016:GLN:HB3	1:D:1020:HIS:HB2	2.01	0.42
1:A:898:LEU:O	1:A:945:VAL:HA	2.20	0.41
1:A:521:VAL:HG23	1:A:721:ALA:HB1	2.02	0.41
1:B:1002:LEU:HB3	1:B:1061:GLN:HB2	2.03	0.41
1:A:505:ARG:HG2	5:A:3024:HOH:O	2.21	0.41
1:C:898:LEU:O	1:C:945:VAL:HA	2.19	0.41
1:B:1174:GLN:OE1	1:B:1206:PRO:HA	2.21	0.41
1:C:1174:GLN:OE1	1:C:1206:PRO:HA	2.20	0.41
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.56	0.41
1:A:633:ASN:O	1:A:732:LYS:HE2	2.21	0.41
1:C:882:GLU:HB2	1:C:1048:TYR:HE2	1.86	0.40
1:A:901:GLN:OE1	2:B:2001:TD6:H6'	2.21	0.40
1:B:692:SER:HB2	1:B:697:ASP:OD2	2.22	0.40
2:D:2001:TD6:H6	2:D:2001:TD6:HM4	1.97	0.40
1:B:778:LEU:HB3	1:B:784:ILE:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:GLY:O	1:B:741:CYS:HB2	2.22	0.40
1:A:1002:LEU:HB3	1:A:1061:GLN:HB2	2.03	0.40
1:A:530:LEU:HD22	1:A:636:SER:HA	2.03	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	807/868 (93%)	786 (97%)	21 (3%)	0	100	100
1	B	803/868 (92%)	784 (98%)	19 (2%)	0	100	100
1	C	798/868 (92%)	777 (97%)	21 (3%)	0	100	100
1	D	800/868 (92%)	779 (97%)	21 (3%)	0	100	100
All	All	3208/3472 (92%)	3126 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	649/726 (89%)	644 (99%)	5 (1%)	86	91
1	B	638/726 (88%)	630 (99%)	8 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	649/726 (89%)	643 (99%)	6 (1%)	84 89
1	D	634/726 (87%)	627 (99%)	7 (1%)	80 85
All	All	2570/2904 (88%)	2544 (99%)	26 (1%)	82 87

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	682	PHE
1	A	831	LEU
1	A	953	PHE
1	A	976	GLN
1	A	1112	LEU
1	B	394	ASN
1	B	464	GLN
1	B	505	ARG
1	B	682	PHE
1	B	810	LEU
1	B	953	PHE
1	B	976	GLN
1	B	1112	LEU
1	C	682	PHE
1	C	810	LEU
1	C	831	LEU
1	C	953	PHE
1	C	976	GLN
1	C	1131	ASN
1	D	367	ASN
1	D	682	PHE
1	D	810	LEU
1	D	953	PHE
1	D	976	GLN
1	D	979	ASP
1	D	1112	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 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	TD6	A	2001	3	24,34,34	1.50	2 (8%)	36,50,50	1.87	8 (22%)
2	TD6	B	2001	3	24,34,34	1.59	2 (8%)	36,50,50	1.79	8 (22%)
2	TD6	C	2001	3	24,34,34	1.52	2 (8%)	36,50,50	1.74	6 (16%)
2	TD6	D	2001	3	24,34,34	1.61	2 (8%)	36,50,50	1.87	7 (19%)

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	TD6	A	2001	3	-	0/19/26/26	0/2/2/2
2	TD6	B	2001	3	-	0/19/26/26	0/2/2/2
2	TD6	C	2001	3	-	0/19/26/26	0/2/2/2
2	TD6	D	2001	3	-	0/19/26/26	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	TD6	C5-S1	-4.17	1.66	1.74
2	B	2001	TD6	C5-S1	-3.80	1.67	1.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	TD6	C5-S1	-3.70	1.67	1.74
2	A	2001	TD6	C5-S1	-2.61	1.69	1.74
2	C	2001	TD6	C2-N3	6.19	1.49	1.35
2	B	2001	TD6	C2-N3	6.36	1.49	1.35
2	D	2001	TD6	C2-N3	6.40	1.49	1.35
2	A	2001	TD6	C2-N3	6.54	1.50	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	TD6	C6-C5-C4	-4.17	123.83	127.56
2	D	2001	TD6	C6-C5-C4	-3.96	124.01	127.56
2	C	2001	TD6	C6-C5-C4	-3.37	124.54	127.56
2	B	2001	TD6	C6-C5-C4	-3.06	124.83	127.56
2	D	2001	TD6	CM4-C4-C5	-2.27	123.79	128.90
2	B	2001	TD6	CM4-C4-C5	-2.17	124.03	128.90
2	A	2001	TD6	O1B-PB-O3A	-2.12	95.46	105.09
2	A	2001	TD6	CM4-C4-C5	-2.01	124.37	128.90
2	B	2001	TD6	O3B-PB-O2B	2.06	117.20	110.58
2	B	2001	TD6	O1B-PB-O2B	2.12	117.40	110.58
2	C	2001	TD6	C6-C5-S1	2.14	123.23	120.24
2	C	2001	TD6	C5-C4-N3	2.17	112.88	107.83
2	C	2001	TD6	O7-PA-O1A	2.23	118.25	109.62
2	A	2001	TD6	C5-C4-N3	2.31	113.19	107.83
2	D	2001	TD6	C5-C4-N3	2.31	113.20	107.83
2	B	2001	TD6	C5-C4-N3	2.31	113.21	107.83
2	D	2001	TD6	C6-C5-S1	2.35	123.52	120.24
2	A	2001	TD6	O7-PA-O1A	2.50	119.34	109.62
2	C	2001	TD6	O3B-PB-O2B	2.51	118.65	110.58
2	A	2001	TD6	O3B-PB-O2B	2.52	118.69	110.58
2	B	2001	TD6	C13-CLB-C11	2.52	117.70	114.74
2	D	2001	TD6	O3B-PB-O2B	2.57	118.85	110.58
2	B	2001	TD6	O7-PA-O1A	2.66	119.93	109.62
2	D	2001	TD6	O7-PA-O1A	2.78	120.40	109.62
2	A	2001	TD6	C6-C5-S1	2.88	124.28	120.24
2	C	2001	TD6	PA-O3A-PB	7.15	156.63	132.67
2	B	2001	TD6	PA-O3A-PB	7.21	156.84	132.67
2	A	2001	TD6	PA-O3A-PB	7.52	157.89	132.67
2	D	2001	TD6	PA-O3A-PB	7.52	157.89	132.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	TD6	1	0
2	D	2001	TD6	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	817/868 (94%)	0.30	59 (7%)	18	25	15, 32, 59, 82	0
1	B	813/868 (93%)	0.30	56 (6%)	20	27	15, 32, 66, 101	0
1	C	808/868 (93%)	0.32	51 (6%)	23	31	18, 35, 64, 92	0
1	D	810/868 (93%)	0.50	69 (8%)	13	18	17, 35, 66, 96	0
All	All	3248/3472 (93%)	0.35	235 (7%)	18	25	15, 33, 64, 101	0

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	399	SER	7.2
1	C	368	ALA	7.0
1	D	810	LEU	6.7
1	D	368	ALA	6.2
1	B	421	VAL	6.0
1	B	810	LEU	6.0
1	D	574	GLY	5.3
1	D	935	ASP	5.3
1	D	831	LEU	5.1
1	B	779	ILE	5.0
1	C	779	ILE	4.8
1	D	419	PHE	4.8
1	B	371	ILE	4.8
1	A	368	ALA	4.5
1	D	779	ILE	4.5
1	C	784	ILE	4.5
1	A	413	TRP	4.5
1	B	394	ASN	4.5
1	B	368	ALA	4.4
1	A	810	LEU	4.4
1	B	367	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	419	PHE	4.4
1	B	501	VAL	4.4
1	D	631	SER	4.1
1	C	371	ILE	4.0
1	D	367	ASN	4.0
1	C	785	SER	4.0
1	D	373	LEU	3.9
1	B	785	SER	3.9
1	D	501	VAL	3.9
1	D	987	ILE	3.9
1	B	395	THR	3.9
1	B	1102	GLY	3.9
1	C	633	ASN	3.8
1	C	397	PHE	3.8
1	A	626	THR	3.6
1	D	559	SER	3.6
1	C	953	PHE	3.6
1	D	786	MET	3.6
1	B	432	LEU	3.5
1	D	934	PRO	3.5
1	D	653	VAL	3.5
1	D	937	THR	3.5
1	A	371	ILE	3.5
1	B	775	THR	3.5
1	C	983	GLY	3.5
1	D	561	PHE	3.5
1	A	702	ILE	3.4
1	B	472	ASP	3.4
1	A	779	ILE	3.4
1	D	420	LYS	3.4
1	A	419	PHE	3.4
1	D	632	ASP	3.4
1	C	1210	SER	3.3
1	C	413	TRP	3.3
1	C	984	ALA	3.3
1	A	574	GLY	3.3
1	C	812	LYS	3.3
1	C	394	ASN	3.3
1	D	981	VAL	3.3
1	C	629	GLU	3.2
1	B	414	ASP	3.2
1	A	1007	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	419	PHE	3.1
1	A	653	VAL	3.1
1	B	397	PHE	3.1
1	D	432	LEU	3.0
1	D	973	TRP	3.0
1	B	647	ALA	3.0
1	B	556	GLN	3.0
1	D	654	VAL	3.0
1	D	953	PHE	3.0
1	A	365	ASP	3.0
1	B	653	VAL	3.0
1	A	937	THR	2.9
1	D	471	HIS	2.9
1	D	785	SER	2.9
1	B	786	MET	2.9
1	D	472	ASP	2.9
1	D	608	ALA	2.9
1	B	415	LEU	2.9
1	D	807	VAL	2.9
1	B	559	SER	2.8
1	A	1227	GLY	2.8
1	C	1227	GLY	2.8
1	D	938	PRO	2.8
1	D	369	ARG	2.8
1	A	631	SER	2.8
1	D	954	ALA	2.8
1	B	373	LEU	2.8
1	A	953	PHE	2.8
1	A	367	ASN	2.8
1	A	394	ASN	2.8
1	B	648	PHE	2.7
1	A	429	ARG	2.7
1	C	417	ARG	2.7
1	B	793	LEU	2.7
1	C	653	VAL	2.7
1	B	777	ALA	2.7
1	C	937	THR	2.7
1	C	476	VAL	2.7
1	A	931	ALA	2.7
1	D	1103	GLU	2.7
1	D	797	GLN	2.7
1	B	654	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1125	ALA	2.7
1	C	647	ALA	2.7
1	C	632	ASP	2.7
1	A	428	GLN	2.6
1	B	784	ILE	2.6
1	A	954	ALA	2.6
1	C	981	VAL	2.6
1	A	608	ALA	2.6
1	B	794	ARG	2.6
1	C	628	GLU	2.6
1	A	397	PHE	2.6
1	D	558	PHE	2.6
1	A	1023	GLY	2.6
1	C	646	ALA	2.6
1	B	471	HIS	2.6
1	B	658	LEU	2.6
1	D	626	THR	2.6
1	D	984	ALA	2.6
1	C	1059	GLY	2.5
1	A	633	ASN	2.5
1	C	415	LEU	2.5
1	C	501	VAL	2.5
1	B	1190	ASP	2.5
1	D	657	THR	2.5
1	C	606	LEU	2.5
1	D	397	PHE	2.5
1	C	702	ILE	2.5
1	A	647	ALA	2.5
1	C	786	MET	2.5
1	A	606	LEU	2.5
1	C	1060	ILE	2.5
1	D	606	LEU	2.5
1	A	988	ILE	2.5
1	D	832	ALA	2.4
1	A	416	ASP	2.4
1	C	936	GLY	2.4
1	A	991	PHE	2.4
1	C	831	LEU	2.4
1	D	793	LEU	2.4
1	A	812	LYS	2.4
1	A	1224	THR	2.4
1	B	469	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	395	THR	2.4
1	A	609	VAL	2.4
1	D	1222	LEU	2.4
1	A	1083	ARG	2.4
1	C	986	SER	2.4
1	D	395	THR	2.4
1	D	649	ALA	2.4
1	D	658	LEU	2.4
1	D	983	GLY	2.4
1	B	473	LYS	2.4
1	B	783	ASP	2.3
1	B	420	LYS	2.3
1	C	652	GLY	2.3
1	A	415	LEU	2.3
1	C	793	LEU	2.3
1	A	933	ASN	2.3
1	A	936	GLY	2.3
1	B	1107	ASN	2.3
1	D	476	VAL	2.3
1	A	469	THR	2.3
1	C	852	GLU	2.3
1	D	394	ASN	2.3
1	A	951	SER	2.3
1	A	934	PRO	2.3
1	A	992	ILE	2.3
1	B	702	ILE	2.3
1	B	836	ASP	2.3
1	D	940	GLY	2.2
1	D	986	SER	2.2
1	B	589	MET	2.2
1	B	475	THR	2.2
1	D	634	ARG	2.2
1	A	414	ASP	2.2
1	C	608	ALA	2.2
1	D	630	GLY	2.2
1	D	642	LEU	2.2
1	A	852	GLU	2.2
1	A	561	PHE	2.2
1	C	561	PHE	2.2
1	B	1223	ASP	2.2
1	A	987	ILE	2.2
1	C	954	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	606	LEU	2.2
1	D	660	LEU	2.2
1	A	657	THR	2.2
1	A	981	VAL	2.2
1	B	981	VAL	2.2
1	C	475	THR	2.2
1	D	648	PHE	2.2
1	B	780	GLY	2.2
1	B	803	VAL	2.2
1	C	657	THR	2.2
1	C	590	PHE	2.2
1	C	987	ILE	2.2
1	B	561	PHE	2.1
1	B	608	ALA	2.1
1	C	414	ASP	2.1
1	A	632	ASP	2.1
1	A	986	SER	2.1
1	C	626	THR	2.1
1	A	808	ARG	2.1
1	B	429	ARG	2.1
1	D	1024	ARG	2.1
1	D	647	ALA	2.1
1	D	936	GLY	2.1
1	B	954	ALA	2.1
1	A	1028	PHE	2.1
1	D	417	ARG	2.1
1	B	1060	ILE	2.1
1	C	810	LEU	2.1
1	D	858	PRO	2.1
1	D	1130	GLU	2.1
1	A	634	ARG	2.1
1	B	986	SER	2.1
1	D	956	VAL	2.1
1	A	813	HIS	2.0
1	B	430	LYS	2.0
1	B	983	GLY	2.0
1	A	956	VAL	2.0
1	D	803	VAL	2.0
1	C	934	PRO	2.0
1	A	973	TRP	2.0
1	B	987	ILE	2.0
1	D	702	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	978	GLY	2.0
1	D	792	ALA	2.0
1	A	698	VAL	2.0
1	D	1060	ILE	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
2	TD6	C	2001	33/33	0.96	0.15	-0.40	19,23,46,49	0
2	TD6	A	2001	33/33	0.97	0.14	-0.42	15,21,46,48	0
2	TD6	B	2001	33/33	0.96	0.15	-0.48	12,23,48,50	0
2	TD6	D	2001	33/33	0.97	0.14	-0.51	13,24,48,53	0
3	MG	C	2002	1/1	0.97	0.12	-0.61	14,14,14,14	0
3	MG	A	2002	1/1	0.98	0.10	-1.34	12,12,12,12	0
4	CA	C	2003	1/1	0.96	0.05	-1.59	33,33,33,33	0
4	CA	B	2003	1/1	0.99	0.04	-1.74	29,29,29,29	0
3	MG	D	2002	1/1	0.96	0.10	-2.17	19,19,19,19	0
3	MG	B	2002	1/1	0.96	0.06	-2.59	17,17,17,17	0
4	CA	D	2003	1/1	0.99	0.03	-2.68	31,31,31,31	0
4	CA	A	2003	1/1	0.98	0.05	-2.84	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.