



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:27 PM GMT

PDB ID : 3ZHV
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis KGD,
post-decarboxylation intermediate from pyruvate (2-hydroxyethyl-ThDP)
Authors : Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.
Deposited on : 2012-12-24
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 ⓘ symbol.

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

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

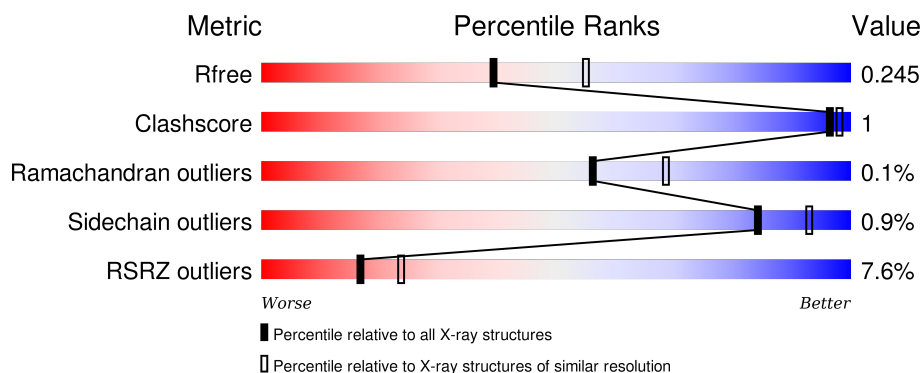
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. 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	868	<div> <div>7%</div> <div>90%</div> <div>6%</div> </div>
1	B	868	<div> <div>6%</div> <div>89%</div> <div>6%</div> </div>
1	C	868	<div> <div>7%</div> <div>88%</div> <div>5% 7%</div> </div>
1	D	868	<div> <div>8%</div> <div>90%</div> <div>6%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26141 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.

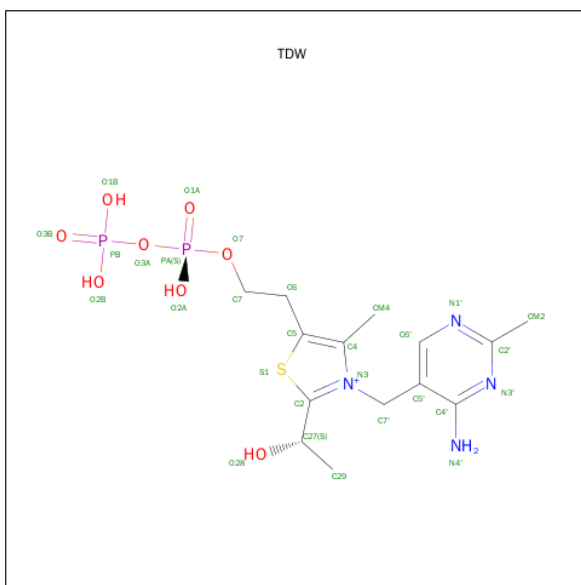
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	820	Total	C	N	O	S	0	0	0
			6332	3988	1118	1204	22			
1	B	813	Total	C	N	O	S	0	1	0
			6252	3946	1106	1177	23			
1	C	803	Total	C	N	O	S	0	0	0
			6234	3935	1102	1174	23			
1	D	812	Total	C	N	O	S	0	0	0
			6230	3928	1102	1176	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 2-[3-[(4-AZANYL-2-METHYL-PYRIMIDIN-5-YL)METHYL]-4-METHYL-2-[(1S)-1-OXIDANYLETHYL]-1,3-THIAZOL-3-IUM-5-YL]ETHYL PHOSPHONO HYDROGEN PHOSPHATE (three-letter code: TDW) (formula: C₁₄H₂₃N₄O₈P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 29	C 14	N 4	O 8	P 2	S 1	0	0
2	B	1	Total 29	C 14	N 4	O 8	P 2	S 1	0	0
2	C	1	Total 29	C 14	N 4	O 8	P 2	S 1	0	0
2	D	1	Total 29	C 14	N 4	O 8	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	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 1	Ca 1	0	0
4	D	1	Total 1	Ca 1	0	0
4	C	1	Total 1	Ca 1	0	0

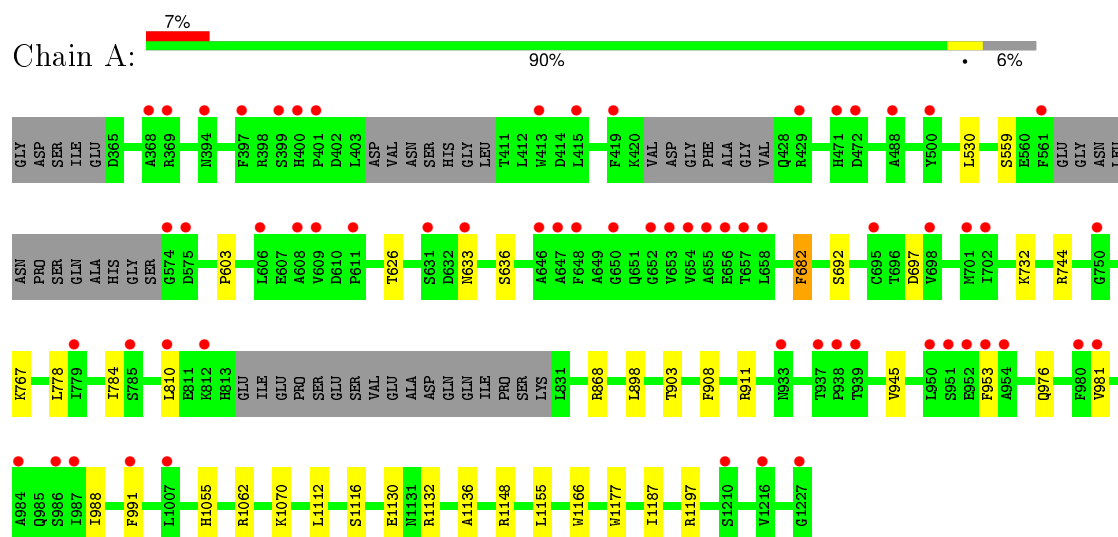
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	289	Total 289	O 289	0	0
5	B	218	Total 218	O 218	0	0
5	C	260	Total 260	O 260	0	0
5	D	202	Total 202	O 202	0	0

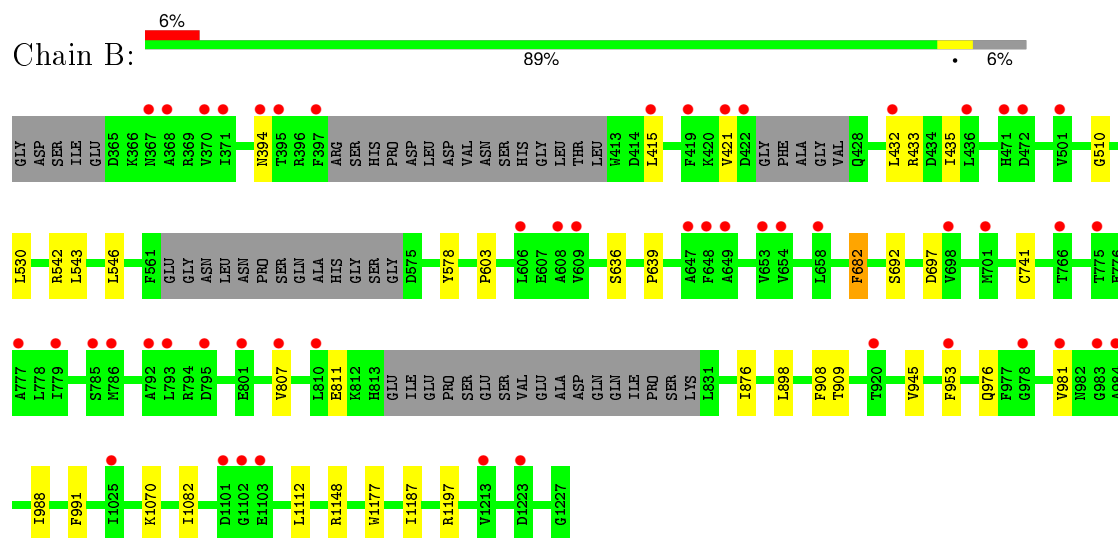
3 Residue-property plots

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.

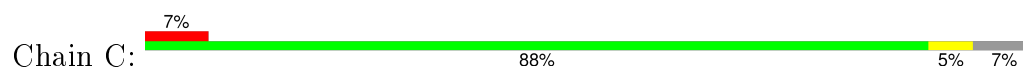
- Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

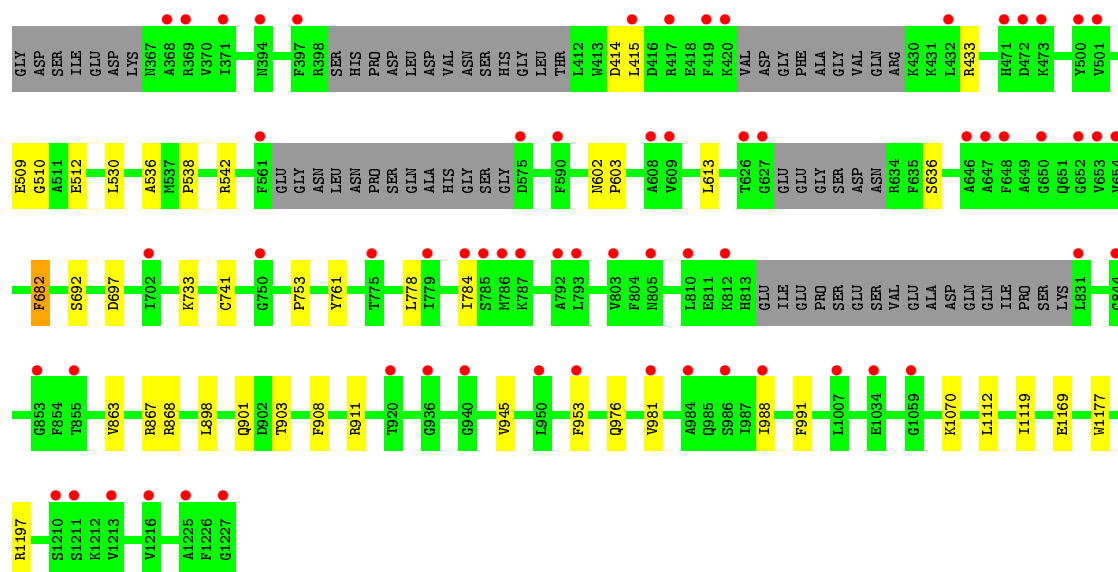


- Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



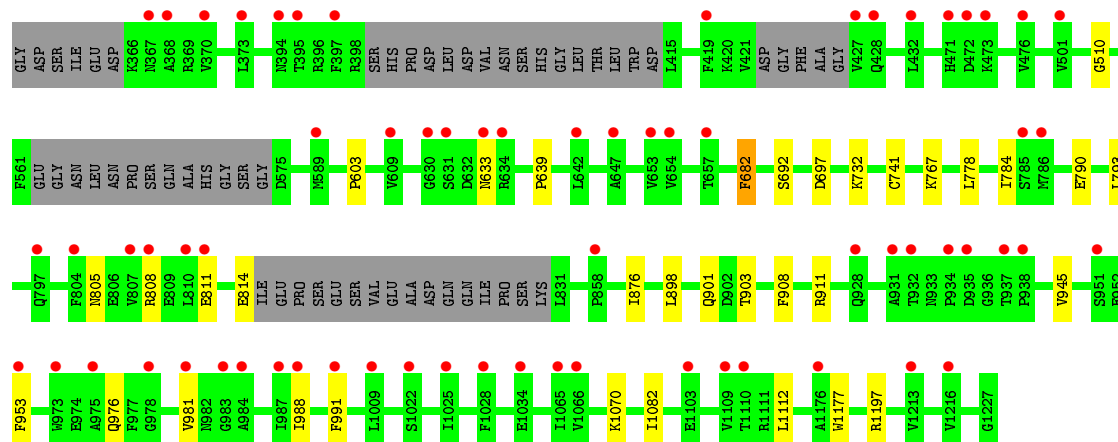
- Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME





● Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

Chain D: 8% 90% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.46 Å 83.70 Å 160.33 Å 99.68° 98.87° 100.63°	Depositor
Resolution (Å)	41.06 – 2.30 41.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (41.06-2.30) 91.1 (41.06-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.29 Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.203 , 0.235 0.213 , 0.245	Depositor DCC
R_{free} test set	8627 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.4	EDS
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 172548 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26141	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	0/6462	0.62	0/8770
1	B	0.48	0/6382	0.62	0/8663
1	C	0.49	0/6360	0.62	0/8620
1	D	0.49	0/6356	0.62	0/8624
All	All	0.49	0/25560	0.62	0/34677

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	6332	0	6078	20	0
1	B	6252	0	6023	16	0
1	C	6234	0	6050	20	0
1	D	6230	0	5987	15	0
2	A	29	0	20	0	0
2	B	29	0	20	0	0
2	C	29	0	20	1	0
2	D	29	0	20	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	289	0	0	0	0
5	B	218	0	0	0	0
5	C	260	0	0	2	0
5	D	202	0	0	0	0
All	All	26141	0	24218	71	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 (71) 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:778:LEU:HB3	1:A:784:ILE:HG12	1.81	0.61
1:B:415:LEU:HA	1:B:432:LEU:HB3	1.84	0.60
1:A:744:ARG:NH2	1:A:767:LYS:O	2.39	0.56
1:C:778:LEU:HB3	1:C:784:ILE:HG12	1.88	0.55
1:A:1112:LEU:HD21	1:A:1155:LEU:HD22	1.88	0.55
1:B:1148:ARG:HG3	1:B:1187:ILE:HD12	1.91	0.53
1:B:542:ARG:HD3	1:B:578:TYR:HA	1.92	0.52
1:C:542:ARG:NH1	1:C:602:ASN:OD1	2.35	0.52
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.93	0.51
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.92	0.50
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.93	0.49
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.94	0.49
1:A:1148:ARG:HG3	1:A:1187:ILE:HD12	1.94	0.49
1:D:778:LEU:HB3	1:D:784:ILE:HG12	1.95	0.48
1:C:415:LEU:HB3	1:C:433:ARG:HB3	1.95	0.48
1:A:559:SER:HA	1:A:810:LEU:HD11	1.96	0.47
1:D:510:GLY:O	1:D:741:CYS:HB2	2.15	0.47
1:C:510:GLY:O	1:C:741:CYS:HB2	2.15	0.46
1:A:626:THR:HG21	1:A:636:SER:OG	2.14	0.46
1:A:692:SER:HB2	1:A:697:ASP:OD2	2.16	0.46
1:D:633:ASN:O	1:D:732:LYS:HE3	2.16	0.46
1:C:692:SER:HB2	1:C:697:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:GLY:O	1:B:741:CYS:HB2	2.15	0.46
1:A:1116:SER:HG	1:A:1166:TRP:HH2	1.63	0.45
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.52	0.45
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.52	0.45
1:A:1112:LEU:CD2	1:A:1155:LEU:HD22	2.47	0.45
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.52	0.45
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.51	0.45
1:B:807:VAL:O	1:B:811:GLU:HG3	2.17	0.45
1:C:898:LEU:O	1:C:945:VAL:HA	2.16	0.45
1:B:898:LEU:O	1:B:945:VAL:HA	2.18	0.44
1:D:898:LEU:O	1:D:945:VAL:HA	2.18	0.44
1:C:753:PRO:HB2	1:C:761:TYR:CE1	2.53	0.44
1:B:421:VAL:HG11	1:B:435:ILE:HD12	2.00	0.44
1:A:898:LEU:O	1:A:945:VAL:HA	2.18	0.44
1:C:509:GLU:HA	1:C:512:GLU:OE2	2.18	0.43
1:C:908:PHE:CZ	1:C:1070:LYS:HG2	2.53	0.43
1:B:692:SER:HB2	1:B:697:ASP:OD2	2.18	0.43
1:C:863:VAL:O	1:C:867:ARG:HG3	2.19	0.43
1:A:903:THR:O	1:A:911:ARG:HD2	2.19	0.43
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.53	0.43
1:A:908:PHE:CZ	1:A:1070:LYS:HG2	2.53	0.43
1:D:692:SER:HB2	1:D:697:ASP:OD2	2.18	0.43
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.54	0.43
1:A:1112:LEU:HD12	1:A:1136:ALA:HB3	2.01	0.42
1:A:1130:GLU:HB2	1:A:1132:ARG:HG2	2.01	0.42
1:A:1055:HIS:HE1	1:A:1062:ARG:O	2.02	0.42
1:B:415:LEU:HB3	1:B:433:ARG:HB3	2.01	0.42
1:D:603:PRO:HD3	1:D:991:PHE:CZ	2.54	0.42
1:A:530:LEU:HD22	1:A:636:SER:HA	2.02	0.42
1:D:876:ILE:HD11	1:D:1082:ILE:HD13	2.02	0.42
1:A:633:ASN:O	1:A:732:LYS:HE2	2.20	0.42
1:C:538:PRO:HB2	5:C:3033:HOH:O	2.18	0.42
1:D:903:THR:O	1:D:911:ARG:HD2	2.20	0.42
1:D:811:GLU:HA	1:D:814:GLU:HG2	2.02	0.42
1:C:733:LYS:HE3	5:C:3014:HOH:O	2.19	0.41
1:D:805:ASN:HA	1:D:808:ARG:NH1	2.35	0.41
1:B:603:PRO:HD3	1:B:991:PHE:CZ	2.56	0.41
1:C:530:LEU:HD22	1:C:636:SER:HA	2.02	0.41
2:C:2001:TDW:H6'	1:D:901:GLN:OE1	2.21	0.41
1:C:903:THR:O	1:C:911:ARG:HD2	2.20	0.41
1:C:536:ALA:HB3	1:C:613:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:603:PRO:HD3	1:C:991:PHE:CZ	2.56	0.41
1:B:543:LEU:HD23	1:B:546:LEU:HD12	2.03	0.41
1:B:876:ILE:HD11	1:B:1082:ILE:HD13	2.03	0.40
1:C:1119:ILE:HD12	1:C:1169:GLU:HG3	2.03	0.40
1:C:901:GLN:OE1	2:D:2001:TDW:H6'	2.21	0.40
1:A:603:PRO:HD3	1:A:991:PHE:CZ	2.57	0.40
1:B:530:LEU:HD22	1:B:636:SER:HA	2.03	0.40
1:D:790:GLU:HA	1:D:793:LEU:HD12	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	810/868 (93%)	790 (98%)	19 (2%)	1 (0%)	56	68
1	B	804/868 (93%)	786 (98%)	17 (2%)	1 (0%)	56	68
1	C	791/868 (91%)	774 (98%)	16 (2%)	1 (0%)	56	68
1	D	802/868 (92%)	784 (98%)	17 (2%)	1 (0%)	56	68
All	All	3207/3472 (92%)	3134 (98%)	69 (2%)	4 (0%)	56	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	682	PHE
1	D	682	PHE
1	B	682	PHE
1	C	682	PHE

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	648/726 (89%)	644 (99%)	4 (1%)	90	96
1	B	637/726 (88%)	630 (99%)	7 (1%)	80	90
1	C	642/726 (88%)	636 (99%)	6 (1%)	84	93
1	D	632/726 (87%)	626 (99%)	6 (1%)	84	93
All	All	2559/2904 (88%)	2536 (99%)	23 (1%)	84	93

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	682	PHE
1	A	868	ARG
1	A	953	PHE
1	A	976	GLN
1	B	394	ASN
1	B	639	PRO
1	B	682	PHE
1	B	909	THR
1	B	953	PHE
1	B	976	GLN
1	B	1112	LEU
1	C	414	ASP
1	C	682	PHE
1	C	868	ARG
1	C	953	PHE
1	C	976	GLN
1	C	1112	LEU
1	D	639	PRO
1	D	682	PHE
1	D	767	LYS
1	D	953	PHE
1	D	976	GLN
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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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	TDW	A	2001	3	23,30,30	1.47	2 (8%)	34,45,45	1.63	5 (14%)
2	TDW	B	2001	3	23,30,30	1.41	3 (13%)	34,45,45	1.64	4 (11%)
2	TDW	C	2001	3	23,30,30	1.23	2 (8%)	34,45,45	1.91	3 (8%)
2	TDW	D	2001	3	23,30,30	1.51	2 (8%)	34,45,45	1.58	3 (8%)

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	TDW	A	2001	3	-	0/18/21/21	0/2/2/2
2	TDW	B	2001	3	-	0/18/21/21	0/2/2/2
2	TDW	C	2001	3	-	0/18/21/21	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TDW	D	2001	3	-	0/18/21/21	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TDW	C5-S1	-4.78	1.65	1.74
2	A	2001	TDW	C5-S1	-4.54	1.65	1.74
2	B	2001	TDW	C5-S1	-4.49	1.65	1.74
2	C	2001	TDW	C5-S1	-3.51	1.67	1.74
2	B	2001	TDW	PB-O1B	-2.10	1.47	1.54
2	B	2001	TDW	C2-N3	4.31	1.45	1.35
2	C	2001	TDW	C2-N3	4.47	1.45	1.35
2	D	2001	TDW	C2-N3	4.79	1.46	1.35
2	A	2001	TDW	C2-N3	5.09	1.46	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	TDW	C6-C5-C4	-3.66	124.28	127.56
2	A	2001	TDW	C6-C5-C4	-2.55	125.28	127.56
2	B	2001	TDW	O3A-PA-O7	-2.41	96.55	102.94
2	D	2001	TDW	O3A-PA-O7	-2.34	96.74	102.94
2	A	2001	TDW	O3A-PA-O7	-2.31	96.80	102.94
2	B	2001	TDW	C5-C4-N3	2.00	112.48	107.83
2	B	2001	TDW	O1B-PB-O3B	2.13	117.42	110.58
2	D	2001	TDW	O7-PA-O1A	2.17	118.04	109.62
2	A	2001	TDW	O1B-PB-O2B	2.25	115.96	107.38
2	A	2001	TDW	O7-PA-O1A	2.32	118.61	109.62
2	C	2001	TDW	C6-C5-S1	3.08	124.55	120.24
2	B	2001	TDW	PA-O3A-PB	6.89	155.76	132.67
2	A	2001	TDW	PA-O3A-PB	6.99	156.10	132.67
2	D	2001	TDW	PA-O3A-PB	7.36	157.35	132.67
2	C	2001	TDW	PA-O3A-PB	8.55	161.33	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	C	2001	TDW	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2001	TDW	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

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, 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	820/868 (94%)	0.36	63 (7%) 16 23	30, 47, 80, 112	0
1	B	813/868 (93%)	0.31	51 (6%) 23 31	29, 47, 80, 118	0
1	C	803/868 (92%)	0.33	65 (8%) 15 21	30, 47, 77, 108	0
1	D	812/868 (93%)	0.43	67 (8%) 14 20	30, 46, 78, 109	0
All	All	3248/3472 (93%)	0.36	246 (7%) 17 24	29, 47, 79, 118	0

All (246) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	371	ILE	6.7
1	D	368	ALA	6.5
1	B	421	VAL	6.0
1	D	419	PHE	5.9
1	C	779	ILE	5.8
1	A	401	PRO	5.7
1	C	561	PHE	5.6
1	D	472	ASP	5.3
1	B	472	ASP	5.1
1	C	368	ALA	5.1
1	B	419	PHE	5.0
1	B	368	ALA	4.8
1	B	786	MET	4.7
1	B	394	ASN	4.6
1	C	775	THR	4.6
1	D	810	LEU	4.6
1	A	394	ASN	4.5
1	C	1213	VAL	4.4
1	C	1210	SER	4.4
1	B	653	VAL	4.3
1	C	786	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	413	TRP	4.1
1	A	953	PHE	4.1
1	B	395	THR	4.0
1	B	785	SER	4.0
1	A	472	ASP	4.0
1	C	371	ILE	4.0
1	D	785	SER	4.0
1	B	647	ALA	4.0
1	D	501	VAL	3.9
1	C	953	PHE	3.9
1	D	807	VAL	3.9
1	B	397	PHE	3.9
1	A	698	VAL	3.9
1	D	934	PRO	3.8
1	B	984	ALA	3.8
1	D	797	GLN	3.7
1	A	471	HIS	3.7
1	A	400	HIS	3.7
1	A	750	GLY	3.7
1	A	655	ALA	3.7
1	D	427	VAL	3.6
1	D	367	ASN	3.6
1	A	702	ILE	3.5
1	D	471	HIS	3.5
1	B	810	LEU	3.5
1	A	561	PHE	3.5
1	D	953	PHE	3.5
1	D	633	ASN	3.5
1	B	415	LEU	3.5
1	A	1210	SER	3.5
1	A	653	VAL	3.5
1	B	648	PHE	3.5
1	D	931	ALA	3.5
1	C	415	LEU	3.4
1	B	367	ASN	3.4
1	C	750	GLY	3.4
1	C	472	ASP	3.4
1	B	649	ALA	3.4
1	B	1103	GLU	3.4
1	D	1025	ILE	3.3
1	B	501	VAL	3.3
1	D	473	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	953	PHE	3.3
1	B	654	VAL	3.3
1	D	981	VAL	3.3
1	C	397	PHE	3.3
1	A	368	ALA	3.2
1	C	792	ALA	3.2
1	A	986	SER	3.2
1	D	984	ALA	3.2
1	D	647	ALA	3.2
1	D	978	GLY	3.2
1	C	419	PHE	3.2
1	C	652	GLY	3.1
1	C	986	SER	3.1
1	B	981	VAL	3.1
1	A	779	ILE	3.1
1	C	812	LYS	3.1
1	B	777	ALA	3.1
1	D	808	ARG	3.1
1	C	590	PHE	3.0
1	D	394	ASN	3.0
1	D	609	VAL	3.0
1	A	647	ALA	3.0
1	C	432	LEU	3.0
1	D	786	MET	3.0
1	A	609	VAL	3.0
1	A	399	SER	3.0
1	D	395	THR	3.0
1	C	575	ASP	2.9
1	D	811	GLU	2.9
1	D	631	SER	2.9
1	A	633	ASN	2.9
1	C	394	ASN	2.9
1	C	793	LEU	2.9
1	D	1066	VAL	2.8
1	C	646	ALA	2.8
1	D	983	GLY	2.8
1	B	807	VAL	2.8
1	D	370	VAL	2.8
1	A	419	PHE	2.8
1	B	779	ILE	2.8
1	A	415	LEU	2.8
1	A	933	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	634	ARG	2.8
1	C	1216	VAL	2.8
1	B	1102	GLY	2.7
1	D	938	PRO	2.7
1	A	575	ASP	2.7
1	B	609	VAL	2.7
1	A	701	MET	2.7
1	A	654	VAL	2.7
1	A	950	LEU	2.7
1	D	1103	GLU	2.7
1	C	471	HIS	2.7
1	D	1216	VAL	2.7
1	A	657	THR	2.7
1	C	831	LEU	2.6
1	D	589	MET	2.6
1	D	642	LEU	2.6
1	B	658	LEU	2.6
1	A	646	ALA	2.6
1	A	397	PHE	2.6
1	A	429	ARG	2.6
1	A	951	SER	2.6
1	B	370	VAL	2.6
1	C	784	ILE	2.6
1	A	1216	VAL	2.6
1	B	1101	ASP	2.6
1	C	653	VAL	2.6
1	A	937	THR	2.6
1	D	937	THR	2.6
1	D	987	ILE	2.6
1	A	650	GLY	2.6
1	C	984	ALA	2.6
1	D	432	LEU	2.6
1	C	855	THR	2.6
1	D	653	VAL	2.6
1	C	988	ILE	2.6
1	D	373	LEU	2.5
1	D	654	VAL	2.5
1	A	652	GLY	2.5
1	C	940	GLY	2.5
1	A	810	LEU	2.5
1	B	1025	ILE	2.5
1	C	609	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	626	THR	2.5
1	D	1034	GLU	2.5
1	C	420	LYS	2.5
1	C	920	THR	2.5
1	A	785	SER	2.5
1	C	1034	GLU	2.4
1	C	981	VAL	2.4
1	A	656	GLU	2.4
1	D	630	GLY	2.4
1	B	606	LEU	2.4
1	A	695	CYS	2.4
1	D	973	TRP	2.4
1	A	608	ALA	2.4
1	A	606	LEU	2.4
1	B	432	LEU	2.4
1	B	422	ASP	2.4
1	C	702	ILE	2.4
1	A	939	THR	2.4
1	B	775	THR	2.4
1	A	1227	GLY	2.4
1	D	991	PHE	2.4
1	B	701	MET	2.3
1	C	805	ASN	2.3
1	B	978	GLY	2.3
1	D	932	THR	2.3
1	C	936	GLY	2.3
1	D	428	GLN	2.3
1	D	988	ILE	2.3
1	A	954	ALA	2.3
1	B	1223	ASP	2.3
1	C	1227	GLY	2.3
1	A	1007	LEU	2.3
1	A	981	VAL	2.3
1	B	766	THR	2.3
1	A	658	LEU	2.3
1	B	1213	VAL	2.3
1	C	608	ALA	2.3
1	A	631	SER	2.3
1	D	1022	SER	2.3
1	B	436	LEU	2.3
1	C	803	VAL	2.3
1	A	980	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	397	PHE	2.3
1	B	471	HIS	2.3
1	C	853	GLY	2.2
1	C	647	ALA	2.2
1	D	1110	THR	2.2
1	B	801	GLU	2.2
1	C	1225	ALA	2.2
1	D	1176	ALA	2.2
1	D	951	SER	2.2
1	A	500	TYR	2.2
1	A	369	ARG	2.2
1	D	1028	PHE	2.2
1	D	928	GLN	2.2
1	B	793	LEU	2.2
1	C	1007	LEU	2.2
1	C	417	ARG	2.2
1	B	698	VAL	2.2
1	D	1065	ILE	2.2
1	C	654	VAL	2.2
1	A	574	GLY	2.2
1	C	650	GLY	2.2
1	A	812	LYS	2.2
1	C	787	LYS	2.2
1	C	810	LEU	2.1
1	C	844	GLY	2.1
1	C	785	SER	2.1
1	B	792	ALA	2.1
1	C	1059	GLY	2.1
1	A	987	ILE	2.1
1	A	938	PRO	2.1
1	C	473	LYS	2.1
1	D	858	PRO	2.1
1	C	369	ARG	2.1
1	B	920	THR	2.1
1	D	1009	LEU	2.1
1	A	488	ALA	2.1
1	D	935	ASP	2.1
1	A	648	PHE	2.1
1	D	804	PHE	2.1
1	C	950	LEU	2.1
1	A	984	ALA	2.1
1	B	608	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	975	ALA	2.1
1	D	1109	VAL	2.1
1	C	627	GLY	2.0
1	C	648	PHE	2.0
1	D	657	THR	2.0
1	B	795	ASP	2.0
1	A	952	GLU	2.0
1	B	983	GLY	2.0
1	D	476	VAL	2.0
1	D	1213	VAL	2.0
1	A	991	PHE	2.0
1	C	1211	SER	2.0
1	C	501	VAL	2.0
1	A	611	PRO	2.0
1	C	500	TYR	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	C	2002	1/1	0.99	0.16	0.11	24,24,24,24	0
2	TDW	B	2001	29/29	0.96	0.20	-0.04	28,37,47,49	0
2	TDW	D	2001	29/29	0.98	0.19	-0.10	28,35,44,47	0
2	TDW	C	2001	29/29	0.96	0.17	-0.12	32,37,47,48	0
2	TDW	A	2001	29/29	0.96	0.17	-0.32	27,36,48,50	0
3	MG	A	2002	1/1	0.96	0.13	-0.46	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	B	2002	1/1	0.97	0.15	-0.99	34,34,34,34	0
4	CA	C	2003	1/1	0.98	0.08	-1.43	48,48,48,48	0
4	CA	B	2003	1/1	0.97	0.04	-1.71	52,52,52,52	0
3	MG	D	2002	1/1	0.97	0.11	-1.94	27,27,27,27	0
4	CA	D	2003	1/1	0.98	0.03	-2.89	44,44,44,44	0
4	CA	A	2003	1/1	0.99	0.03	-6.69	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.