



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:46 PM GMT

PDB ID : 4G5Y  
Title : Crystal Structure of Mycobacterium tuberculosis Pantothenate synthetase in a ternary complex with ATP and N,N-DIMETHYLTHIOPHENE-3-SULFONAMIDE  
Authors : Ciulli, A.; Silvestre, H.L.; Blundell, T.L.; Abell, C.  
Deposited on : 2012-07-18  
Resolution : 1.80 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

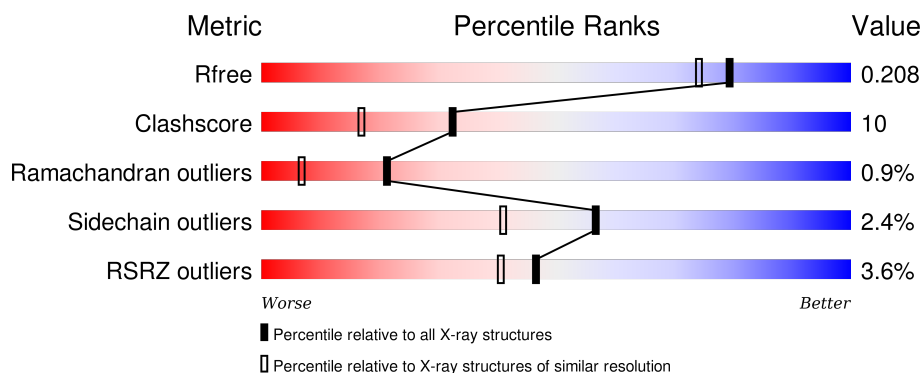
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	301	
1	B	301	

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
4	0OC	A	403	-	-	-	X
4	0OC	B	404	-	-	X	-
5	GOL	B	405	-	-	X	X
6	EOH	A	405	-	-	X	-
6	EOH	A	406	-	-	-	X
6	EOH	B	406	-	-	-	X
6	EOH	B	407	-	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 4688 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.

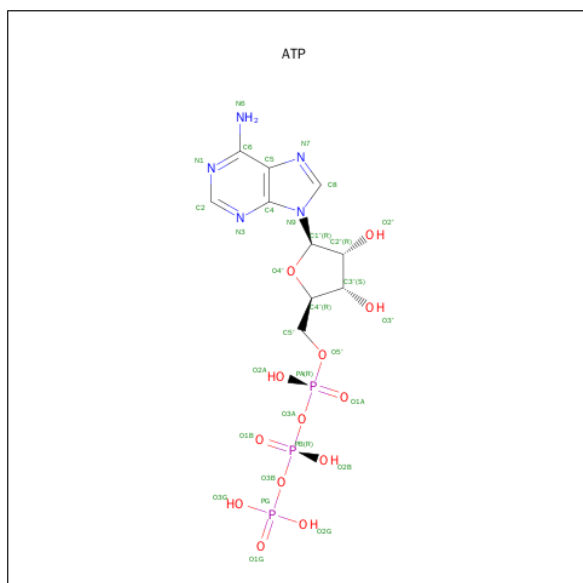
- Molecule 1 is a protein called Pantothenate synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	4	0
			2134	1350	385	393	6			
1	B	272	Total	C	N	O	S	0	4	0
			2029	1287	369	368	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	EXPRESSION TAG	UNP P0A5R0
A	2	ALA	THR	ENGINEERED MUTATION	UNP P0A5R0
A	77	GLY	GLU	ENGINEERED MUTATION	UNP P0A5R0
B	0	ALA	-	EXPRESSION TAG	UNP P0A5R0
B	2	ALA	THR	ENGINEERED MUTATION	UNP P0A5R0
B	77	GLY	GLU	ENGINEERED MUTATION	UNP P0A5R0

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

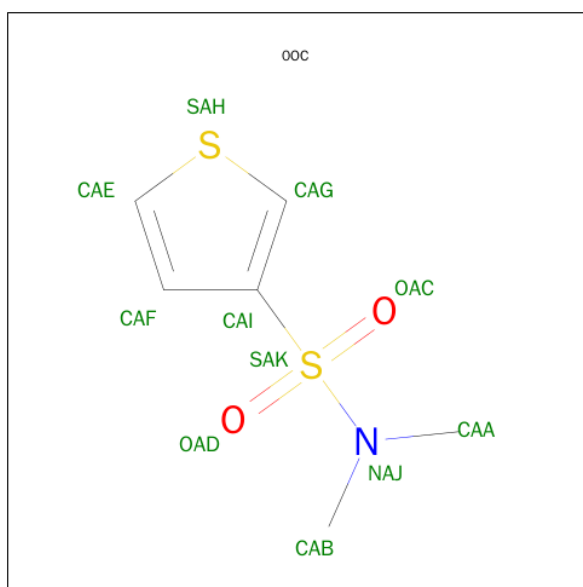


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- 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		

- Molecule 4 is N,N-DIMETHYLTHIOPHENE-3-SULFONAMIDE (three-letter code: OOC) (formula: C<sub>6</sub>H<sub>9</sub>NO<sub>2</sub>S<sub>2</sub>).



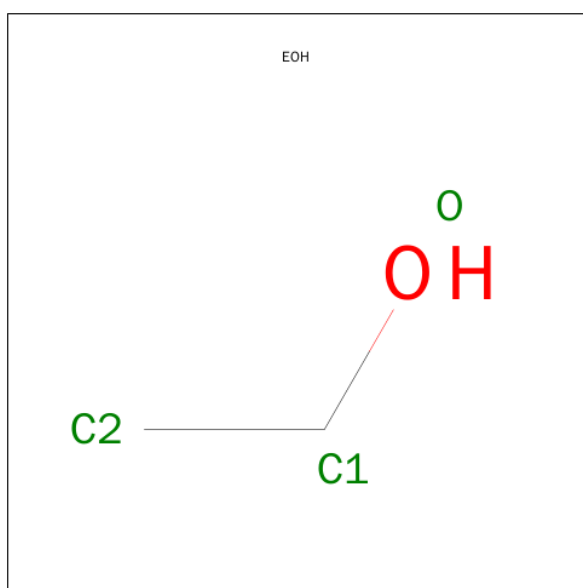
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			11	6	1	2	2		
4	B	1	Total	C	N	O	S	0	0
			11	6	1	2	2		
4	B	1	Total	C	N	O	S	0	0
			11	6	1	2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is ETHANOL (three-letter code: EOH) (formula:  $C_2H_6O$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	2	1		
6	A	1	Total	C	O	0	0
			3	2	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			3	2	1		
6	B	1	Total	C	O	0	0
			3	2	1		

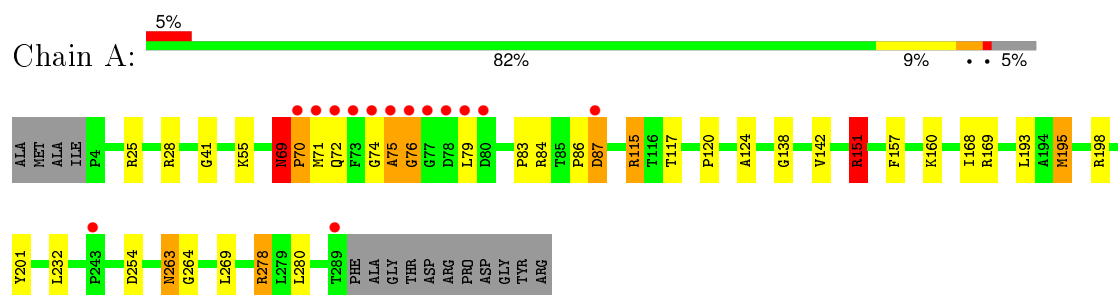
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	196	Total	O	0	0
			196	196		
7	B	208	Total	O	0	0
			208	208		

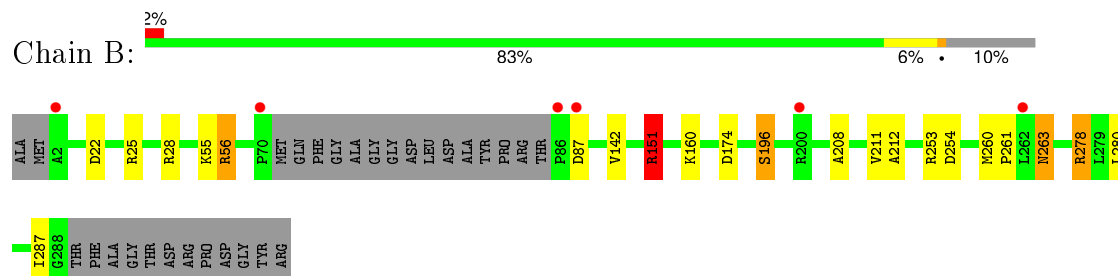
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Pantothenate synthetase



#### • Molecule 1: Pantothenate synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	48.26 Å 71.06 Å 81.65 Å 90.00° 99.35° 90.00°	Depositor
Resolution (Å)	37.57 – 1.80 37.57 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (37.57-1.80) 99.6 (37.57-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.13 (at 1.79 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.158 , 0.208 0.158 , 0.208	Depositor DCC
$R_{free}$ test set	2533 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.8	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 50748 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4688	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, EOH, OOC, ATP

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	1.08	1/2179 (0.0%)	1.15	14/2975 (0.5%)
1	B	1.08	0/2072	1.13	6/2828 (0.2%)
All	All	1.08	1/4251 (0.0%)	1.14	20/5803 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	ASN	C-O	6.17	1.35	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	ARG	NE-CZ-NH2	-12.32	114.14	120.30
1	B	253	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	254	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	B	151	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	A	151	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	115	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	A	280	LEU	CB-CG-CD2	-6.43	100.06	111.00
1	A	169	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	278	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	28[A]	ARG	NE-CZ-NH2	-5.94	117.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28[B]	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	269	LEU	CB-CG-CD1	-5.83	101.08	111.00
1	B	174	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	56[A]	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	56[B]	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	193	LEU	CB-CG-CD1	5.31	120.02	111.00
1	A	69	ASN	C-N-CD	-5.26	109.03	120.60
1	A	169	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	195	MET	CA-CB-CG	-5.08	104.66	113.30
1	A	232	LEU	CB-CG-CD1	-5.01	102.48	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	69	ASN	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2134	0	2183	39	0
1	B	2029	0	2105	44	0
2	A	31	0	12	0	0
2	B	31	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	11	0	8	4	0
4	B	22	0	18	8	0
5	A	6	0	8	0	0
5	B	6	0	8	26	0
6	A	6	0	12	2	0
6	B	6	0	12	3	0
7	A	196	0	0	5	0
7	B	208	0	0	7	0
All	All	4688	0	4378	91	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 10.

All (91) 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:280[B]:LEU:CD1	5:B:405:GOL:H32	1.51	1.38
1:B:196:SER:HB2	5:B:405:GOL:O1	1.25	1.27
1:B:196:SER:CB	5:B:405:GOL:O1	1.95	1.14
1:A:70[B]:PRO:HB3	1:A:79:LEU:HD22	1.14	1.13
1:B:160:LYS:HE3	5:B:405:GOL:H31	1.34	1.09
1:B:280[B]:LEU:CD1	5:B:405:GOL:C3	2.33	1.07
1:B:280[B]:LEU:HD11	5:B:405:GOL:H32	1.10	1.05
1:B:280[B]:LEU:HD12	5:B:405:GOL:H32	1.40	1.03
1:A:70[B]:PRO:HB3	1:A:79:LEU:CD2	1.89	1.02
1:A:115:ARG:O	6:A:405:EOH:H22	1.61	1.00
5:B:405:GOL:H2	7:B:504:HOH:O	1.64	0.97
1:A:70[B]:PRO:CB	1:A:79:LEU:HD22	1.93	0.97
4:B:404:0OC:H5	7:B:587:HOH:O	1.63	0.96
1:B:280[B]:LEU:HD11	5:B:405:GOL:C3	1.97	0.93
1:A:142[A]:VAL:HG11	4:A:403:0OC:CAF	1.97	0.93
1:B:160:LYS:HD2	5:B:405:GOL:O3	1.70	0.92
1:B:280[B]:LEU:HD12	5:B:405:GOL:C3	2.02	0.85
1:B:208:ALA:HB1	4:B:404:0OC:H3	1.58	0.85
1:A:117:THR:OG1	6:A:405:EOH:H21	1.81	0.79
1:A:142[A]:VAL:CG1	4:A:403:0OC:CAF	2.61	0.78
1:A:75:ALA:HA	1:A:76:GLY:C	2.07	0.76
1:B:208:ALA:CB	4:B:404:0OC:H3	2.18	0.73
1:B:160:LYS:HE3	5:B:405:GOL:C3	2.15	0.73
1:B:142[A]:VAL:HG11	4:B:403:0OC:CAF	2.21	0.70
1:B:196:SER:CB	5:B:405:GOL:HO1	2.04	0.70
5:B:405:GOL:C2	7:B:504:HOH:O	2.29	0.70
1:B:160:LYS:CD	5:B:405:GOL:O3	2.40	0.69
4:B:404:0OC:CAB	7:B:587:HOH:O	2.28	0.69
1:A:75:ALA:HA	1:A:76:GLY:O	1.93	0.68
1:A:263:ASN:CG	1:A:264:GLY:H	1.98	0.68
7:A:613:HOH:O	6:B:407:EOH:H23	1.93	0.68
1:A:142[A]:VAL:HG11	4:A:403:0OC:CAE	2.23	0.67
7:A:613:HOH:O	6:B:407:EOH:C2	2.42	0.67
1:A:69:ASN:HD22	1:A:72:GLN:N	1.95	0.63
1:B:278:ARG:HH21	1:B:278:ARG:HG2	1.64	0.63
1:B:278:ARG:NH2	1:B:278:ARG:HG2	2.14	0.62
1:B:196:SER:OG	5:B:405:GOL:O1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:ASP:HB3	1:B:261:PRO:HD3	1.81	0.61
1:B:212:ALA:HB2	4:B:404:OOC:H8	1.84	0.60
1:B:260:MET:SD	1:B:261:PRO:HD2	2.42	0.60
1:B:160:LYS:CE	5:B:405:GOL:H31	2.20	0.60
1:A:69:ASN:HD22	1:A:72:GLN:H	1.52	0.57
1:A:41:GLY:O	7:A:678:HOH:O	2.17	0.56
1:A:263:ASN:CG	1:A:264:GLY:N	2.59	0.56
1:A:70[B]:PRO:CB	1:A:79:LEU:CD2	2.69	0.55
1:A:151:ARG:NH2	1:B:151:ARG:HG3	2.22	0.55
1:B:160:LYS:NZ	5:B:405:GOL:H11	2.22	0.54
1:A:151:ARG:NH2	1:B:151:ARG:CG	2.71	0.54
1:A:70[B]:PRO:HG3	1:A:79:LEU:HD21	1.91	0.52
1:B:212:ALA:HB2	4:B:404:OOC:CAE	2.39	0.52
1:B:260:MET:CE	1:B:287:ILE:HG12	2.40	0.52
1:A:79:LEU:O	1:A:79:LEU:HD12	2.09	0.51
1:A:25:ARG:NH1	7:A:614:HOH:O	2.38	0.51
1:B:56[A]:ARG:NH1	7:B:637:HOH:O	2.42	0.51
1:A:69:ASN:ND2	1:A:72:GLN:N	2.59	0.51
1:B:160:LYS:CE	5:B:405:GOL:C3	2.86	0.50
1:B:208:ALA:HB1	4:B:404:OOC:CAA	2.36	0.50
1:B:160:LYS:HZ2	5:B:405:GOL:C1	2.24	0.50
1:B:25:ARG:NH2	1:B:151:ARG:HH22	2.11	0.49
1:A:160:LYS:HE2	1:A:195:MET:O	2.13	0.49
1:A:75:ALA:CA	1:A:76:GLY:C	2.80	0.49
1:B:263:ASN:N	1:B:263:ASN:OD1	2.45	0.48
5:B:405:GOL:C1	7:B:691:HOH:O	2.62	0.47
1:A:84:ARG:O	1:A:86:PRO:HD3	2.14	0.47
1:B:160:LYS:NZ	5:B:405:GOL:C1	2.78	0.47
1:B:22:ASP:OD1	1:B:25:ARG:NH1	2.47	0.47
1:A:198:ARG:HD3	1:A:278:ARG:O	2.15	0.46
1:A:69:ASN:ND2	1:A:72:GLN:H	2.14	0.45
1:B:287:ILE:HA	1:B:287:ILE:HD13	1.60	0.45
1:B:160:LYS:HZ2	1:B:196:SER:HB2	1.81	0.45
1:A:83:PRO:HD3	1:A:201:TYR:OH	2.16	0.45
1:A:74:GLY:O	1:A:75:ALA:O	2.35	0.45
1:B:160:LYS:HE2	1:B:160:LYS:HB3	1.79	0.44
1:B:260:MET:HE2	1:B:287:ILE:HG12	2.00	0.44
1:B:25:ARG:NH2	1:B:151:ARG:NH2	2.66	0.44
1:A:157:PHE:CZ	1:A:168:ILE:HD13	2.52	0.44
1:B:208:ALA:O	1:B:211:VAL:HG12	2.17	0.44
7:A:613:HOH:O	6:B:407:EOH:H21	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:405:GOL:H11	7:B:691:HOH:O	2.18	0.42
1:A:71:MET:SD	1:A:138:GLY:HA2	2.59	0.42
1:A:79:LEU:HD12	1:A:79:LEU:C	2.41	0.42
1:B:280[B]:LEU:HD12	5:B:405:GOL:O3	2.19	0.41
1:A:69:ASN:HB3	1:A:70[B]:PRO:C	2.40	0.41
1:A:71:MET:O	1:A:71:MET:HG2	2.19	0.41
1:A:75:ALA:CA	1:A:76:GLY:O	2.66	0.41
1:B:280[B]:LEU:CD1	5:B:405:GOL:O3	2.67	0.41
1:A:120:PRO:HB2	1:A:124:ALA:HB2	2.04	0.40
1:A:142[A]:VAL:HG11	4:A:403:OOC:CAI	2.47	0.40
2:B:401:ATP:O3G	5:B:405:GOL:H12	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	288/301 (96%)	273 (95%)	9 (3%)	6 (2%)	9	1
1	B	272/301 (90%)	267 (98%)	5 (2%)	0	100	100
All	All	560/602 (93%)	540 (96%)	14 (2%)	6 (1%)	21	5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ALA
1	A	76	GLY
1	A	87	ASP
1	A	69	ASN
1	A	70[A]	PRO
1	A	70[B]	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	217/223 (97%)	213 (98%)	4 (2%)	66	54
1	B	207/223 (93%)	201 (97%)	6 (3%)	50	34
All	All	424/446 (95%)	414 (98%)	10 (2%)	57	41

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	87	ASP
1	A	151	ARG
1	A	263	ASN
1	B	28	ARG
1	B	55	LYS
1	B	87	ASP
1	B	151	ARG
1	B	196	SER
1	B	263	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	148	GLN
1	A	222	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	ATP	A	401	3	24,33,33	1.05	1 (4%)	31,52,52	2.32	6 (19%)
4	0OC	A	403	-	9,11,11	3.16	5 (55%)	11,16,16	5.16	6 (54%)
5	GOL	A	404	-	5,5,5	0.94	0	5,5,5	1.01	0
6	EOH	A	405	-	2,2,2	0.32	0	1,1,1	0.75	0
6	EOH	A	406	-	2,2,2	0.54	0	1,1,1	0.55	0
2	ATP	B	401	3	24,33,33	1.47	4 (16%)	31,52,52	2.72	12 (38%)
4	0OC	B	403	-	9,11,11	3.26	4 (44%)	11,16,16	7.14	7 (63%)
4	0OC	B	404	-	9,11,11	3.39	5 (55%)	11,16,16	6.01	7 (63%)
5	GOL	B	405	-	5,5,5	0.41	0	5,5,5	1.17	0
6	EOH	B	406	-	2,2,2	0.65	0	1,1,1	0.18	0
6	EOH	B	407	-	2,2,2	0.44	0	1,1,1	0.45	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	ATP	A	401	3	-	0/18/38/38	0/3/3/3
4	0OC	A	403	-	-	0/6/12/12	0/1/1/1
5	GOL	A	404	-	-	0/4/4/4	0/0/0/0
6	EOH	A	405	-	-	0/0/0/0	0/0/0/0
6	EOH	A	406	-	-	0/0/0/0	0/0/0/0
2	ATP	B	401	3	-	0/18/38/38	0/3/3/3
4	0OC	B	403	-	-	0/6/12/12	0/1/1/1
4	0OC	B	404	-	-	0/6/12/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	405	-	-	0/4/4/4	0/0/0/0
6	EOH	B	406	-	-	0/0/0/0	0/0/0/0
6	EOH	B	407	-	-	0/0/0/0	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	0OC	CAI-SAK	-4.99	1.69	1.76
4	B	404	0OC	CAG-CAI	-4.81	1.34	1.37
4	A	403	0OC	CAG-CAI	-4.73	1.34	1.37
4	B	404	0OC	CAI-SAK	-3.24	1.71	1.76
4	B	403	0OC	CAG-CAI	-2.67	1.35	1.37
4	B	404	0OC	SAK-NAJ	-2.62	1.53	1.62
4	A	403	0OC	CAG-SAH	-2.32	1.68	1.70
2	B	401	ATP	C5'-C4'	2.14	1.58	1.51
2	B	401	ATP	C8-N7	2.18	1.38	1.34
2	B	401	ATP	C2-N1	2.45	1.38	1.33
4	A	403	0OC	OAD-SAK	2.92	1.47	1.43
2	A	401	ATP	C5-C4	3.16	1.47	1.40
4	B	403	0OC	SAK-NAJ	3.43	1.75	1.62
2	B	401	ATP	C5-C4	4.09	1.49	1.40
4	B	403	0OC	OAC-SAK	4.45	1.49	1.43
4	A	403	0OC	OAC-SAK	4.85	1.49	1.43
4	B	404	0OC	OAD-SAK	5.34	1.50	1.43
4	B	404	0OC	OAC-SAK	5.66	1.50	1.43
4	B	403	0OC	OAD-SAK	7.43	1.53	1.43

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	0OC	CAI-CAG-SAH	-18.23	100.53	112.29
4	B	404	0OC	CAI-CAG-SAH	-11.87	104.63	112.29
4	A	403	0OC	CAI-CAG-SAH	-11.27	105.02	112.29
4	A	403	0OC	CAI-SAK-NAJ	-10.82	94.36	106.99
2	B	401	ATP	N3-C2-N1	-10.44	120.90	128.89
2	A	401	ATP	N3-C2-N1	-9.64	121.52	128.89
4	B	403	0OC	CAI-SAK-NAJ	-9.05	96.42	106.99
4	B	403	0OC	OAD-SAK-OAC	-8.01	105.65	119.47
4	B	404	0OC	CAA-NAJ-SAK	-6.49	99.93	116.59
4	B	404	0OC	CAB-NAJ-SAK	-6.19	100.68	116.59
4	B	404	0OC	OAD-SAK-OAC	-5.79	109.47	119.47
2	B	401	ATP	C1'-N9-C4	-4.61	119.99	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	0OC	CAB-NAJ-CAA	-3.14	107.65	114.74
2	B	401	ATP	C2'-C1'-N9	-3.10	109.55	114.29
2	A	401	ATP	PB-O3B-PG	-3.07	122.36	132.67
2	B	401	ATP	O2A-PA-O3A	-3.05	91.28	105.09
2	B	401	ATP	PB-O3B-PG	-3.00	122.61	132.67
2	B	401	ATP	O5'-PA-O1A	-2.91	98.31	109.62
4	A	403	0OC	OAD-SAK-OAC	-2.82	114.60	119.47
2	A	401	ATP	O3'-C3'-C4'	-2.41	103.83	111.05
2	B	401	ATP	C4-C5-N7	-2.16	107.49	109.48
2	B	401	ATP	O3A-PA-O5'	-2.12	97.32	102.94
2	A	401	ATP	O3A-PA-O5'	-2.10	97.37	102.94
2	B	401	ATP	O2B-PB-O3B	-2.06	95.73	105.09
4	B	404	0OC	CAE-SAH-CAG	2.01	96.46	92.37
4	A	403	0OC	OAD-SAK-CAI	2.18	110.84	108.00
2	A	401	ATP	N6-C6-N1	2.29	124.12	119.20
2	B	401	ATP	C2-N1-C6	2.33	122.93	118.77
2	B	401	ATP	O2A-PA-O5'	2.68	121.95	108.46
4	A	403	0OC	CAB-NAJ-CAA	3.25	122.08	114.74
4	B	403	0OC	OAD-SAK-CAI	3.36	112.37	108.00
2	B	401	ATP	O2A-PA-O1A	3.41	131.03	112.53
2	A	401	ATP	O2A-PA-O1A	3.87	133.51	112.53
4	A	403	0OC	OAC-SAK-NAJ	4.11	116.11	106.69
4	B	403	0OC	CAE-SAH-CAG	4.37	101.28	92.37
4	B	403	0OC	OAD-SAK-NAJ	4.55	117.11	106.69
4	B	403	0OC	OAC-SAK-NAJ	5.23	118.68	106.69
4	B	404	0OC	CAI-SAK-NAJ	10.87	119.68	106.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	0OC	4	0
6	A	405	EOH	2	0
2	B	401	ATP	1	0
4	B	403	0OC	1	0
4	B	404	0OC	7	0
5	B	405	GOL	26	0
6	B	407	EOH	3	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	286/301 (95%)	-0.10	14 (4%)	33 27	14, 28, 59, 85	10 (3%)
1	B	272/301 (90%)	-0.37	6 (2%)	65 60	16, 25, 53, 86	0
All	All	558/602 (92%)	-0.23	20 (3%)	46 40	14, 26, 59, 86	10 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	76	GLY	6.6
1	A	77	GLY	6.5
1	A	75	ALA	6.1
1	A	71	MET	4.6
1	A	73	PHE	4.2
1	A	74	GLY	4.0
1	A	70[A]	PRO	3.9
1	B	86	PRO	3.6
1	B	2	ALA	3.5
1	A	243	PRO	3.2
1	B	70	PRO	3.2
1	A	72	GLN	3.2
1	A	79	LEU	3.1
1	A	78	ASP	3.0
1	A	289	THR	2.8
1	A	80	ASP	2.7
1	A	87	ASP	2.3
1	B	87	ASP	2.2
1	B	262	LEU	2.1
1	B	200	ARG	2.1

## 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
6	EOH	A	406	3/3	0.84	0.29	21.18	41,41,42,42	0
5	GOL	B	405	6/6	0.86	0.27	6.73	18,39,46,62	6
6	EOH	B	406	3/3	0.90	0.12	4.94	33,33,33,34	0
4	0OC	A	403	11/11	0.94	0.25	2.21	14,23,28,30	11
4	0OC	B	404	11/11	0.86	0.26	1.72	21,33,61,64	11
4	0OC	B	403	11/11	0.94	0.14	1.22	28,42,48,52	0
2	ATP	B	401	31/31	0.95	0.09	0.70	20,24,46,50	0
6	EOH	A	405	3/3	0.94	0.11	0.40	22,22,38,63	0
5	GOL	A	404	6/6	0.97	0.10	0.21	18,23,24,24	0
2	ATP	A	401	31/31	0.98	0.07	-0.89	21,30,44,46	0
6	EOH	B	407	3/3	0.87	0.13	-	39,39,40,45	0
3	MG	A	402	1/1	0.95	0.04	-	43,43,43,43	0
3	MG	B	402	1/1	0.92	0.24	-	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.