



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 12:14 AM GMT

PDB ID : 3Q1K
Title : The Crystal Structure of the D-alanyl-alanine Synthetase A from Salmonella enterica Typhimurium Complexed with ADP
Authors : Zhang, R.; Maltseva, N.; Papazisi, L.; Anderson, W.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2010-12-17
Resolution : 2.20 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

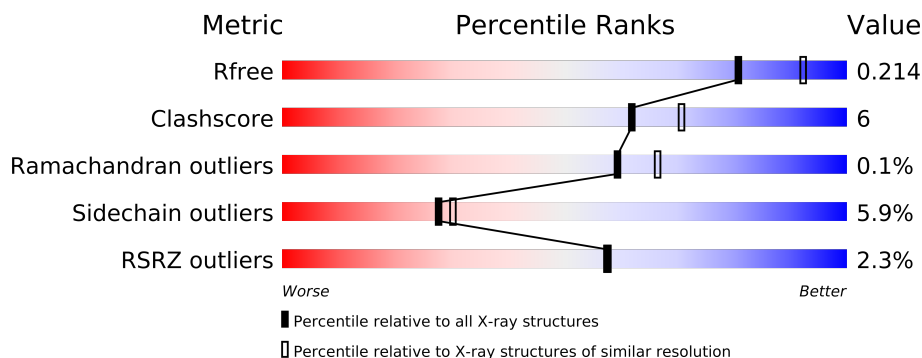
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	367	
1	B	367	
1	C	367	
1	D	367	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	FMT	A	371	-	X
3	FMT	B	373	-	X
4	MG	A	372	-	X
4	MG	B	371	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	A	373	-	X
5	GOL	B	376	-	X
5	GOL	C	371	-	X
5	GOL	C	372	-	X
6	SO4	B	375	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11376 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

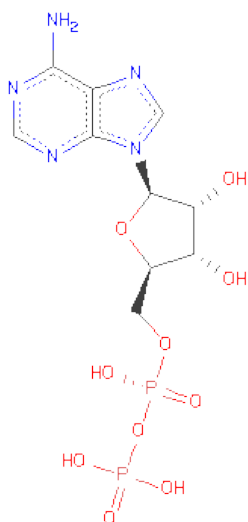
- Molecule 1 is a protein called D-alanine–D-alanine ligase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	Se	0	3	0
			2737	1726	480	522	4	5			
1	B	346	Total	C	N	O	S	Se	0	1	0
			2626	1655	464	498	4	5			
1	C	345	Total	C	N	O	S	Se	0	4	0
			2646	1669	468	499	4	6			
1	D	355	Total	C	N	O	S	Se	0	4	0
			2731	1718	481	524	4	4			

There are 12 discrepancies between the modelled and reference sequences:

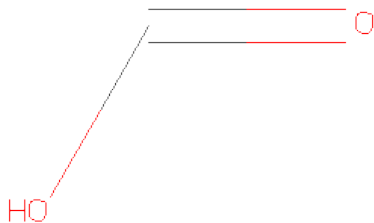
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP P0A1F0
A	-1	ASN	-	EXPRESSION TAG	UNP P0A1F0
A	0	ALA	-	EXPRESSION TAG	UNP P0A1F0
B	-2	SER	-	EXPRESSION TAG	UNP P0A1F0
B	-1	ASN	-	EXPRESSION TAG	UNP P0A1F0
B	0	ALA	-	EXPRESSION TAG	UNP P0A1F0
C	-2	SER	-	EXPRESSION TAG	UNP P0A1F0
C	-1	ASN	-	EXPRESSION TAG	UNP P0A1F0
C	0	ALA	-	EXPRESSION TAG	UNP P0A1F0
D	-2	SER	-	EXPRESSION TAG	UNP P0A1F0
D	-1	ASN	-	EXPRESSION TAG	UNP P0A1F0
D	0	ALA	-	EXPRESSION TAG	UNP P0A1F0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).

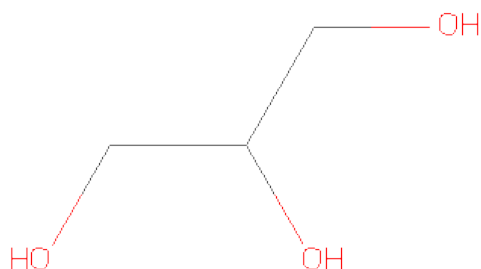


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	B	1	Total	C	O	0	0
			3	1	2		
3	D	1	Total	C	O	0	0
			3	1	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



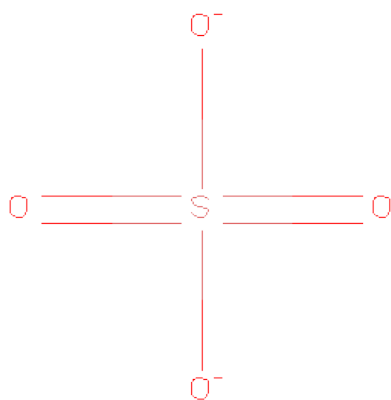
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 6 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

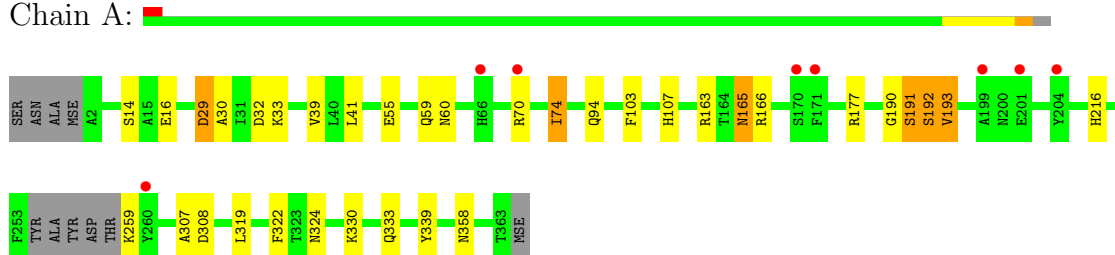
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	144	Total	O	0	0
			144	144		
7	B	113	Total	O	0	0
			113	113		
7	C	109	Total	O	0	0
			109	109		
7	D	115	Total	O	0	0
			115	115		

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.

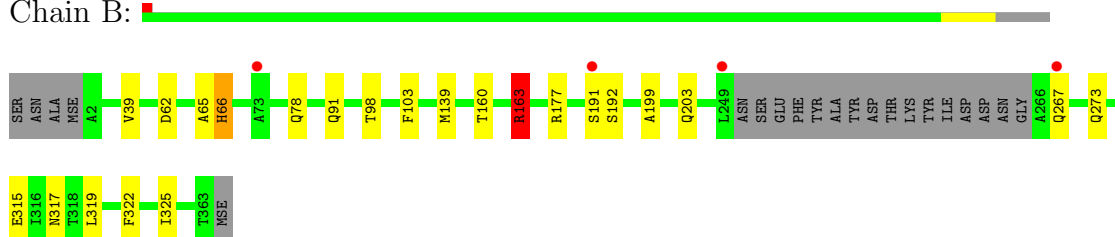
• Molecule 1: D-alanine–D-alanine ligase A

Chain A:



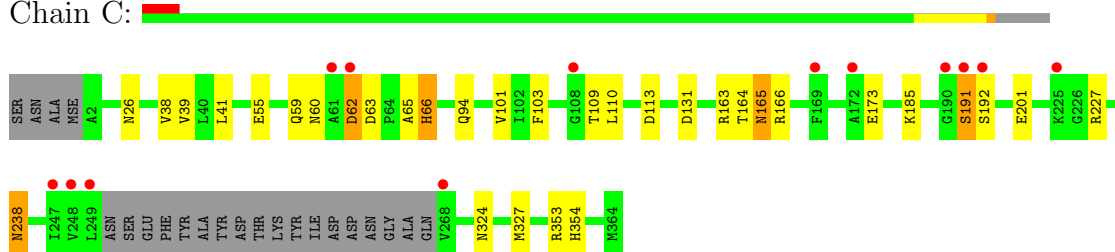
• Molecule 1: D-alanine–D-alanine ligase A

Chain B:



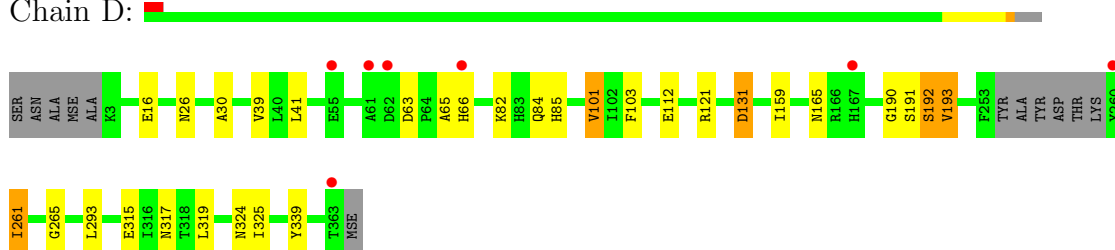
• Molecule 1: D-alanine–D-alanine ligase A

Chain C:



• Molecule 1: D-alanine–D-alanine ligase A

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.15Å 85.81Å 230.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.54 – 2.20 47.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.54-2.20) 99.9 (47.54-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.176 , 0.221 0.169 , 0.214	Depositor DCC
R_{free} test set	4328 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.4	EDS
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 86405 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11376	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, FMT, ADP, SO4

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	0.48	0/2779	0.60	0/3769
1	B	0.48	0/2665	0.62	1/3615 (0.0%)
1	C	0.43	0/2684	0.59	0/3639
1	D	0.48	0/2773	0.60	1/3763 (0.0%)
All	All	0.47	0/10901	0.60	2/14786 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	VAL	CB-CA-C	-5.29	101.34	111.40
1	B	163	ARG	NE-CZ-NH2	5.29	122.94	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2737	0	0	19	0
1	B	2626	0	0	6	0
1	C	2646	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2731	0	0	17	0
2	A	27	0	0	1	0
2	B	27	0	0	2	0
2	C	27	0	0	1	0
2	D	27	0	0	2	0
3	A	3	0	0	0	0
3	B	9	0	0	0	0
3	D	3	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	12	0	0	4	0
6	B	5	0	0	0	0
7	A	144	0	0	3	0
7	B	113	0	0	1	0
7	C	109	0	0	1	0
7	D	115	0	0	3	0
All	All	11376	0	0	62	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

The worst 5 of 62 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:33:LYS:CE	7:A:435:HOH:O	2.14	0.94
1:A:74:ILE:O	1:A:74:ILE:CD1	2.30	0.80
1:C:238:ASN:CG	1:C:238:ASN:O	2.30	0.70
1:C:65:ALA:O	1:C:66:HIS:CB	2.39	0.69
1:C:113:ASP:OD2	1:D:121:ARG:NH1	2.29	0.66

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	356/367 (97%)	347 (98%)	9 (2%)	0	100	100
1	B	343/367 (94%)	329 (96%)	13 (4%)	1 (0%)	50	53
1	C	345/367 (94%)	335 (97%)	10 (3%)	0	100	100
1	D	355/367 (97%)	346 (98%)	9 (2%)	0	100	100
All	All	1399/1468 (95%)	1357 (97%)	41 (3%)	1 (0%)	59	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	HIS

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	294/293 (100%)	276 (94%)	18 (6%)	26	28
1	B	282/293 (96%)	265 (94%)	17 (6%)	27	29
1	C	285/293 (97%)	265 (93%)	20 (7%)	21	22
1	D	294/293 (100%)	280 (95%)	14 (5%)	35	41
All	All	1155/1172 (98%)	1086 (94%)	69 (6%)	28	29

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	317	ASN
1	C	55	GLU
1	D	192	SER
1	B	319	LEU
1	C	38	VAL

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

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	ADP	A	370	4	29,29,29	1.13	3 (10%)	45,45,45	1.72	7 (15%)
3	FMT	A	371	-	2,2,2	0.66	0	1,1,1	0.12	0
5	GOL	A	373	-	5,5,5	0.30	0	5,5,5	0.78	0
2	ADP	B	370	4	29,29,29	1.08	2 (6%)	45,45,45	1.81	7 (15%)
3	FMT	B	372	-	2,2,2	0.59	0	1,1,1	0.12	0
3	FMT	B	373	-	2,2,2	0.66	0	1,1,1	0.04	0
3	FMT	B	374	-	2,2,2	0.63	0	1,1,1	0.22	0
6	SO4	B	375	-	4,4,4	0.16	0	6,6,6	0.19	0
5	GOL	B	376	-	5,5,5	0.35	0	5,5,5	0.41	0
2	ADP	C	370	-	29,29,29	1.13	2 (6%)	45,45,45	1.73	8 (17%)
5	GOL	C	371	-	5,5,5	0.38	0	5,5,5	0.72	0
5	GOL	C	372	-	5,5,5	0.48	0	5,5,5	0.62	0
2	ADP	D	370	4	29,29,29	1.11	2 (6%)	45,45,45	1.77	6 (13%)
3	FMT	D	371	-	2,2,2	0.70	0	1,1,1	0.12	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	ADP	A	370	4	-	0/16/32/32	0/1/3/3
3	FMT	A	371	-	-	0/0/0/0	0/0/0/0
5	GOL	A	373	-	-	0/4/4/4	0/0/0/0
2	ADP	B	370	4	-	0/16/32/32	0/1/3/3
3	FMT	B	372	-	-	0/0/0/0	0/0/0/0
3	FMT	B	373	-	-	0/0/0/0	0/0/0/0
3	FMT	B	374	-	-	0/0/0/0	0/0/0/0
6	SO4	B	375	-	-	0/0/0/0	0/0/0/0
5	GOL	B	376	-	-	0/4/4/4	0/0/0/0
2	ADP	C	370	-	-	0/16/32/32	0/1/3/3
5	GOL	C	371	-	-	0/4/4/4	0/0/0/0
5	GOL	C	372	-	-	0/4/4/4	0/0/0/0
2	ADP	D	370	4	-	0/16/32/32	0/1/3/3
3	FMT	D	371	-	-	0/0/0/0	0/0/0/0

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	370	ADP	C5-C4	3.40	1.48	1.40
2	C	370	ADP	C5-C4	3.33	1.48	1.40
2	A	370	ADP	C5-C4	3.29	1.47	1.40
2	B	370	ADP	C5-C4	2.78	1.46	1.40
2	A	370	ADP	C4-N9	-2.53	1.34	1.37

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	370	ADP	N3-C2-N1	-6.20	123.52	128.71
2	D	370	ADP	N3-C2-N1	-6.12	123.59	128.71
2	B	370	ADP	N3-C4-N9	6.03	136.32	125.43
2	B	370	ADP	N3-C2-N1	-5.81	123.85	128.71
2	D	370	ADP	N3-C4-N9	5.68	135.68	125.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	357/367 (97%)	-0.34	8 (2%) 59 59	24, 41, 88, 121	0
1	B	346/367 (94%)	-0.35	4 (1%) 75 76	22, 40, 73, 110	0
1	C	345/367 (94%)	-0.28	13 (3%) 38 39	26, 44, 87, 128	0
1	D	355/367 (96%)	-0.38	7 (1%) 62 62	25, 40, 79, 119	0
All	All	1403/1468 (95%)	-0.34	32 (2%) 57 58	22, 41, 84, 128	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	LEU	10.0
1	D	260	TYR	6.3
1	B	249	LEU	5.0
1	B	191	SER	3.9
1	C	108	GLY	3.7

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	B	371	1/1	0.38	17.36	85,85,85,85	0
6	SO4	B	375	5/5	0.23	11.50	126,127,129,132	0
5	GOL	B	376	6/6	0.24	5.22	67,72,77,78	0
3	FMT	A	371	3/3	0.20	4.93	35,35,46,47	0
4	MG	A	372	1/1	0.16	3.11	35,35,35,35	0
5	GOL	C	372	6/6	0.17	2.80	43,63,66,71	0
3	FMT	B	373	3/3	0.15	2.74	40,40,53,53	0
5	GOL	A	373	6/6	0.23	2.50	39,65,69,71	0
5	GOL	C	371	6/6	0.13	2.25	69,74,79,80	0
3	FMT	B	374	3/3	0.15	1.97	55,55,60,60	0
3	FMT	D	371	3/3	0.16	1.74	36,36,43,46	0
4	MG	D	372	1/1	0.10	-0.10	36,36,36,36	0
2	ADP	B	370	27/27	0.11	-0.17	34,51,116,120	0
2	ADP	C	370	27/27	0.10	-0.44	43,65,149,158	0
3	FMT	B	372	3/3	0.10	-0.57	48,48,52,57	0
2	ADP	A	370	27/27	0.08	-0.65	36,48,54,58	0
2	ADP	D	370	27/27	0.08	-0.89	37,46,54,61	0

6.5 Other polymers ⓘ

There are no such residues in this entry.