Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 02:15 am BST

PDB ID	:	4CP8
Title	:	Structure of the amidase domain of allophanate hydrolase from Pseudomonas sp strain ADP
Authors	:	Balotra, S.; Newman, J.; French, N.; French, L.; Peat, T.S.; Scott, C.
Deposited on	:	2014-02-03
Resolution	:	2.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

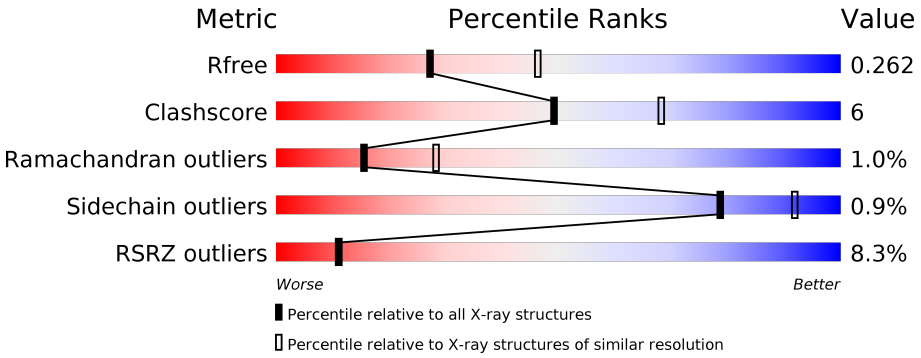
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	487	2% 84% 7% • 8%
1	B	487	2% 86% 6% 8%
1	C	487	3% 86% 6% 8%
1	D	487	2% 85% 6% • 8%
1	E	487	18% 80% 11% • 8%
1	F	487	19% 78% 12% • 9%

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLI	A	1466	-	-	X	-
2	MLI	B	1465	-	-	X	-
2	MLI	C	1466	-	-	X	-
2	MLI	D	1465	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20462 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 ALLOPHANATE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	2	0
			3375	2146	580	639	10			
1	B	447	Total	C	N	O	S	0	0	0
			3345	2126	574	635	10			
1	C	448	Total	C	N	O	S	0	0	0
			3355	2132	577	636	10			
1	D	447	Total	C	N	O	S	0	1	0
			3356	2132	577	637	10			
1	E	450	Total	C	N	O	S	0	1	0
			3373	2144	580	639	10			
1	F	444	Total	C	N	O	S	0	0	0
			3318	2110	568	630	10			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q936X2
A	-18	GLY	-	expression tag	UNP Q936X2
A	-17	SER	-	expression tag	UNP Q936X2
A	-16	SER	-	expression tag	UNP Q936X2
A	-15	HIS	-	expression tag	UNP Q936X2
A	-14	HIS	-	expression tag	UNP Q936X2
A	-13	HIS	-	expression tag	UNP Q936X2
A	-12	HIS	-	expression tag	UNP Q936X2
A	-11	HIS	-	expression tag	UNP Q936X2
A	-10	HIS	-	expression tag	UNP Q936X2
A	-9	SER	-	expression tag	UNP Q936X2
A	-8	SER	-	expression tag	UNP Q936X2
A	-7	GLY	-	expression tag	UNP Q936X2
A	-6	LEU	-	expression tag	UNP Q936X2
A	-5	VAL	-	expression tag	UNP Q936X2
A	-4	PRO	-	expression tag	UNP Q936X2
A	-3	ARG	-	expression tag	UNP Q936X2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q936X2
A	-1	SER	-	expression tag	UNP Q936X2
A	0	HIS	-	expression tag	UNP Q936X2
B	-19	MET	-	expression tag	UNP Q936X2
B	-18	GLY	-	expression tag	UNP Q936X2
B	-17	SER	-	expression tag	UNP Q936X2
B	-16	SER	-	expression tag	UNP Q936X2
B	-15	HIS	-	expression tag	UNP Q936X2
B	-14	HIS	-	expression tag	UNP Q936X2
B	-13	HIS	-	expression tag	UNP Q936X2
B	-12	HIS	-	expression tag	UNP Q936X2
B	-11	HIS	-	expression tag	UNP Q936X2
B	-10	HIS	-	expression tag	UNP Q936X2
B	-9	SER	-	expression tag	UNP Q936X2
B	-8	SER	-	expression tag	UNP Q936X2
B	-7	GLY	-	expression tag	UNP Q936X2
B	-6	LEU	-	expression tag	UNP Q936X2
B	-5	VAL	-	expression tag	UNP Q936X2
B	-4	PRO	-	expression tag	UNP Q936X2
B	-3	ARG	-	expression tag	UNP Q936X2
B	-2	GLY	-	expression tag	UNP Q936X2
B	-1	SER	-	expression tag	UNP Q936X2
B	0	HIS	-	expression tag	UNP Q936X2
C	-19	MET	-	expression tag	UNP Q936X2
C	-18	GLY	-	expression tag	UNP Q936X2
C	-17	SER	-	expression tag	UNP Q936X2
C	-16	SER	-	expression tag	UNP Q936X2
C	-15	HIS	-	expression tag	UNP Q936X2
C	-14	HIS	-	expression tag	UNP Q936X2
C	-13	HIS	-	expression tag	UNP Q936X2
C	-12	HIS	-	expression tag	UNP Q936X2
C	-11	HIS	-	expression tag	UNP Q936X2
C	-10	HIS	-	expression tag	UNP Q936X2
C	-9	SER	-	expression tag	UNP Q936X2
C	-8	SER	-	expression tag	UNP Q936X2
C	-7	GLY	-	expression tag	UNP Q936X2
C	-6	LEU	-	expression tag	UNP Q936X2
C	-5	VAL	-	expression tag	UNP Q936X2
C	-4	PRO	-	expression tag	UNP Q936X2
C	-3	ARG	-	expression tag	UNP Q936X2
C	-2	GLY	-	expression tag	UNP Q936X2
C	-1	SER	-	expression tag	UNP Q936X2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q936X2
D	-19	MET	-	expression tag	UNP Q936X2
D	-18	GLY	-	expression tag	UNP Q936X2
D	-17	SER	-	expression tag	UNP Q936X2
D	-16	SER	-	expression tag	UNP Q936X2
D	-15	HIS	-	expression tag	UNP Q936X2
D	-14	HIS	-	expression tag	UNP Q936X2
D	-13	HIS	-	expression tag	UNP Q936X2
D	-12	HIS	-	expression tag	UNP Q936X2
D	-11	HIS	-	expression tag	UNP Q936X2
D	-10	HIS	-	expression tag	UNP Q936X2
D	-9	SER	-	expression tag	UNP Q936X2
D	-8	SER	-	expression tag	UNP Q936X2
D	-7	GLY	-	expression tag	UNP Q936X2
D	-6	LEU	-	expression tag	UNP Q936X2
D	-5	VAL	-	expression tag	UNP Q936X2
D	-4	PRO	-	expression tag	UNP Q936X2
D	-3	ARG	-	expression tag	UNP Q936X2
D	-2	GLY	-	expression tag	UNP Q936X2
D	-1	SER	-	expression tag	UNP Q936X2
D	0	HIS	-	expression tag	UNP Q936X2
E	-19	MET	-	expression tag	UNP Q936X2
E	-18	GLY	-	expression tag	UNP Q936X2
E	-17	SER	-	expression tag	UNP Q936X2
E	-16	SER	-	expression tag	UNP Q936X2
E	-15	HIS	-	expression tag	UNP Q936X2
E	-14	HIS	-	expression tag	UNP Q936X2
E	-13	HIS	-	expression tag	UNP Q936X2
E	-12	HIS	-	expression tag	UNP Q936X2
E	-11	HIS	-	expression tag	UNP Q936X2
E	-10	HIS	-	expression tag	UNP Q936X2
E	-9	SER	-	expression tag	UNP Q936X2
E	-8	SER	-	expression tag	UNP Q936X2
E	-7	GLY	-	expression tag	UNP Q936X2
E	-6	LEU	-	expression tag	UNP Q936X2
E	-5	VAL	-	expression tag	UNP Q936X2
E	-4	PRO	-	expression tag	UNP Q936X2
E	-3	ARG	-	expression tag	UNP Q936X2
E	-2	GLY	-	expression tag	UNP Q936X2
E	-1	SER	-	expression tag	UNP Q936X2
E	0	HIS	-	expression tag	UNP Q936X2
F	-19	MET	-	expression tag	UNP Q936X2

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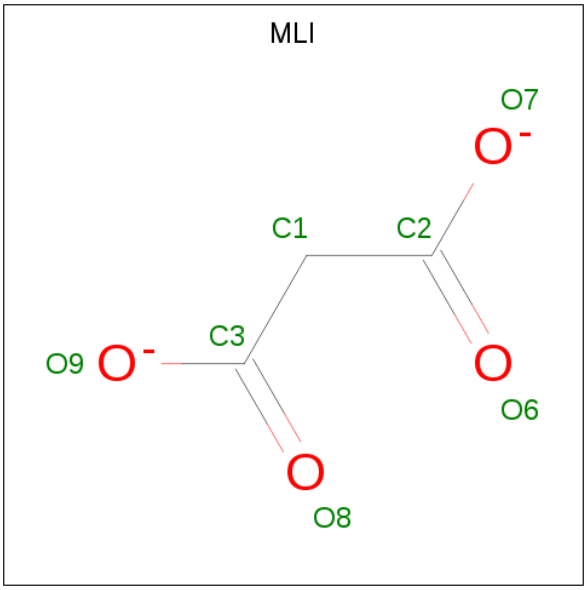
Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP Q936X2
F	-17	SER	-	expression tag	UNP Q936X2
F	-16	SER	-	expression tag	UNP Q936X2
F	-15	HIS	-	expression tag	UNP Q936X2
F	-14	HIS	-	expression tag	UNP Q936X2
F	-13	HIS	-	expression tag	UNP Q936X2
F	-12	HIS	-	expression tag	UNP Q936X2
F	-11	HIS	-	expression tag	UNP Q936X2
F	-10	HIS	-	expression tag	UNP Q936X2
F	-9	SER	-	expression tag	UNP Q936X2
F	-8	SER	-	expression tag	UNP Q936X2
F	-7	GLY	-	expression tag	UNP Q936X2
F	-6	LEU	-	expression tag	UNP Q936X2
F	-5	VAL	-	expression tag	UNP Q936X2
F	-4	PRO	-	expression tag	UNP Q936X2
F	-3	ARG	-	expression tag	UNP Q936X2
F	-2	GLY	-	expression tag	UNP Q936X2
F	-1	SER	-	expression tag	UNP Q936X2
F	0	HIS	-	expression tag	UNP Q936X2

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 3 4	0	0
2	B	1	Total C O 7 3 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 7 3 4	0	0
2	D	1	Total C O 7 3 4	0	0

- Molecule 3 is water.

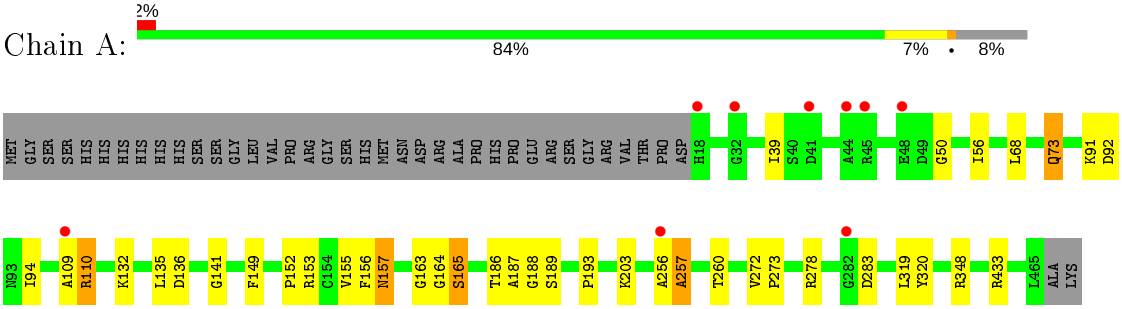
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	86	Total O 86 86	0	0
3	B	71	Total O 71 71	0	0
3	C	84	Total O 84 84	0	0
3	D	51	Total O 51 51	0	0
3	E	18	Total O 18 18	0	0
3	F	2	Total O 2 2	0	0

3 Residue-property plots (i)

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.

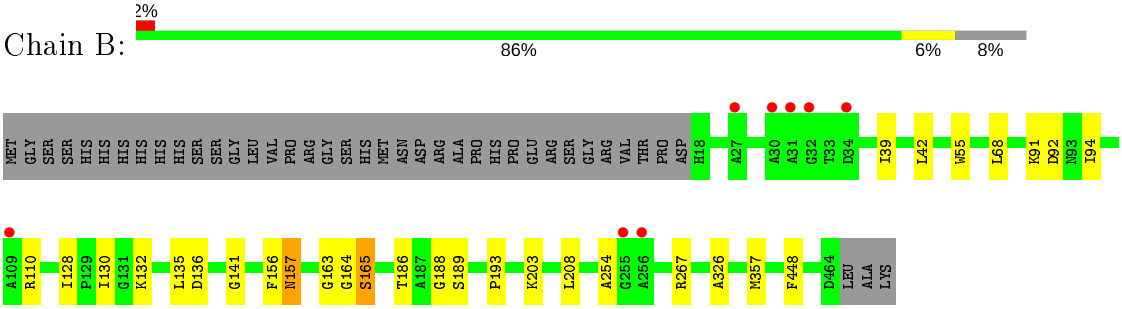
- Molecule 1: ALLOPHANATE HYDROLASE

Chain A:



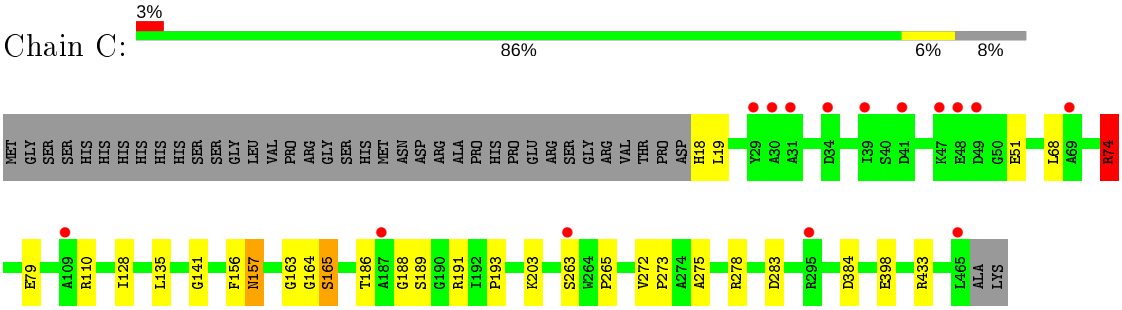
- Molecule 1: ALLOPHANATE HYDROLASE

Chain B:



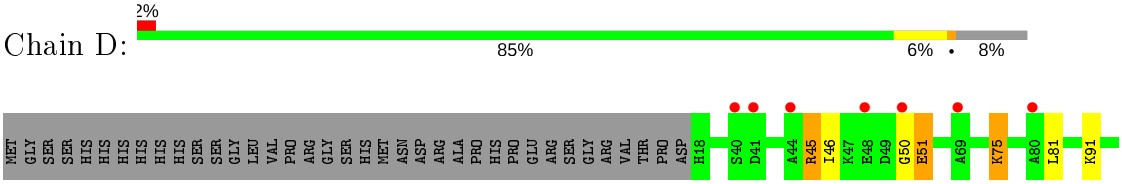
- Molecule 1: ALLOPHANATE HYDROLASE

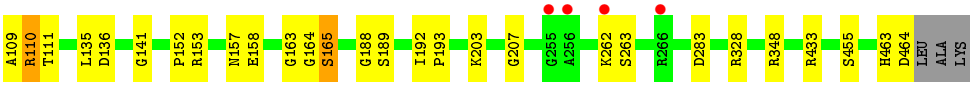
Chain C:



- Molecule 1: ALLOPHANATE HYDROLASE

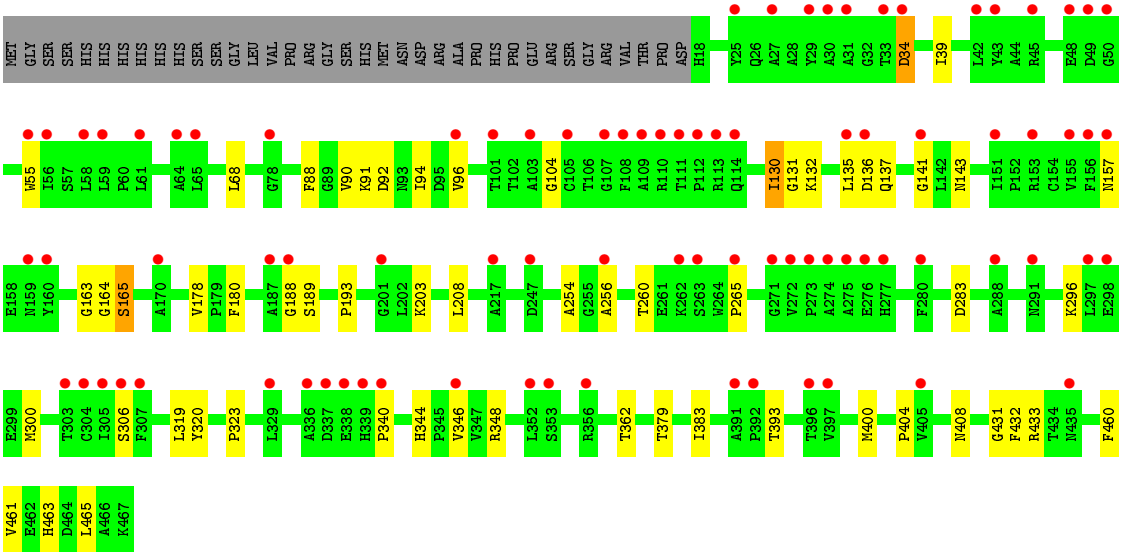
Chain D:





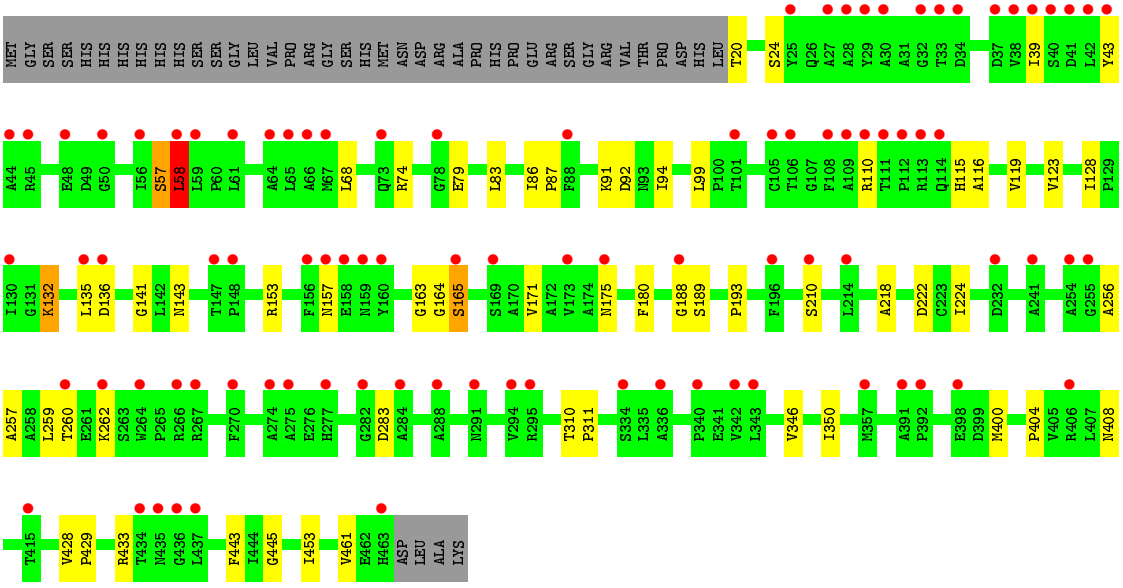
• Molecule 1: ALLOPHANATE HYDROLASE

Chain E:



• Molecule 1: ALLOPHANATE HYDROLASE

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.45Å 179.23Å 112.61Å 90.00° 106.63° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 39.59 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.50) 100.0 (39.59-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.224 , 0.259 0.226 , 0.262	Depositor DCC
R_{free} test set	5383 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 32.3	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	0.92	EDS
Total number of atoms	20462	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.37% 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: MLI

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	0.50	0/3449	0.69	1/4696 (0.0%)
1	B	0.51	0/3418	0.67	0/4654
1	C	0.52	0/3429	0.68	1/4669 (0.0%)
1	D	0.50	0/3430	0.66	1/4670 (0.0%)
1	E	0.44	0/3447	0.67	1/4694 (0.0%)
1	F	0.44	0/3391	0.70	2/4618 (0.0%)
All	All	0.49	0/20564	0.68	6/28001 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	6

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	74	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	E	34	ASP	N-CA-CB	5.99	121.38	110.60
1	F	57	SER	CB-CA-C	-5.83	99.02	110.10
1	F	58	LEU	CA-CB-CG	5.17	127.19	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	348	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	348	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	GLY	Peptide
1	B	163	GLY	Peptide
1	C	163	GLY	Peptide
1	D	163	GLY	Peptide
1	E	163	GLY	Peptide
1	F	163	GLY	Peptide

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	3375	0	3328	35	0
1	B	3345	0	3295	27	0
1	C	3355	0	3302	28	0
1	D	3356	0	3304	25	0
1	E	3373	0	3318	59	0
1	F	3318	0	3267	64	0
2	A	7	0	2	5	0
2	B	7	0	2	5	0
2	C	7	0	2	6	0
2	D	7	0	2	5	0
3	A	86	0	0	2	0
3	B	71	0	0	0	0
3	C	84	0	0	2	0
3	D	51	0	0	1	0
3	E	18	0	0	2	0
3	F	2	0	0	1	0
All	All	20462	0	19822	235	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 6.

All (235) 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:94:ILE:O	1:E:132:LYS:NZ	1.58	1.34
1:F:115:HIS:HB3	1:F:119:VAL:HG13	1.39	1.02
1:F:86:ILE:HD12	1:F:180:PHE:HE1	1.27	0.95
1:E:340:PRO:HB2	1:E:348:ARG:HE	1.35	0.92
1:D:189:SER:HG	2:D:1465:MLI:C2	1.83	0.90
1:E:92:ASP:OD1	1:E:132:LYS:HD3	1.72	0.90
1:F:218:ALA:O	1:F:222:ASP:OD1	1.89	0.90
1:A:165:SER:HB3	1:A:189:SER:HB3	1.54	0.89
1:D:189:SER:OG	2:D:1465:MLI:C2	2.20	0.89
1:E:165:SER:HB3	1:E:189:SER:HB3	1.55	0.89
1:D:165:SER:HB3	1:D:189:SER:HB3	1.56	0.87
1:F:92:ASP:OD1	1:F:132:LYS:CD	2.22	0.87
1:F:115:HIS:HB3	1:F:119:VAL:CG1	2.05	0.86
1:E:92:ASP:OD1	1:E:132:LYS:CD	2.23	0.86
1:B:165:SER:HB3	1:B:189:SER:HB3	1.57	0.85
1:F:165:SER:HB3	1:F:189:SER:HB3	1.55	0.85
1:C:165:SER:HB3	1:C:189:SER:HB3	1.56	0.85
1:E:344:HIS:CE1	1:E:346:VAL:HG22	2.11	0.85
1:E:400:MET:HE1	1:E:408:ASN:HB2	1.59	0.83
1:F:400:MET:HE1	1:F:408:ASN:HB2	1.59	0.83
1:B:94:ILE:O	1:B:132:LYS:NZ	2.13	0.80
1:A:257:ALA:HA	1:A:260:THR:OG1	1.81	0.80
1:A:94:ILE:O	1:A:132:LYS:NZ	2.14	0.80
1:F:92:ASP:OD1	1:F:132:LYS:HD3	1.82	0.79
1:F:92:ASP:OD1	1:F:132:LYS:HD2	1.81	0.79
1:F:116:ALA:O	1:F:119:VAL:HG12	1.82	0.78
1:F:86:ILE:HD12	1:F:180:PHE:CE1	2.17	0.77
1:E:88:PHE:HA	1:E:178:VAL:HG11	1.69	0.74
1:F:189:SER:OG	3:F:2001:HOH:O	2.05	0.73
1:A:165:SER:HB3	1:A:189:SER:CB	2.19	0.73
1:E:256:ALA:O	1:E:260:THR:OG1	2.07	0.73
1:C:165:SER:HB3	1:C:189:SER:CB	2.19	0.72
1:A:256:ALA:O	1:A:257:ALA:HB3	1.87	0.72
1:B:165:SER:HB3	1:B:189:SER:CB	2.20	0.72
1:E:165:SER:HB3	1:E:189:SER:CB	2.19	0.72
1:F:165:SER:HB3	1:F:189:SER:CB	2.19	0.72
1:F:83:LEU:HB3	1:F:86:ILE:HD11	1.70	0.71
1:E:88:PHE:HA	1:E:178:VAL:CG1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:SER:HB3	1:D:189:SER:CB	2.20	0.71
1:F:83:LEU:HB3	1:F:86:ILE:CD1	2.21	0.71
1:C:273:PRO:O	1:C:278:ARG:NH1	2.24	0.70
1:A:73[B]:GLN:NE2	3:A:2006:HOH:O	2.25	0.70
1:E:265:PRO:O	3:E:2011:HOH:O	2.11	0.68
1:A:273:PRO:O	1:A:278:ARG:NH1	2.25	0.68
1:E:178:VAL:HG12	1:E:180:PHE:O	1.92	0.68
1:F:428:VAL:HG21	1:F:461:VAL:CG2	2.23	0.68
1:E:379:THR:O	1:E:383:ILE:HG12	1.93	0.68
1:E:400:MET:CE	1:E:408:ASN:HB2	2.23	0.68
1:F:400:MET:CE	1:F:408:ASN:HB2	2.23	0.68
1:E:283:ASP:OD2	1:E:393:THR:HG23	1.93	0.68
1:F:210:SER:O	1:F:224:ILE:HD13	1.93	0.67
1:B:55:TRP:CH2	1:B:130:ILE:HD11	2.29	0.67
1:E:400:MET:HE3	1:E:404:PRO:O	1.95	0.67
1:F:83:LEU:O	1:F:86:ILE:HG12	1.94	0.66
1:E:90:VAL:HG11	1:E:96:VAL:HG21	1.77	0.66
1:F:400:MET:HE3	1:F:404:PRO:O	1.96	0.65
1:E:92:ASP:OD1	1:E:132:LYS:HD2	1.94	0.65
1:A:56[A]:ILE:HD12	1:A:149:PHE:CD2	2.31	0.65
1:E:178:VAL:CG1	1:E:180:PHE:O	2.45	0.65
1:F:86:ILE:CD1	1:F:180:PHE:HE1	2.05	0.65
1:A:164:GLY:HA3	1:A:193:PRO:HG3	1.80	0.64
1:E:344:HIS:HE1	1:E:346:VAL:HG22	1.63	0.64
1:F:428:VAL:HG21	1:F:461:VAL:HG23	1.80	0.63
1:C:164:GLY:HA3	1:C:193:PRO:HG3	1.81	0.62
1:E:300:MET:HE2	1:E:463:HIS:HB3	1.80	0.62
1:C:265:PRO:HA	1:E:348:ARG:NH2	2.15	0.62
1:A:56[A]:ILE:HD12	1:A:149:PHE:CG	2.35	0.62
1:E:431:GLY:C	1:E:432:PHE:HD1	2.03	0.62
1:A:256:ALA:O	1:A:257:ALA:CB	2.48	0.62
1:F:164:GLY:HA3	1:F:193:PRO:HG3	1.82	0.61
1:B:164:GLY:HA3	1:B:193:PRO:HG3	1.82	0.61
1:F:428:VAL:CG2	1:F:461:VAL:CG2	2.79	0.61
1:E:164:GLY:HA3	1:E:193:PRO:HG3	1.82	0.61
1:F:218:ALA:C	1:F:222:ASP:OD1	2.38	0.60
1:D:45:ARG:HG3	1:D:46:ILE:N	2.16	0.60
1:B:186:THR:HB	2:B:1465:MLI:C1	2.33	0.59
1:D:164:GLY:HA3	1:D:193:PRO:HG3	1.83	0.59
1:F:74:ARG:O	1:F:79:GLU:HB2	2.03	0.58
1:B:189:SER:OG	2:B:1465:MLI:O7	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:SER:O	1:F:224:ILE:CD1	2.52	0.58
1:F:283:ASP:OD2	1:F:433:ARG:NH1	2.37	0.58
1:E:55:TRP:CH2	1:E:130:ILE:CD1	2.88	0.57
1:A:283:ASP:OD2	1:A:433:ARG:NH1	2.38	0.57
1:D:283:ASP:OD2	1:D:433:ARG:NH1	2.37	0.57
1:E:283:ASP:OD2	1:E:433:ARG:NH1	2.37	0.57
1:F:94:ILE:O	1:F:132:LYS:HE2	2.05	0.57
1:F:257:ALA:O	1:F:260:THR:N	2.25	0.56
1:C:283:ASP:OD2	1:C:433:ARG:NH1	2.39	0.56
1:E:90:VAL:HG11	1:E:96:VAL:CG2	2.35	0.56
1:E:55:TRP:CH2	1:E:130:ILE:HD11	2.41	0.56
1:C:272:VAL:HG12	1:C:278:ARG:NH1	2.21	0.55
1:F:428:VAL:CG2	1:F:429:PRO:HD2	2.36	0.55
1:A:50:GLY:HA3	3:A:2003:HOH:O	2.06	0.55
1:D:189:SER:OG	2:D:1465:MLI:C1	2.54	0.55
1:D:463:HIS:O	1:D:464:ASP:HB2	2.08	0.54
1:C:74:ARG:HG2	1:C:79:GLU:CD	2.27	0.53
1:E:323:PRO:HB2	1:E:362:THR:HG22	1.91	0.53
1:F:428:VAL:HG23	1:F:429:PRO:HD2	1.89	0.53
1:F:83:LEU:HD22	1:F:86:ILE:HD13	1.89	0.53
1:E:104:GLY:O	1:E:137:GLN:HG3	2.08	0.53
1:F:20:THR:N	1:F:24:SER:HG	2.07	0.52
1:B:186:THR:HB	2:B:1465:MLI:H12	1.90	0.52
1:F:143:ASN:ND2	1:F:400:MET:HE1	2.25	0.52
1:A:272:VAL:HG12	1:A:278:ARG:NH1	2.23	0.52
1:C:189:SER:OG	2:C:1466:MLI:O7	2.22	0.52
1:C:164:GLY:O	1:C:189:SER:HA	2.09	0.52
1:C:18:HIS:CG	1:C:19:LEU:H	2.28	0.52
1:E:300:MET:CE	1:E:460:PHE:HA	2.40	0.52
1:E:143:ASN:ND2	1:E:400:MET:HE1	2.25	0.52
1:C:141:GLY:O	1:C:165:SER:HB2	2.10	0.52
1:B:254:ALA:HB2	1:B:448:PHE:CE1	2.45	0.52
1:E:300:MET:HE2	1:E:460:PHE:HA	1.91	0.52
1:F:164:GLY:O	1:F:189:SER:HA	2.10	0.52
1:A:189:SER:OG	2:A:1466:MLI:C2	2.57	0.51
1:D:141:GLY:O	1:D:165:SER:HB2	2.10	0.51
1:D:189:SER:HG	2:D:1465:MLI:C1	2.22	0.51
1:B:164:GLY:O	1:B:189:SER:HA	2.10	0.51
1:B:326:ALA:HB2	1:B:357:MET:CE	2.41	0.51
1:D:164:GLY:O	1:D:189:SER:HA	2.11	0.51
1:A:164:GLY:O	1:A:189:SER:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:PRO:HB2	1:E:348:ARG:NE	2.16	0.51
1:E:164:GLY:O	1:E:189:SER:HA	2.11	0.51
1:A:141:GLY:O	1:A:165:SER:HB2	2.11	0.50
1:B:141:GLY:O	1:B:165:SER:HB2	2.11	0.50
1:B:42:LEU:HD21	1:B:130:ILE:HD13	1.94	0.50
1:C:186:THR:HB	2:C:1466:MLI:C1	2.42	0.50
1:A:186:THR:HB	2:A:1466:MLI:C1	2.42	0.50
1:E:90:VAL:HG12	1:E:131:GLY:O	2.11	0.50
1:E:208:LEU:CD1	1:E:254:ALA:HB2	2.40	0.50
1:F:141:GLY:O	1:F:165:SER:HB2	2.11	0.50
1:B:189:SER:OG	2:B:1465:MLI:C2	2.60	0.50
1:E:344:HIS:ND1	1:E:346:VAL:HG22	2.26	0.50
1:F:445:GLY:HA3	1:F:453:ILE:HD11	1.93	0.50
1:E:141:GLY:O	1:E:165:SER:HB2	2.11	0.49
1:C:189:SER:HG	2:C:1466:MLI:C2	2.21	0.49
1:C:189:SER:OG	2:C:1466:MLI:C2	2.60	0.49
1:C:51:GLU:HB2	3:C:2004:HOH:O	2.13	0.49
1:E:300:MET:CE	1:E:463:HIS:HB3	2.42	0.48
1:A:319:LEU:HD22	1:A:320:TYR:CE2	2.48	0.48
1:F:86:ILE:O	1:F:86:ILE:HG13	2.13	0.48
1:D:207:GLY:HA2	3:D:2027:HOH:O	2.12	0.48
1:E:55:TRP:CH2	1:E:130:ILE:HD12	2.49	0.48
1:E:135:LEU:HD13	1:E:136:ASP:O	2.14	0.48
1:E:344:HIS:CE1	1:E:346:VAL:CG2	2.91	0.48
1:F:135:LEU:HD13	1:F:136:ASP:O	2.14	0.48
1:A:92:ASP:OD1	1:A:132:LYS:HE2	2.14	0.48
1:D:75:LYS:HB2	1:D:81:LEU:HD12	1.95	0.48
1:A:109:ALA:O	1:A:110:ARG:HB2	2.13	0.48
1:B:39:ILE:HD12	1:B:68:LEU:HD22	1.96	0.48
1:E:90:VAL:HG13	1:E:90:VAL:O	2.13	0.48
1:A:189:SER:HG	2:A:1466:MLI:C2	2.27	0.47
1:A:39:ILE:HD12	1:A:68:LEU:HD22	1.96	0.47
1:F:346:VAL:O	1:F:350:ILE:HG12	2.14	0.47
1:D:135:LEU:HD13	1:D:136:ASP:O	2.14	0.47
1:F:39:ILE:CD1	1:F:128:ILE:CD1	2.93	0.47
1:B:92:ASP:OD1	1:B:132:LYS:HE2	2.15	0.47
1:D:109:ALA:O	1:D:110:ARG:HB2	2.15	0.47
1:E:296:LYS:HG2	1:E:300:MET:HE1	1.97	0.47
1:E:306:SER:HA	3:E:2013:HOH:O	2.15	0.47
1:F:428:VAL:CG2	1:F:429:PRO:CD	2.93	0.47
1:A:135:LEU:HD13	1:A:136:ASP:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:171:VAL:O	1:F:175:ASN:HB2	2.16	0.46
1:E:319:LEU:HD22	1:E:320:TYR:CE2	2.51	0.46
1:B:135:LEU:HD13	1:B:136:ASP:O	2.15	0.46
1:F:119:VAL:O	1:F:123:VAL:HG13	2.16	0.46
1:A:189:SER:OG	2:A:1466:MLI:O7	2.32	0.46
1:C:68:LEU:HD13	1:C:128:ILE:HD11	1.98	0.45
1:D:164:GLY:HA3	1:D:193:PRO:CG	2.46	0.45
1:A:187:ALA:H	2:A:1466:MLI:C2	2.30	0.45
1:E:130:ILE:HD11	1:E:178:VAL:HG21	1.99	0.45
1:B:91:LYS:HG2	1:B:135:LEU:HD23	1.98	0.45
1:A:91:LYS:HG2	1:A:135:LEU:HD23	1.99	0.45
1:F:164:GLY:O	1:F:165:SER:CB	2.65	0.45
1:C:191:ARG:HD2	3:C:2031:HOH:O	2.16	0.45
1:D:50:GLY:O	1:D:51:GLU:HB2	2.17	0.45
1:E:39:ILE:HD12	1:E:68:LEU:HD22	1.98	0.45
1:F:39:ILE:HD12	1:F:68:LEU:HD22	1.99	0.45
1:B:55:TRP:CH2	1:B:130:ILE:CD1	2.98	0.45
1:A:257:ALA:HA	1:A:260:THR:HG1	1.82	0.44
1:C:164:GLY:O	1:C:165:SER:CB	2.65	0.44
1:E:91:LYS:HG2	1:E:135:LEU:HD23	1.99	0.44
1:F:39:ILE:HD11	1:F:128:ILE:CD1	2.47	0.44
1:F:443:PHE:HB3	1:F:453:ILE:HG23	1.98	0.44
1:D:91:LYS:HG2	1:D:135:LEU:HD23	2.00	0.44
1:B:164:GLY:O	1:B:165:SER:CB	2.65	0.44
1:B:68:LEU:HD13	1:B:128:ILE:HD11	2.00	0.44
1:C:186:THR:HB	2:C:1466:MLI:H12	1.99	0.44
1:E:164:GLY:O	1:E:165:SER:CB	2.65	0.44
1:F:43:TYR:HD2	1:F:58:LEU:HD21	1.83	0.44
1:F:57:SER:HB3	1:F:99:LEU:HD22	1.99	0.44
1:A:164:GLY:O	1:A:165:SER:CB	2.65	0.43
1:E:164:GLY:HA3	1:E:193:PRO:CG	2.48	0.43
1:F:164:GLY:HA3	1:F:193:PRO:CG	2.48	0.43
1:D:262:LYS:O	1:D:455[B]:SER:OG	2.18	0.43
1:A:164:GLY:HA3	1:A:193:PRO:CG	2.48	0.43
1:D:152:PRO:C	1:D:153:ARG:HG2	2.39	0.43
1:D:164:GLY:O	1:D:165:SER:CB	2.66	0.43
1:E:88:PHE:HA	1:E:178:VAL:HG13	1.98	0.43
1:F:83:LEU:HB3	1:F:86:ILE:CG1	2.49	0.43
1:A:135:LEU:C	1:A:135:LEU:HD12	2.39	0.43
1:F:257:ALA:HA	1:F:260:THR:CG2	2.48	0.43
1:C:74:ARG:HH11	1:C:74:ARG:HG2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:ILE:CD1	1:F:128:ILE:HD13	2.48	0.42
1:A:56[A]:ILE:CD1	1:A:149:PHE:CG	3.03	0.42
1:B:267:ARG:NH2	1:C:384:ASP:OD1	2.52	0.42
1:E:461:VAL:O	1:E:465:LEU:HD22	2.19	0.42
1:B:135:LEU:HD12	1:B:135:LEU:C	2.40	0.42
1:F:87:PRO:HA	1:F:128:ILE:HG13	2.02	0.42
1:F:43:TYR:CD2	1:F:58:LEU:HD21	2.55	0.42
1:B:208:LEU:CD1	1:B:254:ALA:HB3	2.49	0.42
1:C:156:PHE:O	1:C:157:ASN:HB2	2.20	0.42
1:F:39:ILE:HD11	1:F:128:ILE:HD13	2.02	0.42
1:C:164:GLY:HA3	1:C:193:PRO:CG	2.47	0.42
1:F:91:LYS:HG2	1:F:135:LEU:HD23	2.00	0.42
1:D:153:ARG:HD2	1:D:158:GLU:O	2.20	0.41
1:B:164:GLY:HA3	1:B:193:PRO:CG	2.48	0.41
1:E:208:LEU:CD1	1:E:254:ALA:CB	2.98	0.41
1:C:275:ALA:HA	1:C:278:ARG:HG3	2.02	0.41
1:C:263:SER:O	1:E:348:ARG:NH1	2.54	0.41
1:C:186:THR:HB	2:C:1466:MLI:C2	2.50	0.41
1:C:74:ARG:CG	1:C:79:GLU:CD	2.89	0.41
1:F:445:GLY:CA	1:F:453:ILE:HD11	2.50	0.41
1:A:152:PRO:C	1:A:153:ARG:HG2	2.41	0.41
1:B:156:PHE:O	1:B:157:ASN:HB2	2.20	0.41
1:F:428:VAL:HG23	1:F:429:PRO:CD	2.51	0.41
1:F:257:ALA:O	1:F:259:LEU:N	2.54	0.41
1:F:453:ILE:O	1:F:453:ILE:HG22	2.20	0.41
1:A:135:LEU:HD12	1:A:135:LEU:O	2.21	0.40
1:E:296:LYS:HG2	1:E:300:MET:CE	2.52	0.40
1:F:310:THR:HB	1:F:311:PRO:CD	2.51	0.40
1:A:156:PHE:O	1:A:157:ASN:HB2	2.22	0.40
1:B:186:THR:HB	2:B:1465:MLI:C2	2.52	0.40
1:D:328:ARG:NH2	2:D:1465:MLI:O9	2.46	0.40
1:D:192:ILE:HB	1:D:193:PRO:HD3	2.04	0.40
1:E:431:GLY:O	1:E:432:PHE:HD1	2.05	0.40

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	448/487 (92%)	429 (96%)	14 (3%)	5 (1%)	14	26
1	B	445/487 (91%)	427 (96%)	14 (3%)	4 (1%)	17	31
1	C	446/487 (92%)	426 (96%)	16 (4%)	4 (1%)	17	31
1	D	446/487 (92%)	429 (96%)	12 (3%)	5 (1%)	14	26
1	E	449/487 (92%)	431 (96%)	14 (3%)	4 (1%)	17	31
1	F	442/487 (91%)	421 (95%)	16 (4%)	5 (1%)	14	26
All	All	2676/2922 (92%)	2563 (96%)	86 (3%)	27 (1%)	15	28

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	B	165	SER
1	C	165	SER
1	D	51	GLU
1	D	165	SER
1	E	165	SER
1	F	165	SER
1	A	110	ARG
1	B	110	ARG
1	B	157	ASN
1	C	110	ARG
1	D	110	ARG
1	E	34	ASP
1	F	110	ARG
1	A	157	ASN
1	A	188	GLY
1	A	257	ALA
1	B	188	GLY
1	C	157	ASN
1	C	188	GLY

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Mol	Chain	Res	Type
1	D	157	ASN
1	D	188	GLY
1	E	157	ASN
1	E	188	GLY
1	F	157	ASN
1	F	188	GLY
1	F	256	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	344/375 (92%)	340 (99%)	4 (1%)	71	88
1	B	340/375 (91%)	339 (100%)	1 (0%)	92	97
1	C	341/375 (91%)	337 (99%)	4 (1%)	71	88
1	D	342/375 (91%)	337 (98%)	5 (2%)	65	85
1	E	342/375 (91%)	340 (99%)	2 (1%)	86	95
1	F	337/375 (90%)	333 (99%)	4 (1%)	71	88
All	All	2046/2250 (91%)	2026 (99%)	20 (1%)	78	90

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73[A]	GLN
1	A	73[B]	GLN
1	A	155	VAL
1	A	203	LYS
1	B	203	LYS
1	C	74	ARG
1	C	135	LEU
1	C	203	LYS
1	C	398	GLU
1	D	45	ARG
1	D	75	LYS

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Mol	Chain	Res	Type
1	D	111	THR
1	D	203	LYS
1	D	263	SER
1	E	130	ILE
1	E	203	LYS
1	F	58	LEU
1	F	132	LYS
1	F	153	ARG
1	F	262	LYS

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

Mol	Chain	Res	Type
1	C	72	GLN

5.3.3 RNA (i)

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 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	$\#\|Z\|>2$
2	MLI	C	1466	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	B	1465	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	A	1466	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	D	1465	-	0,6,6	0.00	-	0,7,7	0.00	-

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	MLI	C	1466	-	-	0/0/4/4	-
2	MLI	B	1465	-	-	0/0/4/4	-
2	MLI	A	1466	-	-	0/0/4/4	-
2	MLI	D	1465	-	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1466	MLI	6	0
2	B	1465	MLI	5	0
2	A	1466	MLI	5	0
2	D	1465	MLI	5	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	448/487 (91%)	-0.00	9 (2%) 65 68	16, 26, 59, 96	0
1	B	447/487 (91%)	-0.04	8 (1%) 68 71	16, 28, 59, 84	0
1	C	448/487 (91%)	0.07	15 (3%) 46 50	14, 25, 61, 81	0
1	D	447/487 (91%)	0.12	11 (2%) 57 61	15, 28, 58, 95	0
1	E	450/487 (92%)	1.22	86 (19%) 1 1	35, 63, 90, 115	0
1	F	444/487 (91%)	1.34	93 (20%) 1 0	43, 74, 100, 117	0
All	All	2684/2922 (91%)	0.45	222 (8%) 11 11	14, 35, 87, 117	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	50	GLY	6.5
1	F	78	GLY	5.8
1	E	108	PHE	5.8
1	F	434	THR	5.6
1	F	436	GLY	5.4
1	F	109	ALA	5.3
1	E	336	ALA	5.3
1	D	50	GLY	4.9
1	E	109	ALA	4.8
1	F	437	LEU	4.7
1	F	130	ILE	4.6
1	E	153	ARG	4.5
1	E	276	GLU	4.5
1	E	159	ASN	4.4
1	D	262	LYS	4.3
1	F	108	PHE	4.3
1	A	109	ALA	4.2
1	F	25	TYR	4.2
1	A	256	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	340	PRO	4.0
1	E	291	ASN	4.0
1	E	48	GLU	3.9
1	F	266	ARG	3.9
1	F	159	ASN	3.9
1	F	40	SER	3.9
1	F	73	GLN	3.9
1	F	29	TYR	3.8
1	F	113	ARG	3.7
1	F	114	GLN	3.7
1	F	48	GLU	3.7
1	D	256	ALA	3.7
1	E	114	GLN	3.7
1	E	306	SER	3.7
1	E	160	TYR	3.6
1	E	43	TYR	3.6
1	B	255	GLY	3.6
1	F	435	ASN	3.6
1	D	48	GLU	3.5
1	F	175	ASN	3.5
1	E	274	ALA	3.5
1	F	42	LEU	3.5
1	E	262	LYS	3.5
1	F	274	ALA	3.4
1	E	64	ALA	3.4
1	F	50	GLY	3.4
1	F	157	ASN	3.4
1	F	28	ALA	3.3
1	F	64	ALA	3.3
1	C	465	LEU	3.3
1	E	33	THR	3.3
1	E	27	ALA	3.3
1	F	111	THR	3.2
1	E	337	ASP	3.2
1	F	32	GLY	3.2
1	F	158	GLU	3.2
1	D	69	ALA	3.1
1	F	277	HIS	3.1
1	F	262	LYS	3.1
1	E	256	ALA	3.1
1	F	33	THR	3.1
1	F	284	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	48	GLU	3.1
1	E	396	THR	3.1
1	F	58	LEU	3.1
1	F	275	ALA	3.1
1	E	307	PHE	3.0
1	F	295	ARG	3.0
1	E	42	LEU	3.0
1	F	27	ALA	3.0
1	D	266	ARG	3.0
1	B	30	ALA	3.0
1	E	305	ILE	3.0
1	A	48	GLU	3.0
1	E	111	THR	3.0
1	F	61	LEU	2.9
1	E	25	TYR	2.9
1	E	113	ARG	2.9
1	E	135	LEU	2.9
1	E	265	PRO	2.9
1	F	148	PRO	2.9
1	F	391	ALA	2.9
1	F	88	PHE	2.9
1	F	260	THR	2.9
1	E	30	ALA	2.9
1	E	170	ALA	2.9
1	E	105	CYS	2.9
1	F	294	VAL	2.9
1	E	107	GLY	2.9
1	A	44	ALA	2.9
1	E	157	ASN	2.8
1	F	188	GLY	2.8
1	C	49	ASP	2.8
1	F	334	SER	2.8
1	F	38	VAL	2.8
1	F	34	ASP	2.8
1	E	187	ALA	2.8
1	E	273	PRO	2.8
1	C	31	ALA	2.8
1	F	255	GLY	2.7
1	E	103	ALA	2.7
1	E	151	ILE	2.7
1	F	398	GLU	2.7
1	F	39	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	339	HIS	2.7
1	E	397	VAL	2.7
1	F	336	ALA	2.7
1	F	210	SER	2.7
1	E	110	ARG	2.7
1	E	45	ARG	2.7
1	C	69	ALA	2.6
1	C	295	ARG	2.6
1	E	303	THR	2.6
1	E	61	LEU	2.6
1	F	135	LEU	2.6
1	E	155	VAL	2.6
1	C	47	LYS	2.6
1	E	29	TYR	2.6
1	E	112	PRO	2.6
1	E	356	ARG	2.6
1	B	27	ALA	2.6
1	E	391	ALA	2.6
1	F	214	LEU	2.6
1	F	291	ASN	2.6
1	F	43	TYR	2.6
1	F	147	THR	2.5
1	E	34	ASP	2.5
1	F	67	MET	2.5
1	F	270	PHE	2.5
1	E	277	HIS	2.5
1	A	41	ASP	2.5
1	F	156	PHE	2.5
1	F	112	PRO	2.5
1	E	297	LEU	2.5
1	D	255	GLY	2.5
1	D	44	ALA	2.5
1	E	55	TRP	2.5
1	C	29	TYR	2.5
1	E	405	VAL	2.5
1	E	263	SER	2.5
1	F	66	ALA	2.5
1	F	101	THR	2.5
1	F	254	ALA	2.5
1	F	160	TYR	2.5
1	F	41	ASP	2.5
1	F	267	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	288	ALA	2.4
1	F	173	VAL	2.4
1	F	45	ARG	2.4
1	F	196	PHE	2.4
1	B	32	GLY	2.4
1	F	288	ALA	2.4
1	E	156	PHE	2.4
1	F	44	ALA	2.4
1	F	165	SER	2.4
1	E	78	GLY	2.4
1	F	463	HIS	2.4
1	E	298	GLU	2.4
1	B	256	ALA	2.3
1	B	109	ALA	2.3
1	D	40	SER	2.3
1	E	188	GLY	2.3
1	A	45	ARG	2.3
1	F	105	CYS	2.3
1	C	263	SER	2.3
1	F	415	THR	2.3
1	E	304	CYS	2.3
1	E	435	ASN	2.3
1	E	49	ASP	2.3
1	F	59	LEU	2.3
1	F	406	ARG	2.3
1	C	109	ALA	2.3
1	F	232	ASP	2.3
1	E	217	ALA	2.3
1	E	275	ALA	2.3
1	F	343	LEU	2.3
1	E	96	VAL	2.2
1	F	282	GLY	2.2
1	B	34	ASP	2.2
1	C	30	ALA	2.2
1	E	352	LEU	2.2
1	F	65	LEU	2.2
1	F	392	PRO	2.2
1	F	136	ASP	2.2
1	F	106	THR	2.2
1	E	65[A]	LEU	2.2
1	E	346	VAL	2.2
1	E	59	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	271	GLY	2.2
1	E	329	LEU	2.2
1	A	18	HIS	2.2
1	E	338	GLU	2.2
1	E	272	VAL	2.2
1	B	31	ALA	2.2
1	A	282	GLY	2.2
1	F	342	VAL	2.1
1	E	392	PRO	2.1
1	E	58	LEU	2.1
1	F	37	ASP	2.1
1	F	340	PRO	2.1
1	F	110	ARG	2.1
1	E	201	GLY	2.1
1	F	30	ALA	2.1
1	F	169	SER	2.1
1	A	32	GLY	2.1
1	F	357	MET	2.1
1	E	280	PHE	2.1
1	D	80	ALA	2.1
1	E	101	THR	2.1
1	D	41	ASP	2.1
1	E	247	ASP	2.1
1	F	264	TRP	2.1
1	E	141	GLY	2.0
1	E	31	ALA	2.0
1	F	241	ALA	2.0
1	E	353	SER	2.0
1	F	56	ILE	2.0
1	C	34	ASP	2.0
1	E	136	ASP	2.0
1	C	187	ALA	2.0
1	C	39	ILE	2.0
1	E	56	ILE	2.0
1	C	41	ASP	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 carbohydrates 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	MLI	A	1466	7/7	0.92	0.18	24,28,30,31	0
2	MLI	B	1465	7/7	0.93	0.17	29,30,36,40	0
2	MLI	C	1466	7/7	0.95	0.17	21,26,28,33	0
2	MLI	D	1465	7/7	0.95	0.15	25,31,35,36	0

6.5 Other polymers (i)

There are no such residues in this entry.