



# wwPDB X-ray Structure Validation Summary Report i

Feb 26, 2014 – 02:41 PM GMT

PDB ID : 3KP1  
Title : Crystal structure of ornithine 4,5 aminomutase (Resting State)  
Authors : Wolthers, K.R.; Levy, C.W.; Scrutton, N.S.; Leys, D.  
Deposited on : 2009-11-14  
Resolution : 2.01 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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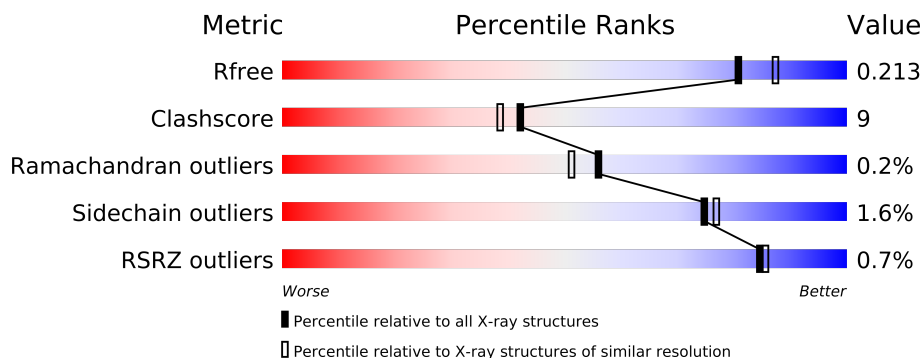
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 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 2.01 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	4888 (2.00-2.00)
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  $\geq 3$ , 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	763	
1	B	763	
1	C	763	
1	D	763	
2	E	121	
2	F	121	
2	G	121	
2	H	121	

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	PLP	D	1802	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 29625 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-ornithine aminomutase E component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5634	3550	978	1072	34			
1	B	726	Total	C	N	O	S	0	0	0
			5655	3568	981	1072	34			
1	D	726	Total	C	N	O	S	0	0	0
			5647	3564	981	1068	34			
1	C	726	Total	C	N	O	S	0	0	0
			5633	3557	978	1064	34			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
A	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
A	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
A	744	SER	-	EXPRESSION TAG	UNP Q8VPJ5
A	745	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
A	746	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
A	747	PRO	-	EXPRESSION TAG	UNP Q8VPJ5
A	748	ASN	-	EXPRESSION TAG	UNP Q8VPJ5
A	749	SER	-	EXPRESSION TAG	UNP Q8VPJ5
A	750	SER	-	EXPRESSION TAG	UNP Q8VPJ5
A	751	SER	-	EXPRESSION TAG	UNP Q8VPJ5
A	752	VAL	-	EXPRESSION TAG	UNP Q8VPJ5
A	753	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
A	754	LYS	-	EXPRESSION TAG	UNP Q8VPJ5
A	755	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
A	756	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
A	757	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
A	758	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
A	759	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
A	760	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
A	761	HIS	-	EXPRESSION TAG	UNP Q8VPJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	762	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
A	763	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
A	764	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
A	765	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
A	766	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
B	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
B	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
B	744	SER	-	EXPRESSION TAG	UNP Q8VPJ5
B	745	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
B	746	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
B	747	PRO	-	EXPRESSION TAG	UNP Q8VPJ5
B	748	ASN	-	EXPRESSION TAG	UNP Q8VPJ5
B	749	SER	-	EXPRESSION TAG	UNP Q8VPJ5
B	750	SER	-	EXPRESSION TAG	UNP Q8VPJ5
B	751	SER	-	EXPRESSION TAG	UNP Q8VPJ5
B	752	VAL	-	EXPRESSION TAG	UNP Q8VPJ5
B	753	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
B	754	LYS	-	EXPRESSION TAG	UNP Q8VPJ5
B	755	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
B	756	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
B	757	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
B	758	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
B	759	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
B	760	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
B	761	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	762	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	763	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	764	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	765	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
B	766	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
D	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
D	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
D	744	SER	-	EXPRESSION TAG	UNP Q8VPJ5
D	745	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
D	746	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
D	747	PRO	-	EXPRESSION TAG	UNP Q8VPJ5
D	748	ASN	-	EXPRESSION TAG	UNP Q8VPJ5
D	749	SER	-	EXPRESSION TAG	UNP Q8VPJ5
D	750	SER	-	EXPRESSION TAG	UNP Q8VPJ5
D	751	SER	-	EXPRESSION TAG	UNP Q8VPJ5

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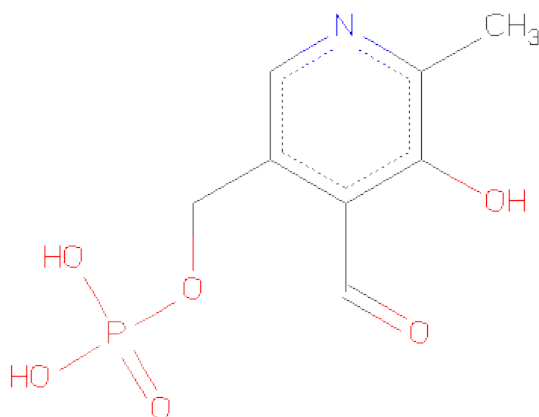
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Chain	Residue	Modelled	Actual	Comment	Reference
D	752	VAL	-	EXPRESSION TAG	UNP Q8VPJ5
D	753	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
D	754	LYS	-	EXPRESSION TAG	UNP Q8VPJ5
D	755	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
D	756	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
D	757	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
D	758	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
D	759	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
D	760	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
D	761	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	762	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	763	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	764	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	765	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
D	766	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	?	-	ILE	SEE REMARK 999	UNP Q8VPJ5
C	?	-	ASP	SEE REMARK 999	UNP Q8VPJ5
C	?	-	GLY	SEE REMARK 999	UNP Q8VPJ5
C	744	SER	-	EXPRESSION TAG	UNP Q8VPJ5
C	745	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
C	746	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
C	747	PRO	-	EXPRESSION TAG	UNP Q8VPJ5
C	748	ASN	-	EXPRESSION TAG	UNP Q8VPJ5
C	749	SER	-	EXPRESSION TAG	UNP Q8VPJ5
C	750	SER	-	EXPRESSION TAG	UNP Q8VPJ5
C	751	SER	-	EXPRESSION TAG	UNP Q8VPJ5
C	752	VAL	-	EXPRESSION TAG	UNP Q8VPJ5
C	753	ASP	-	EXPRESSION TAG	UNP Q8VPJ5
C	754	LYS	-	EXPRESSION TAG	UNP Q8VPJ5
C	755	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
C	756	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
C	757	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
C	758	ALA	-	EXPRESSION TAG	UNP Q8VPJ5
C	759	LEU	-	EXPRESSION TAG	UNP Q8VPJ5
C	760	GLU	-	EXPRESSION TAG	UNP Q8VPJ5
C	761	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	762	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	763	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	764	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	765	HIS	-	EXPRESSION TAG	UNP Q8VPJ5
C	766	HIS	-	EXPRESSION TAG	UNP Q8VPJ5

- Molecule 2 is a protein called D-ornithine aminomutase S component.

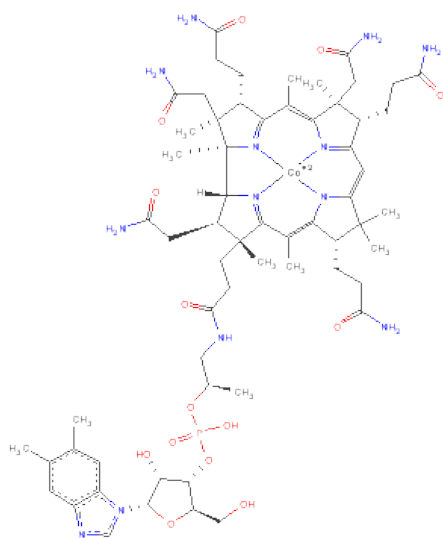
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	F	109	Total	C	N	O	S	0	0	0
			858	539	152	163	4			
2	H	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			
2	G	109	Total	C	N	O	S	0	0	0
			855	538	152	161	4			

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



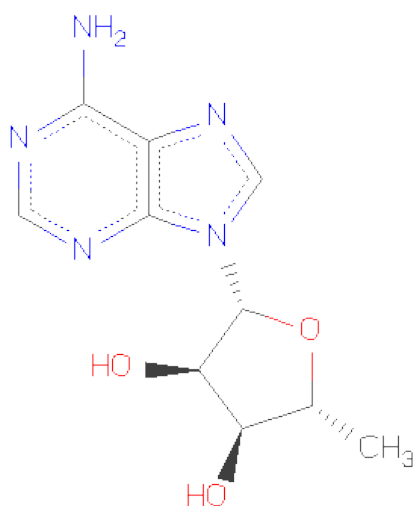
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula:  $C_{62}H_{89}CoN_{13}O_{14}P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
4	B	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
4	D	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0
4	C	1	Total 91	C 62	Co 1	N 13	O 14	P 1	0	0

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $C_{10}H_{13}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			18	10	5	3		
5	B	1	Total	C	N	O	0	0
			18	10	5	3		
5	D	1	Total	C	N	O	0	0
			18	10	5	3		
5	C	1	Total	C	N	O	0	0
			18	10	5	3		

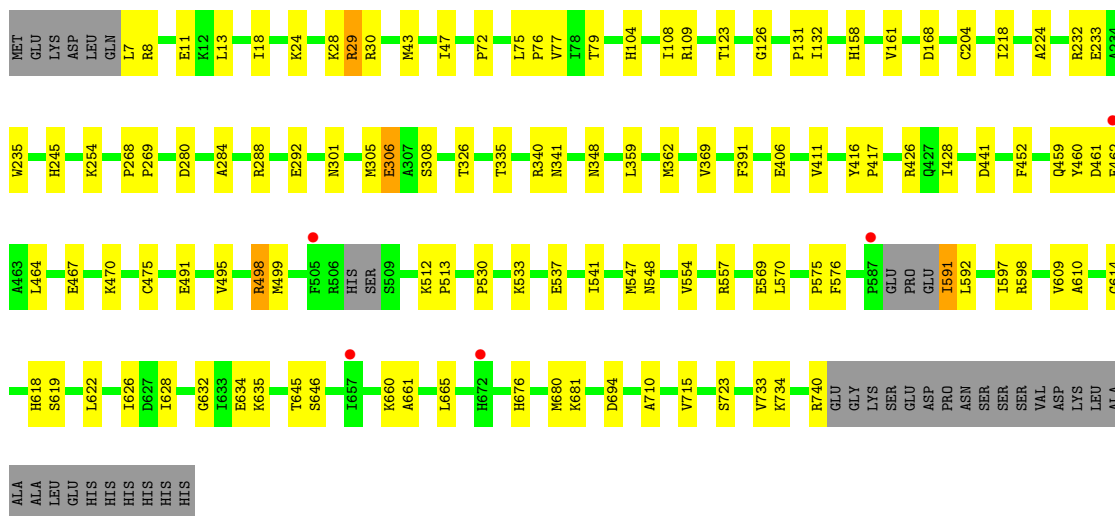
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	618	Total	O	0	0
			618	618		
6	E	108	Total	O	0	0
			108	108		
6	B	722	Total	O	0	0
			722	722		
6	F	139	Total	O	0	0
			139	139		
6	D	731	Total	O	0	0
			731	731		
6	H	111	Total	O	0	0
			111	111		
6	C	633	Total	O	0	0
			633	633		
6	G	75	Total	O	0	0
			75	75		



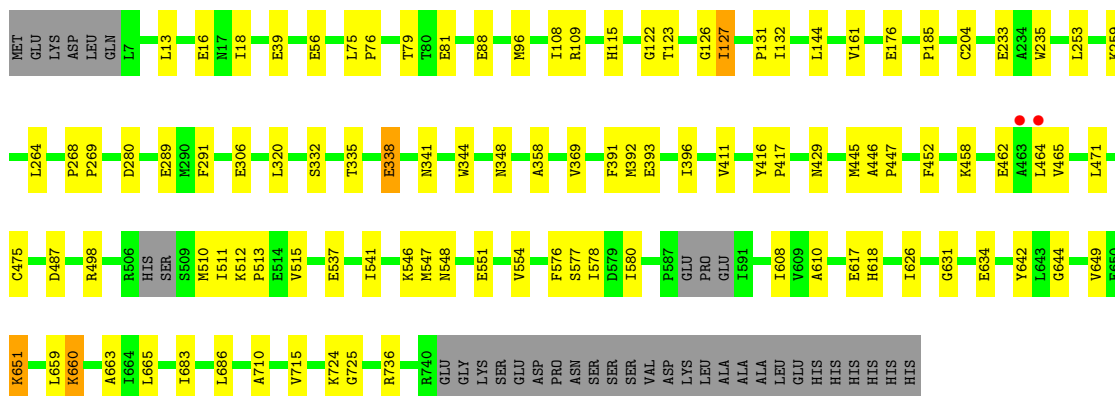


Chain D:



- Molecule 1: D-ornithine aminomutase E component

Chain C:



- Molecule 2: D-ornithine aminomutase S component

Chain E:



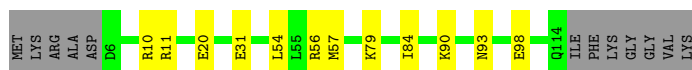
- Molecule 2: D-ornithine aminomutase S component

Chain F:

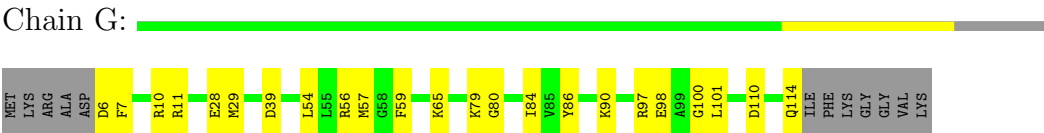


- Molecule 2: D-ornithine aminomutase S component

Chain H:



● Molecule 2: D-ornithine aminomutase S component



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.43Å 234.51Å 124.56Å 90.00° 103.51° 90.00°	Depositor
Resolution (Å)	43.74 – 2.01 49.28 – 2.01	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.74-2.01) 99.3 (49.28-2.01)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, $R_{free}$	0.163 , 0.216 0.162 , 0.213	Depositor DCC
$R_{free}$ test set	12199 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.573	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 40.2	EDS
Estimated twinning fraction	0.027 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 243067 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	29625	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: B12, 5AD, PLP

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	0.36	0/5739	0.52	0/7771
1	B	0.40	0/5760	0.55	1/7795 (0.0%)
1	C	0.33	0/5738	0.51	0/7768
1	D	0.38	0/5752	0.54	1/7785 (0.0%)
2	E	0.36	0/867	0.46	0/1163
2	F	0.40	0/870	0.51	0/1167
2	G	0.30	0/867	0.43	0/1163
2	H	0.37	0/867	0.47	0/1163
All	All	0.37	0/26460	0.52	2/35775 (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	498	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	153	ARG	NE-CZ-NH2	-5.05	117.78	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	5634	0	5563	110	0
1	B	5655	0	5622	91	0
1	C	5633	0	5596	84	0
1	D	5647	0	5616	84	0
2	E	855	0	863	13	0
2	F	858	0	865	20	0
2	G	855	0	863	24	0
2	H	855	0	863	18	0
3	A	15	0	7	0	0
3	B	15	0	7	0	0
3	C	15	0	7	0	0
3	D	15	0	7	0	0
4	A	91	0	87	23	0
4	B	91	0	87	10	0
4	C	91	0	87	15	0
4	D	91	0	87	23	0
5	A	18	0	10	1	0
5	B	18	0	10	0	0
5	C	18	0	10	1	0
5	D	18	0	10	0	0
6	A	618	0	0	17	0
6	B	722	0	0	17	0
6	C	633	0	0	14	0
6	D	731	0	0	15	1
6	E	108	0	0	6	0
6	F	139	0	0	10	1
6	G	75	0	0	2	0
6	H	111	0	0	8	0
All	All	29625	0	26267	473	1

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 9.

The worst 5 of 473 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:93:ARG:HA	1:A:96:MET:HE2	1.18	1.12
2:H:54:LEU:HD23	2:H:57:MET:HE1	1.29	1.09
1:D:43:MET:SD	6:D:3158:HOH:O	2.21	0.98
1:D:428:ILE:HB	6:D:1191:HOH:O	1.65	0.96
1:B:393:GLU:HG2	2:F:29:MET:HE2	1.48	0.96

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:3045:HOH:O	6:D:834:HOH:O[1.656]	1.99	0.21

## 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	720/763 (94%)	703 (98%)	16 (2%)	1 (0%)	59	55
1	B	720/763 (94%)	704 (98%)	14 (2%)	2 (0%)	50	44
1	C	720/763 (94%)	705 (98%)	14 (2%)	1 (0%)	59	55
1	D	720/763 (94%)	705 (98%)	14 (2%)	1 (0%)	59	55
2	E	107/121 (88%)	106 (99%)	1 (1%)	0	100	100
2	F	107/121 (88%)	107 (100%)	0	0	100	100
2	G	107/121 (88%)	105 (98%)	2 (2%)	0	100	100
2	H	107/121 (88%)	107 (100%)	0	0	100	100
All	All	3308/3536 (94%)	3242 (98%)	61 (2%)	5 (0%)	56	51

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	738	GLU
1	B	411	VAL
1	C	411	VAL
1	D	411	VAL
1	A	411	VAL

### 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	596/644 (92%)	586 (98%)	10 (2%)	73	75
1	B	602/644 (94%)	597 (99%)	5 (1%)	89	92
1	C	597/644 (93%)	586 (98%)	11 (2%)	71	73
1	D	600/644 (93%)	588 (98%)	12 (2%)	68	69
2	E	89/100 (89%)	86 (97%)	3 (3%)	49	45
2	F	90/100 (90%)	87 (97%)	3 (3%)	50	46
2	G	89/100 (89%)	88 (99%)	1 (1%)	84	86
2	H	89/100 (89%)	89 (100%)	0	100	100
All	All	2752/2976 (92%)	2707 (98%)	45 (2%)	75	77

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	97	ARG
1	D	341	ASN
1	C	651	LYS
1	D	168	ASP
1	D	391	PHE

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

Mol	Chain	Res	Type
2	G	9	GLN

### 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 ⓘ

12 ligands are modelled in this entry.

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	$\# Z  > 2$
4	B12	A	1801	1,5	101,101,101	8.71	12 (11%)	152,166,166	2.17	25 (16%)
3	PLP	A	1802	1	14,15,16	1.24	1 (7%)	20,22,23	1.04	0
5	5AD	A	767	4	20,20,20	2.29	5 (25%)	30,30,30	4.43	16 (53%)
4	B12	B	1801	1,5	101,101,101	8.18	12 (11%)	152,166,166	2.10	27 (17%)
3	PLP	B	1802	1	14,15,16	1.33	1 (7%)	20,22,23	1.06	2 (10%)
5	5AD	B	767	4	20,20,20	2.32	6 (30%)	30,30,30	4.45	14 (46%)
4	B12	C	1801	1,5	101,101,101	8.46	13 (12%)	152,166,166	2.20	22 (14%)
3	PLP	C	1802	1	14,15,16	1.32	1 (7%)	20,22,23	0.96	1 (5%)
5	5AD	C	767	4	20,20,20	2.33	6 (30%)	30,30,30	4.57	16 (53%)
4	B12	D	1801	1,5	101,101,101	7.92	13 (12%)	152,166,166	2.14	26 (17%)
3	PLP	D	1802	1	14,15,16	1.33	1 (7%)	20,22,23	1.06	1 (5%)
5	5AD	D	767	4	20,20,20	2.34	6 (30%)	30,30,30	4.50	17 (56%)

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
4	B12	A	1801	1,5	1/1/36/38	0/56/223/223	0/1/11/11
3	PLP	A	1802	1	-	0/6/6/8	0/1/1/1
5	5AD	A	767	4	1/1/4/4	0/4/20/20	0/1/3/3
4	B12	B	1801	1,5	1/1/36/38	0/56/223/223	0/1/11/11
3	PLP	B	1802	1	-	0/6/6/8	0/1/1/1
5	5AD	B	767	4	1/1/4/4	0/4/20/20	0/1/3/3
4	B12	C	1801	1,5	-	0/56/223/223	0/1/11/11
3	PLP	C	1802	1	-	0/6/6/8	0/1/1/1
5	5AD	C	767	4	1/1/4/4	0/4/20/20	0/1/3/3
4	B12	D	1801	1,5	1/1/36/38	0/56/223/223	0/1/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PLP	D	1802	1	-	0/6/6/8	0/1/1/1
5	5AD	D	767	4	1/1/4/4	0/4/20/20	0/1/3/3

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	B12	CO-N21	62.66	1.92	1.79
4	B	1801	B12	CO-N21	61.56	1.91	1.79
4	C	1801	B12	CO-N24	59.70	1.91	1.79
4	A	1801	B12	CO-N24	59.59	1.91	1.79
4	C	1801	B12	CO-N21	59.10	1.91	1.79

The worst 5 of 167 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1801	B12	C2-C1-N21	13.82	108.09	101.05
5	C	767	5AD	O4'-C1'-N9	12.86	120.40	108.44
5	B	767	5AD	O4'-C4'-C5'	12.50	132.16	109.36
4	D	1801	B12	C2-C1-N21	12.18	107.26	101.05
5	D	767	5AD	O4'-C1'-N9	12.08	119.68	108.44

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	767	5AD	C1'
5	C	767	5AD	C1'
4	D	1801	B12	C19
4	B	1801	B12	C19
5	B	767	5AD	C1'

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, 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	726/763 (95%)	-0.09	17 (2%) 57 57	14, 26, 56, 73	0
1	B	726/763 (95%)	-0.32	1 (0%) 93 94	11, 23, 45, 63	0
1	C	726/763 (95%)	-0.32	2 (0%) 91 93	15, 28, 45, 61	0
1	D	726/763 (95%)	-0.32	5 (0%) 84 85	11, 23, 47, 61	0
2	E	109/121 (90%)	-0.38	0 100 100	20, 30, 47, 56	0
2	F	109/121 (90%)	-0.54	0 100 100	16, 25, 37, 47	0
2	G	109/121 (90%)	-0.13	0 100 100	24, 36, 49, 57	0
2	H	109/121 (90%)	-0.34	0 100 100	17, 29, 46, 56	0
All	All	3340/3536 (94%)	-0.27	25 (0%) 84 85	11, 26, 49, 73	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	672	HIS	3.3
1	A	587	PRO	3.3
1	A	661	ALA	3.2
1	A	580	ILE	3.0
1	D	672	HIS	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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	PLP	D	1802	15/16	0.16	2.20	17,20,27,28	0
5	5AD	B	767	18/18	0.13	1.83	28,38,45,46	0
3	PLP	A	1802	15/16	0.14	1.36	22,26,33,34	0
5	5AD	C	767	18/18	0.15	1.30	37,43,48,50	0
3	PLP	C	1802	15/16	0.16	1.03	17,21,23,26	0
5	5AD	D	767	18/18	0.11	0.94	27,34,40,41	0
5	5AD	A	767	18/18	0.10	0.69	26,34,43,44	0
3	PLP	B	1802	15/16	0.14	0.45	14,20,24,25	0
4	B12	C	1801	91/91	0.11	0.41	16,24,34,40	0
4	B12	B	1801	91/91	0.10	-0.02	18,24,35,43	0
4	B12	D	1801	91/91	0.10	-0.16	20,27,36,41	0
4	B12	A	1801	91/91	0.10	-0.40	29,37,46,52	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.