



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:27 PM GMT

PDB ID : 3ZHT  
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis KGD, first post-decarboxylation intermediate from 2-oxoadipate  
Authors : Wagner, T.; Barilone, N.; Bellinzoni, M.; Alzari, P.M.  
Deposited on : 2012-12-24  
Resolution : 2.15 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](mailto: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.

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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

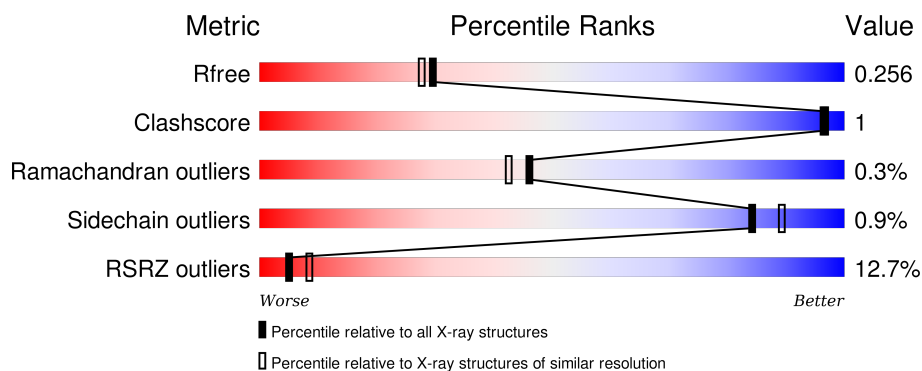
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




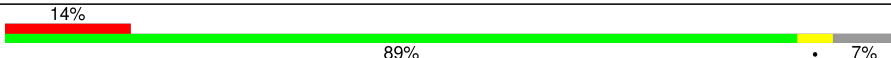
The reported resolution of this entry is 2.15 Å.

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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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  $\geq 3$ , 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	
1	B	868	
1	C	868	
1	D	868	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26205 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.

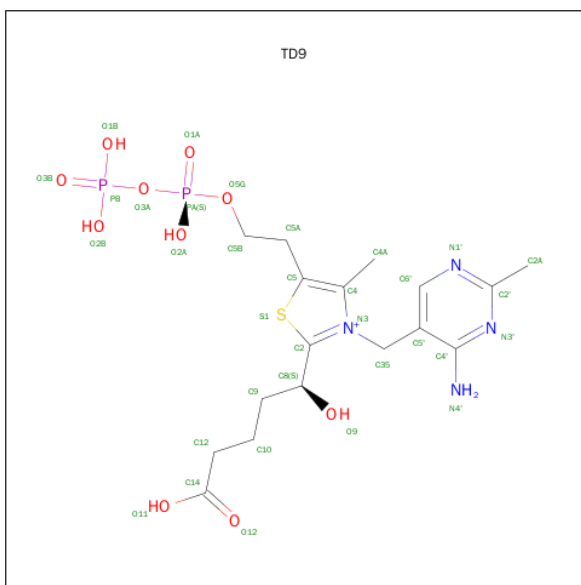
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	814	Total	C	N	O	S	0	1	0
			6292	3963	1111	1194	24			
1	B	809	Total	C	N	O	S	0	2	0
			6224	3922	1101	1176	25			
1	C	808	Total	C	N	O	S	0	0	0
			6258	3940	1104	1191	23			
1	D	807	Total	C	N	O	S	0	0	0
			6199	3905	1091	1180	23			

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 (5S)-5-{3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-4-METHYL-5-(2-{[(PHOSPHONATOXY)PHOSPHINATO]OXY}ETHYL)-1,3-THIAZOL-3-IUM-2-YL}-5-HYDROXPENTANOATE (three-letter code: TD9) (formula: C<sub>17</sub>H<sub>27</sub>N<sub>4</sub>O<sub>10</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 34	C 17	N 4	O 10	P 2	S 1	0	0
2	B	1	Total 34	C 17	N 4	O 10	P 2	S 1	0	0
2	C	1	Total 34	C 17	N 4	O 10	P 2	S 1	0	0
2	D	1	Total 34	C 17	N 4	O 10	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 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

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

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

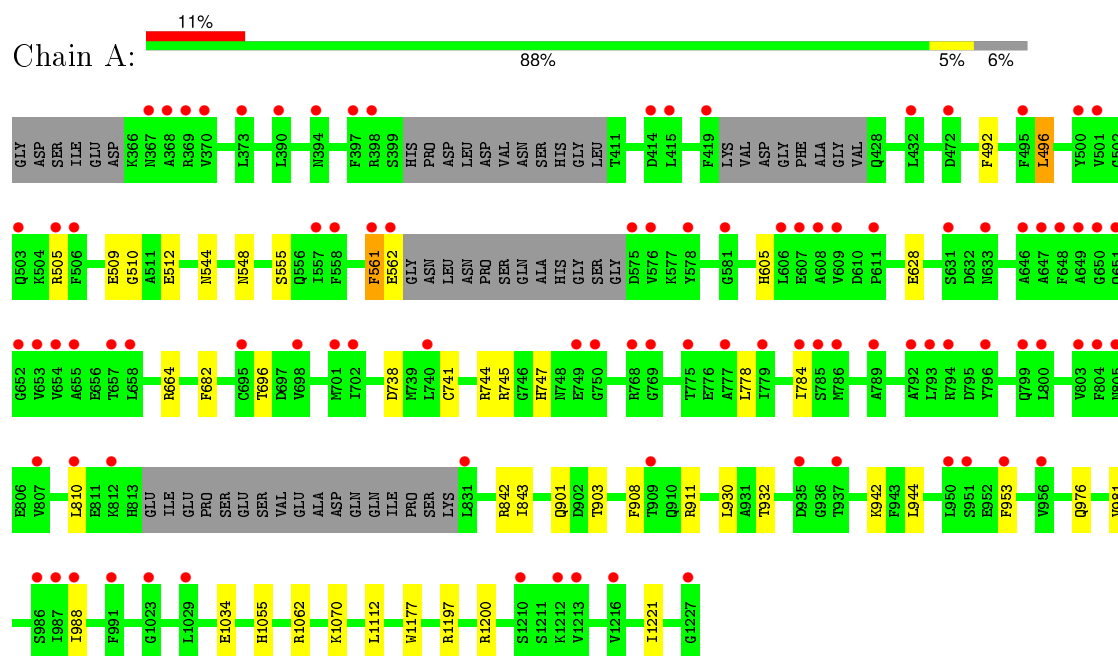
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	339	Total 339	O 339	0	0
5	B	223	Total 223	O 223	0	0
5	C	305	Total 305	O 305	0	0
5	D	221	Total 221	O 221	0	0

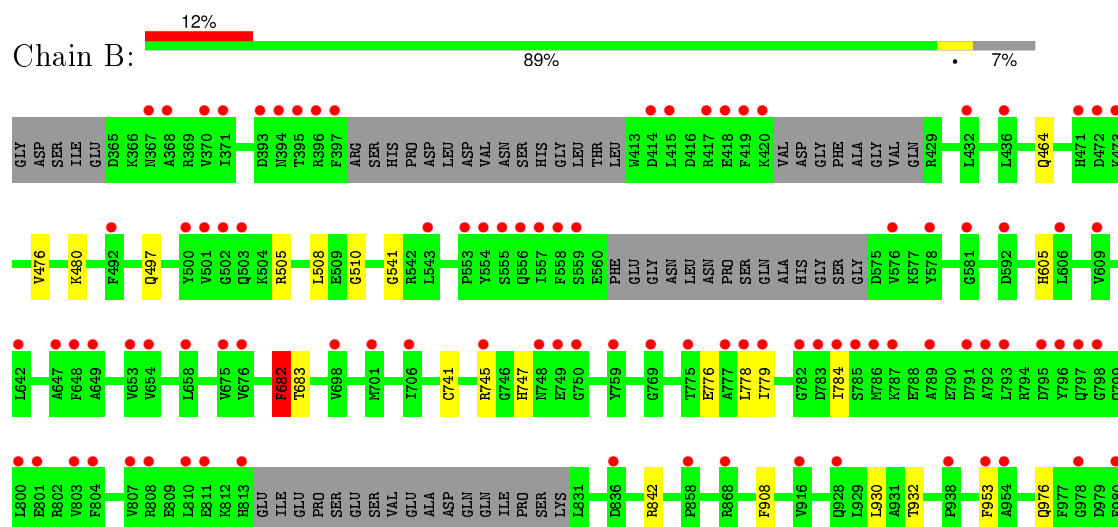
### 3 Residue-property plots

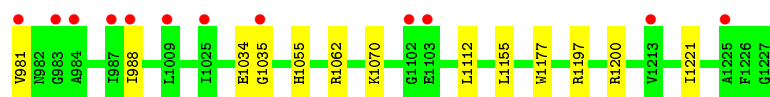
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

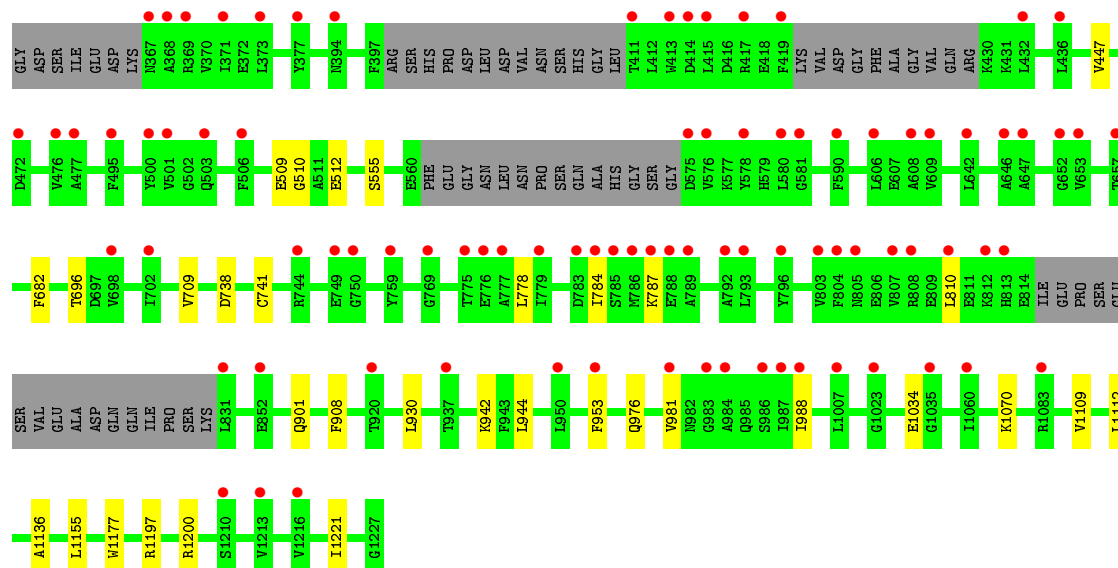
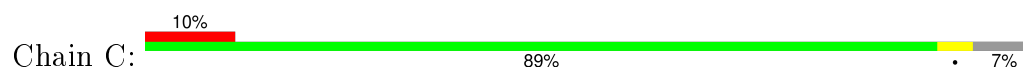


#### • Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

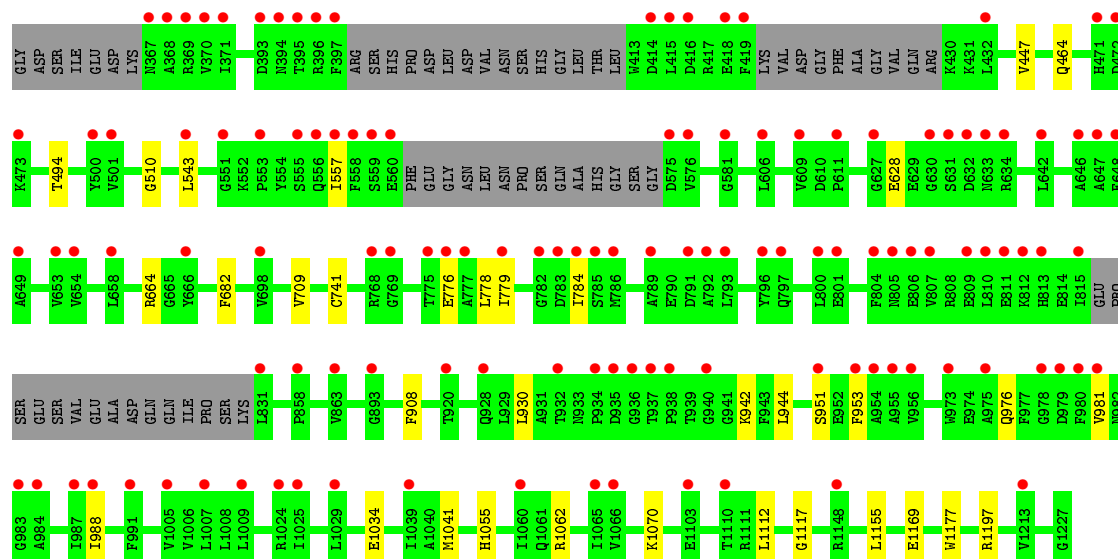
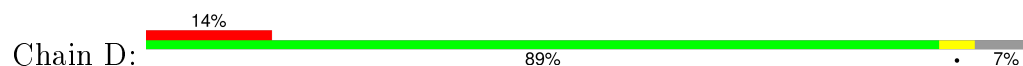




• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.37Å 83.80Å 159.51Å 99.76° 99.06° 100.61°	Depositor
Resolution (Å)	41.11 – 2.15 41.11 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.5 (41.11-2.15) 90.8 (41.11-2.15)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 2.16Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.223 , 0.246 0.228 , 0.256	Depositor DCC
$R_{free}$ test set	10531 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.6	EDS
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 209669 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	26205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	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 23.99 % 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 4.1817e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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: MG, TD9, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.50	0/6422	0.62	0/8710
1	B	0.48	0/6356	0.62	0/8627
1	C	0.50	0/6384	0.61	0/8657
1	D	0.48	0/6324	0.62	0/8584
All	All	0.49	0/25486	0.62	0/34578

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	6292	0	6064	23	0
1	B	6224	0	5986	18	0
1	C	6258	0	6043	15	0
1	D	6199	0	5953	15	0
2	A	34	0	23	0	0
2	B	34	0	23	1	0
2	C	34	0	23	0	0
2	D	34	0	23	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	339	0	0	0	0
5	B	223	0	0	1	0
5	C	305	0	0	0	0
5	D	221	0	0	1	0
All	All	26205	0	24138	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:B:1035:GLY:O	1:B:1062:ARG:HD2	1.90	0.71
1:D:1112:LEU:HD21	1:D:1155:LEU:HD22	1.84	0.59
1:B:497:GLN:HG3	1:B:745:ARG:HH12	1.68	0.59
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	1.85	0.57
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.87	0.56
1:B:476:VAL:HG12	1:B:480:LYS:HE2	1.87	0.55
1:A:544:ASN:OD1	1:A:548:ASN:ND2	2.41	0.54
1:C:509:GLU:HA	1:C:512:GLU:OE2	2.09	0.53
1:D:942:LYS:HE2	1:D:944:LEU:HD21	1.90	0.53
1:B:497:GLN:HG3	1:B:745:ARG:NH1	2.26	0.51
1:A:555:SER:HA	1:A:810:LEU:HD22	1.92	0.51
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	0.51
1:A:843:ILE:HG12	1:A:930:LEU:HD21	1.94	0.50
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.93	0.50
1:B:505:ARG:HA	1:B:747:HIS:O	2.12	0.49
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.94	0.49
1:A:744:ARG:HG3	1:A:745:ARG:HG3	1.96	0.48
1:D:1041:MET:HE2	1:D:1117:GLY:HA3	1.96	0.48
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.49	0.47
1:B:778:LEU:HB3	1:B:784:ILE:HG12	1.95	0.47
1:A:901:GLN:OE1	2:B:2001:TD9:H6'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ARG:HA	1:A:747:HIS:O	2.15	0.47
1:A:778:LEU:HB3	1:A:784:ILE:HG12	1.97	0.46
1:C:555:SER:HA	1:C:810:LEU:HD22	1.98	0.46
1:A:561:PHE:O	1:A:562:GLU:HB2	2.16	0.46
1:A:908:PHE:CZ	1:A:1070:LYS:HG2	2.51	0.46
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.52	0.45
1:D:1169:GLU:OE1	5:D:3208:HOH:O	2.21	0.45
1:C:510:GLY:O	1:C:741:CYS:HB2	2.17	0.45
1:C:908:PHE:CZ	1:C:1070:LYS:HG2	2.52	0.45
1:A:492:PHE:CE1	1:A:496:LEU:HD13	2.53	0.44
1:D:776:GLU:HA	1:D:779:ILE:HD12	1.99	0.44
1:C:1112:LEU:CD2	1:C:1155:LEU:HD22	2.48	0.44
1:A:843:ILE:HG12	1:A:930:LEU:CD2	2.47	0.44
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.53	0.44
1:A:510:GLY:O	1:A:741:CYS:HB2	2.18	0.43
1:B:776:GLU:HA	1:B:779:ILE:HD12	1.98	0.43
1:A:843:ILE:CG1	1:A:930:LEU:HD21	2.48	0.43
1:B:1055:HIS:HE1	1:B:1062:ARG:O	2.01	0.43
1:D:510:GLY:O	1:D:741:CYS:HB2	2.18	0.43
1:B:510:GLY:O	1:B:741:CYS:HB2	2.18	0.43
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.54	0.43
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.53	0.43
1:D:628:GLU:HG2	1:D:664:ARG:O	2.19	0.42
1:B:682:PHE:CD1	1:B:683:THR:HG23	2.54	0.42
1:A:509:GLU:HA	1:A:512:GLU:OE2	2.20	0.42
1:C:1109:VAL:HG21	1:C:1136:ALA:HB2	2.00	0.42
1:D:778:LEU:HB3	1:D:784:ILE:HG12	2.01	0.42
1:B:1177:TRP:CD1	1:B:1197:ARG:HD3	2.54	0.42
1:D:1055:HIS:HE1	1:D:1062:ARG:O	2.03	0.42
1:A:628:GLU:HG2	1:A:664:ARG:O	2.20	0.41
1:D:543:LEU:HD22	1:D:557:ILE:HG23	2.01	0.41
1:C:778:LEU:HB3	1:C:784:ILE:HG12	2.02	0.41
1:C:447:VAL:HG22	1:C:709:VAL:HG12	2.01	0.41
1:A:903:THR:O	1:A:911:ARG:HD2	2.21	0.41
1:D:447:VAL:HG22	1:D:709:VAL:HG12	2.02	0.41
1:D:1112:LEU:CD2	1:D:1155:LEU:HD22	2.50	0.41
1:B:842:ARG:NH2	1:B:932:THR:O	2.53	0.41
1:A:1200:ARG:HG3	1:A:1221:ILE:HD11	2.03	0.41
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.02	0.41
1:B:1200:ARG:HG3	1:B:1221:ILE:HD11	2.03	0.41
1:C:1200:ARG:HG3	1:C:1221:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:ARG:NH2	1:A:932:THR:O	2.54	0.41
1:A:1055:HIS:HE1	1:A:1062:ARG:O	2.03	0.40
1:B:747:HIS:HA	5:B:3035:HOH:O	2.21	0.40
1:B:508:LEU:HD13	1:B:541:GLY:HA3	2.03	0.40
1:C:696:THR:HG21	1:C:738:ASP:HB2	2.03	0.40
1:A:942:LYS:HE3	1:A:944:LEU:HD21	2.03	0.40
1:C:942:LYS:HE3	1:C:944:LEU:HD21	2.04	0.40
1:C:901:GLN:OE1	2:D:2001:TD9:H6'	2.21	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	805/868 (93%)	784 (97%)	18 (2%)	3 (0%)	39	34
1	B	801/868 (92%)	780 (97%)	18 (2%)	3 (0%)	39	34
1	C	798/868 (92%)	776 (97%)	21 (3%)	1 (0%)	56	57
1	D	797/868 (92%)	778 (98%)	18 (2%)	1 (0%)	56	57
All	All	3201/3472 (92%)	3118 (97%)	75 (2%)	8 (0%)	46	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	561	PHE
1	B	1034	GLU
1	D	1034	GLU
1	A	1034	GLU
1	C	1034	GLU
1	A	605	HIS
1	B	605	HIS

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Mol	Chain	Res	Type
1	B	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	646/726 (89%)	641 (99%)	5 (1%)	86	91
1	B	635/726 (88%)	630 (99%)	5 (1%)	86	91
1	C	645/726 (89%)	640 (99%)	5 (1%)	86	91
1	D	633/726 (87%)	626 (99%)	7 (1%)	80	85
All	All	2559/2904 (88%)	2537 (99%)	22 (1%)	84	89

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	496	LEU
1	A	682	PHE
1	A	953	PHE
1	A	976	GLN
1	A	1112	LEU
1	B	464	GLN
1	B	682	PHE
1	B	930	LEU
1	B	953	PHE
1	B	976	GLN
1	C	682	PHE
1	C	787	LYS
1	C	930	LEU
1	C	953	PHE
1	C	976	GLN
1	D	464	GLN
1	D	494	THR
1	D	682	PHE
1	D	930	LEU
1	D	951	SER

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Mol	Chain	Res	Type
1	D	953	PHE
1	D	976	GLN

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

### 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	TD9	A	2001	3	25,35,35	1.48	2 (8%)	37,51,51	1.57	3 (8%)
2	TD9	B	2001	3	25,35,35	1.32	2 (8%)	37,51,51	1.45	2 (5%)
2	TD9	C	2001	3	25,35,35	1.47	2 (8%)	37,51,51	1.55	3 (8%)
2	TD9	D	2001	3	25,35,35	1.43	3 (12%)	37,51,51	1.47	4 (10%)

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	TD9	A	2001	3	-	0/20/27/27	0/2/2/2
2	TD9	B	2001	3	-	0/20/27/27	0/2/2/2
2	TD9	C	2001	3	-	0/20/27/27	0/2/2/2
2	TD9	D	2001	3	-	0/20/27/27	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	TD9	C5-S1	-5.37	1.64	1.74
2	A	2001	TD9	C5-S1	-4.97	1.64	1.74
2	B	2001	TD9	C5-S1	-4.14	1.66	1.74
2	D	2001	TD9	C5-S1	-4.09	1.66	1.74
2	D	2001	TD9	PB-O1B	2.13	1.62	1.54
2	C	2001	TD9	C2-N3	4.67	1.45	1.35
2	B	2001	TD9	C2-N3	4.85	1.46	1.35
2	D	2001	TD9	C2-N3	4.97	1.46	1.35
2	A	2001	TD9	C2-N3	5.28	1.47	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	TD9	O1B-PB-O3A	-2.56	93.46	105.09
2	D	2001	TD9	O3A-PA-O5G	-2.49	96.34	102.94
2	A	2001	TD9	C5A-C5-C4	-2.39	125.42	127.56
2	C	2001	TD9	O1B-PB-O3A	-2.38	94.30	105.09
2	D	2001	TD9	O1B-PB-O3A	-2.05	95.80	105.09
2	C	2001	TD9	C5A-C5-C4	-2.04	125.74	127.56
2	D	2001	TD9	C5-C4-N3	2.02	112.52	107.83
2	B	2001	TD9	O2B-PB-O3B	2.78	119.54	110.58
2	B	2001	TD9	PA-O3A-PB	5.98	152.72	132.67
2	D	2001	TD9	PA-O3A-PB	6.24	153.59	132.67
2	A	2001	TD9	PA-O3A-PB	6.72	155.20	132.67
2	C	2001	TD9	PA-O3A-PB	6.89	155.78	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	TD9	1	0
2	D	2001	TD9	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	814/868 (93%)	0.62	94 (11%) <b>6</b> <b>11</b>	23, 39, 71, 113	0
1	B	809/868 (93%)	0.74	106 (13%) <b>5</b> <b>8</b>	24, 43, 76, 111	0
1	C	808/868 (93%)	0.58	87 (10%) <b>8</b> <b>12</b>	23, 39, 70, 97	0
1	D	807/868 (92%)	0.78	124 (15%) <b>3</b> <b>4</b>	23, 42, 76, 105	0
All	All	3238/3472 (93%)	0.68	411 (12%) <b>5</b> <b>8</b>	23, 41, 74, 113	0

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	VAL	13.4
1	D	501	VAL	11.8
1	A	368	ALA	9.0
1	B	368	ALA	8.5
1	D	368	ALA	8.5
1	B	367	ASN	7.7
1	D	810	LEU	7.6
1	B	810	LEU	7.5
1	C	779	ILE	7.5
1	B	777	ALA	7.2
1	A	561	PHE	7.2
1	B	807	VAL	6.7
1	B	793	LEU	6.5
1	C	368	ALA	6.3
1	B	419	PHE	6.3
1	C	769	GLY	6.2
1	B	394	ASN	6.1
1	C	785	SER	5.9
1	D	785	SER	5.9
1	C	810	LEU	5.8
1	B	785	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	419	PHE	5.7
1	D	793	LEU	5.5
1	D	395	THR	5.4
1	C	415	LEU	5.4
1	D	779	ILE	5.3
1	D	813	HIS	5.2
1	B	397	PHE	5.2
1	B	779	ILE	5.1
1	C	394	ASN	5.1
1	B	775	THR	5.1
1	B	786	MET	5.1
1	B	432	LEU	5.1
1	D	419	PHE	5.0
1	A	1210	SER	5.0
1	B	581	GLY	5.0
1	A	785	SER	5.0
1	B	500	TYR	5.0
1	C	369	ARG	4.9
1	A	750	GLY	4.8
1	B	576	VAL	4.8
1	A	702	ILE	4.7
1	C	576	VAL	4.7
1	D	953	PHE	4.7
1	C	500	TYR	4.7
1	A	800	LEU	4.6
1	A	792	ALA	4.6
1	D	797	GLN	4.6
1	B	371	ILE	4.6
1	D	631	SER	4.6
1	C	1213	VAL	4.5
1	D	394	ASN	4.5
1	D	815	ILE	4.5
1	D	371	ILE	4.4
1	A	793	LEU	4.4
1	B	953	PHE	4.4
1	D	987	ILE	4.4
1	B	654	VAL	4.4
1	A	812	LYS	4.3
1	A	653	VAL	4.3
1	A	575	ASP	4.3
1	A	394	ASN	4.3
1	B	395	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	775	THR	4.2
1	A	784	ILE	4.1
1	A	804	PHE	4.1
1	B	370	VAL	4.1
1	A	807	VAL	4.1
1	D	988	ILE	4.0
1	D	804	PHE	4.0
1	C	367	ASN	4.0
1	A	953	PHE	4.0
1	B	647	ALA	4.0
1	D	575	ASP	4.0
1	D	369	ARG	3.9
1	A	810	LEU	3.9
1	A	698	VAL	3.9
1	D	500	TYR	3.9
1	A	779	ILE	3.9
1	C	792	ALA	3.9
1	C	803	VAL	3.9
1	D	581	GLY	3.8
1	A	419	PHE	3.8
1	B	648	PHE	3.8
1	B	804	PHE	3.8
1	D	786	MET	3.8
1	C	813	HIS	3.8
1	C	501	VAL	3.8
1	C	812	LYS	3.8
1	C	786	MET	3.7
1	B	557	ILE	3.7
1	C	784	ILE	3.7
1	B	502	GLY	3.7
1	B	658	LEU	3.7
1	B	796	TYR	3.7
1	C	578	TYR	3.7
1	D	551	GLY	3.6
1	C	804	PHE	3.6
1	B	803	VAL	3.6
1	A	562	GLU	3.6
1	B	606	LEU	3.6
1	D	647	ALA	3.6
1	B	414	ASP	3.6
1	C	652	GLY	3.6
1	C	1210	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	415	LEU	3.6
1	D	559	SER	3.5
1	B	653	VAL	3.5
1	D	978	GLY	3.5
1	A	576	VAL	3.5
1	D	983	GLY	3.5
1	D	576	VAL	3.5
1	B	984	ALA	3.5
1	C	805	ASN	3.5
1	D	811	GLU	3.4
1	D	938	PRO	3.4
1	C	953	PHE	3.4
1	C	575	ASP	3.4
1	B	418	GLU	3.4
1	C	807	VAL	3.4
1	A	805	ASN	3.4
1	B	787	LYS	3.4
1	D	633	ASN	3.4
1	C	653	VAL	3.4
1	C	702	ILE	3.4
1	D	981	VAL	3.3
1	B	813	HIS	3.3
1	D	654	VAL	3.3
1	C	852	GLU	3.3
1	A	803	VAL	3.3
1	D	807	VAL	3.3
1	D	936	GLY	3.3
1	A	367	ASN	3.3
1	D	1103	GLU	3.3
1	C	646	ALA	3.3
1	A	501	VAL	3.3
1	B	981	VAL	3.3
1	B	556	GLN	3.3
1	B	978	GLY	3.2
1	B	553	PRO	3.2
1	A	472	ASP	3.2
1	A	986	SER	3.2
1	A	1227	GLY	3.2
1	A	991	PHE	3.2
1	B	649	ALA	3.2
1	A	987	ILE	3.2
1	A	581	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	796	TYR	3.2
1	D	1110	THR	3.2
1	A	609	VAL	3.2
1	A	631	SER	3.2
1	A	646	ALA	3.2
1	A	652	GLY	3.2
1	D	556	GLN	3.2
1	B	417	ARG	3.1
1	B	789	ALA	3.1
1	D	984	ALA	3.1
1	D	932	THR	3.1
1	A	1213	VAL	3.1
1	D	653	VAL	3.1
1	D	768	ARG	3.1
1	D	611	PRO	3.1
1	D	775	THR	3.1
1	D	367	ASN	3.1
1	B	472	ASP	3.1
1	A	370	VAL	3.1
1	B	436	LEU	3.1
1	B	987	ILE	3.1
1	B	811	GLU	3.1
1	A	658	LEU	3.1
1	C	432	LEU	3.1
1	B	791	ASP	3.1
1	C	581	GLY	3.1
1	D	471	HIS	3.1
1	C	987	ILE	3.1
1	D	769	GLY	3.1
1	D	557	ILE	3.0
1	D	472	ASP	3.0
1	C	986	SER	3.0
1	B	609	VAL	3.0
1	B	543	LEU	3.0
1	B	1213	VAL	3.0
1	D	831	LEU	3.0
1	B	792	ALA	3.0
1	B	1025	ILE	3.0
1	D	1025	ILE	3.0
1	B	555	SER	3.0
1	B	801	GLU	2.9
1	C	787	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	506	PHE	2.9
1	D	809	GLU	2.9
1	C	984	ALA	2.9
1	D	777	ALA	2.9
1	A	606	LEU	2.9
1	B	642	LEU	2.9
1	A	654	VAL	2.9
1	D	396	ARG	2.9
1	D	609	VAL	2.9
1	D	782	GLY	2.9
1	D	858	PRO	2.9
1	B	784	ILE	2.9
1	D	784	ILE	2.9
1	D	1066	VAL	2.9
1	A	657	THR	2.9
1	D	632	ASP	2.9
1	C	436	LEU	2.9
1	C	1216	VAL	2.9
1	D	937	THR	2.9
1	A	398	ARG	2.9
1	C	777	ALA	2.9
1	C	988	ILE	2.8
1	D	642	LEU	2.8
1	C	377	TYR	2.8
1	D	893	GLY	2.8
1	B	393	ASP	2.8
1	A	373	LEU	2.8
1	C	417	ARG	2.8
1	C	580	LEU	2.8
1	C	793	LEU	2.8
1	D	658	LEU	2.8
1	A	796	TYR	2.8
1	D	812	LYS	2.8
1	A	777	ALA	2.8
1	B	749	GLU	2.8
1	A	1216	VAL	2.8
1	D	1213	VAL	2.8
1	A	655	ALA	2.7
1	D	649	ALA	2.7
1	B	698	VAL	2.7
1	B	795	ASP	2.7
1	A	701	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	988	ILE	2.7
1	A	506	PHE	2.7
1	A	414	ASP	2.7
1	A	794	ARG	2.7
1	B	420	LYS	2.7
1	B	983	GLY	2.7
1	C	983	GLY	2.7
1	D	418	GLU	2.7
1	C	373	LEU	2.6
1	C	950	LEU	2.6
1	C	414	ASP	2.6
1	C	609	VAL	2.6
1	A	633	ASN	2.6
1	B	759	TYR	2.6
1	D	634	ARG	2.6
1	A	397	PHE	2.6
1	A	740	LEU	2.6
1	D	955	ALA	2.6
1	A	799	GLN	2.6
1	B	1103	GLU	2.6
1	C	831	LEU	2.6
1	D	1009	LEU	2.6
1	D	416	ASP	2.6
1	D	558	PHE	2.6
1	B	988	ILE	2.6
1	D	796	TYR	2.5
1	D	473	LYS	2.5
1	A	1023	GLY	2.5
1	D	940	GLY	2.5
1	C	1007	LEU	2.5
1	D	415	LEU	2.5
1	C	981	VAL	2.5
1	D	1060	ILE	2.5
1	C	783	ASP	2.5
1	A	650	GLY	2.5
1	B	954	ALA	2.5
1	A	768	ARG	2.5
1	A	500	TYR	2.5
1	A	578	TYR	2.5
1	B	471	HIS	2.5
1	B	701	MET	2.5
1	D	1065	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	657	THR	2.5
1	A	608	ALA	2.5
1	C	789	ALA	2.5
1	D	801	GLU	2.5
1	D	553	PRO	2.5
1	D	414	ASP	2.5
1	C	503	GLN	2.5
1	B	1225	ALA	2.5
1	C	371	ILE	2.5
1	C	1060	ILE	2.5
1	A	695	CYS	2.5
1	C	937	THR	2.5
1	D	975	ALA	2.4
1	D	991	PHE	2.4
1	D	934	PRO	2.4
1	B	473	LYS	2.4
1	B	916	VAL	2.4
1	D	791	ASP	2.4
1	D	863	VAL	2.4
1	D	935	ASP	2.4
1	D	973	TRP	2.4
1	A	390	LEU	2.4
1	A	950	LEU	2.4
1	B	558	PHE	2.4
1	C	776	GLU	2.4
1	B	559	SER	2.4
1	B	676	VAL	2.4
1	A	789	ALA	2.4
1	D	789	ALA	2.4
1	B	938	PRO	2.4
1	C	606	LEU	2.4
1	A	503	GLN	2.3
1	B	503	GLN	2.3
1	B	800	LEU	2.3
1	C	642	LEU	2.3
1	D	805	ASN	2.3
1	A	647	ALA	2.3
1	D	928	GLN	2.3
1	C	476	VAL	2.3
1	D	776	GLU	2.3
1	D	555	SER	2.3
1	B	396	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1035	GLY	2.3
1	D	951	SER	2.3
1	D	783	ASP	2.3
1	D	954	ALA	2.3
1	A	369	ARG	2.3
1	D	630	GLY	2.3
1	A	649	ALA	2.3
1	C	759	TYR	2.3
1	D	698	VAL	2.3
1	A	775	THR	2.3
1	B	797	GLN	2.3
1	B	778	LEU	2.3
1	D	1007	LEU	2.3
1	B	798	GLY	2.2
1	A	611	PRO	2.2
1	C	920	THR	2.2
1	A	495	PHE	2.2
1	B	578	TYR	2.2
1	A	1212	LYS	2.2
1	A	432	LEU	2.2
1	C	1083	ARG	2.2
1	D	1148	ARG	2.2
1	B	858	PRO	2.2
1	A	558	PHE	2.2
1	D	648	PHE	2.2
1	C	750	GLY	2.2
1	C	608	ALA	2.2
1	A	831	LEU	2.2
1	D	543	LEU	2.2
1	A	769	GLY	2.2
1	B	782	GLY	2.2
1	D	979	ASP	2.2
1	A	1029	LEU	2.2
1	C	413	TRP	2.2
1	B	928	GLN	2.2
1	C	411	THR	2.2
1	B	836	ASP	2.2
1	C	749	GLU	2.2
1	D	432	LEU	2.1
1	D	606	LEU	2.1
1	B	592	ASP	2.1
1	B	783	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1023	GLY	2.1
1	D	627	GLY	2.1
1	B	554	TYR	2.1
1	D	956	VAL	2.1
1	D	920	THR	2.1
1	B	980	PHE	2.1
1	D	397	PHE	2.1
1	D	1024	ARG	2.1
1	D	646	ALA	2.1
1	A	935	ASP	2.1
1	C	1035	GLY	2.1
1	A	909	THR	2.1
1	D	800	LEU	2.1
1	C	495	PHE	2.1
1	C	590	PHE	2.1
1	D	980	PHE	2.1
1	B	675	VAL	2.1
1	D	370	VAL	2.1
1	D	1005	VAL	2.1
1	B	808	ARG	2.1
1	B	706	ILE	2.1
1	B	415	LEU	2.1
1	C	477	ALA	2.1
1	B	1102	GLY	2.1
1	A	951	SER	2.1
1	A	557	ILE	2.1
1	C	472	ASP	2.1
1	A	749	GLU	2.1
1	D	560	GLU	2.1
1	D	806	GLU	2.1
1	B	748	ASN	2.1
1	C	647	ALA	2.1
1	C	744	ARG	2.1
1	B	769	GLY	2.1
1	D	792	ALA	2.1
1	A	786	MET	2.1
1	D	666	TYR	2.1
1	A	937	THR	2.0
1	A	607	GLU	2.0
1	A	505	ARG	2.0
1	B	745	ARG	2.0
1	B	1009	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	1029	LEU	2.0
1	B	750	GLY	2.0
1	B	492	PHE	2.0
1	B	868	ARG	2.0
1	A	651	GLN	2.0
1	D	1039	ILE	2.0
1	C	808	ARG	2.0
1	A	648	PHE	2.0
1	A	956	VAL	2.0
1	C	698	VAL	2.0
1	C	788	GLU	2.0
1	D	393	ASP	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	MG	A	2002	1/1	0.93	0.16	0.12	25,25,25,25	0
2	TD9	D	2001	34/34	0.97	0.18	-0.14	18,29,63,65	0
3	MG	C	2002	1/1	0.99	0.15	-0.14	22,22,22,22	0
2	TD9	B	2001	34/34	0.95	0.18	-0.25	20,32,69,73	0
2	TD9	A	2001	34/34	0.96	0.17	-0.26	24,32,63,65	0
2	TD9	C	2001	34/34	0.96	0.17	-0.36	23,30,57,58	0
3	MG	D	2002	1/1	0.97	0.11	-1.45	24,24,24,24	0
3	MG	B	2002	1/1	0.95	0.12	-1.63	28,28,28,28	0
4	CA	D	2003	1/1	0.96	0.06	-1.80	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	B	2003	1/1	0.96	0.05	-1.98	43,43,43,43	0
4	CA	C	2003	1/1	0.99	0.04	-2.10	38,38,38,38	0
4	CA	A	2003	1/1	0.98	0.06	-2.83	38,38,38,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.