



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 13, 2018 – 05:43 PM EDT

PDB ID : 3K5I
Title : Crystal structure of N5-carboxyaminoimidazole synthase from aspergillus clavatus in complex with ADP and 5-aminoimidazole ribonucleotide
Authors : Thoden, J.B.; Holden, H.M.; Paritala, H.; Firestine, S.M.
Deposited on : 2009-10-07
Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

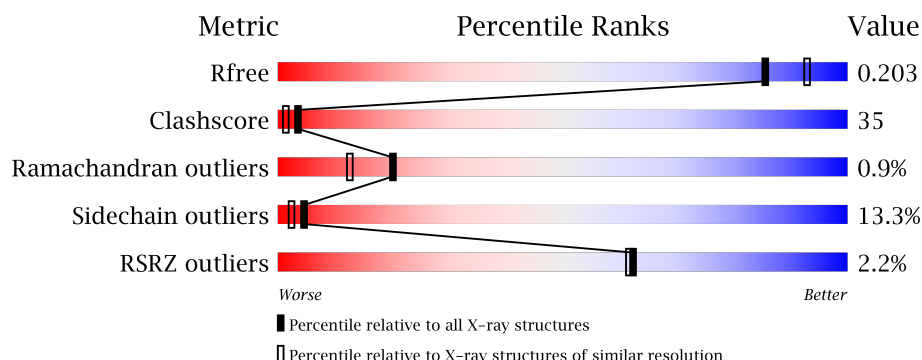
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	403	
1	B	403	
1	C	403	
1	D	403	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NHE	A	385	-	-	-	X
3	NHE	C	384	-	-	-	X
6	AIR	A	402	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13147 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 Phosphoribosyl-aminoimidazole carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	5	0
			2975	1870	523	566	16			
1	B	376	Total	C	N	O	S	0	6	0
			2944	1850	516	563	15			
1	C	382	Total	C	N	O	S	0	6	0
			2995	1881	529	569	16			
1	D	373	Total	C	N	O	S	0	1	0
			2888	1816	506	550	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	HIS	-	EXPRESSION TAG	UNP A1CII2
A	-18	GLY	-	EXPRESSION TAG	UNP A1CII2
A	-17	SER	-	EXPRESSION TAG	UNP A1CII2
A	-16	SER	-	EXPRESSION TAG	UNP A1CII2
A	-15	HIS	-	EXPRESSION TAG	UNP A1CII2
A	-14	HIS	-	EXPRESSION TAG	UNP A1CII2
A	-13	HIS	-	EXPRESSION TAG	UNP A1CII2
A	-12	HIS	-	EXPRESSION TAG	UNP A1CII2
A	-11	HIS	-	EXPRESSION TAG	UNP A1CII2
A	-10	HIS	-	EXPRESSION TAG	UNP A1CII2
A	-9	SER	-	EXPRESSION TAG	UNP A1CII2
A	-8	SER	-	EXPRESSION TAG	UNP A1CII2
A	-7	GLU	-	EXPRESSION TAG	UNP A1CII2
A	-6	ASN	-	EXPRESSION TAG	UNP A1CII2
A	-5	LEU	-	EXPRESSION TAG	UNP A1CII2
A	-4	TYR	-	EXPRESSION TAG	UNP A1CII2
A	-3	PHE	-	EXPRESSION TAG	UNP A1CII2
A	-2	GLN	-	EXPRESSION TAG	UNP A1CII2
A	-1	GLY	-	EXPRESSION TAG	UNP A1CII2
A	0	HIS	-	EXPRESSION TAG	UNP A1CII2
B	-19	HIS	-	EXPRESSION TAG	UNP A1CII2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP A1CII2
B	-17	SER	-	EXPRESSION TAG	UNP A1CII2
B	-16	SER	-	EXPRESSION TAG	UNP A1CII2
B	-15	HIS	-	EXPRESSION TAG	UNP A1CII2
B	-14	HIS	-	EXPRESSION TAG	UNP A1CII2
B	-13	HIS	-	EXPRESSION TAG	UNP A1CII2
B	-12	HIS	-	EXPRESSION TAG	UNP A1CII2
B	-11	HIS	-	EXPRESSION TAG	UNP A1CII2
B	-10	HIS	-	EXPRESSION TAG	UNP A1CII2
B	-9	SER	-	EXPRESSION TAG	UNP A1CII2
B	-8	SER	-	EXPRESSION TAG	UNP A1CII2
B	-7	GLU	-	EXPRESSION TAG	UNP A1CII2
B	-6	ASN	-	EXPRESSION TAG	UNP A1CII2
B	-5	LEU	-	EXPRESSION TAG	UNP A1CII2
B	-4	TYR	-	EXPRESSION TAG	UNP A1CII2
B	-3	PHE	-	EXPRESSION TAG	UNP A1CII2
B	-2	GLN	-	EXPRESSION TAG	UNP A1CII2
B	-1	GLY	-	EXPRESSION TAG	UNP A1CII2
B	0	HIS	-	EXPRESSION TAG	UNP A1CII2
C	-19	HIS	-	EXPRESSION TAG	UNP A1CII2
C	-18	GLY	-	EXPRESSION TAG	UNP A1CII2
C	-17	SER	-	EXPRESSION TAG	UNP A1CII2
C	-16	SER	-	EXPRESSION TAG	UNP A1CII2
C	-15	HIS	-	EXPRESSION TAG	UNP A1CII2
C	-14	HIS	-	EXPRESSION TAG	UNP A1CII2
C	-13	HIS	-	EXPRESSION TAG	UNP A1CII2
C	-12	HIS	-	EXPRESSION TAG	UNP A1CII2
C	-11	HIS	-	EXPRESSION TAG	UNP A1CII2
C	-10	HIS	-	EXPRESSION TAG	UNP A1CII2
C	-9	SER	-	EXPRESSION TAG	UNP A1CII2
C	-8	SER	-	EXPRESSION TAG	UNP A1CII2
C	-7	GLU	-	EXPRESSION TAG	UNP A1CII2
C	-6	ASN	-	EXPRESSION TAG	UNP A1CII2
C	-5	LEU	-	EXPRESSION TAG	UNP A1CII2
C	-4	TYR	-	EXPRESSION TAG	UNP A1CII2
C	-3	PHE	-	EXPRESSION TAG	UNP A1CII2
C	-2	GLN	-	EXPRESSION TAG	UNP A1CII2
C	-1	GLY	-	EXPRESSION TAG	UNP A1CII2
C	0	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-19	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-18	GLY	-	EXPRESSION TAG	UNP A1CII2
D	-17	SER	-	EXPRESSION TAG	UNP A1CII2

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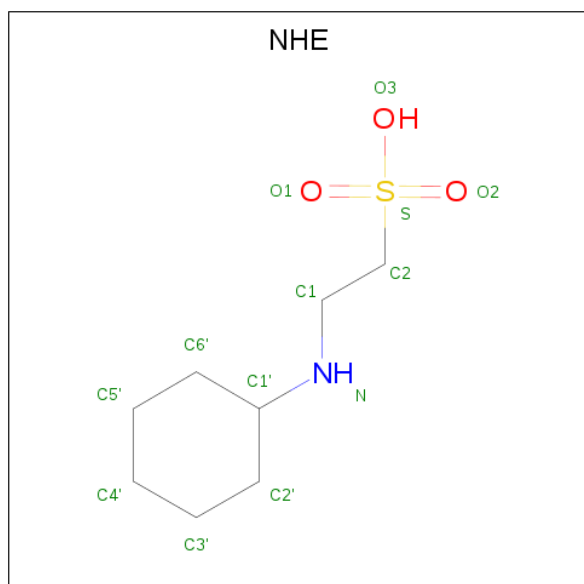
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP A1CII2
D	-15	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-14	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-13	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-12	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-11	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-10	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-9	SER	-	EXPRESSION TAG	UNP A1CII2
D	-8	SER	-	EXPRESSION TAG	UNP A1CII2
D	-7	GLU	-	EXPRESSION TAG	UNP A1CII2
D	-6	ASN	-	EXPRESSION TAG	UNP A1CII2
D	-5	LEU	-	EXPRESSION TAG	UNP A1CII2
D	-4	TYR	-	EXPRESSION TAG	UNP A1CII2
D	-3	PHE	-	EXPRESSION TAG	UNP A1CII2
D	-2	GLN	-	EXPRESSION TAG	UNP A1CII2
D	-1	GLY	-	EXPRESSION TAG	UNP A1CII2
D	0	HIS	-	EXPRESSION TAG	UNP A1CII2

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

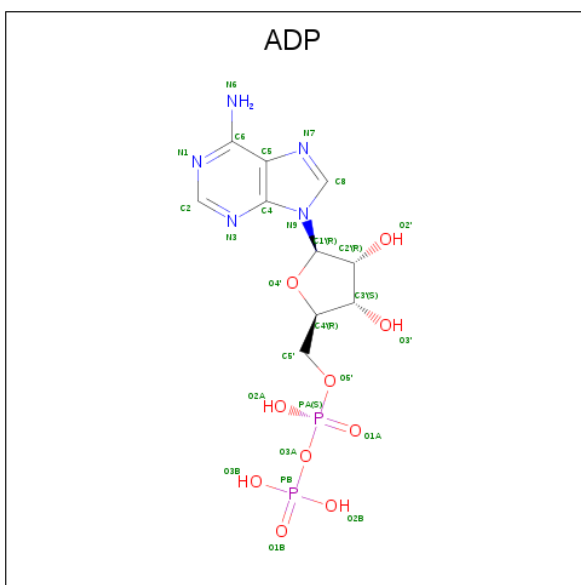
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C₈H₁₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		
3	C	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

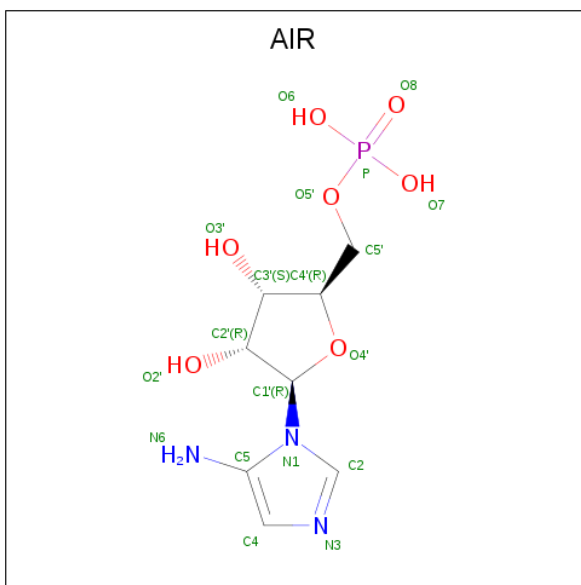
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 5-AMINOIMIDAZOLE RIBONUCLEOTIDE (three-letter code: AIR) (formula: $C_8H_{14}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			19	8	3	7	1		
6	B	1	Total	C	N	O	P	0	0
			19	8	3	7	1		
6	C	1	Total	C	N	O	P	0	0
			19	8	3	7	1		
6	D	1	Total	C	N	O	P	0	0
			19	8	3	7	1		

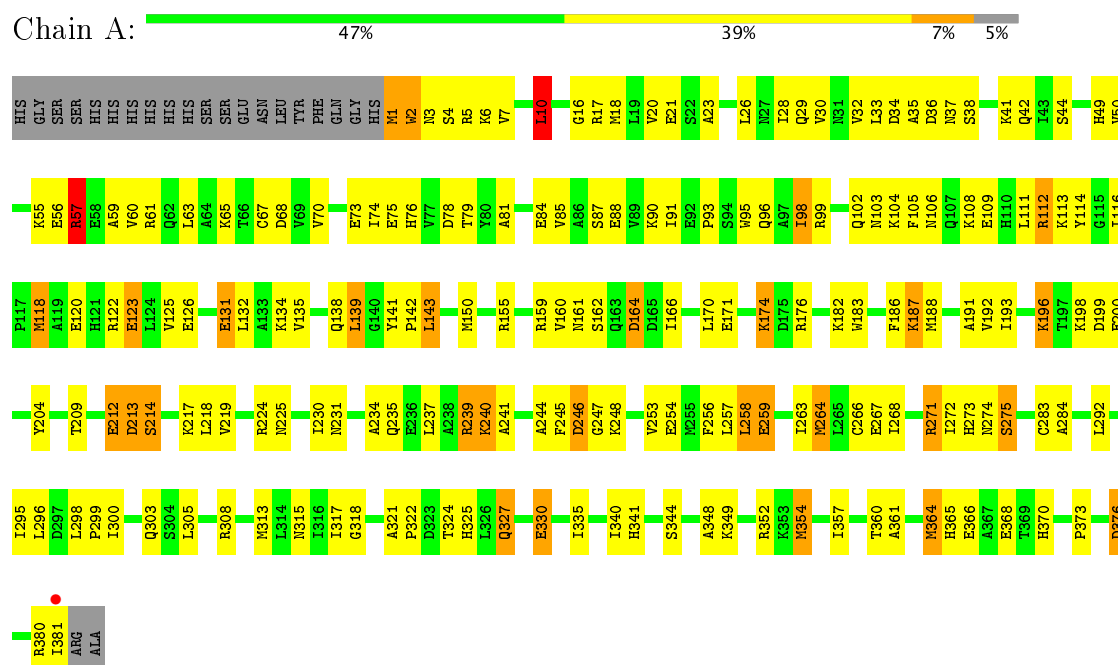
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	322	Total	O	0	0
			322	322		
7	B	266	Total	O	0	0
			266	266		
7	C	299	Total	O	0	0
			299	299		
7	D	243	Total	O	0	0
			243	243		

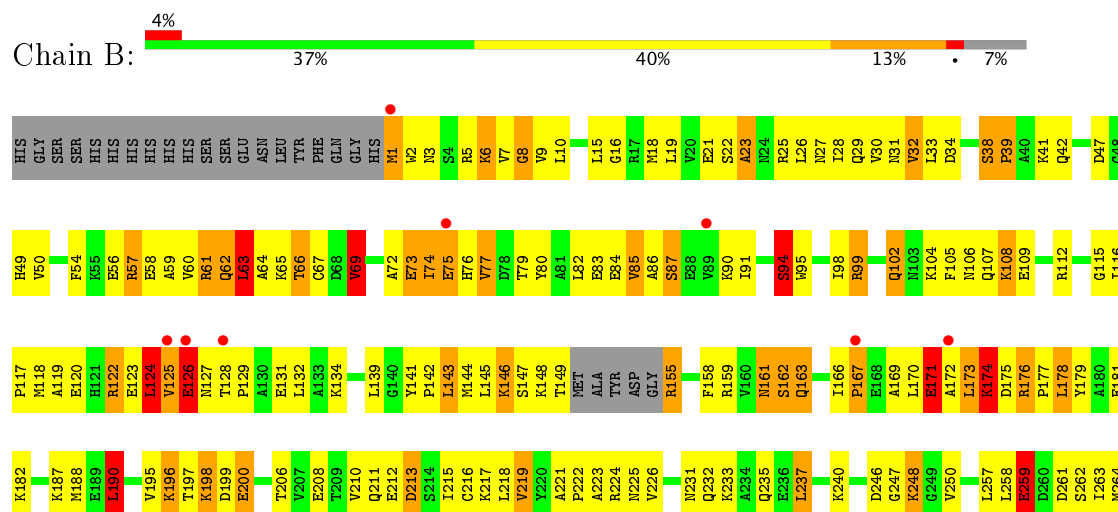
3 Residue-property plots

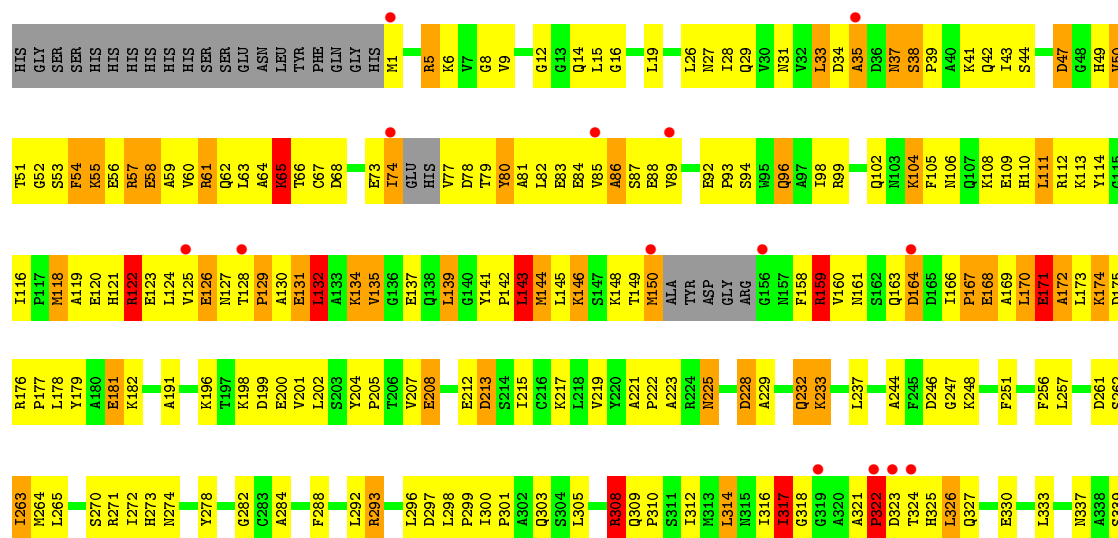
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Phosphoribosyl-aminoimidazole carboxylase



- Molecule 1: Phosphoribosyl-aminoimidazole carboxylase





I340	I341	I342	I343	S344
A347	A348	R349	P350	G351
R352	K353	H354	G355	I357
A361	M364	H365	E366	A367
E368	Q372	P373	I374	I375
D376	V377	V378	D379	R380
ILE	ARG	ALA		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.50 Å 134.20 Å 98.50 Å 90.00° 105.60° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 44.73 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-2.00) 91.9 (44.73-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.00 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.203 , 0.269 0.206 , 0.203	Depositor DCC
R_{free} test set	11666 reflections (10.92%)	DCC
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 136.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13147	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NHE, NA, MG, ADP, AIR

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	0.85	2/3049 (0.1%)	1.67	38/4128 (0.9%)
1	B	0.80	0/3019	1.68	58/4086 (1.4%)
1	C	0.83	0/3072	1.69	47/4157 (1.1%)
1	D	0.81	0/2941	1.68	48/3980 (1.2%)
All	All	0.83	2/12081 (0.0%)	1.68	191/16351 (1.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	ALA	CA-CB	6.50	1.66	1.52
1	A	192	VAL	CB-CG1	5.80	1.65	1.52

The worst 5 of 191 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	ARG	NE-CZ-NH1	-22.98	108.81	120.30
1	A	57	ARG	NE-CZ-NH2	-18.40	111.10	120.30
1	C	308	ARG	NE-CZ-NH2	14.93	127.77	120.30
1	A	57	ARG	NE-CZ-NH1	13.26	126.93	120.30
1	B	352	ARG	NE-CZ-NH1	12.95	126.77	120.30

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	2975	0	2984	162	0
1	B	2944	0	2953	200	0
1	C	2995	0	3008	208	0
1	D	2888	0	2908	278	0
2	A	1	0	0	0	0
3	A	13	0	17	1	0
3	C	13	0	17	5	0
4	A	27	0	10	1	0
4	B	27	0	12	1	0
4	C	27	0	12	2	0
4	D	27	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	19	0	11	0	0
6	B	19	0	11	2	0
6	C	19	0	12	2	0
6	D	19	0	12	2	0
7	A	322	0	0	18	0
7	B	266	0	0	22	0
7	C	299	0	0	18	0
7	D	243	0	0	26	0
All	All	13147	0	11979	841	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 35.

The worst 5 of 841 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:C:324:THR:HG23	1:C:381:ILE:HG21	1.25	1.17
1:D:53:SER:HB3	1:D:56:GLU:HG3	1.20	1.16
1:C:62:GLN:HE22	1:C:65[A]:LYS:HE3	1.09	1.12
1:A:116:ILE:HD11	1:A:240:LYS:HD3	1.28	1.12
1:A:187:LYS:HE2	1:A:259:GLU:HA	1.35	1.08

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	384/403 (95%)	365 (95%)	18 (5%)	1 (0%)	44	40
1	B	378/403 (94%)	346 (92%)	28 (7%)	4 (1%)	17	9
1	C	386/403 (96%)	368 (95%)	16 (4%)	2 (0%)	32	26
1	D	368/403 (91%)	344 (94%)	18 (5%)	6 (2%)	11	5
All	All	1516/1612 (94%)	1423 (94%)	80 (5%)	13 (1%)	20	12

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	ALA
1	B	174	LYS
1	C	322	PRO
1	D	171	GLU
1	D	172	ALA

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	322/336 (96%)	295 (92%)	27 (8%)	13	8
1	B	320/336 (95%)	260 (81%)	60 (19%)	2	1
1	C	324/336 (96%)	286 (88%)	38 (12%)	6	3
1	D	312/336 (93%)	265 (85%)	47 (15%)	3	1
All	All	1278/1344 (95%)	1106 (86%)	172 (14%)	4	2

5 of 172 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	311	SER
1	C	75	GLU
1	D	198	LYS
1	B	326	LEU
1	C	5	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	232	GLN
1	C	327	GLN
1	D	106	ASN
1	C	225	ASN
1	D	110	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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
3	NHE	A	385	-	13,13,13	1.15	1 (7%)	15,17,17	2.67	6 (40%)
4	ADP	A	400	5	25,29,29	1.06	2 (8%)	24,45,45	3.59	10 (41%)
6	AIR	A	402	-	16,20,20	0.82	0	18,30,30	2.18	6 (33%)
4	ADP	B	400	5	25,29,29	0.99	2 (8%)	24,45,45	2.58	8 (33%)
6	AIR	B	402	-	16,20,20	0.62	0	18,30,30	2.08	6 (33%)
3	NHE	C	384	-	13,13,13	1.07	1 (7%)	15,17,17	4.57	6 (40%)
4	ADP	C	400	5	25,29,29	0.95	1 (4%)	24,45,45	2.47	5 (20%)
6	AIR	C	402	-	16,20,20	0.81	0	18,30,30	1.79	6 (33%)
4	ADP	D	400	5	25,29,29	1.00	2 (8%)	24,45,45	2.41	9 (37%)
6	AIR	D	402	-	16,20,20	0.82	0	18,30,30	1.80	4 (22%)

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
3	NHE	A	385	-	-	0/7/15/15	0/1/1/1
4	ADP	A	400	5	-	0/12/32/32	0/3/3/3
6	AIR	A	402	-	1/1/5/5	0/6/26/26	0/2/2/2
4	ADP	B	400	5	-	0/12/32/32	0/3/3/3
6	AIR	B	402	-	-	0/6/26/26	0/2/2/2
3	NHE	C	384	-	-	0/7/15/15	0/1/1/1
4	ADP	C	400	5	-	0/12/32/32	0/3/3/3
6	AIR	C	402	-	-	0/6/26/26	0/2/2/2
4	ADP	D	400	5	-	0/12/32/32	0/3/3/3
6	AIR	D	402	-	-	0/6/26/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	ADP	C6-N6	-3.11	1.21	1.34
4	D	400	ADP	C6-N6	-2.21	1.25	1.34
4	B	400	ADP	C6-N6	-2.17	1.25	1.34
4	C	400	ADP	C2-N1	2.21	1.38	1.33
3	C	384	NHE	C2-S	2.54	1.81	1.77

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	400	ADP	N3-C2-N1	-10.15	120.02	128.86
4	C	400	ADP	N3-C2-N1	-9.48	120.60	128.86
4	B	400	ADP	N3-C2-N1	-8.50	121.45	128.86
3	A	385	NHE	O3-S-O2	-5.86	97.92	111.37
4	B	400	ADP	O2'-C2'-C1'	-5.25	95.20	111.61

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	402	AIR	C4'

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	385	NHE	1	0
4	A	400	ADP	1	0
4	B	400	ADP	1	0
6	B	402	AIR	2	0
3	C	384	NHE	5	0
4	C	400	ADP	2	0
6	C	402	AIR	2	0
4	D	400	ADP	2	0
6	D	402	AIR	2	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	381/403 (94%)	-0.24	1 (0%) 93 93	7, 25, 59, 79	0
1	B	376/403 (93%)	0.03	15 (3%) 39 39	8, 28, 72, 93	0
1	C	382/403 (94%)	-0.24	3 (0%) 86 85	10, 27, 61, 84	0
1	D	373/403 (92%)	0.04	14 (3%) 41 41	10, 29, 71, 90	0
All	All	1512/1612 (93%)	-0.11	33 (2%) 62 61	7, 27, 67, 93	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	5.4
1	D	322	PRO	5.3
1	B	323	ASP	3.8
1	D	324	THR	3.6
1	B	172	ALA	3.6

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NHE	C	384	13/13	0.96	0.13	2.65	17,37,56,77	0
3	NHE	A	385	13/13	0.97	0.12	2.35	15,30,99,99	0
6	AIR	D	402	19/19	0.88	0.17	1.01	14,45,99,99	0
6	AIR	C	402	19/19	0.96	0.10	-0.17	4,13,32,38	0
6	AIR	A	402	19/19	0.95	0.10	-0.26	1,15,23,23	0
6	AIR	B	402	19/19	0.95	0.11	-0.33	2,34,99,99	0
4	ADP	D	400	27/27	0.94	0.10	-0.44	8,29,56,98	0
4	ADP	B	400	27/27	0.94	0.10	-0.58	4,35,63,99	0
4	ADP	A	400	27/27	0.97	0.08	-0.90	6,19,31,99	0
4	ADP	C	400	27/27	0.97	0.09	-1.07	4,21,41,47	0
2	NA	A	384	1/1	0.88	0.13	-	37,37,37,37	0
5	MG	B	401	1/1	0.93	0.05	-	27,27,27,27	0
5	MG	D	401	1/1	0.84	0.10	-	31,31,31,31	0
5	MG	A	401	1/1	0.97	0.04	-	14,14,14,14	0
5	MG	C	401	1/1	0.97	0.03	-	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.