Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 07:29 AM EDT

PDB ID	:	4XAU
Title	:	Crystal structure of AtS13 from Actinomadura melliaura
Authors	:	Wang, F.; Singh, S.; Xu, W.; Thorson, J.S.; Phillips Jr., G.N.; Enzyme Discovery for Natural Product Biosynthesis (NatPro)
Deposited on	:	2014-12-15
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

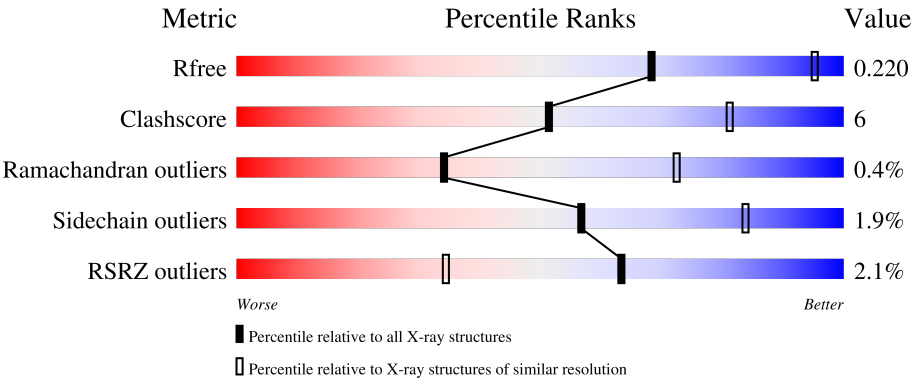
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	389	82% 13% ·
1	B	389	85% 12% ·
1	C	389	79% 16% · ·
1	D	389	% 82% 15% · ·
1	E	389	% 82% 13% · ·

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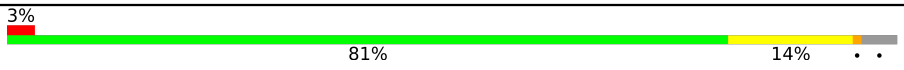
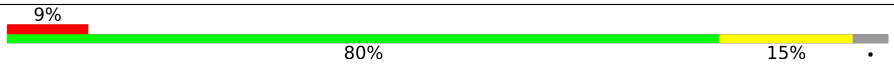
Mol	Chain	Length	Quality of chain
1	F	389	
1	G	389	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20714 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 Putative aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			2909	1830	527	539	13			
1	B	378	Total	C	N	O	S	0	0	0
			2938	1847	533	545	13			
1	C	374	Total	C	N	O	S	0	0	0
			2919	1836	529	541	13			
1	D	378	Total	C	N	O	S	0	0	0
			2938	1847	533	545	13			
1	E	373	Total	C	N	O	S	0	0	0
			2914	1833	528	540	13			
1	F	373	Total	C	N	O	S	0	0	0
			2914	1833	528	540	13			
1	G	373	Total	C	N	O	S	0	0	0
			2914	1833	528	540	13			

There are 140 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q0H2X1
A	-18	GLY	-	expression tag	UNP Q0H2X1
A	-17	SER	-	expression tag	UNP Q0H2X1
A	-16	SER	-	expression tag	UNP Q0H2X1
A	-15	HIS	-	expression tag	UNP Q0H2X1
A	-14	HIS	-	expression tag	UNP Q0H2X1
A	-13	HIS	-	expression tag	UNP Q0H2X1
A	-12	HIS	-	expression tag	UNP Q0H2X1
A	-11	HIS	-	expression tag	UNP Q0H2X1
A	-10	HIS	-	expression tag	UNP Q0H2X1
A	-9	SER	-	expression tag	UNP Q0H2X1
A	-8	SER	-	expression tag	UNP Q0H2X1
A	-7	GLY	-	expression tag	UNP Q0H2X1
A	-6	LEU	-	expression tag	UNP Q0H2X1
A	-5	VAL	-	expression tag	UNP Q0H2X1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	PRO	-	expression tag	UNP Q0H2X1
A	-3	ARG	-	expression tag	UNP Q0H2X1
A	-2	GLY	-	expression tag	UNP Q0H2X1
A	-1	SER	-	expression tag	UNP Q0H2X1
A	0	HIS	-	expression tag	UNP Q0H2X1
B	-19	MET	-	initiating methionine	UNP Q0H2X1
B	-18	GLY	-	expression tag	UNP Q0H2X1
B	-17	SER	-	expression tag	UNP Q0H2X1
B	-16	SER	-	expression tag	UNP Q0H2X1
B	-15	HIS	-	expression tag	UNP Q0H2X1
B	-14	HIS	-	expression tag	UNP Q0H2X1
B	-13	HIS	-	expression tag	UNP Q0H2X1
B	-12	HIS	-	expression tag	UNP Q0H2X1
B	-11	HIS	-	expression tag	UNP Q0H2X1
B	-10	HIS	-	expression tag	UNP Q0H2X1
B	-9	SER	-	expression tag	UNP Q0H2X1
B	-8	SER	-	expression tag	UNP Q0H2X1
B	-7	GLY	-	expression tag	UNP Q0H2X1
B	-6	LEU	-	expression tag	UNP Q0H2X1
B	-5	VAL	-	expression tag	UNP Q0H2X1
B	-4	PRO	-	expression tag	UNP Q0H2X1
B	-3	ARG	-	expression tag	UNP Q0H2X1
B	-2	GLY	-	expression tag	UNP Q0H2X1
B	-1	SER	-	expression tag	UNP Q0H2X1
B	0	HIS	-	expression tag	UNP Q0H2X1
C	-19	MET	-	initiating methionine	UNP Q0H2X1
C	-18	GLY	-	expression tag	UNP Q0H2X1
C	-17	SER	-	expression tag	UNP Q0H2X1
C	-16	SER	-	expression tag	UNP Q0H2X1
C	-15	HIS	-	expression tag	UNP Q0H2X1
C	-14	HIS	-	expression tag	UNP Q0H2X1
C	-13	HIS	-	expression tag	UNP Q0H2X1
C	-12	HIS	-	expression tag	UNP Q0H2X1
C	-11	HIS	-	expression tag	UNP Q0H2X1
C	-10	HIS	-	expression tag	UNP Q0H2X1
C	-9	SER	-	expression tag	UNP Q0H2X1
C	-8	SER	-	expression tag	UNP Q0H2X1
C	-7	GLY	-	expression tag	UNP Q0H2X1
C	-6	LEU	-	expression tag	UNP Q0H2X1
C	-5	VAL	-	expression tag	UNP Q0H2X1
C	-4	PRO	-	expression tag	UNP Q0H2X1
C	-3	ARG	-	expression tag	UNP Q0H2X1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q0H2X1
C	-1	SER	-	expression tag	UNP Q0H2X1
C	0	HIS	-	expression tag	UNP Q0H2X1
D	-19	MET	-	initiating methionine	UNP Q0H2X1
D	-18	GLY	-	expression tag	UNP Q0H2X1
D	-17	SER	-	expression tag	UNP Q0H2X1
D	-16	SER	-	expression tag	UNP Q0H2X1
D	-15	HIS	-	expression tag	UNP Q0H2X1
D	-14	HIS	-	expression tag	UNP Q0H2X1
D	-13	HIS	-	expression tag	UNP Q0H2X1
D	-12	HIS	-	expression tag	UNP Q0H2X1
D	-11	HIS	-	expression tag	UNP Q0H2X1
D	-10	HIS	-	expression tag	UNP Q0H2X1
D	-9	SER	-	expression tag	UNP Q0H2X1
D	-8	SER	-	expression tag	UNP Q0H2X1
D	-7	GLY	-	expression tag	UNP Q0H2X1
D	-6	LEU	-	expression tag	UNP Q0H2X1
D	-5	VAL	-	expression tag	UNP Q0H2X1
D	-4	PRO	-	expression tag	UNP Q0H2X1
D	-3	ARG	-	expression tag	UNP Q0H2X1
D	-2	GLY	-	expression tag	UNP Q0H2X1
D	-1	SER	-	expression tag	UNP Q0H2X1
D	0	HIS	-	expression tag	UNP Q0H2X1
E	-19	MET	-	initiating methionine	UNP Q0H2X1
E	-18	GLY	-	expression tag	UNP Q0H2X1
E	-17	SER	-	expression tag	UNP Q0H2X1
E	-16	SER	-	expression tag	UNP Q0H2X1
E	-15	HIS	-	expression tag	UNP Q0H2X1
E	-14	HIS	-	expression tag	UNP Q0H2X1
E	-13	HIS	-	expression tag	UNP Q0H2X1
E	-12	HIS	-	expression tag	UNP Q0H2X1
E	-11	HIS	-	expression tag	UNP Q0H2X1
E	-10	HIS	-	expression tag	UNP Q0H2X1
E	-9	SER	-	expression tag	UNP Q0H2X1
E	-8	SER	-	expression tag	UNP Q0H2X1
E	-7	GLY	-	expression tag	UNP Q0H2X1
E	-6	LEU	-	expression tag	UNP Q0H2X1
E	-5	VAL	-	expression tag	UNP Q0H2X1
E	-4	PRO	-	expression tag	UNP Q0H2X1
E	-3	ARG	-	expression tag	UNP Q0H2X1
E	-2	GLY	-	expression tag	UNP Q0H2X1
E	-1	SER	-	expression tag	UNP Q0H2X1

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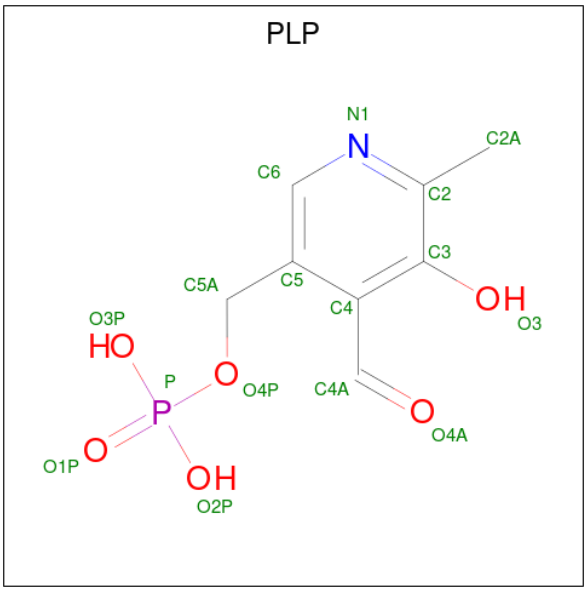
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP Q0H2X1
F	-19	MET	-	initiating methionine	UNP Q0H2X1
F	-18	GLY	-	expression tag	UNP Q0H2X1
F	-17	SER	-	expression tag	UNP Q0H2X1
F	-16	SER	-	expression tag	UNP Q0H2X1
F	-15	HIS	-	expression tag	UNP Q0H2X1
F	-14	HIS	-	expression tag	UNP Q0H2X1
F	-13	HIS	-	expression tag	UNP Q0H2X1
F	-12	HIS	-	expression tag	UNP Q0H2X1
F	-11	HIS	-	expression tag	UNP Q0H2X1
F	-10	HIS	-	expression tag	UNP Q0H2X1
F	-9	SER	-	expression tag	UNP Q0H2X1
F	-8	SER	-	expression tag	UNP Q0H2X1
F	-7	GLY	-	expression tag	UNP Q0H2X1
F	-6	LEU	-	expression tag	UNP Q0H2X1
F	-5	VAL	-	expression tag	UNP Q0H2X1
F	-4	PRO	-	expression tag	UNP Q0H2X1
F	-3	ARG	-	expression tag	UNP Q0H2X1
F	-2	GLY	-	expression tag	UNP Q0H2X1
F	-1	SER	-	expression tag	UNP Q0H2X1
F	0	HIS	-	expression tag	UNP Q0H2X1
G	-19	MET	-	initiating methionine	UNP Q0H2X1
G	-18	GLY	-	expression tag	UNP Q0H2X1
G	-17	SER	-	expression tag	UNP Q0H2X1
G	-16	SER	-	expression tag	UNP Q0H2X1
G	-15	HIS	-	expression tag	UNP Q0H2X1
G	-14	HIS	-	expression tag	UNP Q0H2X1
G	-13	HIS	-	expression tag	UNP Q0H2X1
G	-12	HIS	-	expression tag	UNP Q0H2X1
G	-11	HIS	-	expression tag	UNP Q0H2X1
G	-10	HIS	-	expression tag	UNP Q0H2X1
G	-9	SER	-	expression tag	UNP Q0H2X1
G	-8	SER	-	expression tag	UNP Q0H2X1
G	-7	GLY	-	expression tag	UNP Q0H2X1
G	-6	LEU	-	expression tag	UNP Q0H2X1
G	-5	VAL	-	expression tag	UNP Q0H2X1
G	-4	PRO	-	expression tag	UNP Q0H2X1
G	-3	ARG	-	expression tag	UNP Q0H2X1
G	-2	GLY	-	expression tag	UNP Q0H2X1
G	-1	SER	-	expression tag	UNP Q0H2X1
G	0	HIS	-	expression tag	UNP Q0H2X1

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is water.

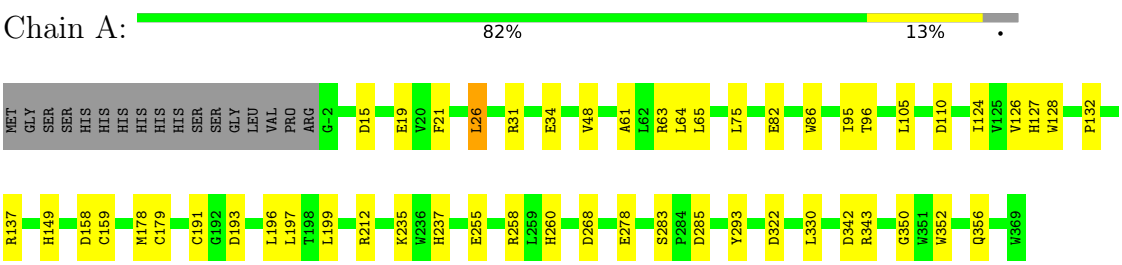
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total	O	0	0
			50	50		
3	B	54	Total	O	0	0
			54	54		
3	C	49	Total	O	0	0
			49	49		
3	D	20	Total	O	0	0
			20	20		
3	E	41	Total	O	0	0
			41	41		
3	F	29	Total	O	0	0
			29	29		
3	G	9	Total	O	0	0
			9	9		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

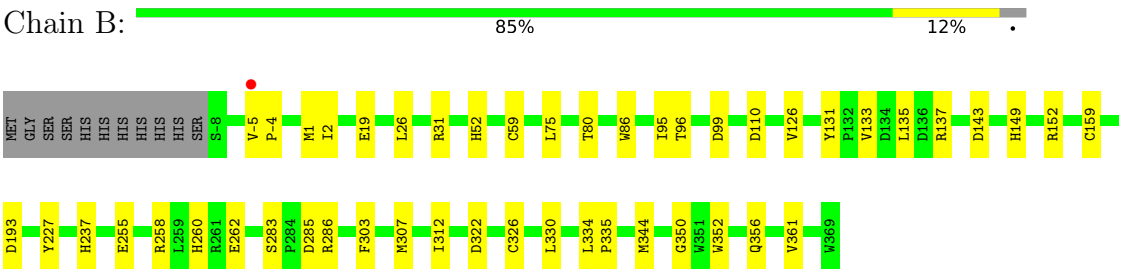
• Molecule 1: Putative aminotransferase

Chain A:



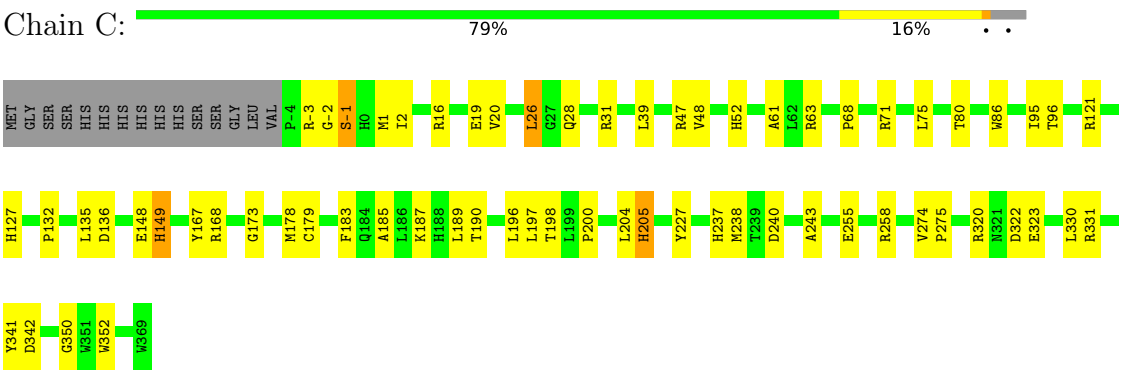
• Molecule 1: Putative aminotransferase

Chain B:



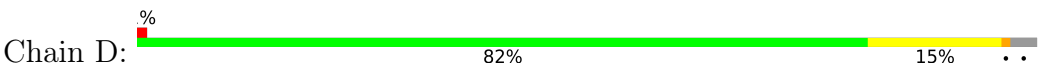
• Molecule 1: Putative aminotransferase

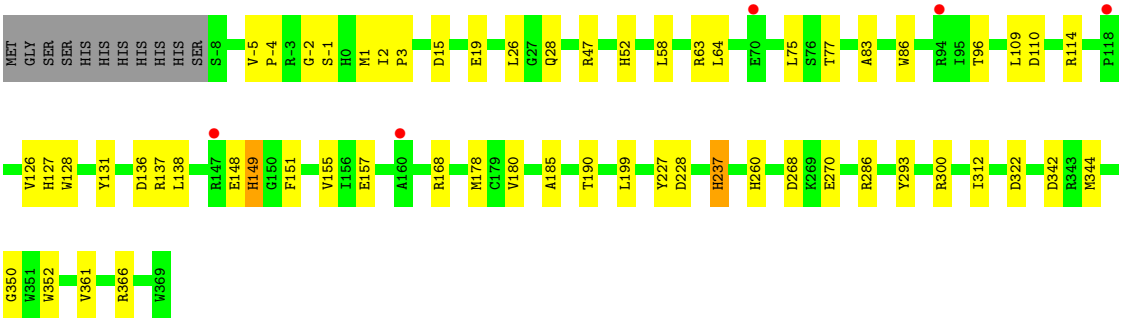
Chain C:



• Molecule 1: Putative aminotransferase

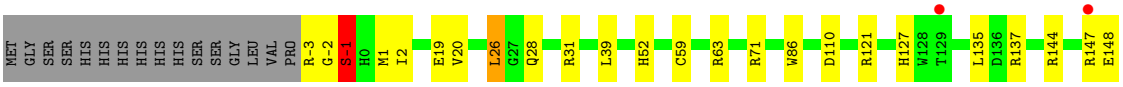
Chain D:

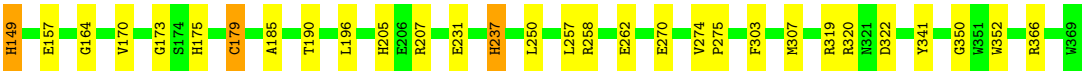




• Molecule 1: Putative aminotransferase

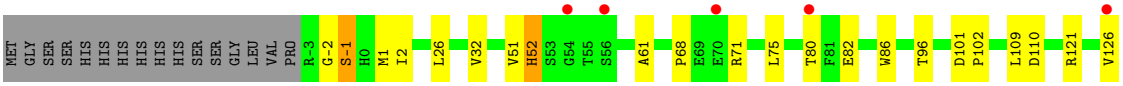
Chain E:

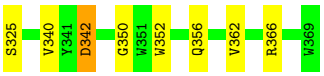




• Molecule 1: Putative aminotransferase

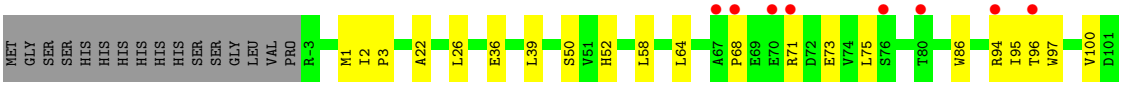
Chain F:

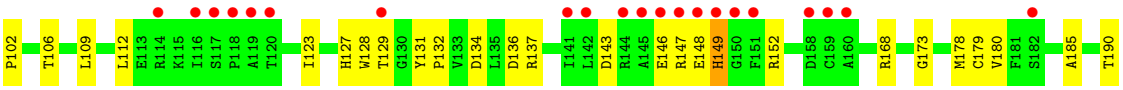




• Molecule 1: Putative aminotransferase

Chain G:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	233.15Å 233.15Å 460.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.95 – 3.00 29.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.95-3.00) 91.1 (29.95-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	0.87 (at 3.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.220 0.187 , 0.220	Depositor DCC
R_{free} test set	2000 reflections (2.08%)	wwPDB-VP
Wilson B-factor (Å^2)	78.3	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 72.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20714	wwPDB-VP
Average B, all atoms (Å^2)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.84	3/2977 (0.1%)	0.66	0/4046
1	B	0.82	3/3006 (0.1%)	0.65	0/4086
1	C	0.77	0/2987	0.65	0/4060
1	D	0.48	0/3006	0.57	0/4086
1	E	0.72	2/2982 (0.1%)	0.66	0/4053
1	F	0.49	0/2982	0.57	0/4053
1	G	0.37	0/2982	0.51	0/4053
All	All	0.66	8/20922 (0.0%)	0.61	0/28437

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	CYS	CB-SG	-6.06	1.72	1.82
1	E	179	CYS	CB-SG	-5.89	1.72	1.81
1	B	326	CYS	CB-SG	-5.79	1.72	1.81
1	A	159	CYS	CB-SG	-5.53	1.72	1.81
1	A	179	CYS	CB-SG	-5.38	1.73	1.81
1	E	59	CYS	CB-SG	-5.35	1.73	1.81
1	B	59	CYS	CB-SG	-5.19	1.73	1.81
1	A	191	CYS	CB-SG	-5.19	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2909	0	2850	30	0
1	B	2938	0	2862	26	0
1	C	2919	0	2851	41	1
1	D	2938	0	2862	36	0
1	E	2914	0	2852	29	0
1	F	2914	0	2852	38	0
1	G	2914	0	2852	33	0
2	C	16	0	8	3	0
3	A	50	0	0	2	0
3	B	54	0	0	4	0
3	C	49	0	0	5	0
3	D	20	0	0	2	0
3	E	41	0	0	2	0
3	F	29	0	0	7	0
3	G	9	0	0	0	0
All	All	20714	0	19989	226	1

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 6.

All (226) 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:E:31:ARG:HD3	3:E:403:HOH:O	1.86	0.75
1:A:110:ASP:OD1	1:A:137:ARG:NH2	2.19	0.75
1:F:356:GLN:NE2	3:F:401:HOH:O	2.19	0.74
1:C:187:LYS:NZ	2:C:500:PLP:H4A	2.03	0.73
1:B:133:VAL:HB	3:B:445:HOH:O	1.90	0.72
1:D:322:ASP:O	3:D:411:HOH:O	2.09	0.71
1:C:136:ASP:OD2	1:C:168:ARG:NH1	2.25	0.70
1:E:-3:ARG:O	1:E:-1:SER:N	2.22	0.70
1:A:268:ASP:OD1	1:A:293:TYR:OH	2.08	0.69
1:C:19:GLU:OE1	1:C:31:ARG:NH1	2.26	0.68
1:C:63:ARG:NE	3:C:632:HOH:O	2.27	0.68
1:A:278:GLU:OE1	1:A:343:ARG:NH2	2.28	0.66
1:C:255:GLU:OE2	1:C:258:ARG:NH2	2.20	0.65
1:B:255:GLU:OE2	1:B:258:ARG:NH2	2.16	0.65
1:C:80:THR:HB	3:C:614:HOH:O	1.96	0.65
1:A:255:GLU:OE2	1:A:258:ARG:NH2	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:350:GLY:HA3	1:G:352:TRP:CZ3	2.32	0.65
1:D:350:GLY:HA3	1:D:352:TRP:CZ3	2.33	0.64
1:B:356:GLN:HB2	3:B:415:HOH:O	1.98	0.64
1:F:283:SER:OG	1:F:285:ASP:OD1	2.12	0.63
1:F:270:GLU:O	1:F:366:ARG:NH1	2.32	0.63
1:E:39:LEU:HD13	1:E:196:LEU:HD22	1.80	0.62
1:F:148:GLU:HG2	1:F:149:HIS:ND1	2.15	0.62
1:G:75:LEU:HD23	1:G:96:THR:HB	1.82	0.62
1:D:-2:GLY:O	1:D:-1:SER:OG	2.18	0.62
1:E:258:ARG:NH1	1:E:262:GLU:OE1	2.33	0.62
1:D:110:ASP:OD1	1:D:137:ARG:NH2	2.33	0.61
1:A:212:ARG:NH1	3:A:434:HOH:O	2.34	0.61
1:A:31:ARG:NH2	1:A:34:GLU:OE1	2.33	0.60
1:C:16:ARG:NH2	3:C:601:HOH:O	2.34	0.60
1:F:350:GLY:HA3	1:F:352:TRP:CZ3	2.36	0.60
1:E:270:GLU:O	1:E:366:ARG:NH1	2.35	0.59
1:G:136:ASP:OD2	1:G:168:ARG:NH1	2.36	0.59
1:D:64:LEU:HD12	1:D:178:MET:HE1	1.85	0.59
1:D:227:TYR:OH	1:F:82:GLU:OE2	2.11	0.58
1:A:31:ARG:HD3	3:A:401:HOH:O	2.01	0.58
1:A:126:VAL:HG22	1:A:158:ASP:HB3	1.86	0.58
1:E:110:ASP:OD1	1:E:137:ARG:NH2	2.38	0.57
1:F:110:ASP:OD1	1:F:137:ARG:NH2	2.38	0.56
1:A:178:MET:HE2	1:A:197:LEU:HD11	1.86	0.56
1:C:47:ARG:HA	1:C:205:HIS:CD2	2.40	0.56
1:A:283:SER:OG	1:A:285:ASP:OD1	2.14	0.56
1:B:350:GLY:HA3	1:B:352:TRP:CZ3	2.41	0.56
1:G:68:PRO:HG2	1:G:71:ARG:HG3	1.87	0.56
1:A:126:VAL:O	1:A:128:TRP:N	2.40	0.54
1:F:322:ASP:N	1:F:322:ASP:OD1	2.38	0.54
1:A:75:LEU:HD23	1:A:96:THR:HB	1.90	0.54
1:E:250:LEU:O	3:E:421:HOH:O	2.19	0.54
1:F:255:GLU:OE2	1:F:258:ARG:NH2	2.25	0.53
1:A:64:LEU:HD12	1:A:178:MET:HE1	1.90	0.53
1:B:19:GLU:OE1	1:B:31:ARG:NH1	2.39	0.53
1:C:168:ARG:HD3	3:C:648:HOH:O	2.08	0.53
1:A:350:GLY:HA3	1:A:352:TRP:CZ3	2.43	0.53
1:D:138:LEU:HD21	1:D:155:VAL:HG11	1.91	0.53
1:G:39:LEU:HD13	1:G:196:LEU:HD22	1.90	0.52
1:E:148:GLU:HG2	1:E:149:HIS:ND1	2.24	0.52
1:D:228:ASP:OD2	1:F:325:SER:OG	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:HIS:ND1	1:F:132:PRO:HA	2.24	0.52
1:F:52:HIS:N	3:F:425:HOH:O	2.39	0.52
1:F:75:LEU:HD23	1:F:96:THR:HB	1.92	0.52
1:D:149:HIS:O	1:D:151:PHE:N	2.43	0.51
1:F:51:VAL:HB	3:F:425:HOH:O	2.10	0.51
1:B:95:ILE:HB	1:B:330:LEU:HD13	1.92	0.51
1:G:1:MET:HG3	1:G:2:ILE:N	2.26	0.51
1:E:350:GLY:HA3	1:E:352:TRP:CZ3	2.44	0.51
1:C:16:ARG:HD3	3:C:608:HOH:O	2.09	0.51
1:C:322:ASP:N	1:C:322:ASP:OD1	2.43	0.51
1:F:342:ASP:OD1	1:F:342:ASP:N	2.43	0.51
1:G:143:ASP:HB3	1:G:147:ARG:HH22	1.76	0.51
1:G:322:ASP:OD1	1:G:322:ASP:N	2.41	0.51
1:G:52:HIS:N	1:G:236:TRP:O	2.43	0.50
1:D:127:HIS:HE2	1:D:157:GLU:HB3	1.75	0.50
1:B:80:THR:HG21	1:B:126:VAL:HG21	1.92	0.50
1:C:-2:GLY:O	1:C:-1:SER:HB2	2.12	0.50
1:F:262:GLU:HB2	3:F:415:HOH:O	2.11	0.50
1:G:106:THR:HG21	1:G:131:TYR:HD2	1.77	0.50
1:G:148:GLU:HG2	1:G:149:HIS:ND1	2.26	0.50
1:G:58:LEU:HG	1:G:180:VAL:HG11	1.94	0.50
1:D:110:ASP:HB3	1:D:114:ARG:HH12	1.77	0.49
1:D:312:ILE:HD13	1:D:361:VAL:HG22	1.93	0.49
1:E:320:ARG:HG2	1:E:341:TYR:CZ	2.48	0.49
1:F:126:VAL:O	1:F:128:TRP:N	2.45	0.49
1:B:19:GLU:O	3:B:401:HOH:O	2.19	0.49
1:A:356:GLN:HG2	1:G:22:ALA:HA	1.94	0.49
1:F:80:THR:HG21	1:F:126:VAL:HG21	1.94	0.49
1:E:322:ASP:OD1	1:E:322:ASP:N	2.46	0.49
1:A:95:ILE:HB	1:A:330:LEU:HD13	1.95	0.48
1:D:77:THR:HG22	3:D:415:HOH:O	2.13	0.48
1:G:127:HIS:ND1	1:G:132:PRO:HA	2.28	0.48
1:B:283:SER:OG	1:B:285:ASP:OD1	2.28	0.48
1:D:268:ASP:OD1	1:D:293:TYR:OH	2.23	0.48
1:F:109:LEU:HB3	1:F:141:ILE:HD11	1.96	0.48
1:C:135:LEU:HB2	1:C:167:TYR:CE2	2.49	0.48
1:B:75:LEU:HD23	1:B:96:THR:HB	1.96	0.48
1:C:28:GLN:HB2	1:C:237:HIS:HD1	1.78	0.48
1:A:260:HIS:CE1	1:A:350:GLY:HA2	2.49	0.48
1:B:1:MET:HG3	1:B:2:ILE:N	2.28	0.48
1:C:148:GLU:HG2	1:C:149:HIS:ND1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:20:VAL:HG12	1:E:26:LEU:HD12	1.96	0.48
1:C:39:LEU:HD13	1:C:196:LEU:HD22	1.95	0.47
1:D:148:GLU:HG2	1:D:149:HIS:ND1	2.29	0.47
1:C:71:ARG:O	1:C:121:ARG:HB2	2.15	0.47
1:F:184:GLN:HB2	3:F:427:HOH:O	2.13	0.47
1:D:270:GLU:O	1:D:366:ARG:NH1	2.43	0.47
1:B:303:PHE:O	1:B:307:MET:HG2	2.14	0.47
1:F:-2:GLY:HA2	3:F:402:HOH:O	2.14	0.47
1:B:143:ASP:OD1	1:B:152:ARG:NH1	2.36	0.47
1:D:109:LEU:HD12	1:D:137:ARG:HD3	1.96	0.47
1:G:73:GLU:HB2	1:G:94:ARG:NH2	2.30	0.47
1:E:19:GLU:OE1	1:E:31:ARG:NH1	2.47	0.47
1:F:173:GLY:HA2	1:F:179:CYS:SG	2.55	0.47
1:C:185:ALA:HA	1:C:190:THR:OG1	2.15	0.47
1:C:95:ILE:HB	1:C:330:LEU:HD13	1.97	0.46
1:D:110:ASP:HB3	1:D:114:ARG:NH1	2.29	0.46
1:F:303:PHE:O	1:F:307:MET:HG2	2.14	0.46
1:G:95:ILE:HB	1:G:330:LEU:HD13	1.97	0.46
1:G:75:LEU:HB2	1:G:123:ILE:HG12	1.96	0.46
1:G:100:VAL:O	1:G:102:PRO:HD3	2.16	0.46
1:G:173:GLY:HA2	1:G:179:CYS:SG	2.55	0.46
1:B:322:ASP:OD1	1:B:322:ASP:N	2.49	0.46
1:B:312:ILE:HD13	1:B:361:VAL:HG22	1.98	0.46
1:B:110:ASP:OD1	1:B:137:ARG:NH2	2.49	0.46
1:C:20:VAL:HG12	1:C:26:LEU:HD12	1.97	0.46
1:C:178:MET:HE2	1:C:197:LEU:HD11	1.97	0.46
1:D:75:LEU:HD23	1:D:96:THR:HB	1.98	0.46
1:B:99:ASP:HA	1:B:334:LEU:HD22	1.97	0.46
1:C:173:GLY:HA2	1:C:179:CYS:SG	2.55	0.46
1:A:322:ASP:N	1:A:322:ASP:OD1	2.48	0.46
1:B:131:TYR:CZ	1:B:286:ARG:HD2	2.50	0.46
1:C:187:LYS:HZ3	2:C:500:PLP:H4A	1.77	0.45
1:G:185:ALA:HA	1:G:190:THR:OG1	2.16	0.45
1:A:82:GLU:OE2	1:B:227:TYR:OH	2.15	0.45
1:D:300:ARG:NH1	1:D:344:MET:O	2.48	0.45
1:D:109:LEU:HB2	1:D:137:ARG:CZ	2.45	0.45
1:A:127:HIS:ND1	1:A:132:PRO:HA	2.30	0.45
1:B:307:MET:HE3	1:B:312:ILE:HB	1.97	0.45
1:G:303:PHE:O	1:G:307:MET:HG2	2.16	0.45
1:F:68:PRO:O	1:F:121:ARG:NH2	2.50	0.45
1:E:185:ALA:HA	1:E:190:THR:OG1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:GLY:HA3	1:E:352:TRP:CH2	2.52	0.45
1:G:64:LEU:HD12	1:G:178:MET:HE1	1.98	0.45
1:F:32:VAL:HG21	1:F:238:MET:O	2.15	0.45
1:C:47:ARG:HG2	1:C:205:HIS:HD2	1.82	0.44
1:D:58:LEU:HD23	1:D:180:VAL:HG21	1.99	0.44
1:D:322:ASP:OD1	1:D:322:ASP:N	2.50	0.44
1:A:21:PHE:CD1	1:A:26:LEU:HD11	2.52	0.44
1:G:342:ASP:OD1	1:G:342:ASP:N	2.50	0.44
1:C:227:TYR:O	1:E:319:ARG:NH1	2.46	0.44
1:C:320:ARG:HG2	1:C:341:TYR:CZ	2.53	0.44
1:E:71:ARG:O	1:E:121:ARG:HB2	2.18	0.44
1:E:207:ARG:NH2	1:E:231:GLU:OE2	2.38	0.44
1:D:136:ASP:OD2	1:D:168:ARG:NH1	2.51	0.44
1:F:260:HIS:CE1	1:F:350:GLY:HA2	2.53	0.44
1:G:3:PRO:HG2	1:G:352:TRP:NE1	2.33	0.44
1:D:3:PRO:HG2	1:D:352:TRP:NE1	2.32	0.44
1:D:83:ALA:HB2	1:F:214:TYR:CE1	2.52	0.44
1:F:297:VAL:HG11	1:F:303:PHE:CE1	2.53	0.43
1:A:48:VAL:HB	1:A:196:LEU:HD11	2.01	0.43
1:A:235:LYS:NZ	1:B:193:ASP:OD2	2.48	0.43
1:G:146:GLU:HB2	1:G:152:ARG:HB2	2.01	0.43
1:A:61:ALA:HA	1:A:178:MET:HE1	2.00	0.43
1:C:68:PRO:HG2	1:C:71:ARG:HG3	2.00	0.43
1:C:127:HIS:ND1	1:C:132:PRO:HA	2.32	0.43
1:C:187:LYS:CE	2:C:500:PLP:H4A	2.49	0.43
1:A:342:ASP:OD1	1:A:342:ASP:N	2.49	0.43
1:B:334:LEU:HA	1:B:335:PRO:HD2	1.83	0.43
1:D:131:TYR:CZ	1:D:286:ARG:HD2	2.53	0.43
1:G:274:VAL:HA	1:G:275:PRO:HD3	1.89	0.43
1:E:164:GLY:HA3	1:E:257:LEU:HD21	2.00	0.43
1:B:260:HIS:CE1	1:B:350:GLY:HA2	2.54	0.43
1:E:303:PHE:O	1:E:307:MET:HG2	2.18	0.43
1:D:28:GLN:OE1	1:D:237:HIS:ND1	2.49	0.43
1:C:48:VAL:HB	1:C:196:LEU:HD11	2.01	0.42
1:D:126:VAL:O	1:D:128:TRP:N	2.52	0.42
1:G:112:LEU:HD11	1:G:123:ILE:HD13	1.99	0.42
1:B:258:ARG:NH1	1:B:262:GLU:OE1	2.53	0.42
1:C:135:LEU:HA	1:C:135:LEU:HD23	1.75	0.42
1:F:1:MET:HG3	1:F:2:ILE:N	2.33	0.42
1:C:31:ARG:HB2	1:C:240:ASP:CG	2.39	0.42
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:ARG:HG2	1:E:147:ARG:HH21	1.84	0.42
1:F:101:ASP:HA	1:F:102:PRO:HD3	1.84	0.42
1:F:266:PHE:HE2	1:F:362:VAL:HG21	1.85	0.42
1:F:266:PHE:CE2	1:F:362:VAL:HG21	2.54	0.42
1:C:200:PRO:HD2	1:C:204:LEU:HD12	2.02	0.42
1:E:173:GLY:HA2	1:E:179:CYS:SG	2.60	0.42
1:F:-2:GLY:O	1:F:-1:SER:HB2	2.20	0.42
1:F:61:ALA:HA	1:F:178:MET:HE1	2.01	0.42
1:F:102:PRO:HB3	1:F:340:VAL:CG1	2.50	0.42
1:F:236:TRP:O	3:F:425:HOH:O	2.22	0.42
1:E:127:HIS:HE2	1:E:157:GLU:HB3	1.84	0.42
1:G:204:LEU:HD23	1:G:204:LEU:HA	1.86	0.42
1:C:183:PHE:HA	1:C:189:LEU:O	2.20	0.42
1:G:36:GLU:OE2	1:G:50:SER:OG	2.32	0.42
1:G:109:LEU:HD12	1:G:137:ARG:HD3	2.02	0.42
1:D:15:ASP:O	1:D:19:GLU:HG3	2.20	0.41
1:E:1:MET:HG3	1:E:2:ILE:N	2.33	0.41
1:C:61:ALA:HA	1:C:178:MET:HE1	2.01	0.41
1:E:170:VAL:HB	1:E:175:HIS:CE1	2.55	0.41
1:A:63:ARG:HD3	1:A:63:ARG:HA	1.80	0.41
1:B:344:MET:HB2	3:B:452:HOH:O	2.19	0.41
1:D:47:ARG:NE	1:D:199:LEU:O	2.41	0.41
1:A:15:ASP:O	1:A:19:GLU:HG3	2.20	0.41
1:F:71:ARG:O	1:F:121:ARG:HD2	2.21	0.41
1:G:128:TRP:CD1	1:G:129:THR:HG23	2.56	0.41
1:A:65:LEU:HD23	1:A:65:LEU:HA	1.78	0.41
1:D:185:ALA:HA	1:D:190:THR:OG1	2.20	0.41
1:E:63:ARG:HA	1:E:63:ARG:HD3	1.89	0.41
1:C:75:LEU:HD23	1:C:96:THR:HB	2.03	0.41
1:C:238:MET:HE3	1:C:243:ALA:HB2	2.03	0.41
1:D:1:MET:HG3	1:D:2:ILE:N	2.36	0.41
1:E:28:GLN:OE1	1:E:237:HIS:ND1	2.47	0.41
1:E:135:LEU:HD23	1:E:135:LEU:HA	1.88	0.41
1:D:260:HIS:CE1	1:D:350:GLY:HA2	2.56	0.41
1:D:342:ASP:OD1	1:D:342:ASP:N	2.55	0.40
1:F:127:HIS:HE2	1:F:157:GLU:HB3	1.86	0.40
1:A:124:ILE:HD13	1:A:124:ILE:HG21	1.86	0.40
1:C:350:GLY:HA3	1:C:352:TRP:CZ3	2.55	0.40
1:E:274:VAL:HA	1:E:275:PRO:HD3	1.83	0.40
1:G:97:TRP:HB2	1:G:332:THR:CG2	2.52	0.40
1:G:350:GLY:HA3	1:G:352:TRP:CH2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:VAL:HA	1:C:275:PRO:HD3	1.83	0.40
1:C:342:ASP:OD1	1:C:342:ASP:N	2.54	0.40
1:B:135:LEU:HD23	1:B:135:LEU:HA	1.83	0.40
1:C:1:MET:HG3	1:C:2:ILE:N	2.35	0.40
1:D:63:ARG:HD3	1:D:63:ARG:HA	1.93	0.40

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	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:GLU:OE2	1:C:331:ARG:NH1[4_555]	2.12	0.08

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	370/389 (95%)	354 (96%)	16 (4%)	0	100	100
1	B	376/389 (97%)	356 (95%)	18 (5%)	2 (0%)	29	68
1	C	372/389 (96%)	354 (95%)	16 (4%)	2 (0%)	29	68
1	D	376/389 (97%)	355 (94%)	19 (5%)	2 (0%)	29	68
1	E	371/389 (95%)	354 (95%)	15 (4%)	2 (0%)	29	68
1	F	371/389 (95%)	352 (95%)	18 (5%)	1 (0%)	41	76
1	G	371/389 (95%)	353 (95%)	17 (5%)	1 (0%)	41	76
All	All	2607/2723 (96%)	2478 (95%)	119 (5%)	10 (0%)	34	72

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-5	VAL

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Mol	Chain	Res	Type
1	B	-4	PRO
1	C	-3	ARG
1	D	-5	VAL
1	D	-4	PRO
1	E	-2	GLY
1	C	-1	SER
1	E	-1	SER
1	F	-1	SER
1	G	134	ASP

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	303/318 (95%)	297 (98%)	6 (2%)	55	83
1	B	303/318 (95%)	298 (98%)	5 (2%)	60	85
1	C	303/318 (95%)	297 (98%)	6 (2%)	55	83
1	D	303/318 (95%)	298 (98%)	5 (2%)	60	85
1	E	303/318 (95%)	296 (98%)	7 (2%)	50	80
1	F	303/318 (95%)	296 (98%)	7 (2%)	50	80
1	G	303/318 (95%)	299 (99%)	4 (1%)	69	89
All	All	2121/2226 (95%)	2081 (98%)	40 (2%)	57	84

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	86	TRP
1	A	149	HIS
1	A	193	ASP
1	A	199	LEU
1	A	237	HIS
1	B	26	LEU
1	B	52	HIS

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Mol	Chain	Res	Type
1	B	86	TRP
1	B	149	HIS
1	B	237	HIS
1	C	26	LEU
1	C	52	HIS
1	C	86	TRP
1	C	149	HIS
1	C	198	THR
1	C	205	HIS
1	D	26	LEU
1	D	52	HIS
1	D	86	TRP
1	D	149	HIS
1	D	237	HIS
1	E	-1	SER
1	E	26	LEU
1	E	52	HIS
1	E	86	TRP
1	E	149	HIS
1	E	205	HIS
1	E	237	HIS
1	F	26	LEU
1	F	52	HIS
1	F	86	TRP
1	F	149	HIS
1	F	193	ASP
1	F	237	HIS
1	F	342	ASP
1	G	26	LEU
1	G	86	TRP
1	G	149	HIS
1	G	237	HIS

Sometimes 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 molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
2	PLP	C	500	-	16,16,16	1.35	2 (12%)	20,23,23	1.35	3 (15%)

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	PLP	C	500	-	-	4/8/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	PLP	C3-C2	-2.87	1.38	1.40
2	C	500	PLP	C2-N1	2.16	1.37	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	PLP	C3-C4-C4A	-3.14	115.45	119.90
2	C	500	PLP	C2A-C2-C3	-2.71	117.54	120.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	PLP	C2A-C2-N1	2.39	122.33	117.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	PLP	C3-C4-C4A-O4A
2	C	500	PLP	C4-C5-C5A-O4P
2	C	500	PLP	C6-C5-C5A-O4P
2	C	500	PLP	C5-C4-C4A-O4A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	PLP	3	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, 95^{th} 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	372/389 (95%)	-0.39	0 100 100	63, 82, 110, 196	0
1	B	378/389 (97%)	-0.44	1 (0%) 94 84	62, 79, 107, 171	0
1	C	374/389 (96%)	-0.40	0 100 100	71, 86, 110, 150	0
1	D	378/389 (97%)	-0.13	5 (1%) 77 51	82, 126, 182, 251	0
1	E	373/389 (95%)	-0.31	2 (0%) 91 75	70, 92, 128, 188	0
1	F	373/389 (95%)	-0.03	11 (2%) 51 23	90, 119, 161, 197	0
1	G	373/389 (95%)	0.32	35 (9%) 8 3	89, 160, 235, 277	0
All	All	2621/2723 (96%)	-0.20	54 (2%) 63 34	62, 99, 184, 277	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	150	GLY	5.6
1	G	144	ARG	4.4
1	G	70	GLU	4.0
1	D	118	PRO	3.8
1	F	129	THR	3.8
1	G	329	HIS	3.6
1	D	70	GLU	3.6
1	F	160	ALA	3.6
1	G	114	ARG	3.6
1	G	129	THR	3.5
1	F	158	ASP	3.4
1	G	76	SER	3.4
1	G	158	ASP	3.3
1	G	80	THR	3.3
1	G	68	PRO	3.2
1	G	118	PRO	3.1
1	G	220	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	147	ARG	2.9
1	G	146	GLU	2.9
1	G	151	PHE	2.9
1	F	159	CYS	2.8
1	F	70	GLU	2.7
1	G	116	ILE	2.7
1	G	182	SER	2.7
1	G	142	LEU	2.6
1	G	160	ALA	2.6
1	G	148	GLU	2.5
1	F	80	THR	2.5
1	G	94	ARG	2.5
1	G	335	PRO	2.5
1	G	120	THR	2.5
1	G	141	ILE	2.4
1	D	147	ARG	2.4
1	F	56	SER	2.4
1	G	285	ASP	2.4
1	F	161	HIS	2.4
1	F	54	GLY	2.4
1	G	149	HIS	2.3
1	E	129	THR	2.3
1	F	182	SER	2.3
1	G	71	ARG	2.3
1	G	331	ARG	2.2
1	G	119	ALA	2.2
1	G	159	CYS	2.2
1	D	160	ALA	2.2
1	D	94	ARG	2.2
1	G	201	GLY	2.2
1	B	-5	VAL	2.1
1	E	147	ARG	2.1
1	G	67	ALA	2.1
1	G	145	ALA	2.1
1	F	126	VAL	2.1
1	G	96	THR	2.1
1	G	117	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	B-factors(Å^2)	Q<0.9
2	PLP	C	500	16/16	0.89	0.57	70,71,78,79	16

6.5 Other polymers (i)

There are no such residues in this entry.