



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:05 PM UTC

PDB ID : 4CP8 / pdb_00004cp8
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 ⓘ 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:

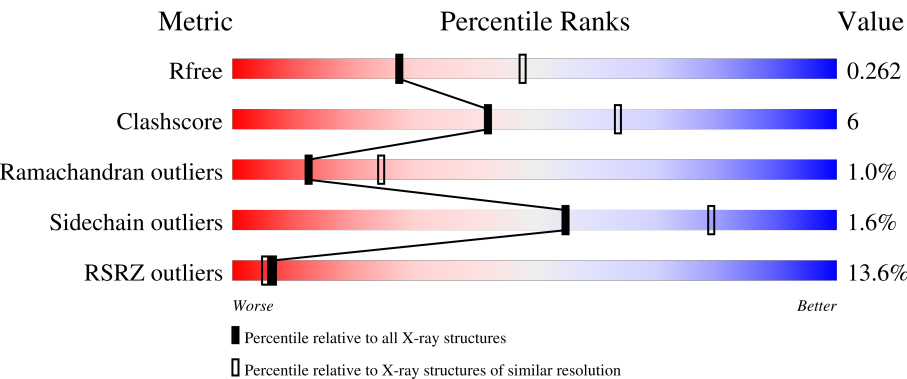
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	487	2% 82% 8% 8%
1	B	487	2% 84% 7% 8%
1	C	487	% 84% 7% 8%
1	D	487	2% 84% 7% 8%
1	E	487	31% 79% 13% 8%

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Mol	Chain	Length	Quality of chain
1	F	487	

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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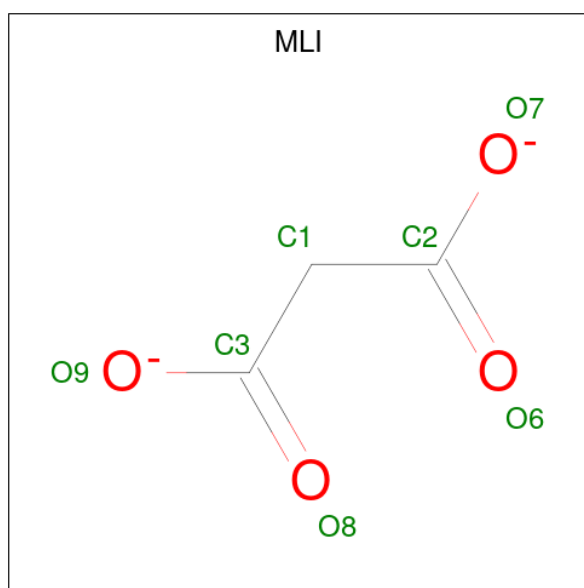
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q936X2
D	-19	MET	-	expression tag	UNP Q936X2
D	-18	GLY	-	expression tag	UNP Q936X2
D	-17	SER	-	expression tag	UNP Q936X2
D	-16	SER	-	expression tag	UNP Q936X2
D	-15	HIS	-	expression tag	UNP Q936X2
D	-14	HIS	-	expression tag	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 (CCD ID: MLI) (formula: $C_3H_2O_4$).



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

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

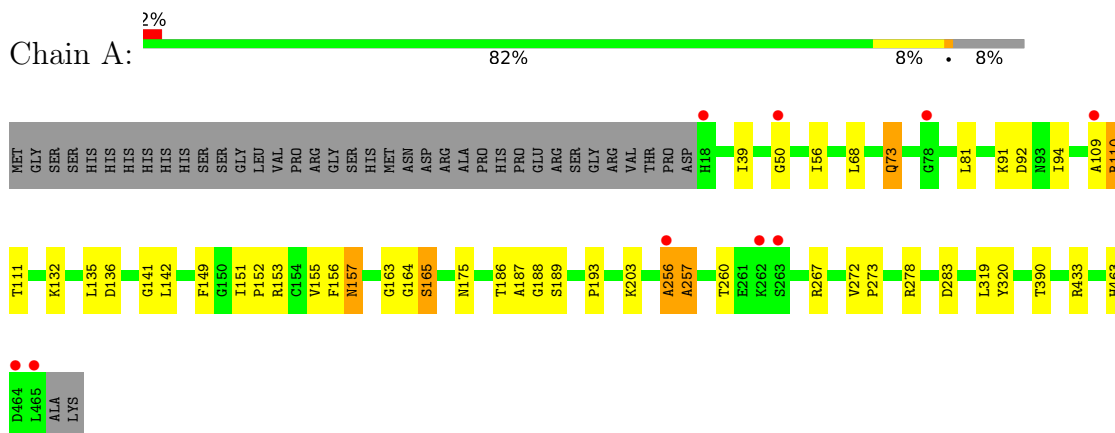
- Molecule 3 is water.

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

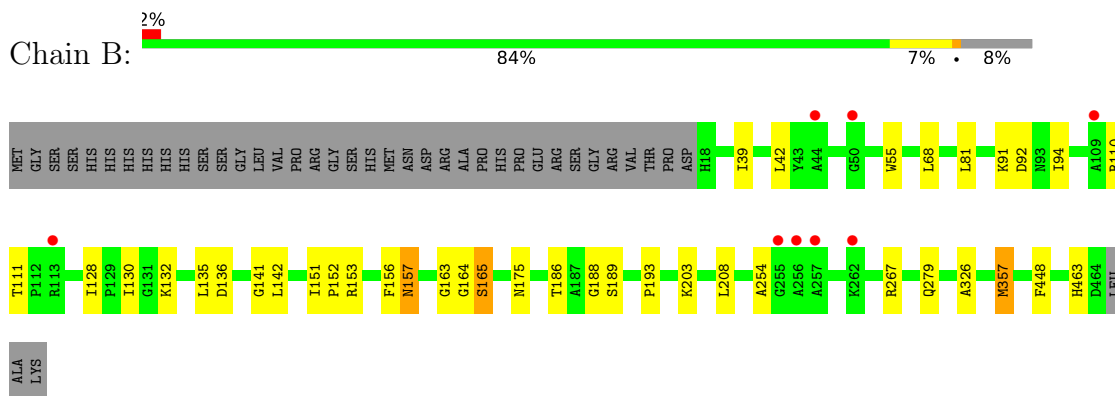
3 Residue-property plots [i](#)

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.

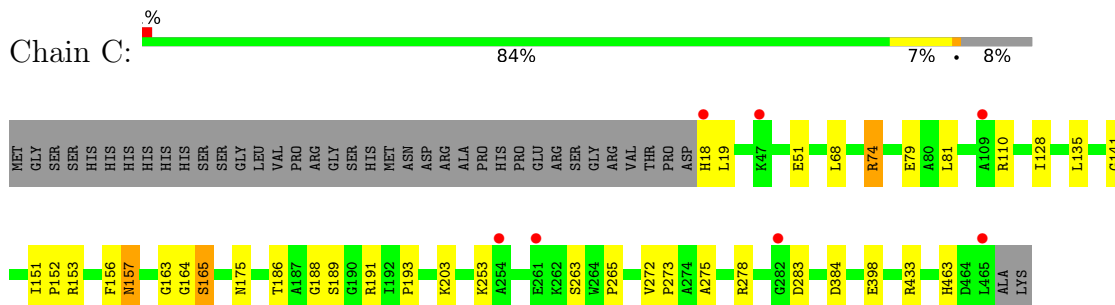
• Molecule 1: ALLOPHANATE HYDROLASE



• Molecule 1: ALLOPHANATE HYDROLASE

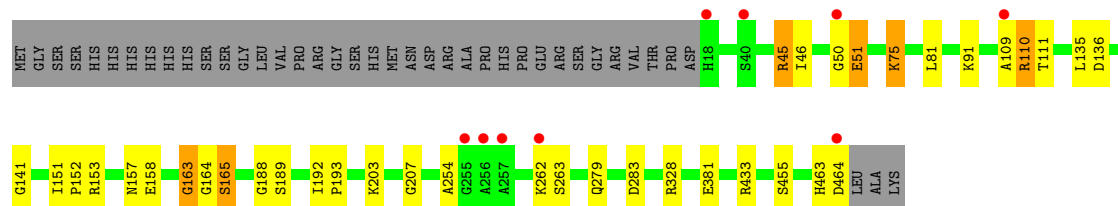


• Molecule 1: ALLOPHANATE HYDROLASE



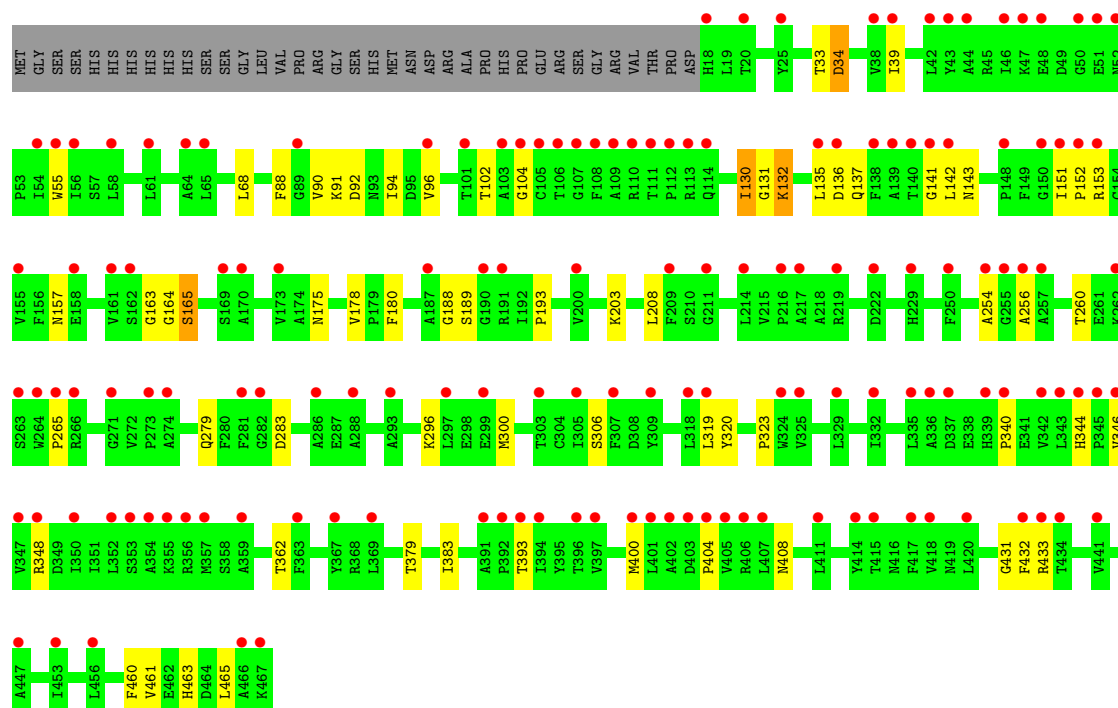
● Molecule 1: ALLOPHANATE HYDROLASE

Chain D:  2% 84% 7% 8%



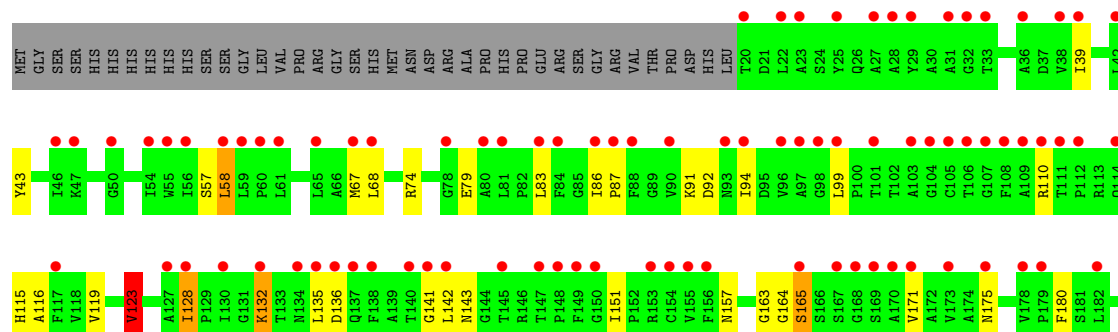
● Molecule 1: ALLOPHANATE HYDROLASE

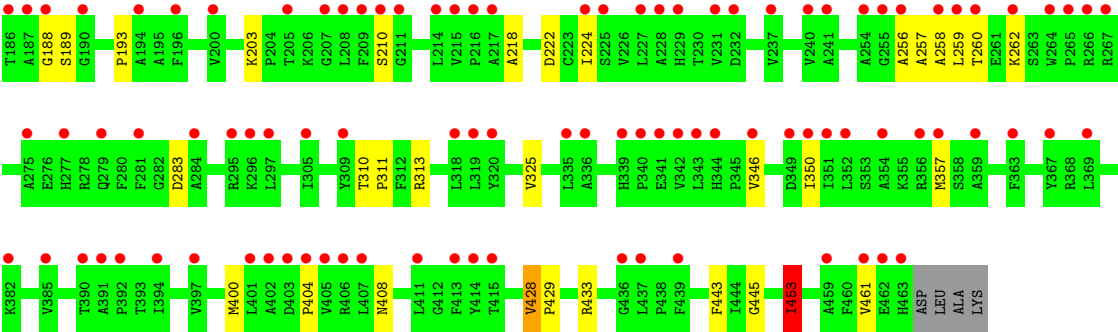
Chain E:  31% 79% 13% 8%



● Molecule 1: ALLOPHANATE HYDROLASE

Chain F:  38% 77% 12% 9%





4 Data and refinement statistics

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 40.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.50) 100.0 (40.00-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.69	0/3449	0.87	5/4696 (0.1%)
1	B	0.71	0/3418	0.87	3/4654 (0.1%)
1	C	0.72	0/3429	0.87	3/4669 (0.1%)
1	D	0.70	0/3430	0.86	3/4670 (0.1%)
1	E	0.62	0/3447	0.88	3/4694 (0.1%)
1	F	0.63	1/3391 (0.0%)	0.90	4/4618 (0.1%)
All	All	0.68	1/20564 (0.0%)	0.87	21/28001 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	128	ILE	CA-CB	-5.55	1.50	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	33	THR	N-CA-C	10.78	124.05	111.11
1	A	151	ILE	N-CA-C	8.70	115.48	107.56
1	B	151	ILE	N-CA-C	8.35	115.16	107.56
1	D	151	ILE	N-CA-C	7.94	114.78	107.56
1	C	253	LYS	N-CA-C	7.69	121.93	112.54
1	C	151	ILE	N-CA-C	7.00	113.93	107.56
1	A	256	ALA	N-CA-C	-6.96	101.32	110.43
1	B	463	HIS	N-CA-C	6.63	118.39	111.03
1	E	34	ASP	N-CA-CB	6.45	121.38	110.49
1	F	151	ILE	N-CA-C	6.26	113.26	107.56
1	D	254	ALA	N-CA-C	6.17	120.58	112.13
1	E	151	ILE	N-CA-C	6.13	113.14	107.56
1	B	111	THR	CB-CA-C	6.05	118.60	110.13
1	F	123	VAL	N-CA-CB	5.70	118.29	110.54
1	F	453	ILE	CB-CA-C	-5.55	104.56	112.22
1	C	463	HIS	N-CA-C	5.52	117.10	111.14
1	A	111	THR	CB-CA-C	5.37	117.65	110.13
1	A	463	HIS	N-CA-C	5.12	116.67	111.14
1	A	390	THR	N-CA-C	-5.07	105.40	111.03
1	D	163	GLY	N-CA-C	-5.07	106.35	112.48
1	F	428	VAL	N-CA-CB	-5.02	107.40	111.67

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	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3345	0	3295	30	0
1	C	3355	0	3302	30	0
1	D	3356	0	3304	25	0
1	E	3373	0	3318	66	0
1	F	3318	0	3267	68	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	4	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	253	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 (253) 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:E:400:MET:HE1	1:E:408:ASN:HB2	1.38	1.02
1:F:115:HIS:HB3	1:F:119:VAL:HG13	1.39	1.02
1:F:400:MET:HE1	1:F:408:ASN:HB2	1.39	0.98
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: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:E:300:MET:HE2	1:E:463:HIS:HB3	1.56	0.85
1:F:165:SER:HB3	1:F:189:SER:HB3	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:143:ASN:ND2	1:F:400:MET:HE2	1.97	0.79
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:E:300:MET:HE1	1:E:460:PHE:HA	1.66	0.78
1:E:143:ASN:ND2	1:E:400:MET:HE2	1.98	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:E:296:LYS:HG2	1:E:300:MET:HE3	1.71	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
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:300:MET:HE2	1:E:463:HIS:CB	2.22	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: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:E:431:GLY:C	1:E:432:PHE:HD1	2.03	0.67
1:B:55:TRP:CH2	1:B:130:ILE:HD11	2.29	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:E:92:ASP:OD1	1:E:132:LYS:HD2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:218:ALA:C	1:F:222:ASP:OD1	2.38	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: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:F:400:MET:CE	1:F:408:ASN:HB2	2.23	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: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
1:E:400:MET:CE	1:E:408:ASN:HB2	2.23	0.58
1:F:210:SER:O	1:F:224:ILE:CD1	2.52	0.58
1:C:74:ARG:HG2	1:C:79:GLU:CD	2.27	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: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:F:257:ALA:O	1:F:260:THR:N	2.25	0.56
1:D:262:LYS:O	1:D:455[B]:SER:OG	2.18	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:E:296:LYS:CG	1:E:300:MET:HE3	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:186:THR:HB	2:B:1465:MLI:H12	1.90	0.52
1:A:272:VAL:HG12	1:A:278:ARG:NH1	2.23	0.52
1:C:18:HIS:CG	1:C:19:LEU:H	2.28	0.52
1:C:164:GLY:O	1:C:189:SER:HA	2.09	0.52
1:C:189:SER:OG	2:C:1466:MLI:O7	2.22	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: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:F:400:MET:HE3	1:F:404:PRO:HA	1.92	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
1:E:340:PRO:HB2	1:E:348:ARG:NE	2.16	0.51
1:E:300:MET:CE	1:E:460:PHE:HA	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:400:MET:HE3	1:E:404:PRO:HA	1.94	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:D:152:PRO:C	1:D:153:ARG:HG2	2.39	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:A:135:LEU:C	1:A:135:LEU:HD12	2.39	0.47
1:B:135:LEU:HD12	1:B:135:LEU:C	2.40	0.47
1:E:143:ASN:HD21	1:E:400:MET:HE2	1.79	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: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
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:C:74:ARG:CG	1:C:79:GLU:CD	2.89	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:A:152:PRO:C	1:A:153:ARG:HG2	2.41	0.45
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:F:143:ASN:HD21	1:F:400:MET:HE2	1.78	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:TRP:CH2	1:B:130:ILE:CD1	2.98	0.45
1:D:50:GLY:O	1:D:51:GLU:HB2	2.17	0.45
1:E:152:PRO:C	1:E:153:ARG:HG2	2.43	0.44
1:B:152:PRO:C	1:B:153:ARG:HG2	2.42	0.44
1:E:135:LEU:C	1:E:135:LEU:HD12	2.42	0.44
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:D:135:LEU:HD12	1:D:135:LEU:C	2.42	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:A:164:GLY:HA3	1:A:193:PRO:CG	2.48	0.43
1:C:152:PRO:C	1:C:153:ARG:HG2	2.42	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:F:67:MET:HE1	1:F:115:HIS:NE2	2.34	0.43
1:E:175:ASN:OD1	1:E:175:ASN:C	2.62	0.43
1:F:257:ALA:HA	1:F:260:THR:CG2	2.48	0.43
1:C:74:ARG:HG2	1:C:74:ARG:HH11	1.83	0.42
1:F:39:ILE:CD1	1:F:128:ILE:HD13	2.48	0.42
1:E:142:LEU:C	1:E:164:GLY:H	2.27	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:D:189:SER:OG	2:D:1465:MLI:O7	2.38	0.42
1:F:43:TYR:CD2	1:F:58:LEU:HD21	2.55	0.42
1:F:87:PRO:HA	1:F:128:ILE:HG13	2.02	0.42
1:A:175:ASN:OD1	1:A:175:ASN:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:ILE:HD11	1:F:128:ILE:HD13	2.02	0.42
1:B:175:ASN:OD1	1:B:175:ASN:C	2.63	0.42
1:F:325:VAL:HG11	1:F:357:MET:HE1	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:F:135:LEU:C	1:F:135:LEU:HD12	2.45	0.42
1:D:153:ARG:HD2	1:D:158:GLU:O	2.20	0.41
1:E:431:GLY:C	1:E:432:PHE:CD1	2.92	0.41
1:F:257:ALA:O	1:F:258:ALA:C	2.63	0.41
1:A:142:LEU:C	1:A:164:GLY:H	2.29	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:263:SER:O	1:E:348:ARG:NH1	2.54	0.41
1:C:275:ALA:HA	1:C:278:ARG:HG3	2.02	0.41
1:C:186:THR:HB	2:C:1466:MLI:C2	2.50	0.41
1:F:142:LEU:C	1:F:164:GLY:H	2.28	0.41
1:F:445:GLY:CA	1:F:453:ILE:HD11	2.50	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:C:175:ASN:OD1	1:C:175:ASN:C	2.64	0.41
1:F:257:ALA:O	1:F:259:LEU:N	2.54	0.41
1:A:135:LEU:HD12	1:A:135:LEU:O	2.21	0.40
1:F:310:THR:HB	1:F:311:PRO:CD	2.51	0.40
1:B:142:LEU:C	1:B:164:GLY:H	2.29	0.40
1:E:92:ASP:OD2	1:E:102:THR:OG1	2.39	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:192:ILE:HB	1:D:193:PRO:HD3	2.04	0.40
1:D:328:ARG:NH2	2:D:1465:MLI:O9	2.46	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%)	11	22
1	B	445/487 (91%)	427 (96%)	14 (3%)	4 (1%)	14	27
1	C	446/487 (92%)	426 (96%)	16 (4%)	4 (1%)	14	27
1	D	446/487 (92%)	429 (96%)	12 (3%)	5 (1%)	11	22
1	E	449/487 (92%)	431 (96%)	14 (3%)	4 (1%)	14	27
1	F	442/487 (91%)	421 (95%)	16 (4%)	5 (1%)	11	22
All	All	2676/2922 (92%)	2563 (96%)	86 (3%)	27 (1%)	12	24

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
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 ⓘ

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%)	338 (98%)	6 (2%)	53	78
1	B	340/375 (91%)	336 (99%)	4 (1%)	63	83
1	C	341/375 (91%)	336 (98%)	5 (2%)	57	80
1	D	342/375 (91%)	335 (98%)	7 (2%)	48	75
1	E	342/375 (91%)	338 (99%)	4 (1%)	63	83
1	F	337/375 (90%)	330 (98%)	7 (2%)	47	74
All	All	2046/2250 (91%)	2013 (98%)	33 (2%)	55	79

All (33) 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	81	LEU
1	A	155	VAL
1	A	203	LYS
1	A	267	ARG
1	B	81	LEU
1	B	203	LYS
1	B	279	GLN
1	B	357	MET
1	C	74	ARG
1	C	81	LEU
1	C	135	LEU
1	C	203	LYS
1	C	398	GLU
1	D	45	ARG
1	D	75	LYS
1	D	111	THR
1	D	203	LYS
1	D	263	SER
1	D	279	GLN
1	D	381	GLU

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Mol	Chain	Res	Type
1	E	130	ILE
1	E	132	LYS
1	E	203	LYS
1	E	279	GLN
1	F	58	LEU
1	F	123	VAL
1	F	132	LYS
1	F	203	LYS
1	F	262	LYS
1	F	313	ARG
1	F	453	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	HIS
1	A	339	HIS
1	B	339	HIS
1	C	72	GLN
1	C	339	HIS
1	C	344	HIS
1	D	339	HIS
1	E	344	HIS
1	F	314	GLN
1	F	339	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	D	1465	-	6,6,6	1.14	0	7,7,7	1.15	0
2	MLI	C	1466	-	6,6,6	1.35	0	7,7,7	0.89	0
2	MLI	A	1466	-	6,6,6	1.18	0	7,7,7	1.36	1 (14%)
2	MLI	B	1465	-	6,6,6	1.27	0	7,7,7	1.09	1 (14%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1466	MLI	C3-C1-C2	-2.74	103.29	112.95
2	B	1465	MLI	C3-C1-C2	-2.06	105.68	112.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1465	MLI	4	0
2	C	1466	MLI	6	0
2	A	1466	MLI	5	0
2	B	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	448/487 (91%)	-0.12	9 (2%) 65 61	12, 26, 59, 96	2 (0%)
1	B	447/487 (91%)	-0.01	8 (1%) 67 64	16, 28, 59, 84	0
1	C	448/487 (91%)	-0.10	7 (1%) 70 67	14, 25, 61, 81	0
1	D	447/487 (91%)	-0.04	9 (2%) 65 61	15, 28, 58, 95	1 (0%)
1	E	450/487 (92%)	1.71	149 (33%) 1 1	34, 63, 90, 115	1 (0%)
1	F	444/487 (91%)	1.96	183 (41%) 0 0	43, 74, 100, 117	0
All	All	2684/2922 (91%)	0.57	365 (13%) 7 5	12, 35, 87, 117	4 (0%)

All (365) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	391	ALA	6.1
1	E	65[A]	LEU	5.6
1	D	256	ALA	5.3
1	E	108	PHE	5.3
1	F	130	ILE	5.2
1	F	463	HIS	5.2
1	E	103	ALA	5.2
1	A	18	HIS	5.1
1	F	80	ALA	5.1
1	F	148	PRO	5.0
1	E	187	ALA	5.0
1	E	109	ALA	4.9
1	E	135	LEU	4.9
1	D	50	GLY	4.9
1	F	25	TYR	4.8
1	F	277	HIS	4.8
1	F	391	ALA	4.8
1	A	465	LEU	4.7
1	E	256	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	105	CYS	4.5
1	A	109	ALA	4.5
1	F	78	GLY	4.4
1	E	344	HIS	4.4
1	E	50	GLY	4.3
1	C	465	LEU	4.3
1	E	336	ALA	4.3
1	F	266	ARG	4.2
1	F	135	LEU	4.2
1	F	108	PHE	4.2
1	E	200	VAL	4.0
1	E	340	PRO	4.0
1	E	352	LEU	3.9
1	F	255	GLY	3.9
1	F	109	ALA	3.8
1	F	175	ASN	3.8
1	E	58	LEU	3.8
1	E	153	ARG	3.8
1	E	170	ALA	3.8
1	E	111	THR	3.7
1	F	210	SER	3.7
1	E	303	THR	3.7
1	B	256	ALA	3.7
1	F	187	ALA	3.7
1	F	58	LEU	3.7
1	E	265	PRO	3.6
1	F	229	HIS	3.6
1	F	20	THR	3.6
1	E	420	LEU	3.6
1	E	136	ASP	3.6
1	F	173	VAL	3.6
1	E	151	ILE	3.6
1	F	342	VAL	3.5
1	F	50	GLY	3.5
1	F	200	VAL	3.5
1	E	106	THR	3.5
1	B	255	GLY	3.5
1	E	190	GLY	3.5
1	F	350	ILE	3.5
1	E	18	HIS	3.5
1	F	22	LEU	3.4
1	F	196	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	101	THR	3.4
1	F	29	TYR	3.4
1	E	56	ILE	3.4
1	F	254	ALA	3.4
1	E	346	VAL	3.3
1	E	356	ARG	3.3
1	F	105	CYS	3.3
1	E	262	LYS	3.3
1	F	414	TYR	3.3
1	F	178	VAL	3.3
1	E	141	GLY	3.2
1	E	255	GLY	3.2
1	F	281	PHE	3.2
1	F	83	LEU	3.2
1	D	255	GLY	3.2
1	F	405	VAL	3.2
1	F	224	ILE	3.2
1	E	392	PRO	3.2
1	F	401	LEU	3.2
1	B	50	GLY	3.2
1	F	127	ALA	3.1
1	F	65	LEU	3.1
1	F	171	VAL	3.1
1	F	211	GLY	3.1
1	E	257	ALA	3.1
1	D	262	LYS	3.1
1	C	18	HIS	3.1
1	E	342	VAL	3.1
1	E	254	ALA	3.1
1	F	402	ALA	3.1
1	F	169	SER	3.1
1	F	267	ARG	3.1
1	E	393	THR	3.0
1	F	258	ALA	3.0
1	E	152	PRO	3.0
1	F	42	LEU	3.0
1	F	215	VAL	3.0
1	F	279	GLN	3.0
1	F	227	LEU	3.0
1	E	263	SER	3.0
1	E	104	GLY	3.0
1	E	397	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	20	THR	3.0
1	F	147	THR	3.0
1	F	462	GLU	3.0
1	F	406	ARG	3.0
1	F	93	ASN	3.0
1	E	307	PHE	2.9
1	F	32	GLY	2.9
1	F	190	GLY	2.9
1	E	46	ILE	2.9
1	F	260	THR	2.9
1	E	217	ALA	2.9
1	F	61	LEU	2.9
1	E	357	MET	2.9
1	F	397	VAL	2.9
1	E	219	ARG	2.9
1	E	467	LYS	2.9
1	F	214	LEU	2.9
1	F	56	ILE	2.9
1	E	173	VAL	2.9
1	F	461	VAL	2.9
1	F	340	PRO	2.9
1	E	138	PHE	2.9
1	F	394	ILE	2.8
1	F	237	VAL	2.8
1	E	273	PRO	2.8
1	F	33	THR	2.8
1	F	98	GLY	2.8
1	E	142	LEU	2.8
1	F	182	LEU	2.8
1	F	357	MET	2.8
1	F	110	ARG	2.8
1	F	165	SER	2.8
1	F	112	PRO	2.8
1	F	114	GLN	2.8
1	F	262	LYS	2.8
1	E	337	ASP	2.8
1	E	339	HIS	2.8
1	F	150	GLY	2.8
1	F	54	ILE	2.8
1	E	363	PHE	2.8
1	F	88	PHE	2.8
1	F	392	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	318	LEU	2.7
1	D	109	ALA	2.7
1	F	137	GLN	2.7
1	F	141	GLY	2.7
1	E	350	ILE	2.7
1	E	297	LEU	2.7
1	F	31	ALA	2.7
1	F	295	ARG	2.7
1	F	344	HIS	2.7
1	A	50	GLY	2.7
1	E	405	VAL	2.7
1	F	437	LEU	2.7
1	E	343	LEU	2.7
1	F	343	LEU	2.7
1	F	415	THR	2.7
1	D	464	ASP	2.6
1	F	363	PHE	2.6
1	B	109	ALA	2.6
1	B	257	ALA	2.6
1	F	145	THR	2.6
1	F	359	ALA	2.6
1	E	432	PHE	2.6
1	F	87	PRO	2.6
1	F	111	THR	2.6
1	F	136	ASP	2.6
1	F	232	ASP	2.6
1	E	406	ARG	2.6
1	F	46	ILE	2.6
1	F	86	ILE	2.6
1	F	149	PHE	2.6
1	F	156	PHE	2.6
1	F	369	LEU	2.6
1	E	169	SER	2.6
1	E	64	ALA	2.6
1	E	354	ALA	2.6
1	E	367	TYR	2.6
1	E	414	TYR	2.6
1	F	55	TRP	2.6
1	E	150	GLY	2.6
1	F	39	ILE	2.6
1	F	94	ILE	2.6
1	F	38	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	229	HIS	2.6
1	E	466	ALA	2.6
1	F	256	ALA	2.6
1	F	336	ALA	2.6
1	F	459	ALA	2.6
1	F	346	VAL	2.5
1	C	109	ALA	2.5
1	F	47	LYS	2.5
1	F	275	ALA	2.5
1	F	104	GLY	2.5
1	E	288	ALA	2.5
1	F	103	ALA	2.5
1	A	263	SER	2.5
1	F	265	PRO	2.5
1	E	407	LEU	2.5
1	F	59	LEU	2.5
1	E	441	VAL	2.5
1	E	110	ARG	2.5
1	F	153	ARG	2.5
1	F	194	ALA	2.5
1	C	261	GLU	2.5
1	E	403	ASP	2.5
1	F	320	TYR	2.5
1	E	411	LEU	2.5
1	F	318	LEU	2.5
1	F	411	LEU	2.5
1	D	18	HIS	2.5
1	E	433	ARG	2.5
1	F	28	ALA	2.5
1	F	241	ALA	2.5
1	F	167	SER	2.5
1	F	84	PHE	2.4
1	F	117	PHE	2.4
1	F	439	PHE	2.4
1	F	264	TRP	2.4
1	F	240	VAL	2.4
1	F	106	THR	2.4
1	E	353	SER	2.4
1	E	211	GLY	2.4
1	F	168	GLY	2.4
1	E	39	ILE	2.4
1	E	42	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	68	LEU	2.4
1	F	413	PHE	2.4
1	E	264	TRP	2.4
1	C	47	LYS	2.4
1	F	99	LEU	2.4
1	E	266	ARG	2.4
1	E	417	PHE	2.4
1	D	257	ALA	2.4
1	F	354	ALA	2.4
1	F	142	LEU	2.4
1	F	403	ASP	2.4
1	E	25	TYR	2.4
1	E	38	VAL	2.4
1	E	293	ALA	2.4
1	E	355	LYS	2.4
1	E	434	THR	2.3
1	E	162	SER	2.3
1	F	436	GLY	2.3
1	E	305	ILE	2.3
1	F	96	VAL	2.3
1	F	155	VAL	2.3
1	F	134	ASN	2.3
1	E	274	ALA	2.3
1	E	402	ALA	2.3
1	F	170	ALA	2.3
1	F	404	PRO	2.3
1	E	319	LEU	2.3
1	F	209	PHE	2.3
1	E	347	VAL	2.3
1	A	256	ALA	2.3
1	E	139	ALA	2.3
1	F	36	ALA	2.3
1	E	324	TRP	2.3
1	E	332	ILE	2.3
1	E	335	LEU	2.3
1	F	259	LEU	2.3
1	F	297	LEU	2.3
1	F	305	ILE	2.3
1	F	335	LEU	2.3
1	E	222	ASP	2.3
1	F	349	ASP	2.3
1	F	138	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	385	VAL	2.3
1	F	27	ALA	2.2
1	E	282	GLY	2.2
1	F	107	GLY	2.2
1	E	400	MET	2.2
1	F	382	LYS	2.2
1	E	51	GLU	2.2
1	E	209	PHE	2.2
1	E	250	PHE	2.2
1	E	148	PRO	2.2
1	E	155	VAL	2.2
1	F	367	TYR	2.2
1	E	47	LYS	2.2
1	E	89	GLY	2.2
1	F	208	LEU	2.2
1	E	54	ILE	2.2
1	E	48	GLU	2.2
1	F	341	GLU	2.2
1	B	113	ARG	2.2
1	F	216	PRO	2.2
1	F	231	VAL	2.2
1	E	61	LEU	2.2
1	F	351	ILE	2.2
1	E	113	ARG	2.2
1	E	404	PRO	2.2
1	E	96	VAL	2.2
1	E	418	VAL	2.2
1	E	52	ASN	2.2
1	E	369	LEU	2.2
1	E	112	PRO	2.2
1	E	216	PRO	2.2
1	B	262	LYS	2.2
1	E	281	PHE	2.2
1	F	90	VAL	2.1
1	E	329	LEU	2.1
1	E	396	THR	2.1
1	F	140	THR	2.1
1	F	207	GLY	2.1
1	F	390	THR	2.1
1	F	225	SER	2.1
1	F	179	PRO	2.1
1	F	67	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	286	ALA	2.1
1	F	284	ALA	2.1
1	E	271	GLY	2.1
1	E	191	ARG	2.1
1	E	299	GLU	2.1
1	F	356	ARG	2.1
1	E	114	GLN	2.1
1	E	325	VAL	2.1
1	B	44	ALA	2.1
1	E	44	ALA	2.1
1	E	359	ALA	2.1
1	F	217	ALA	2.1
1	A	78	GLY	2.1
1	E	107	GLY	2.1
1	F	81	LEU	2.1
1	F	188	GLY	2.1
1	F	319	LEU	2.1
1	E	43	TYR	2.1
1	F	132	LYS	2.1
1	D	40	SER	2.1
1	F	60	PRO	2.1
1	F	339	HIS	2.1
1	F	23	ALA	2.1
1	F	97	ALA	2.1
1	F	228	ALA	2.1
1	E	348	ARG	2.1
1	F	352	LEU	2.1
1	F	128	ILE	2.1
1	A	262	LYS	2.1
1	E	309	TYR	2.1
1	E	345	PRO	2.1
1	F	154	CYS	2.1
1	C	254	ALA	2.0
1	E	447	ALA	2.0
1	E	401	LEU	2.0
1	F	407	LEU	2.0
1	C	282	GLY	2.0
1	E	55	TRP	2.0
1	E	453	ILE	2.0
1	F	186	THR	2.0
1	A	464	ASP	2.0
1	E	161	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	158	GLU	2.0
1	E	214	LEU	2.0
1	E	456	LEU	2.0
1	F	296	LYS	2.0
1	E	101	THR	2.0
1	E	140	THR	2.0
1	E	394	ILE	2.0
1	E	415	THR	2.0
1	F	205	THR	2.0
1	F	309	TYR	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MLI	A	1466	7/7	0.91	0.13	24,28,30,31	0
2	MLI	B	1465	7/7	0.91	0.11	29,30,36,40	0
2	MLI	C	1466	7/7	0.94	0.08	21,26,28,33	0
2	MLI	D	1465	7/7	0.95	0.09	25,31,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.