



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:27 PM GMT

PDB ID : 3ZHR
Title : Crystal structure of the H747A mutant of the SucA domain of Mycobacterium smegmatis KGD showing the active site lid closed
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 ⓘ 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

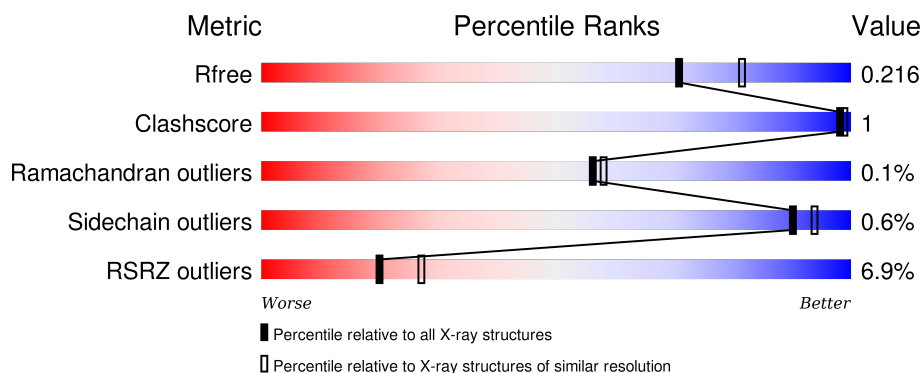
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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 $\leq 5\%$. 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>6%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>
1	B	868	<div> <div>7%</div> <div> <div></div> <div>92%</div> <div>5%</div> </div> </div>
1	C	868	<div> <div>6%</div> <div> <div></div> <div>91%</div> <div>6%</div> </div> </div>
1	D	868	<div> <div>8%</div> <div> <div></div> <div>91%</div> <div>5%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MPD	A	2228	-	-	-	X
5	MPD	C	2228	-	-	-	X
5	MPD	D	2228	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26675 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.

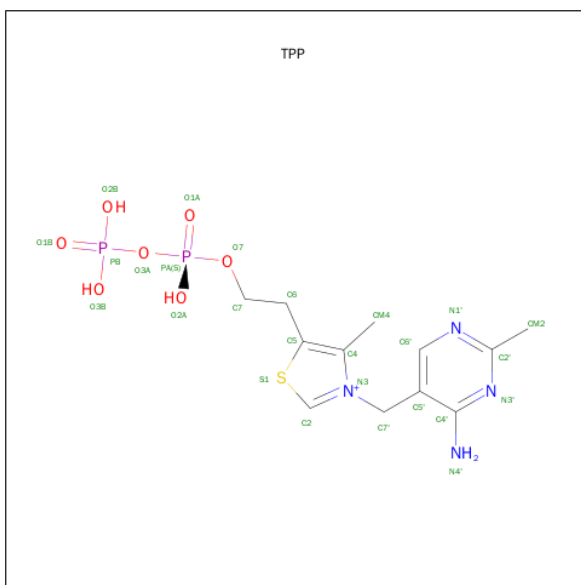
- Molecule 1 is a protein called MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	822	Total	C	N	O	S	0	2	0
			6376	4017	1124	1210	25			
1	B	823	Total	C	N	O	S	0	2	0
			6371	4010	1130	1205	26			
1	C	813	Total	C	N	O	S	0	1	0
			6307	3973	1116	1193	25			
1	D	823	Total	C	N	O	S	0	1	0
			6302	3971	1109	1197	25			

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total 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).

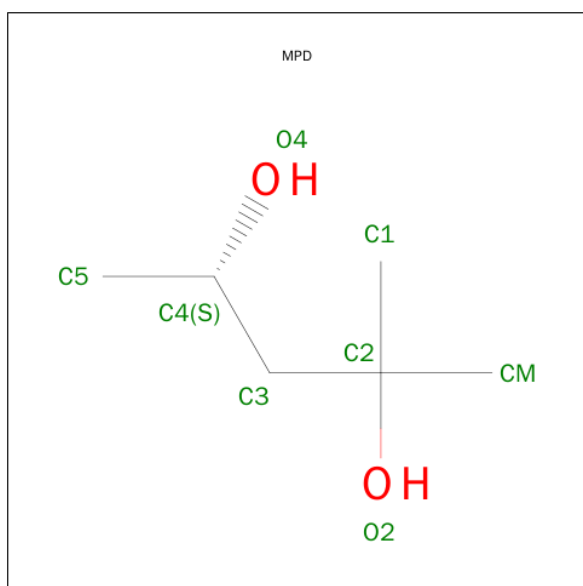
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	C	1	Total	C	O	0	0
			8	6	2		
5	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	339	Total	O	0	0
			339	339		
6	B	259	Total	O	0	0
			259	259		

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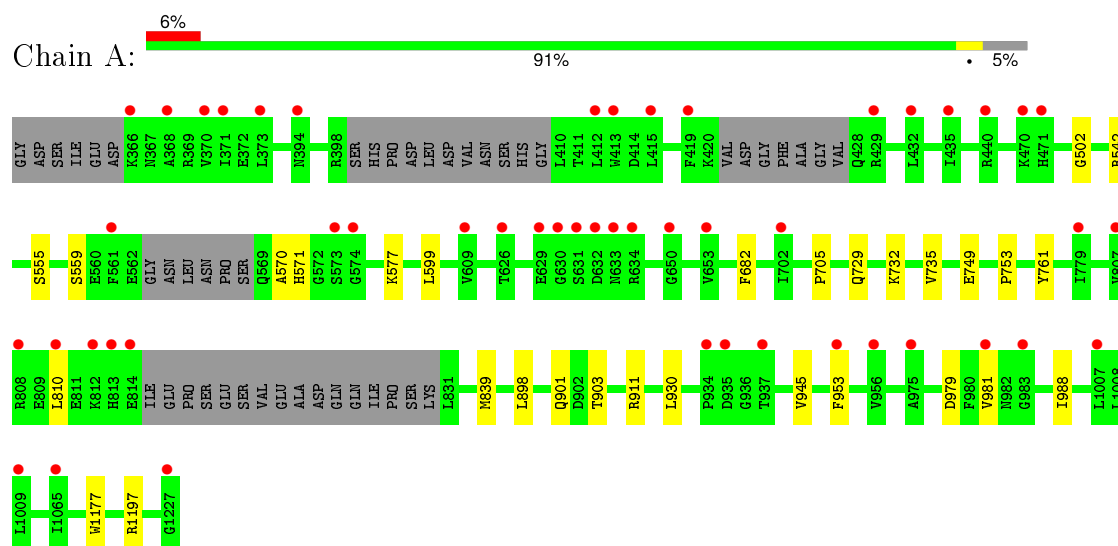
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	326	Total 326	O 326	0	0
6	D	251	Total 251	O 251	0	0

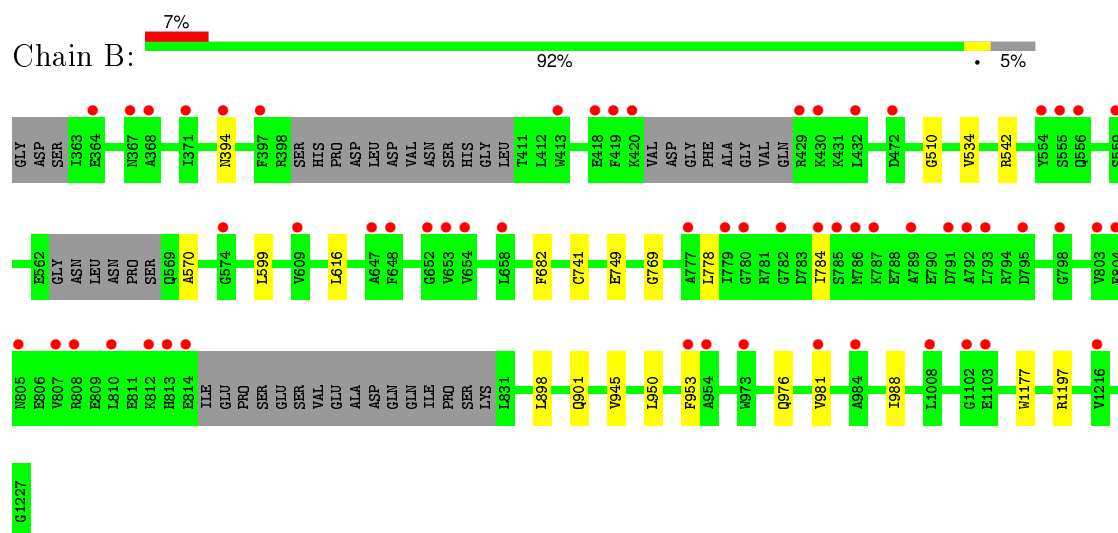
3 Residue-property plots

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

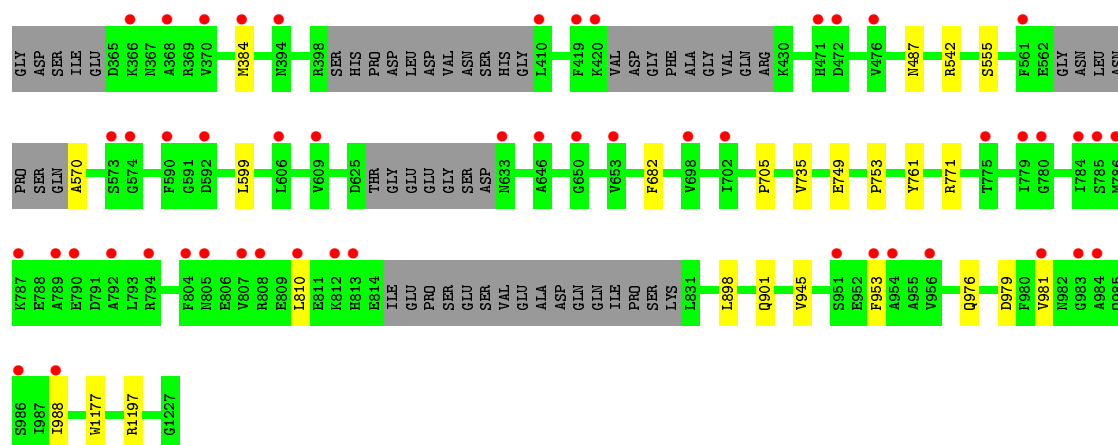


• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME

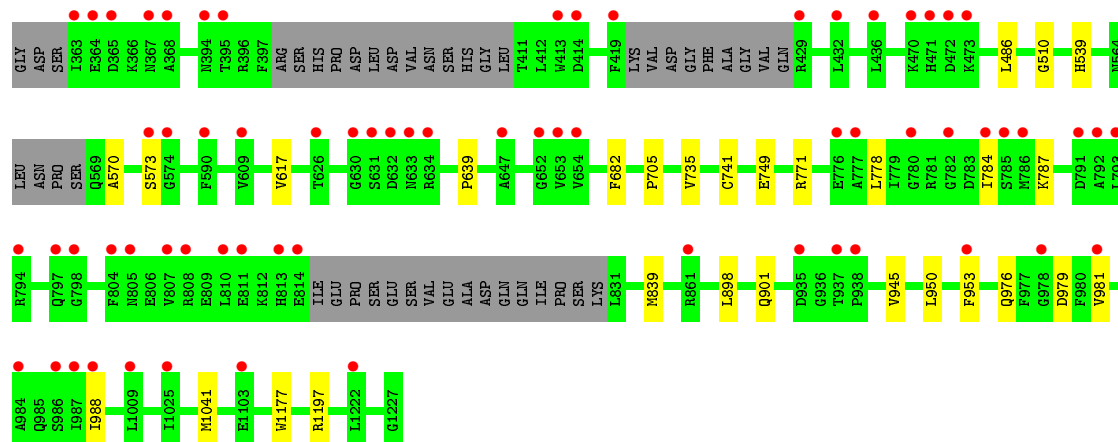


• Molecule 1: MULTIFUNCTIONAL 2-OXOGLUTARATE METABOLISM ENZYME





● 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, α , β , γ	79.97Å 83.45Å 159.67Å 99.64° 98.82° 100.98°	Depositor
Resolution (Å)	30.75 – 2.10 48.75 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.75-2.10) 91.0 (48.75-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.180 , 0.202 0.192 , 0.216	Depositor DCC
R_{free} test set	11122 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.0	EDS
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 221693 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26675	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.34% 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: MPD, CA, MG, TPP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.51	0/6511	0.61	0/8828
1	B	0.49	0/6501	0.60	0/8812
1	C	0.50	0/6436	0.60	0/8724
1	D	0.50	0/6431	0.60	0/8725
All	All	0.50	0/25879	0.60	0/35089

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	6376	0	6164	15	0
1	B	6371	0	6158	10	0
1	C	6307	0	6102	10	0
1	D	6302	0	6048	13	0
2	A	26	0	16	2	0
2	B	26	0	16	1	0
2	C	26	0	16	1	0
2	D	26	0	16	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	8	0	14	0	0
5	B	8	0	14	0	0
5	C	8	0	14	0	0
5	D	8	0	14	0	0
6	A	339	0	0	1	0
6	B	259	0	0	1	0
6	C	326	0	0	0	0
6	D	251	0	0	1	0
All	All	26675	0	24592	49	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 (49) 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:570:ALA:HA	1:A:749:GLU:HB2	1.81	0.62
1:B:542:ARG:NE	1:B:599:LEU:HD21	2.17	0.59
1:C:570:ALA:HA	1:C:749:GLU:HB2	1.87	0.56
1:D:570:ALA:HA	1:D:749:GLU:HB2	1.88	0.56
1:A:705:PRO:HG2	1:A:735:VAL:HG13	1.93	0.51
1:B:534:VAL:HG11	1:B:616:LEU:HD22	1.94	0.50
1:D:981:VAL:HG22	1:D:988:ILE:HD11	1.93	0.50
1:A:981:VAL:HG22	1:A:988:ILE:HD11	1.95	0.49
1:C:981:VAL:HG22	1:C:988:ILE:HD11	1.94	0.49
1:B:981:VAL:HG22	1:B:988:ILE:HD11	1.95	0.48
1:A:559:SER:O	1:A:577:LYS:NZ	2.45	0.48
1:A:901:GLN:OE1	2:B:2001:TPP:H6'	2.15	0.47
1:A:571:HIS:HE1	6:A:3056:HOH:O	1.98	0.47
1:A:898:LEU:O	1:A:945:VAL:HA	2.15	0.46
1:B:570:ALA:HA	1:B:749:GLU:HB2	1.98	0.46
1:A:542:ARG:NE	1:A:599:LEU:HD21	2.30	0.46
1:D:617:VAL:HG11	1:D:639:PRO:HG3	1.98	0.45
1:D:510:GLY:O	1:D:741:CYS:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:898:LEU:O	1:C:945:VAL:HA	2.15	0.45
2:A:2001:TPP:H6'	1:B:901:GLN:OE1	2.16	0.45
1:C:901:GLN:OE1	2:D:2001:TPP:H6'	2.16	0.45
1:D:539:HIS:HE1	1:D:573:SER:HB2	1.81	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
2:C:2001:TPP:H6'	1:D:901:GLN:OE1	2.17	0.44
1:C:542:ARG:NE	1:C:599:LEU:HD21	2.33	0.44
1:B:778:LEU:HB3	1:B:784:ILE:HG12	2.00	0.43
1:B:510:GLY:O	1:B:741:CYS:HB2	2.18	0.43
1:A:839:MET:HE3	1:A:839:MET:O	2.18	0.43
1:D:705:PRO:HG2	1:D:735:VAL:HG13	2.00	0.43
1:A:555:SER:HA	1:A:810:LEU:HD22	2.01	0.43
2:A:2001:TPP:H61	2:A:2001:TPP:HM41	1.94	0.42
1:A:1177:TRP:CD1	1:A:1197:ARG:HD3	2.55	0.42
1:C:555:SER:HA	1:C:810:LEU:HD22	2.01	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	2.55	0.42
1:A:729:GLN:O	1:A:732:LYS:HE3	2.19	0.42
1:C:487:ASN:OD1	1:C:771:ARG:HD2	2.20	0.42
1:D:1041[A]:MET:HE1	6:D:3235:HOH:O	2.20	0.42
1:C:1177:TRP:CD1	1:C:1197:ARG:HD3	2.55	0.42
1:B:769:GLY:HA3	6:B:3024:HOH:O	2.20	0.41
1:D:1177:TRP:CD1	1:D:1197:ARG:HD3	2.55	0.41
1:C:753:PRO:HB2	1:C:761:TYR:CE1	2.56	0.41
1:D:486:LEU:HD13	1:D:771:ARG:HA	2.02	0.41
1:A:502:GLY:HA2	1:A:749:GLU:HG3	2.03	0.41
1:A:753:PRO:HB2	1:A:761:TYR:CE1	2.57	0.40
1:A:903:THR:O	1:A:911:ARG:HD2	2.22	0.40
1:C:705:PRO:HG2	1:C:735:VAL:HG13	2.02	0.40
1:D:839:MET:O	1:D:839:MET:HE2	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	814/868 (94%)	797 (98%)	16 (2%)	1 (0%)	56	58
1	B	815/868 (94%)	798 (98%)	16 (2%)	1 (0%)	56	58
1	C	802/868 (92%)	789 (98%)	12 (2%)	1 (0%)	56	58
1	D	814/868 (94%)	793 (97%)	20 (2%)	1 (0%)	56	58
All	All	3245/3472 (94%)	3177 (98%)	64 (2%)	4 (0%)	56	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	682	PHE
1	B	682	PHE
1	C	682	PHE
1	D	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	657/725 (91%)	654 (100%)	3 (0%)	92	95
1	B	653/725 (90%)	649 (99%)	4 (1%)	90	94
1	C	649/725 (90%)	645 (99%)	4 (1%)	90	94
1	D	639/725 (88%)	634 (99%)	5 (1%)	86	91
All	All	2598/2900 (90%)	2582 (99%)	16 (1%)	90	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	930	LEU
1	A	953	PHE
1	A	979	ASP
1	B	394	ASN

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Mol	Chain	Res	Type
1	B	950	LEU
1	B	953	PHE
1	B	976	GLN
1	C	384	MET
1	C	953	PHE
1	C	976	GLN
1	C	979	ASP
1	D	787	LYS
1	D	950	LEU
1	D	953	PHE
1	D	976	GLN
1	D	979	ASP

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

Mol	Chain	Res	Type
1	B	1020	HIS

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TPP	A	2001	3	20,27,27	1.70	2 (10%)	31,40,40	1.77	8 (25%)
5	MPD	A	2228	-	6,7,7	0.29	0	7,10,10	0.44	0
2	TPP	B	2001	3	20,27,27	1.90	2 (10%)	31,40,40	1.76	9 (29%)
5	MPD	B	2228	-	6,7,7	0.29	0	7,10,10	0.38	0
2	TPP	C	2001	3	20,27,27	1.75	2 (10%)	31,40,40	1.85	8 (25%)
5	MPD	C	2228	-	6,7,7	0.29	0	7,10,10	0.36	0
2	TPP	D	2001	3	20,27,27	2.02	3 (15%)	31,40,40	1.81	9 (29%)
5	MPD	D	2228	-	6,7,7	0.29	0	7,10,10	0.41	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	A	2001	3	-	0/16/17/17	0/2/2/2
5	MPD	A	2228	-	-	0/5/5/5	0/0/0/0
2	TPP	B	2001	3	-	0/16/17/17	0/2/2/2
5	MPD	B	2228	-	-	0/5/5/5	0/0/0/0
2	TPP	C	2001	3	-	0/16/17/17	0/2/2/2
5	MPD	C	2228	-	-	0/5/5/5	0/0/0/0
2	TPP	D	2001	3	-	0/16/17/17	0/2/2/2
5	MPD	D	2228	-	-	0/5/5/5	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	TPP	C4-N3	-7.57	1.33	1.39
2	B	2001	TPP	C4-N3	-6.91	1.33	1.39
2	C	2001	TPP	C4-N3	-6.34	1.34	1.39
2	A	2001	TPP	C4-N3	-6.07	1.34	1.39
2	D	2001	TPP	C4'-N4'	2.19	1.39	1.34
2	C	2001	TPP	PB-O1B	2.37	1.59	1.51
2	D	2001	TPP	PB-O1B	2.39	1.59	1.51
2	A	2001	TPP	PB-O1B	2.55	1.59	1.51
2	B	2001	TPP	PB-O1B	2.92	1.60	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	TPP	CM4-C4-C5	-5.15	117.33	128.90
2	A	2001	TPP	CM4-C4-C5	-4.86	117.97	128.90
2	B	2001	TPP	CM4-C4-C5	-4.54	118.71	128.90
2	D	2001	TPP	CM4-C4-C5	-4.33	119.16	128.90
2	D	2001	TPP	N1'-C2'-N3'	-2.97	120.11	125.60
2	B	2001	TPP	N1'-C2'-N3'	-2.74	120.54	125.60
2	A	2001	TPP	N1'-C2'-N3'	-2.73	120.56	125.60
2	D	2001	TPP	C5'-C6'-N1'	-2.60	119.34	123.86
2	C	2001	TPP	N1'-C2'-N3'	-2.57	120.84	125.60
2	B	2001	TPP	C5'-C6'-N1'	-2.35	119.78	123.86
2	B	2001	TPP	O3A-PA-O7	2.03	108.33	102.94
2	D	2001	TPP	CM2-C2'-N1'	2.04	119.47	117.03
2	D	2001	TPP	CM4-C4-N3	2.04	125.31	122.59
2	B	2001	TPP	CM4-C4-N3	2.08	125.36	122.59
2	B	2001	TPP	CM2-C2'-N1'	2.10	119.55	117.03
2	A	2001	TPP	O3A-PA-O7	2.16	108.67	102.94
2	A	2001	TPP	CM2-C2'-N1'	2.17	119.63	117.03
2	D	2001	TPP	C6-C5-C4	2.21	129.54	127.56
2	C	2001	TPP	C6-C5-S1	2.23	123.35	120.24
2	D	2001	TPP	O3A-PA-O7	2.25	108.90	102.94
2	A	2001	TPP	C6-C5-C4	2.36	129.68	127.56
2	C	2001	TPP	O3A-PA-O7	2.39	109.27	102.94
2	C	2001	TPP	C6-C5-C4	2.80	130.07	127.56
2	A	2001	TPP	CM4-C4-N3	2.84	126.37	122.59
2	C	2001	TPP	CM4-C4-N3	3.02	126.61	122.59
2	B	2001	TPP	C6-C5-C4	3.03	130.28	127.56
2	A	2001	TPP	C6'-N1'-C2'	3.19	121.34	115.77
2	C	2001	TPP	C6'-N1'-C2'	3.25	121.45	115.77
2	B	2001	TPP	C6'-N1'-C2'	3.31	121.55	115.77
2	D	2001	TPP	C5-C4-N3	3.47	115.33	107.69
2	A	2001	TPP	C5-C4-N3	3.54	115.49	107.69
2	B	2001	TPP	C5-C4-N3	3.61	115.64	107.69
2	C	2001	TPP	C5-C4-N3	3.71	115.85	107.69
2	D	2001	TPP	C6'-N1'-C2'	3.82	122.45	115.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	TPP	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	TPP	1	0
2	C	2001	TPP	1	0
2	D	2001	TPP	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	822/868 (94%)	0.19	49 (5%)	25 33	20, 35, 68, 99	0
1	B	823/868 (94%)	0.25	58 (7%)	19 26	20, 35, 73, 121	0
1	C	813/868 (93%)	0.18	51 (6%)	23 31	20, 33, 68, 108	0
1	D	823/868 (94%)	0.26	67 (8%)	15 20	20, 35, 74, 104	0
All	All	3281/3472 (94%)	0.22	225 (6%)	20 27	20, 35, 71, 121	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	574	GLY	16.7
1	D	413	TRP	8.4
1	B	419	PHE	7.7
1	D	807	VAL	6.5
1	D	810	LEU	6.2
1	D	472	ASP	5.9
1	C	779	ILE	5.9
1	C	785	SER	5.9
1	A	415	LEU	5.8
1	D	419	PHE	5.7
1	B	813	HIS	5.5
1	B	413	TRP	5.5
1	A	413	TRP	5.3
1	D	471	HIS	5.2
1	D	630	GLY	5.1
1	B	574	GLY	5.1
1	A	810	LEU	5.1
1	B	807	VAL	5.0
1	C	573	SER	5.0
1	A	633	ASN	4.8
1	B	420	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	420	LYS	4.5
1	A	368	ALA	4.4
1	D	473	LYS	4.3
1	B	368	ALA	4.3
1	A	561	PHE	4.2
1	A	631	SER	4.2
1	D	626	THR	4.1
1	B	791	ASP	4.1
1	D	394	ASN	4.1
1	D	634	ARG	4.0
1	B	367	ASN	4.0
1	C	810	LEU	4.0
1	D	368	ALA	4.0
1	B	785	SER	4.0
1	B	779	ILE	3.9
1	D	632	ASP	3.9
1	A	371	ILE	3.9
1	B	808	ARG	3.9
1	D	429	ARG	3.8
1	C	471	HIS	3.8
1	C	590	PHE	3.8
1	C	786	MET	3.7
1	B	397	PHE	3.7
1	D	414	ASP	3.7
1	B	810	LEU	3.7
1	B	429	ARG	3.7
1	C	784	ILE	3.7
1	D	631	SER	3.6
1	A	807	VAL	3.6
1	B	371	ILE	3.6
1	C	653	VAL	3.6
1	C	419	PHE	3.6
1	B	786	MET	3.5
1	D	590	PHE	3.5
1	D	953	PHE	3.5
1	C	574	GLY	3.4
1	B	430	LYS	3.4
1	A	812	LYS	3.4
1	D	1103	GLU	3.4
1	B	418	GLU	3.4
1	A	419	PHE	3.4
1	C	476	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	364	GLU	3.4
1	B	792	ALA	3.4
1	C	561	PHE	3.3
1	D	804	PHE	3.3
1	B	805	ASN	3.3
1	C	953	PHE	3.3
1	D	785	SER	3.3
1	B	804	PHE	3.3
1	C	807	VAL	3.3
1	A	394	ASN	3.2
1	A	435	ILE	3.2
1	A	412	LEU	3.2
1	A	953	PHE	3.2
1	D	981	VAL	3.1
1	A	440	ARG	3.1
1	D	987	ILE	3.1
1	B	472	ASP	3.1
1	D	805	ASN	3.1
1	A	626	THR	3.1
1	D	791	ASP	3.1
1	C	394	ASN	3.0
1	D	793	LEU	3.0
1	D	808	ARG	3.0
1	D	811	GLU	3.0
1	D	798	GLY	3.0
1	A	981	VAL	3.0
1	A	471	HIS	3.0
1	C	805	ASN	3.0
1	C	986	SER	2.9
1	A	429	ARG	2.9
1	D	786	MET	2.9
1	B	394	ASN	2.9
1	B	648	PHE	2.9
1	C	984	ALA	2.9
1	B	812	LYS	2.9
1	C	808	ARG	2.8
1	A	632	ASP	2.8
1	A	934	PRO	2.8
1	A	366	LYS	2.8
1	B	798	GLY	2.8
1	B	653	VAL	2.8
1	C	609	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	794	ARG	2.8
1	D	633	ASN	2.8
1	A	1007	LEU	2.8
1	B	803	VAL	2.8
1	A	630	GLY	2.7
1	B	647	ALA	2.7
1	A	370	VAL	2.7
1	D	654	VAL	2.7
1	B	954	ALA	2.7
1	C	789	ALA	2.7
1	C	792	ALA	2.7
1	B	1103	GLU	2.6
1	B	1216	VAL	2.6
1	B	953	PHE	2.6
1	D	782	GLY	2.6
1	C	804	PHE	2.6
1	A	935	ASP	2.6
1	A	937	THR	2.6
1	D	777	ALA	2.6
1	D	780	GLY	2.6
1	C	812	LYS	2.6
1	B	789	ALA	2.6
1	B	814	GLU	2.5
1	D	395	THR	2.5
1	C	790	GLU	2.5
1	D	984	ALA	2.5
1	B	432	LEU	2.5
1	B	777	ALA	2.5
1	B	795	ASP	2.5
1	A	573	SER	2.5
1	D	938	PRO	2.5
1	D	652	GLY	2.5
1	D	813	HIS	2.5
1	C	988	ILE	2.5
1	B	559	SER	2.4
1	B	556	GLN	2.4
1	D	797	GLN	2.4
1	A	653	VAL	2.4
1	C	702	ILE	2.4
1	D	363	ILE	2.4
1	A	432	LEU	2.4
1	C	633	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	555	SER	2.4
1	D	814	GLU	2.4
1	A	813	HIS	2.4
1	B	658	LEU	2.4
1	C	368	ALA	2.4
1	D	470	LYS	2.4
1	A	373	LEU	2.4
1	B	782	GLY	2.4
1	D	653	VAL	2.3
1	D	432	LEU	2.3
1	C	775	THR	2.3
1	D	365	ASP	2.3
1	A	814	GLU	2.3
1	B	984	ALA	2.3
1	C	954	ALA	2.3
1	B	654	VAL	2.3
1	C	650	GLY	2.3
1	D	574	GLY	2.3
1	D	784	ILE	2.3
1	D	861	ARG	2.3
1	C	813	HIS	2.3
1	C	983	GLY	2.3
1	B	1102	GLY	2.3
1	A	779	ILE	2.3
1	D	937	THR	2.3
1	C	606	LEU	2.3
1	C	646	ALA	2.2
1	D	792	ALA	2.2
1	D	978	GLY	2.2
1	C	410	LEU	2.2
1	B	554	TYR	2.2
1	B	609	VAL	2.2
1	B	784	ILE	2.2
1	C	780	GLY	2.2
1	C	366	LYS	2.2
1	D	367	ASN	2.2
1	C	698	VAL	2.2
1	C	981	VAL	2.2
1	D	609	VAL	2.2
1	C	951	SER	2.2
1	B	1008	LEU	2.2
1	D	776	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	975	ALA	2.2
1	D	988	ILE	2.2
1	A	629	GLU	2.2
1	A	1065	ILE	2.2
1	D	935	ASP	2.1
1	D	986	SER	2.1
1	B	787	LYS	2.1
1	A	609	VAL	2.1
1	A	634	ARG	2.1
1	C	472	ASP	2.1
1	C	592	ASP	2.1
1	B	652	GLY	2.1
1	B	793	LEU	2.1
1	A	808	ARG	2.1
1	A	983	GLY	2.1
1	C	794	ARG	2.1
1	D	436	LEU	2.1
1	A	470	LYS	2.1
1	B	973	TRP	2.1
1	A	650	GLY	2.1
1	C	370	VAL	2.1
1	C	384	MET	2.1
1	B	364	GLU	2.1
1	D	1025	ILE	2.1
1	D	1009	LEU	2.1
1	D	573	SER	2.1
1	A	956	VAL	2.1
1	A	702	ILE	2.1
1	A	1227	GLY	2.1
1	B	981	VAL	2.1
1	A	1009	LEU	2.0
1	D	647	ALA	2.0
1	C	956	VAL	2.0
1	B	780	GLY	2.0
1	D	1222	LEU	2.0
1	C	787	LYS	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(Å ²)	Q<0.9
5	MPD	C	2228	8/8	0.91	0.16	4.52	64,64,65,66	0
5	MPD	A	2228	8/8	0.91	0.17	4.38	68,69,71,71	0
5	MPD	D	2228	8/8	0.92	0.18	3.70	48,51,52,53	0
3	MG	D	2002	1/1	0.99	0.16	1.54	16,16,16,16	0
5	MPD	B	2228	8/8	0.88	0.15	1.23	47,49,50,50	0
3	MG	A	2002	1/1	0.97	0.14	0.93	12,12,12,12	0
3	MG	C	2002	1/1	0.99	0.15	0.40	11,11,11,11	0
3	MG	B	2002	1/1	0.99	0.14	-0.01	16,16,16,16	0
2	TPP	D	2001	26/26	0.98	0.14	-0.38	14,21,25,28	0
2	TPP	B	2001	26/26	0.97	0.14	-0.70	16,24,28,31	0
2	TPP	A	2001	26/26	0.98	0.11	-0.79	19,22,26,27	0
2	TPP	C	2001	26/26	0.98	0.13	-0.92	17,23,25,26	0
4	CA	B	2003	1/1	0.98	0.05	-1.66	32,32,32,32	0
4	CA	A	2003	1/1	0.99	0.04	-2.01	29,29,29,29	0
4	CA	D	2003	1/1	0.99	0.05	-2.54	30,30,30,30	0
4	CA	C	2003	1/1	0.99	0.04	-2.56	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.