



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 04:38 AM GMT

PDB ID : 3K5I
Title : Crystal structure of N5-carboxyaminoimidazolesynthase 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 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>

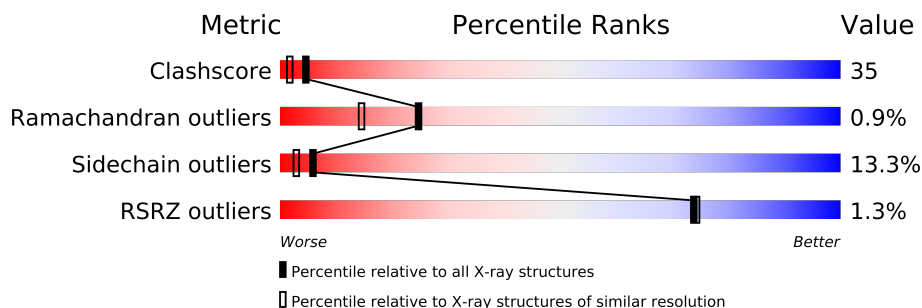
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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. 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	403	
1	B	403	
1	C	403	
1	D	403	

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	NHE	C	384	-	X

2 Entry composition

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

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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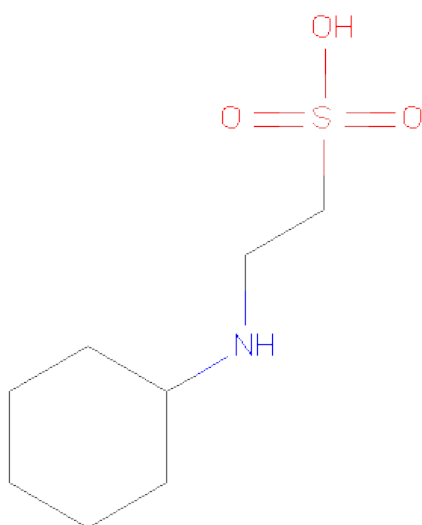
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP A1CII2
D	-15	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-14	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-13	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-12	HIS	-	EXPRESSION TAG	UNP A1CII2
D	-11	HIS	-	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).

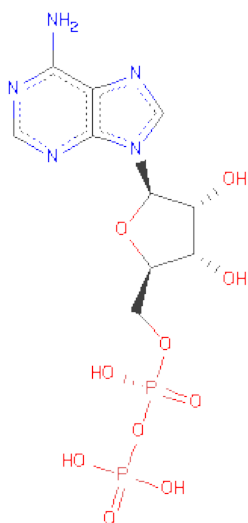
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANESULFONIC 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	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	A	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).

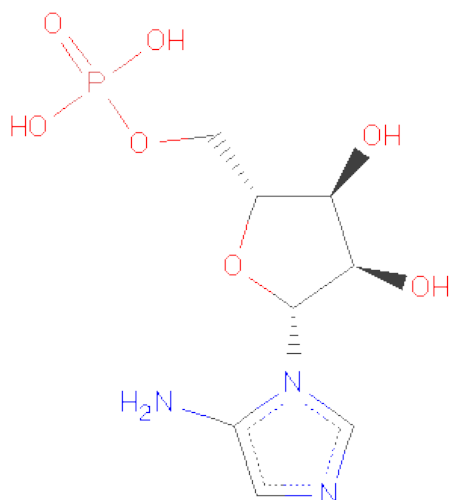
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

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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	B	1	Total	C	N	O	P	0	0
			19	8	3	7	1		
6	A	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		

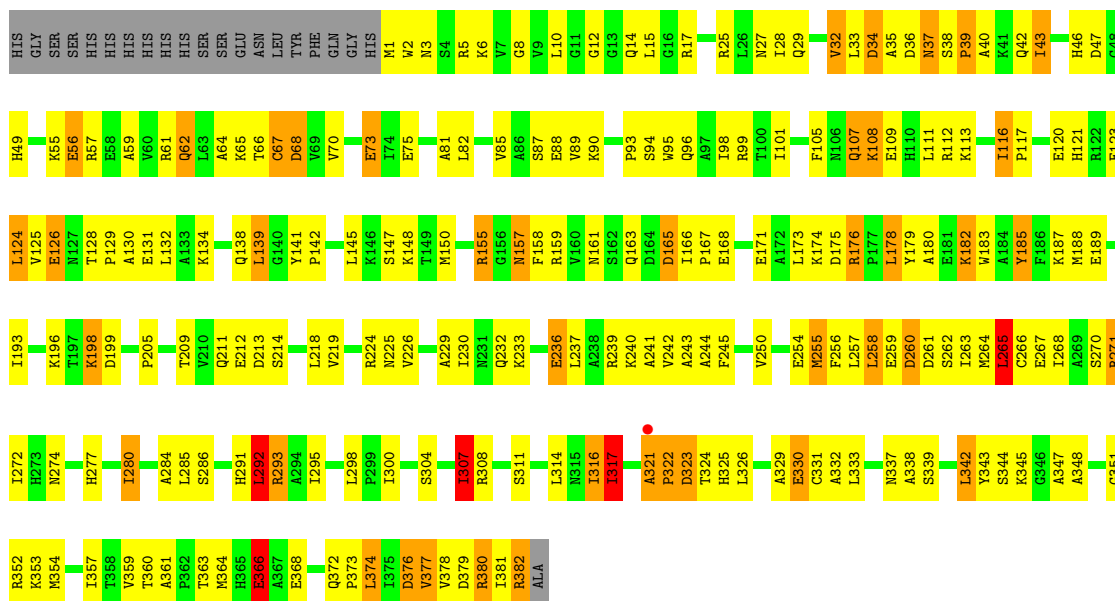
- Molecule 7 is water.

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		



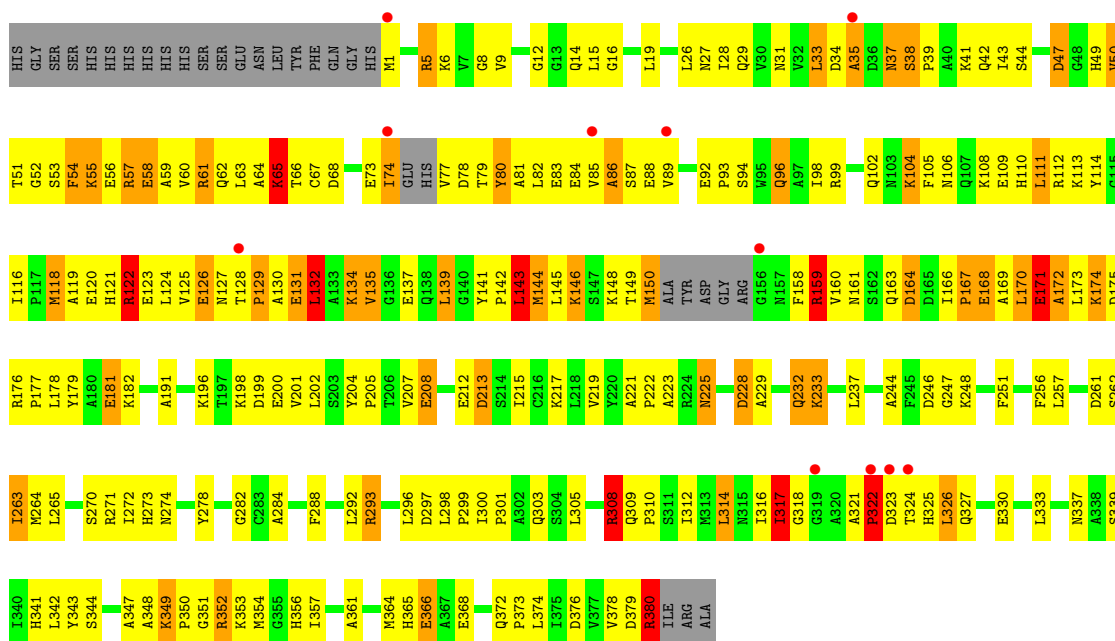
• Molecule 1: Phosphoribosyl-aminoimidazolecarboxylase

Chain C:



• Molecule 1: Phosphoribosyl-aminoimidazolecarboxylase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.50Å 134.20Å 98.50Å 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 2.00Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.203 , 0.269 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 106.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 118600 reflections	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.

5 Model quality

5.1 Standard geometry

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 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	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

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 35.

The worst 5 of 841 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	384/403 (95%)	365 (95%)	18 (5%)	1 (0%)	50	44
1	B	378/403 (94%)	346 (92%)	28 (7%)	4 (1%)	21	10
1	C	386/403 (96%)	368 (95%)	16 (4%)	2 (0%)	38	29
1	D	368/403 (91%)	344 (94%)	18 (5%)	6 (2%)	14	5
All	All	1516/1612 (94%)	1423 (94%)	80 (5%)	13 (1%)	25	14

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 ⓘ

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%)	16	9
1	B	320/336 (95%)	260 (81%)	60 (19%)	2	1
1	C	324/336 (96%)	286 (88%)	38 (12%)	8	4
1	D	312/336 (93%)	265 (85%)	47 (15%)	4	2
All	All	1278/1344 (95%)	1106 (86%)	172 (14%)	6	3

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 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 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	1.29	2 (15%)	17,17,17	2.68	7 (41%)
4	ADP	A	400	5	29,29,29	1.14	2 (6%)	45,45,45	3.39	17 (37%)
6	AIR	A	402	-	20,20,20	1.08	3 (15%)	30,30,30	2.46	12 (40%)
4	ADP	B	400	5	29,29,29	1.03	2 (6%)	45,45,45	2.09	12 (26%)
6	AIR	B	402	-	20,20,20	0.66	0	30,30,30	2.31	11 (36%)
3	NHE	C	384	-	13,13,13	1.14	2 (15%)	17,17,17	4.50	7 (41%)
4	ADP	C	400	5	29,29,29	1.02	2 (6%)	45,45,45	2.27	12 (26%)
6	AIR	C	402	-	20,20,20	1.22	2 (10%)	30,30,30	2.00	10 (33%)
4	ADP	D	400	5	29,29,29	1.01	2 (6%)	45,45,45	1.95	13 (28%)
6	AIR	D	402	-	20,20,20	0.83	0	30,30,30	2.31	8 (26%)

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	-	0/16/32/32	0/1/3/3
6	AIR	A	402	-	1/1/5/5	1/10/26/26	0/2/2/2
4	ADP	B	400	5	-	0/16/32/32	0/1/3/3
6	AIR	B	402	-	-	0/10/26/26	0/2/2/2
3	NHE	C	384	-	-	0/7/15/15	0/1/1/1
4	ADP	C	400	5	-	0/16/32/32	0/1/3/3
6	AIR	C	402	-	-	1/10/26/26	0/2/2/2
4	ADP	D	400	5	-	0/16/32/32	0/1/3/3
6	AIR	D	402	-	-	1/10/26/26	0/2/2/2

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	400	ADP	C6-N6	-4.25	1.21	1.35
6	C	402	AIR	C5-N1	4.09	1.41	1.35
4	D	400	ADP	C6-N6	-3.10	1.25	1.35
3	A	385	NHE	C2-S	3.10	1.82	1.77
4	B	400	ADP	C6-N6	-3.06	1.25	1.35

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	384	NHE	O1-S-C2	15.96	120.48	106.81
4	A	400	ADP	O4'-C1'-N9	10.57	118.27	108.44
4	A	400	ADP	N3-C2-N1	-10.40	120.02	128.71
4	C	400	ADP	N3-C2-N1	-9.70	120.60	128.71
6	D	402	AIR	C4-C5-N1	-9.00	104.73	107.73

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	402	AIR	C4'

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	402	AIR	C2'-C1'-N1-C2
6	A	402	AIR	C2'-C1'-N1-C2
6	D	402	AIR	C2'-C1'-N1-C2

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	381/403 (94%)	-0.23	0 100 100	7, 25, 59, 79	0
1	B	376/403 (93%)	0.03	8 (2%) 60 61	8, 28, 72, 93	0
1	C	382/403 (94%)	-0.23	1 (0%) 91 93	10, 27, 61, 84	0
1	D	373/403 (92%)	0.03	11 (2%) 49 49	10, 29, 71, 90	0
All	All	1512/1612 (93%)	-0.10	20 (1%) 74 74	7, 27, 67, 93	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	322	PRO	4.5
1	D	1	MET	3.9
1	B	172	ALA	3.6
1	B	323	ASP	3.2
1	B	128	THR	3.0

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 ⓘ

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	NHE	C	384	13/13	0.13	2.62	17,37,56,77	0
3	NHE	A	385	13/13	0.11	1.48	15,30,99,99	0
2	NA	A	384	1/1	0.13	0.79	37,37,37,37	0
6	AIR	D	402	19/19	0.16	0.76	14,45,99,99	0
5	MG	D	401	1/1	0.10	0.12	31,31,31,31	0
6	AIR	C	402	19/19	0.10	0.07	4,13,32,38	0
6	AIR	A	402	19/19	0.10	-0.21	1,15,23,23	0
4	ADP	B	400	27/27	0.10	-0.32	4,35,63,99	0
4	ADP	D	400	27/27	0.10	-0.37	8,29,56,98	0
6	AIR	B	402	19/19	0.11	-0.41	2,34,99,99	0
4	ADP	A	400	27/27	0.09	-0.90	6,19,31,99	0
4	ADP	C	400	27/27	0.09	-1.21	4,21,41,47	0
5	MG	B	401	1/1	0.06	-2.54	27,27,27,27	0
5	MG	C	401	1/1	0.03	-3.57	18,18,18,18	0
5	MG	A	401	1/1	0.04	-4.28	14,14,14,14	0

6.5 Other polymers ⓘ

There are no such residues in this entry.