



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:13 am GMT

PDB ID : 3ZHU
Title : Crystal structure of the SucA domain of Mycobacterium smegmatis KGD, second post-decarboxylation intermediate from 2-oxoadipate
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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

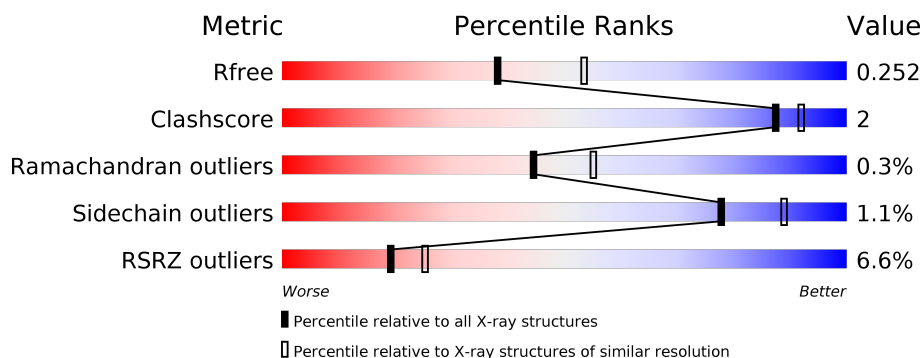
1 Overall quality at a glance

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}	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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>8%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>•</div> </div> </div>
1	B	868	<div> <div>5%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>• •</div> </div> </div>
1	C	868	<div> <div>4%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>•</div> </div> </div>
1	D	868	<div> <div>8%</div> <div> <div></div> <div>92%</div> <div>6%</div> <div>•</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27180 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.

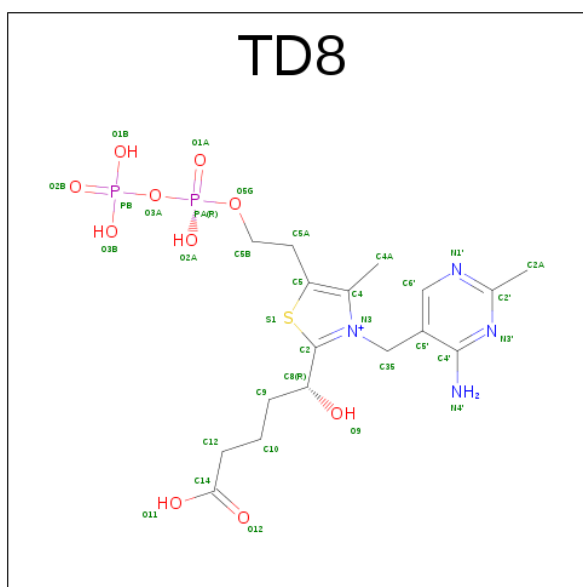
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	847	Total	C	N	O	S	0	1	0
			6531	4106	1156	1245	24			
1	B	836	Total	C	N	O	S	0	0	0
			6463	4067	1142	1230	24			
1	C	845	Total	C	N	O	S	0	1	0
			6530	4108	1157	1241	24			
1	D	852	Total	C	N	O	S	0	0	0
			6578	4138	1163	1253	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 (5R)-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: TD8) (formula: C₁₇H₂₇N₄O₁₀P₂S).



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	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

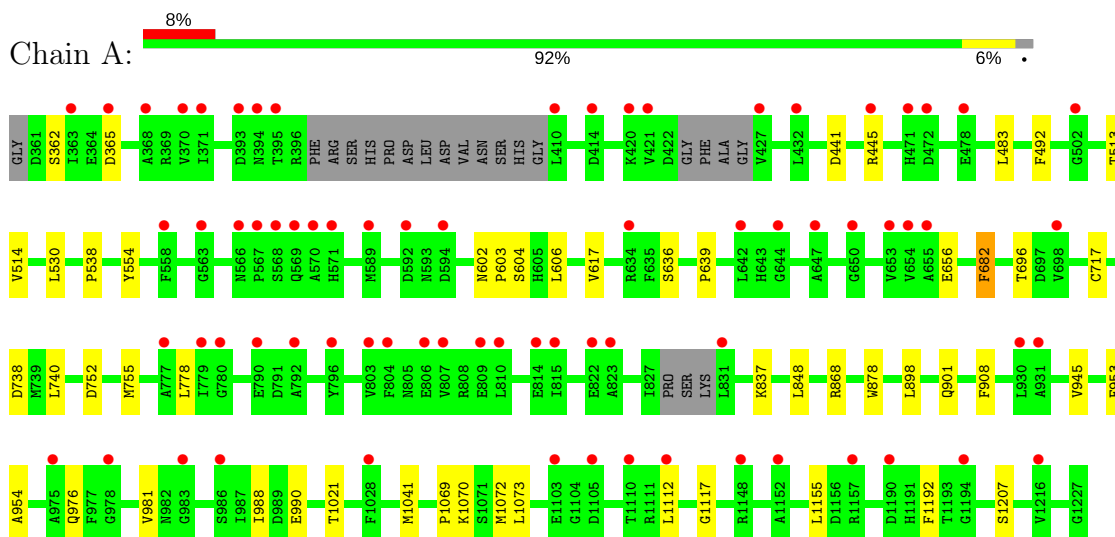
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	239	Total 239	O 239	0	0
5	B	204	Total 204	O 204	0	0
5	C	298	Total 298	O 298	0	0
5	D	193	Total 193	O 193	0	0

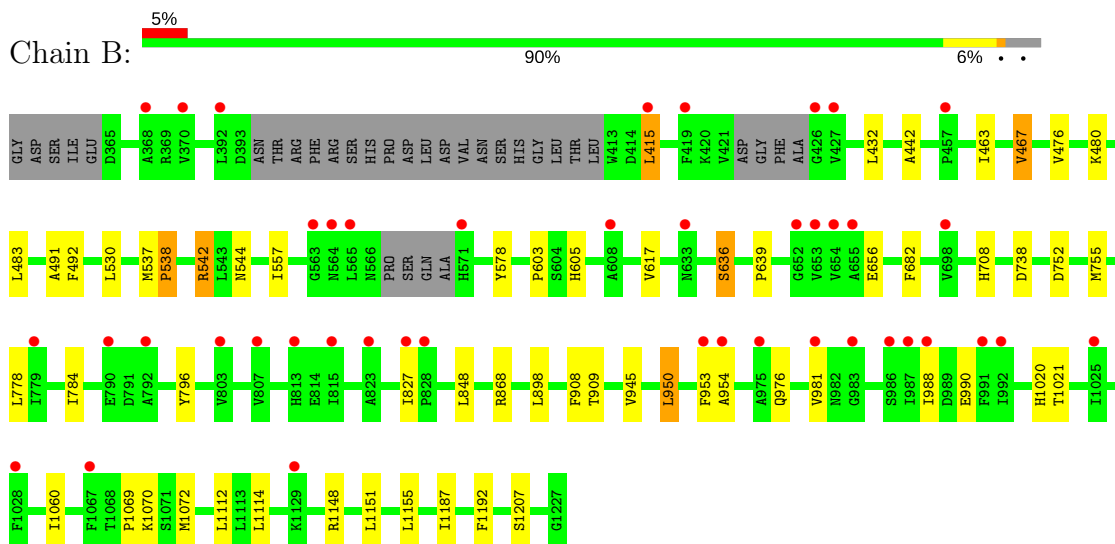
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

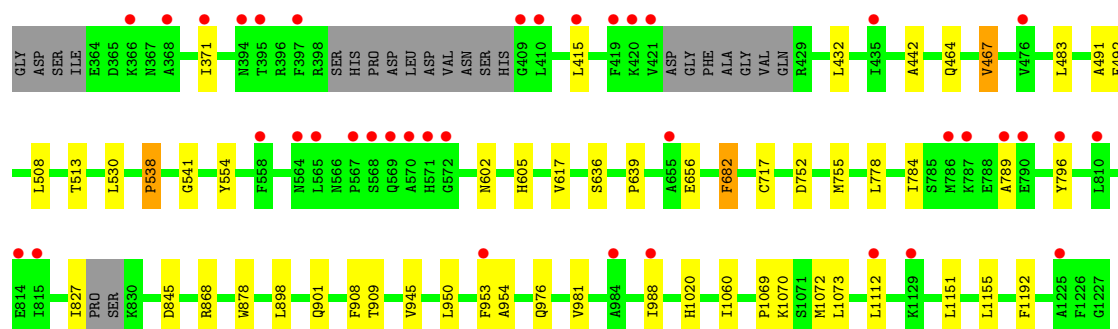


• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

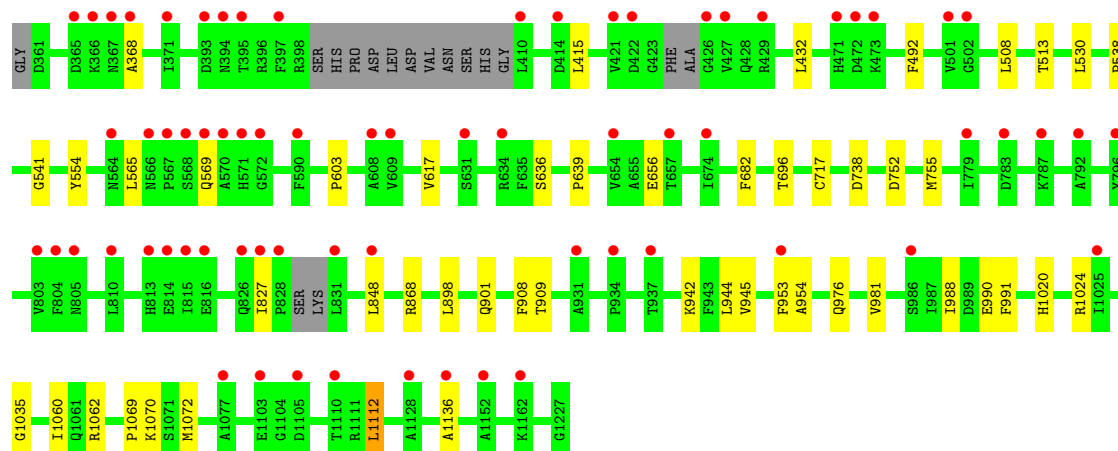


• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME





• 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, α , β , γ	79.78Å 82.29Å 163.04Å 99.19° 99.10° 100.71°	Depositor
Resolution (Å)	40.36 – 2.30 40.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (40.36-2.30) 90.5 (40.36-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.200 , 0.235 0.214 , 0.252	Depositor DCC
R_{free} test set	8505 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27180	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.56% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, TD8, 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	0/6663	0.63	0/9034
1	B	0.50	0/6594	0.63	0/8940
1	C	0.51	0/6661	0.63	0/9032
1	D	0.49	0/6710	0.62	0/9097
All	All	0.50	0/26628	0.63	0/36103

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	6531	0	6302	25	0
1	B	6463	0	6253	34	0
1	C	6530	0	6308	32	0
1	D	6578	0	6362	27	0
2	A	34	0	22	6	0
2	B	34	0	22	2	0
2	C	34	0	22	1	0
2	D	34	0	22	4	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	239	0	0	0	0
5	B	204	0	0	2	0
5	C	298	0	0	2	0
5	D	193	0	0	2	0
All	All	27180	0	25313	121	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 (121) 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:827:ILE:HA	1:B:1060:ILE:HD11	1.66	0.78
1:C:827:ILE:HA	1:C:1060:ILE:HD11	1.69	0.71
1:C:492:PHE:HD1	1:C:554:TYR:HE1	1.38	0.71
1:C:1112:LEU:HD21	1:C:1155:LEU:HD22	1.73	0.70
1:D:827:ILE:HA	1:D:1060:ILE:HD11	1.74	0.70
1:C:371:ILE:HD12	1:D:368:ALA:HB1	1.78	0.66
1:A:1112:LEU:HD21	1:A:1155:LEU:HD22	1.78	0.64
1:C:508:LEU:HD13	1:C:541:GLY:HA3	1.82	0.61
1:D:848:LEU:HD12	1:D:868:ARG:HD3	1.82	0.60
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.84	0.59
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.83	0.59
1:B:537:MET:O	1:B:542:ARG:NH2	2.35	0.58
1:A:848:LEU:HD12	1:A:868:ARG:HD3	1.85	0.58
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.85	0.58
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.85	0.58
1:C:492:PHE:CD1	1:C:554:TYR:HE1	2.21	0.57
2:A:2001:TD8:H5BA	1:B:950:LEU:HD11	1.86	0.57
1:A:901:GLN:OE1	2:B:2001:TD8:H6'	2.06	0.56
1:B:476:VAL:HG12	1:B:480:LYS:HE3	1.88	0.56
1:C:1020:HIS:HD2	5:C:3230:HOH:O	1.89	0.55
1:B:442:ALA:HB1	1:B:467:VAL:HG13	1.88	0.55
1:C:950:LEU:CD1	2:D:2001:TD8:H5BA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:950:LEU:HD11	2:D:2001:TD8:H5BA	1.89	0.55
1:C:901[A]:GLN:OE1	2:D:2001:TD8:H6'	2.07	0.55
1:C:442:ALA:HB1	1:C:467:VAL:HG13	1.89	0.54
1:D:1069:PRO:CB	1:D:1072:MET:HB3	2.37	0.54
2:A:2001:TD8:C2	2:A:2001:TD8:HN4A	2.20	0.54
1:D:1069:PRO:HB2	1:D:1072:MET:HB3	1.89	0.54
1:A:606:LEU:HG	2:A:2001:TD8:N4'	2.23	0.54
1:B:1069:PRO:HB2	1:B:1072:MET:HB3	1.90	0.54
1:A:1069:PRO:CB	1:A:1072:MET:HB3	2.39	0.53
1:B:1069:PRO:CB	1:B:1072:MET:HB3	2.39	0.53
1:C:492:PHE:HD1	1:C:554:TYR:CE1	2.22	0.53
1:A:492:PHE:HD1	1:A:554:TYR:HE1	1.56	0.53
1:D:492:PHE:HD1	1:D:554:TYR:HE1	1.55	0.53
1:C:1069:PRO:HB2	1:C:1072:MET:HB3	1.90	0.52
1:A:1069:PRO:HB2	1:A:1072:MET:HB3	1.91	0.52
1:B:1112:LEU:HD21	1:B:1155:LEU:HD22	1.91	0.52
1:B:1151:LEU:O	1:B:1155:LEU:HG	2.10	0.52
2:C:2001:TD8:H6'	1:D:901:GLN:OE1	2.10	0.51
1:A:441:ASP:HA	1:A:445:ARG:HG3	1.93	0.51
1:C:1069:PRO:CB	1:C:1072:MET:HB3	2.40	0.51
1:C:492:PHE:CD1	1:C:554:TYR:CE1	2.98	0.51
1:B:483:LEU:HD22	1:B:778:LEU:HD12	1.93	0.51
1:C:415:LEU:HA	1:C:432:LEU:HB3	1.93	0.51
1:C:483:LEU:HD22	1:C:778:LEU:HD12	1.93	0.51
1:D:603:PRO:HG3	1:D:990:GLU:HB3	1.93	0.51
1:D:1020:HIS:HD2	5:D:3165:HOH:O	1.93	0.50
1:A:908:PHE:CZ	1:A:1070:LYS:HG2	2.45	0.50
1:B:491:ALA:HB3	1:B:796:TYR:CD2	2.46	0.50
1:A:362:SER:H	1:A:365:ASP:HB3	1.76	0.50
2:A:2001:TD8:H5BA	1:B:950:LEU:CD1	2.42	0.50
2:D:2001:TD8:C2	2:D:2001:TD8:HN4A	2.25	0.50
1:B:415:LEU:HA	1:B:432:LEU:HB3	1.94	0.50
1:B:538:PRO:HD2	5:B:3032:HOH:O	2.12	0.50
1:D:513:THR:HG21	1:D:717:CYS:SG	2.52	0.49
1:B:1155:LEU:HD11	1:B:1192:PHE:CZ	2.47	0.49
1:C:784:ILE:HD12	1:C:789:ALA:HB2	1.94	0.49
1:A:483:LEU:HD22	1:A:778:LEU:HD12	1.95	0.49
1:A:603:PRO:HG3	1:A:990:GLU:HB3	1.94	0.49
1:A:1155:LEU:HD11	1:A:1192:PHE:CZ	2.47	0.48
1:B:1021:THR:HG21	1:B:1207:SER:HB3	1.94	0.48
1:B:530:LEU:HD22	1:B:636:SER:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:PRO:HD2	5:C:3037:HOH:O	2.13	0.48
1:D:656:GLU:HB3	1:D:954:ALA:HB2	1.96	0.48
2:A:2001:TD8:HN4A	2:A:2001:TD8:C8	2.27	0.47
1:B:656:GLU:HB3	1:B:954:ALA:HB2	1.95	0.47
1:B:1148:ARG:HG3	1:B:1187:ILE:HD12	1.95	0.47
1:C:513:THR:HG21	1:C:717:CYS:SG	2.55	0.47
1:C:530:LEU:HD22	1:C:636:SER:HA	1.96	0.47
1:D:1112:LEU:HD12	1:D:1136:ALA:HB3	1.96	0.47
1:C:656:GLU:HB3	1:C:954:ALA:HB2	1.97	0.47
1:A:513:THR:HG21	1:A:717:CYS:SG	2.55	0.47
1:A:752:ASP:O	1:A:755:MET:HE2	2.15	0.46
1:D:752:ASP:O	1:D:755:MET:HE2	2.15	0.46
1:D:508:LEU:HD13	1:D:541:GLY:HA3	1.98	0.46
1:B:908:PHE:CZ	1:B:1070:LYS:HG2	2.51	0.46
1:D:565:LEU:HB3	1:D:569:GLN:HB3	1.98	0.46
1:D:1024:ARG:HB2	5:D:3168:HOH:O	2.16	0.46
1:C:1155:LEU:HD11	1:C:1192:PHE:CZ	2.51	0.46
1:A:898:LEU:O	1:A:945:VAL:HA	2.16	0.45
1:A:530:LEU:HD22	1:A:636:SER:HA	1.98	0.45
1:B:1020:HIS:HD2	5:B:3160:HOH:O	1.99	0.45
1:B:898:LEU:O	1:B:945:VAL:HA	2.16	0.45
1:B:480:LYS:HE2	1:B:784:ILE:HG23	1.99	0.45
1:C:908:PHE:CZ	1:C:1070:LYS:HG2	2.52	0.45
1:D:898:LEU:O	1:D:945:VAL:HA	2.17	0.45
1:B:491:ALA:HB3	1:B:796:TYR:CE2	2.52	0.44
1:A:656:GLU:HB3	1:A:954:ALA:HB2	1.99	0.44
1:C:752:ASP:O	1:C:755:MET:HE2	2.16	0.44
1:B:463:ILE:O	1:B:467:VAL:HB	2.18	0.44
1:A:696:THR:HG21	1:A:738:ASP:HB2	2.01	0.43
1:B:492:PHE:HZ	1:B:557:ILE:HG21	1.84	0.42
1:A:1021:THR:HG21	1:A:1207:SER:HB3	2.01	0.42
1:C:845:ASP:OD1	1:C:868:ARG:NE	2.46	0.42
1:C:898:LEU:O	1:C:945:VAL:HA	2.18	0.42
2:B:2001:TD8:HN4A	2:B:2001:TD8:C8	2.31	0.42
1:C:491:ALA:HB3	1:C:796:TYR:CD2	2.55	0.42
1:D:1035:GLY:O	1:D:1062:ARG:HD3	2.20	0.42
1:B:542:ARG:HE	1:B:542:ARG:HB2	1.70	0.42
1:B:603:PRO:HG3	1:B:990:GLU:HB3	2.01	0.42
1:A:604:SER:O	2:A:2001:TD8:N4'	2.43	0.42
1:B:617:VAL:HG11	1:B:639:PRO:HG3	2.02	0.41
1:D:492:PHE:CD1	1:D:554:TYR:HE1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:MET:HE2	1:A:1117:GLY:HA3	2.03	0.41
1:B:848:LEU:HD12	1:B:868:ARG:HD3	2.01	0.41
1:C:617:VAL:HG11	1:C:639:PRO:HG3	2.03	0.41
1:B:752:ASP:O	1:B:755:MET:HE2	2.21	0.41
1:D:942:LYS:HE3	1:D:944:LEU:HD21	2.02	0.41
1:A:878:TRP:HB3	1:A:1073:LEU:HD23	2.02	0.41
1:D:617:VAL:HG11	1:D:639:PRO:HG3	2.03	0.41
1:D:696:THR:HG21	1:D:738:ASP:HB2	2.02	0.41
1:C:878:TRP:HB3	1:C:1073:LEU:HD23	2.03	0.41
1:B:542:ARG:HG2	1:B:578:TYR:HA	2.03	0.40
1:D:415:LEU:HA	1:D:432:LEU:HB3	2.03	0.40
1:B:708:HIS:HA	1:B:738:ASP:HB3	2.02	0.40
1:D:908:PHE:CZ	1:D:1070:LYS:HG2	2.56	0.40
1:D:530:LEU:HD22	1:D:636:SER:HA	2.02	0.40
1:D:603:PRO:HD3	1:D:991:PHE:CZ	2.57	0.40
1:A:617:VAL:HG11	1:A:639:PRO:HG3	2.03	0.40
1:C:1151:LEU:O	1:C:1155:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	840/868 (97%)	821 (98%)	17 (2%)	2 (0%)	51	63
1	B	828/868 (95%)	806 (97%)	19 (2%)	3 (0%)	38	47
1	C	838/868 (96%)	818 (98%)	17 (2%)	3 (0%)	38	47
1	D	844/868 (97%)	821 (97%)	22 (3%)	1 (0%)	55	67
All	All	3350/3472 (96%)	3266 (98%)	75 (2%)	9 (0%)	44	55

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	636	SER
1	C	605	HIS
1	B	605	HIS
1	A	682	PHE
1	C	682	PHE
1	B	538	PRO
1	C	538	PRO
1	D	538	PRO
1	A	538	PRO

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	671/726 (92%)	664 (99%)	7 (1%)	80	90
1	B	668/726 (92%)	658 (98%)	10 (2%)	70	83
1	C	672/726 (93%)	665 (99%)	7 (1%)	80	90
1	D	679/726 (94%)	674 (99%)	5 (1%)	87	94
All	All	2690/2904 (93%)	2661 (99%)	29 (1%)	78	89

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	514	VAL
1	A	602	ASN
1	A	682	PHE
1	A	740	LEU
1	A	837	LYS
1	A	953	PHE
1	A	976	GLN
1	B	415	LEU
1	B	467	VAL
1	B	542	ARG
1	B	544	ASN
1	B	682	PHE
1	B	909	THR

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Mol	Chain	Res	Type
1	B	950	LEU
1	B	953	PHE
1	B	976	GLN
1	B	1114	LEU
1	C	464	GLN
1	C	467	VAL
1	C	602	ASN
1	C	682	PHE
1	C	909	THR
1	C	953	PHE
1	C	976	GLN
1	D	682	PHE
1	D	909	THR
1	D	953	PHE
1	D	976	GLN
1	D	1112	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1030	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	TD8	A	2001	3	26,35,35	1.15	2 (7%)	28,51,51	2.32	11 (39%)
2	TD8	B	2001	3	26,35,35	0.96	1 (3%)	28,51,51	2.32	7 (25%)
2	TD8	C	2001	3	26,35,35	1.14	2 (7%)	28,51,51	2.53	7 (25%)
2	TD8	D	2001	3	26,35,35	1.07	1 (3%)	28,51,51	2.19	8 (28%)

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	TD8	A	2001	3	-	0/20/27/27	0/2/2/2
2	TD8	B	2001	3	-	0/20/27/27	0/2/2/2
2	TD8	C	2001	3	-	0/20/27/27	0/2/2/2
2	TD8	D	2001	3	-	0/20/27/27	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TD8	O9-C8	-3.81	1.33	1.42
2	A	2001	TD8	O9-C8	-3.73	1.34	1.42
2	C	2001	TD8	O9-C8	-3.63	1.34	1.42
2	B	2001	TD8	O9-C8	-3.44	1.34	1.42
2	A	2001	TD8	PB-O3A	2.45	1.64	1.60
2	C	2001	TD8	PB-O3A	3.13	1.65	1.60

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	TD8	N1'-C2'-N3'	-3.53	119.49	125.59
2	D	2001	TD8	N1'-C2'-N3'	-3.34	119.81	125.59
2	C	2001	TD8	C4A-C4-C5	-3.27	120.96	127.29
2	B	2001	TD8	N1'-C2'-N3'	-3.17	120.10	125.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	TD8	C4A-C4-C5	-2.92	121.64	127.29
2	B	2001	TD8	C4A-C4-C5	-2.90	121.68	127.29
2	A	2001	TD8	N1'-C2'-N3'	-2.86	120.65	125.59
2	A	2001	TD8	C4A-C4-C5	-2.83	121.82	127.29
2	A	2001	TD8	C5'-C6'-N1'	-2.18	120.18	123.87
2	B	2001	TD8	C5'-C6'-N1'	-2.08	120.35	123.87
2	D	2001	TD8	O5G-PA-O1A	-2.06	100.94	109.25
2	A	2001	TD8	C5-C4-N3	2.05	111.95	107.66
2	A	2001	TD8	O3B-PB-O1B	2.23	116.61	107.61
2	A	2001	TD8	O9-C8-C9	2.23	118.40	110.21
2	A	2001	TD8	C6'-C5'-C4'	2.26	118.68	115.68
2	D	2001	TD8	C4A-C4-N3	2.35	125.64	122.69
2	D	2001	TD8	C5-C4-N3	2.37	112.62	107.66
2	C	2001	TD8	C4A-C4-N3	2.43	125.75	122.69
2	A	2001	TD8	C4A-C4-N3	2.47	125.80	122.69
2	A	2001	TD8	C6'-N1'-C2'	2.60	120.38	115.88
2	C	2001	TD8	C5-C4-N3	2.66	113.21	107.66
2	B	2001	TD8	C5-C4-N3	2.76	113.42	107.66
2	A	2001	TD8	C2A-C2'-N1'	3.00	120.45	117.06
2	D	2001	TD8	C6'-N1'-C2'	3.09	121.22	115.88
2	C	2001	TD8	C6'-N1'-C2'	3.13	121.28	115.88
2	B	2001	TD8	C6'-N1'-C2'	3.21	121.44	115.88
2	B	2001	TD8	C2A-C2'-N1'	3.44	120.94	117.06
2	C	2001	TD8	C2A-C2'-N1'	3.63	121.16	117.06
2	D	2001	TD8	C2A-C2'-N1'	3.96	121.54	117.06
2	D	2001	TD8	C5A-C5-C4	7.09	133.12	127.43
2	A	2001	TD8	C5A-C5-C4	8.34	134.13	127.43
2	B	2001	TD8	C5A-C5-C4	8.43	134.20	127.43
2	C	2001	TD8	C5A-C5-C4	9.87	135.35	127.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	TD8	6	0
2	B	2001	TD8	2	0
2	C	2001	TD8	1	0
2	D	2001	TD8	4	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	847/868 (97%)	0.48	73 (8%)	11 16	23, 41, 74, 103	0
1	B	836/868 (96%)	0.27	43 (5%)	29 36	22, 36, 65, 94	0
1	C	845/868 (97%)	0.29	38 (4%)	34 41	22, 36, 65, 114	0
1	D	852/868 (98%)	0.47	69 (8%)	13 17	22, 40, 73, 109	0
All	All	3380/3472 (97%)	0.38	223 (6%)	19 25	22, 38, 70, 114	0

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	421	VAL	10.6
1	A	570	ALA	7.6
1	A	569	GLN	7.4
1	C	570	ALA	7.2
1	C	420	LYS	6.5
1	A	502	GLY	6.1
1	B	368	ALA	5.8
1	A	571	HIS	5.8
1	D	368	ALA	5.8
1	A	568	SER	5.8
1	A	410	LEU	5.7
1	C	569	GLN	5.3
1	A	779	ILE	5.2
1	D	427	VAL	5.1
1	B	571	HIS	4.9
1	D	803	VAL	4.9
1	C	571	HIS	4.8
1	C	397	PHE	4.8
1	C	419	PHE	4.8
1	A	368	ALA	4.7
1	A	807	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	426	GLY	4.7
1	D	371	ILE	4.6
1	D	568	SER	4.4
1	A	394	ASN	4.4
1	A	370	VAL	4.4
1	C	790	GLU	4.2
1	D	410	LEU	4.2
1	A	567	PRO	4.2
1	A	566	ASN	4.2
1	B	815	ILE	4.1
1	A	427	VAL	4.1
1	C	394	ASN	4.1
1	A	790	GLU	4.0
1	D	571	HIS	4.0
1	B	426	GLY	4.0
1	D	567	PRO	3.9
1	D	365	ASP	3.8
1	D	796	TYR	3.8
1	C	568	SER	3.7
1	D	816	GLU	3.7
1	D	569	GLN	3.7
1	D	1152	ALA	3.7
1	C	565	LEU	3.6
1	B	953	PHE	3.6
1	A	1152	ALA	3.5
1	B	807	VAL	3.5
1	D	570	ALA	3.4
1	A	698	VAL	3.4
1	C	395	THR	3.4
1	D	831	LEU	3.4
1	D	471	HIS	3.4
1	D	395	THR	3.4
1	A	810	LEU	3.4
1	A	815	ILE	3.4
1	A	803	VAL	3.3
1	C	366	LYS	3.3
1	C	368	ALA	3.3
1	D	827	ILE	3.3
1	D	564	ASN	3.3
1	D	394	ASN	3.2
1	A	1148	ARG	3.2
1	C	415	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	655	ALA	3.2
1	B	792	ALA	3.2
1	B	653	VAL	3.1
1	A	780	GLY	3.0
1	D	473	LYS	3.0
1	A	831	LEU	3.0
1	B	633	ASN	3.0
1	A	809	GLU	3.0
1	A	421	VAL	2.9
1	D	366	LYS	2.9
1	B	823	ALA	2.9
1	A	558	PHE	2.9
1	B	986	SER	2.9
1	A	589	MET	2.9
1	B	652	GLY	2.9
1	A	395	THR	2.8
1	A	592	ASP	2.8
1	B	392	LEU	2.8
1	C	815	ILE	2.8
1	B	827	ILE	2.8
1	D	804	PHE	2.8
1	D	848	LEU	2.8
1	B	790	GLU	2.8
1	B	983	GLY	2.7
1	A	1190	ASP	2.7
1	B	563	GLY	2.7
1	D	414	ASP	2.7
1	A	983	GLY	2.7
1	D	631	SER	2.7
1	D	828	PRO	2.7
1	D	934	PRO	2.7
1	A	823	ALA	2.7
1	C	655	ALA	2.7
1	D	367	ASN	2.7
1	D	393	ASP	2.7
1	D	783	ASP	2.7
1	D	779	ILE	2.6
1	C	984	ALA	2.6
1	B	803	VAL	2.6
1	D	421	VAL	2.6
1	D	654	VAL	2.6
1	C	435	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	414	ASP	2.6
1	B	698	VAL	2.6
1	D	813	HIS	2.6
1	B	457	PRO	2.6
1	B	427	VAL	2.5
1	C	409	GLY	2.5
1	C	558	PHE	2.5
1	A	796	TYR	2.5
1	A	655	ALA	2.5
1	B	987	ILE	2.5
1	D	931	ALA	2.5
1	A	1110	THR	2.5
1	D	1103	GLU	2.5
1	A	472	ASP	2.5
1	D	805	ASN	2.5
1	A	420	LYS	2.5
1	B	1028	PHE	2.5
1	A	1157	ARG	2.5
1	D	810	LEU	2.5
1	C	814	GLU	2.4
1	B	779	ILE	2.4
1	B	565	LEU	2.4
1	A	432	LEU	2.4
1	B	608	ALA	2.4
1	A	654	VAL	2.4
1	D	953	PHE	2.4
1	C	1225	ALA	2.4
1	D	815	ILE	2.4
1	A	478	GLU	2.4
1	A	986	SER	2.4
1	D	472	ASP	2.3
1	C	810	LEU	2.3
1	B	1067	PHE	2.3
1	D	792	ALA	2.3
1	D	502	GLY	2.3
1	D	397	PHE	2.3
1	A	471	HIS	2.3
1	B	1025	ILE	2.3
1	B	954	ALA	2.3
1	C	410	LEU	2.3
1	B	370	VAL	2.3
1	D	422	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	988	ILE	2.3
1	D	1110	THR	2.3
1	A	445	ARG	2.3
1	B	981	VAL	2.3
1	B	1129	LYS	2.3
1	A	931	ALA	2.3
1	A	634	ARG	2.2
1	A	653	VAL	2.2
1	A	363	ILE	2.2
1	C	564	ASN	2.2
1	D	787	LYS	2.2
1	D	937	THR	2.2
1	A	1105	ASP	2.2
1	A	806	GLU	2.2
1	B	654	VAL	2.2
1	A	1112	LEU	2.2
1	D	826	GLN	2.2
1	C	787	LYS	2.2
1	D	501	VAL	2.2
1	B	813	HIS	2.2
1	B	992	ILE	2.2
1	C	796	TYR	2.2
1	A	1194	GLY	2.2
1	A	792	ALA	2.2
1	A	371	ILE	2.2
1	A	814	GLU	2.2
1	D	1105	ASP	2.2
1	C	476	VAL	2.1
1	A	647	ALA	2.1
1	D	657	THR	2.1
1	C	1129	LYS	2.1
1	C	572	GLY	2.1
1	C	786	MET	2.1
1	A	822	GLU	2.1
1	A	642	LEU	2.1
1	B	828	PRO	2.1
1	A	563	GLY	2.1
1	A	978	GLY	2.1
1	D	814	GLU	2.1
1	C	789	ALA	2.1
1	A	365	ASP	2.1
1	A	393	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	594	ASP	2.1
1	A	1216	VAL	2.1
1	A	804	PHE	2.1
1	D	429	ARG	2.1
1	A	930	LEU	2.1
1	A	1103	GLU	2.1
1	A	777	ALA	2.1
1	D	608	ALA	2.1
1	A	650	GLY	2.1
1	B	419	PHE	2.1
1	B	991	PHE	2.1
1	C	1112	LEU	2.1
1	D	1128	ALA	2.1
1	D	572	GLY	2.1
1	D	986	SER	2.1
1	D	590	PHE	2.1
1	D	634	ARG	2.0
1	D	674	ILE	2.0
1	D	1025	ILE	2.0
1	D	566	ASN	2.0
1	B	975	ALA	2.0
1	D	609	VAL	2.0
1	B	415	LEU	2.0
1	C	371	ILE	2.0
1	C	988	ILE	2.0
1	B	564	ASN	2.0
1	A	644	GLY	2.0
1	A	975	ALA	2.0
1	D	1136	ALA	2.0
1	C	567	PRO	2.0
1	D	1162	LYS	2.0
1	A	1028	PHE	2.0
1	C	953	PHE	2.0
1	D	1077	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(\AA^2)	Q<0.9
2	TD8	C	2001	34/34	0.96	0.14	-0.71	16,28,44,48	0
2	TD8	D	2001	34/34	0.96	0.14	-0.76	19,26,41,43	0
4	CA	C	2003	1/1	0.99	0.10	-0.87	28,28,28,28	0
2	TD8	B	2001	34/34	0.97	0.13	-1.15	17,28,34,37	0
2	TD8	A	2001	34/34	0.97	0.14	-1.26	16,30,40,41	0
3	MG	A	2002	1/1	0.96	0.12	-1.70	26,26,26,26	0
4	CA	D	2003	1/1	0.96	0.08	-1.83	41,41,41,41	0
3	MG	D	2002	1/1	0.96	0.09	-2.04	25,25,25,25	0
4	CA	A	2003	1/1	0.96	0.07	-2.27	41,41,41,41	0
3	MG	C	2002	1/1	0.98	0.10	-2.28	12,12,12,12	0
4	CA	B	2003	1/1	0.99	0.04	-2.80	29,29,29,29	0
3	MG	B	2002	1/1	0.99	0.05	-4.36	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.