



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 04:34 PM GMT

PDB ID : 4HNT
Title : crystal structure of F403A mutant of S. aureus Pyruvate carboxylase
Authors : Yu, L.P.C.; Tong, L.
Deposited on : 2012-10-21
Resolution : 2.80 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>

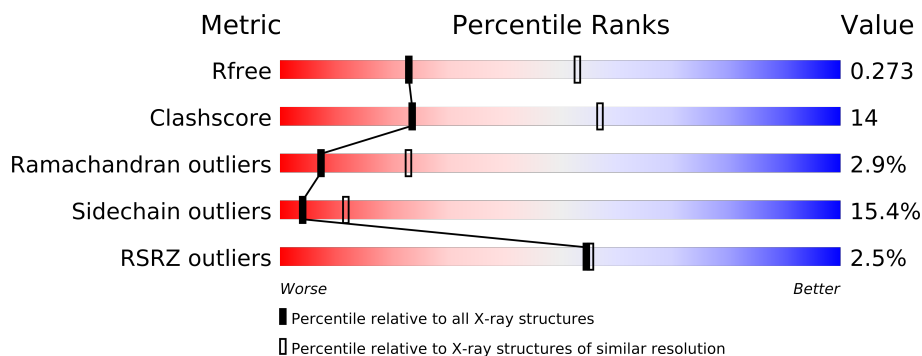
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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 ≥ 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	1173	
1	B	1173	
1	C	1173	
1	D	1173	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32480 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1052	Total	C	N	O	S	0	0	0
			8336	5286	1404	1619	27			
1	B	989	Total	C	N	O	S	0	0	0
			7832	4969	1321	1516	26			
1	C	1059	Total	C	N	O	S	0	0	0
			8373	5307	1412	1626	28			
1	D	989	Total	C	N	O	S	0	0	0
			7832	4969	1321	1516	26			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP Q99UY8
A	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	13	SER	-	EXPRESSION TAG	UNP Q99UY8
A	14	SER	-	EXPRESSION TAG	UNP Q99UY8
A	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	21	SER	-	EXPRESSION TAG	UNP Q99UY8
A	22	SER	-	EXPRESSION TAG	UNP Q99UY8
A	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
A	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
A	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
A	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
A	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
A	29	SER	-	EXPRESSION TAG	UNP Q99UY8
A	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
A	31	MET	-	EXPRESSION TAG	UNP Q99UY8

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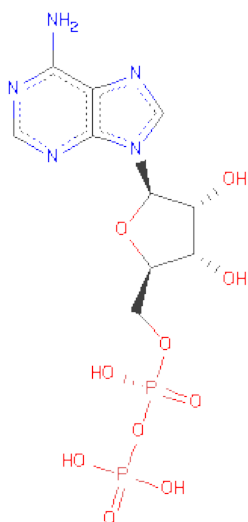
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
A	33	SER	-	EXPRESSION TAG	UNP Q99UY8
B	11	MET	-	EXPRESSION TAG	UNP Q99UY8
B	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	13	SER	-	EXPRESSION TAG	UNP Q99UY8
B	14	SER	-	EXPRESSION TAG	UNP Q99UY8
B	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	21	SER	-	EXPRESSION TAG	UNP Q99UY8
B	22	SER	-	EXPRESSION TAG	UNP Q99UY8
B	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
B	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
B	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
B	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
B	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
B	29	SER	-	EXPRESSION TAG	UNP Q99UY8
B	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
B	31	MET	-	EXPRESSION TAG	UNP Q99UY8
B	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
B	33	SER	-	EXPRESSION TAG	UNP Q99UY8
C	11	MET	-	EXPRESSION TAG	UNP Q99UY8
C	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	13	SER	-	EXPRESSION TAG	UNP Q99UY8
C	14	SER	-	EXPRESSION TAG	UNP Q99UY8
C	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	21	SER	-	EXPRESSION TAG	UNP Q99UY8
C	22	SER	-	EXPRESSION TAG	UNP Q99UY8
C	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
C	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
C	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
C	27	ARG	-	EXPRESSION TAG	UNP Q99UY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
C	29	SER	-	EXPRESSION TAG	UNP Q99UY8
C	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
C	31	MET	-	EXPRESSION TAG	UNP Q99UY8
C	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
C	33	SER	-	EXPRESSION TAG	UNP Q99UY8
D	11	MET	-	EXPRESSION TAG	UNP Q99UY8
D	12	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	13	SER	-	EXPRESSION TAG	UNP Q99UY8
D	14	SER	-	EXPRESSION TAG	UNP Q99UY8
D	15	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	16	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	17	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	18	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	19	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	20	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	21	SER	-	EXPRESSION TAG	UNP Q99UY8
D	22	SER	-	EXPRESSION TAG	UNP Q99UY8
D	23	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	24	LEU	-	EXPRESSION TAG	UNP Q99UY8
D	25	VAL	-	EXPRESSION TAG	UNP Q99UY8
D	26	PRO	-	EXPRESSION TAG	UNP Q99UY8
D	27	ARG	-	EXPRESSION TAG	UNP Q99UY8
D	28	GLY	-	EXPRESSION TAG	UNP Q99UY8
D	29	SER	-	EXPRESSION TAG	UNP Q99UY8
D	30	HIS	-	EXPRESSION TAG	UNP Q99UY8
D	31	MET	-	EXPRESSION TAG	UNP Q99UY8
D	32	ALA	-	EXPRESSION TAG	UNP Q99UY8
D	33	SER	-	EXPRESSION TAG	UNP Q99UY8

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

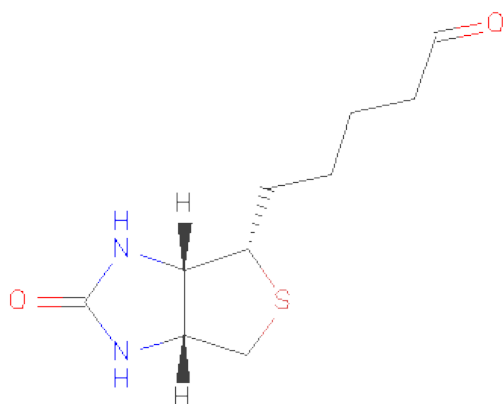


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

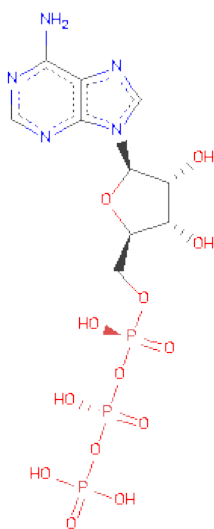
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 5-(HEXAHYDRO-2-OXO-1H-THIENO[3,4-D]IMIDAZOL-6-YL)PENTANAL (three-letter code: BTI) (formula: C₁₀H₁₆N₂O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	B	1	Total	C	N	O	S	0	0
			15	10	2	2	1		
4	D	1	Total	C	N	O	S	0	0
			15	10	2	2	1		

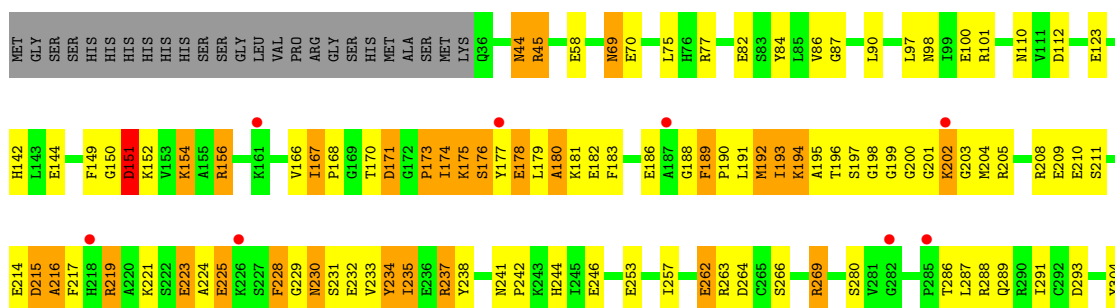
- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

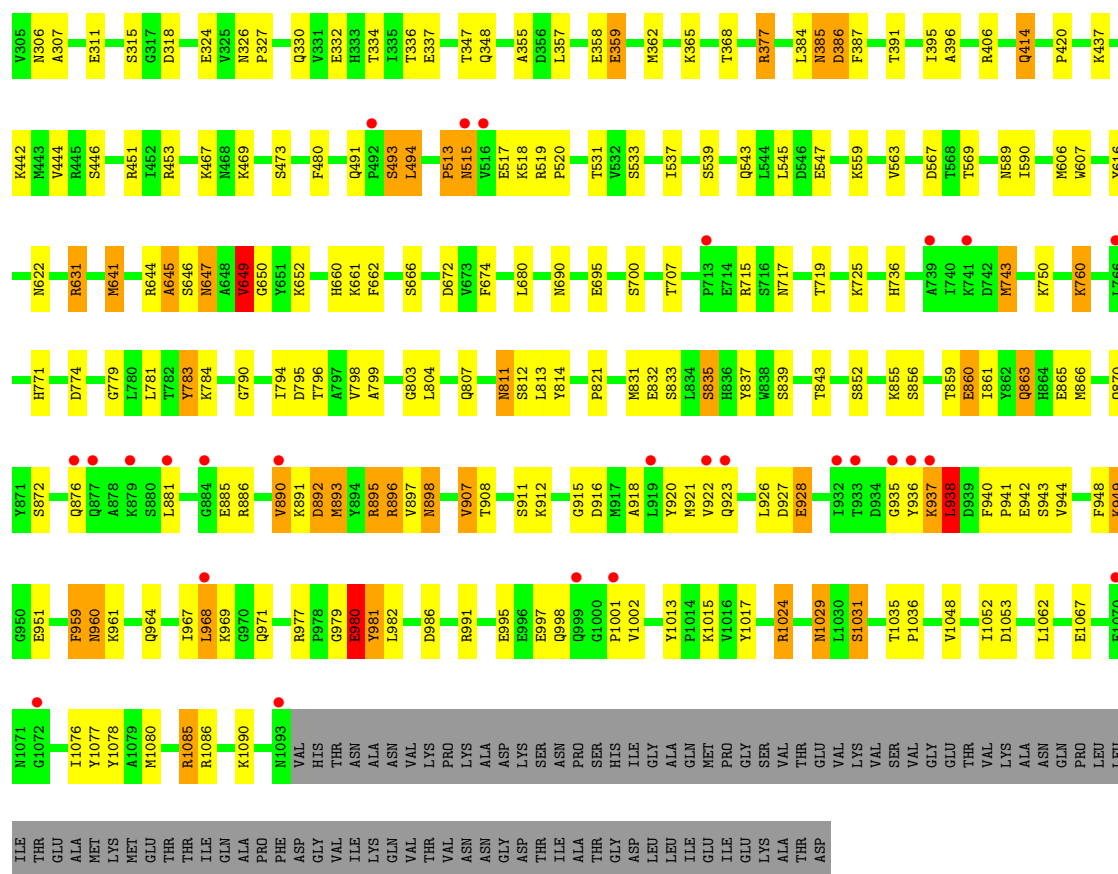


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		



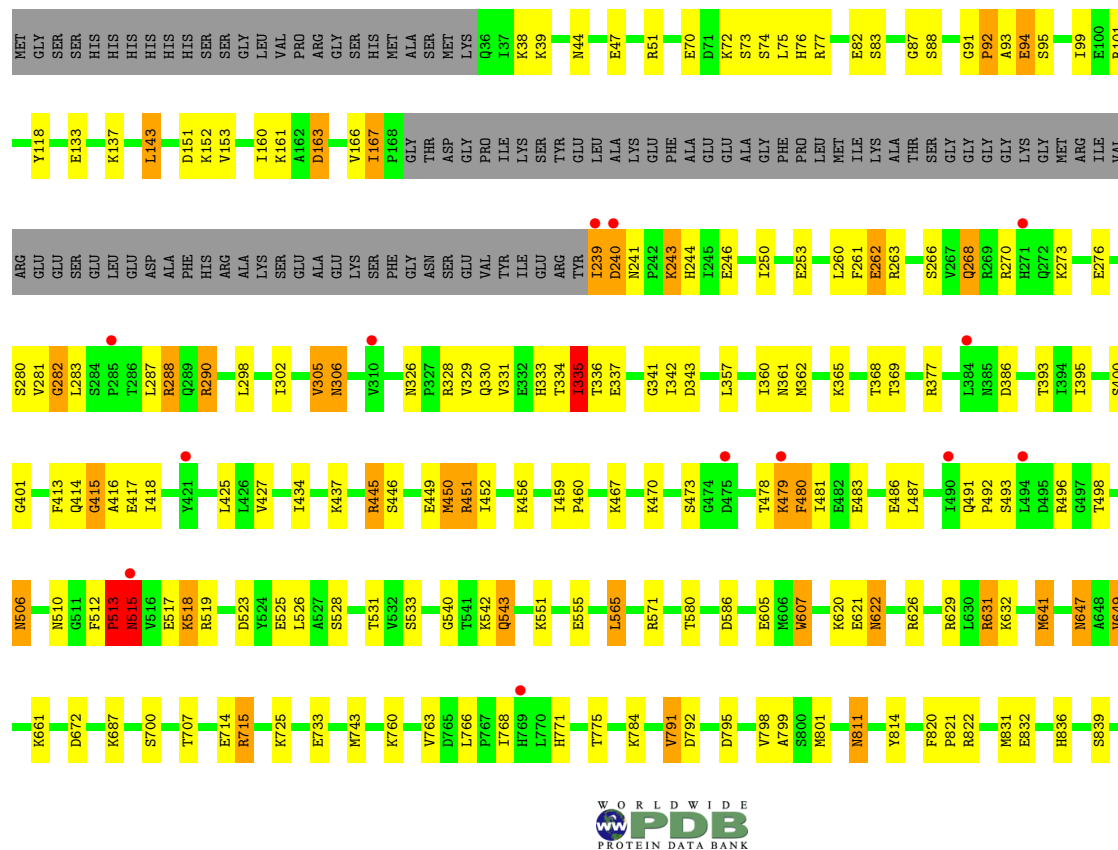
Response	Percentage
Yes	100%
No	0%





• Molecule 1: Pyruvate carboxylase

Chain D:



THR	SER	Y845
GLY	HIS	
ASP	ILE	S852
LEU	GLY	D853
LEU	ALA	I854
ILE	GLN	K855
GLU	MET	S856
ILE	PRO	
ILE	GLY	D986
LYS	SER	Q863
ALA	VAL	H864
THR	THR	E865
ASP	GLU	M866
	VAL	
	LYS	G869
	VAL	K870
	VAL	Y871
	VAL	L874
	GLY	S875
	GLU	
	THR	A879
	VAL	
	LYS	G884
	ALA	F885
	ASN	R886
	GLN	F887
	PRO	D889
	LEU	
	LEU	M893
	ILE	
	THR	R896
	GLU	
	ALA	Y907
	MET	T908
	LYS	P909
	MET	S910
	GLU	S911
	THR	
	THR	M917
	ILE	A918
	GLN	L919
	ALA	Y920
	PRO	M921
	PHE	
	ASP	N1093
	GLY	VAL
	VAL	HIS
	ILE	THR
	LYS	ASN
	GLN	ALA
	VAL	ASN
	THR	VAL
	THR	LYS
	VAL	PRO
	ASN	LYS
	ASN	ALA
	GLY	ASP
	ASP	LYS
	THR	ILE
	ILE	ASN
	ALA	PRO
		L963

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.23Å 256.28Å 126.69Å 90.00° 109.86° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 29.79 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.0 (30.00-2.80) 91.0 (29.79-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.209 , 0.279 0.209 , 0.273	Depositor DCC
R_{free} test set	6458 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	72.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.0	EDS
Estimated twinning fraction	0.030 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 128487 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32480	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: MN, BTI, ATP, ADP

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	0.68	1/8497 (0.0%)	0.73	1/11490 (0.0%)
1	B	0.63	4/7983 (0.1%)	0.66	3/10801 (0.0%)
1	C	0.65	4/8535 (0.0%)	0.68	4/11539 (0.0%)
1	D	0.66	5/7983 (0.1%)	0.70	2/10801 (0.0%)
All	All	0.65	14/32998 (0.0%)	0.69	10/44631 (0.0%)

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	6
1	B	0	3
1	C	0	7
1	D	0	2
All	All	0	18

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	513	PRO	CA-C	14.00	1.80	1.52
1	B	936	TYR	C-N	11.65	1.60	1.34
1	C	513	PRO	C-N	10.85	1.58	1.34
1	C	515	ASN	N-CA	10.62	1.67	1.46
1	B	961	LYS	C-O	10.00	1.42	1.23

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	513	PRO	C-N-CA	8.07	141.87	121.70
1	D	513	PRO	CA-C-N	7.87	134.51	117.20
1	C	513	PRO	CA-C-N	7.83	134.42	117.20
1	B	763	VAL	CA-C-N	7.35	133.38	117.20
1	C	513	PRO	N-CA-CB	-6.11	95.88	102.60

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	GLY	Peptide
1	A	196	THR	Peptide
1	A	271	HIS	Peptide
1	A	415	GLY	Peptide
1	A	490	ILE	Peptide

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	8336	0	488	158	0
1	B	7832	0	7	80	0
1	C	8373	0	526	161	0
1	D	7832	0	7	90	0
2	A	27	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	15	0	16	3	0
4	B	15	0	16	3	0
4	D	15	0	16	2	0
5	C	31	0	12	10	0
All	All	32480	0	1100	482	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 14.

The worst 5 of 482 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:515:ASN:N	1:C:515:ASN:CA	1.67	1.56
1:C:513:PRO:CA	1:C:513:PRO:C	1.80	1.47
1:A:213:LEU:O	1:A:215:ASP:N	1.87	1.07
1:D:607:TRP:CE3	1:D:641:MET:CE	2.40	1.05
1:A:189:PHE:HB3	1:A:190:PRO:HD3	1.41	1.03

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	1048/1173 (89%)	916 (87%)	102 (10%)	30 (3%)	7	23
1	B	985/1173 (84%)	876 (89%)	85 (9%)	24 (2%)	9	29
1	C	1057/1173 (90%)	923 (87%)	96 (9%)	38 (4%)	5	17
1	D	985/1173 (84%)	864 (88%)	94 (10%)	27 (3%)	8	25
All	All	4075/4692 (87%)	3579 (88%)	377 (9%)	119 (3%)	7	23

5 of 119 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	ALA
1	A	211	SER
1	A	213	LEU
1	A	214	GLU
1	A	217	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	907/1005 (90%)	778 (86%)	129 (14%)	5	14
1	B	855/1005 (85%)	726 (85%)	129 (15%)	4	12
1	C	909/1005 (90%)	751 (83%)	158 (17%)	3	8
1	D	855/1005 (85%)	727 (85%)	128 (15%)	4	12
All	All	3526/4020 (88%)	2982 (85%)	544 (15%)	4	12

5 of 544 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	944	VAL
1	C	269	ARG
1	D	714	GLU
1	B	1057	ARG
1	C	154	LYS

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

Mol	Chain	Res	Type
1	C	230	ASN

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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	1201	-	29,29,29	1.19	3 (10%)	45,45,45	1.93	10 (22%)
4	BTI	A	1203	-	16,16,16	1.60	2 (12%)	21,21,21	1.85	4 (19%)
4	BTI	B	1201	-	16,16,16	1.55	3 (18%)	21,21,21	1.90	5 (23%)
5	ATP	C	1202	-	33,33,33	1.14	5 (15%)	52,52,52	1.74	9 (17%)
4	BTI	D	1201	-	16,16,16	1.56	2 (12%)	21,21,21	1.71	5 (23%)

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	1201	-	-	0/16/32/32	0/1/3/3
4	BTI	A	1203	-	-	0/6/27/27	0/0/2/2
4	BTI	B	1201	-	-	0/6/27/27	0/0/2/2
5	ATP	C	1202	-	-	0/22/38/38	0/1/3/3
4	BTI	D	1201	-	-	0/6/27/27	0/0/2/2

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	BTI	O3-C3	4.61	1.34	1.23
4	B	1201	BTI	O3-C3	4.59	1.34	1.23
4	D	1201	BTI	O3-C3	4.41	1.33	1.23
5	C	1202	ATP	C5-C4	3.25	1.47	1.40
4	A	1203	BTI	C2-S1	-3.15	1.76	1.82

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ADP	N3-C2-N1	-6.39	123.36	128.71
4	A	1203	BTI	C5-C6-S1	5.67	110.56	106.04
4	B	1201	BTI	C2-C4-N2	-5.52	105.42	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1202	ATP	N3-C2-N1	-5.49	124.12	128.71
2	A	1201	ADP	N3-C4-N9	5.35	135.09	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	1052/1173 (89%)	-0.24	24 (2%) 57 58	49, 72, 115, 131	0
1	B	989/1173 (84%)	-0.15	28 (2%) 50 52	55, 87, 129, 178	0
1	C	1059/1173 (90%)	-0.08	35 (3%) 44 45	55, 84, 126, 177	0
1	D	989/1173 (84%)	-0.21	14 (1%) 72 72	47, 78, 130, 167	0
All	All	4089/4692 (87%)	-0.17	101 (2%) 54 55	47, 80, 125, 178	0

The worst 5 of 101 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	GLY	5.3
1	D	490	ILE	5.3
1	A	233	VAL	5.0
1	C	877	GLN	4.4
1	A	231	SER	4.4

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(\AA^2)	Q<0.9
3	MN	D	1202	1/1	0.18	-	74,74,74,74	0
3	MN	B	1202	1/1	0.19	-	82,82,82,82	0
3	MN	C	1201	1/1	0.28	-	76,76,76,76	0
2	ADP	A	1201	27/27	0.17	-	86,91,110,110	0
5	ATP	C	1202	31/31	0.16	-	102,108,115,115	0
3	MN	A	1202	1/1	0.20	-	74,74,74,74	0
4	BTI	D	1201	15/15	0.28	-	105,109,113,116	0
4	BTI	B	1201	15/15	0.34	-	105,109,114,115	0
4	BTI	A	1203	15/15	0.33	-	92,99,104,105	0

6.5 Other polymers ⓘ

There are no such residues in this entry.