



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:57 am BST

PDB ID : 3S4T
Title : Crystal structure of putative amidohydrolase-2 (EFI-target 500288) from Polaromonas sp. JS666
Authors : Ramagopal, U.A.; Toro, R.; Girtl, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on : 2011-05-20
Resolution : 1.90 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 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	:	2.11
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

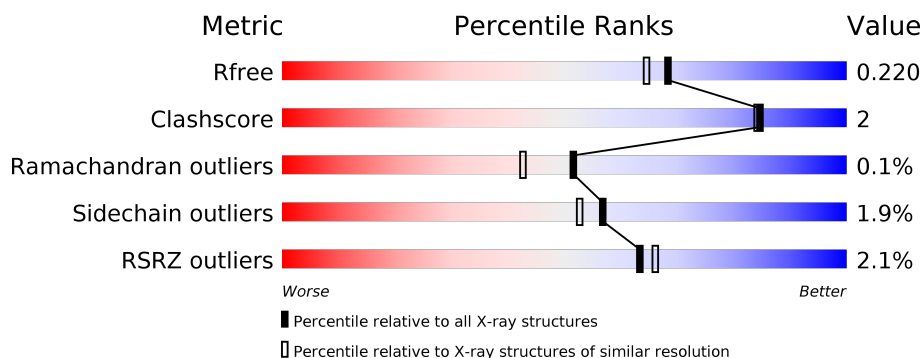
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. 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	348	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>5%</div> </div> </div>
1	B	348	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> </div> </div>
1	C	348	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>6%</div> </div> </div>
1	D	348	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>7%</div> </div> </div>
1	E	348	<div> <div>0%</div> <div> <div></div> <div>89%</div> <div>5%</div> <div>7%</div> </div> </div>
1	F	348	<div> <div>0%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	348	
1	H	348	

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	EPE	F	400	-	-	X	-
2	EPE	G	400	-	-	X	-
3	SO4	E	352	-	-	X	-
6	GOL	F	353	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23306 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 Amidohydrolase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	Se	0	5	0
			2737	1748	478	500	1	10			
1	B	324	Total	C	N	O	S	Se	0	4	0
			2661	1700	468	482	1	10			
1	C	326	Total	C	N	O	S	Se	0	5	0
			2683	1714	471	487	1	10			
1	D	324	Total	C	N	O	S	Se	0	4	0
			2658	1702	462	482	1	11			
1	E	325	Total	C	N	O	S	Se	0	8	0
			2704	1724	476	493	1	10			
1	F	324	Total	C	N	O	S	Se	0	2	0
			2642	1693	458	480	1	10			
1	G	327	Total	C	N	O	S	Se	0	8	0
			2720	1732	483	494	1	10			
1	H	324	Total	C	N	O	S	Se	0	3	0
			2650	1694	464	481	1	10			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
A	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
A	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
A	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
A	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
A	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
A	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
A	334	SER	-	EXPRESSION TAG	UNP Q12BV1
A	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	339	HIS	-	EXPRESSION TAG	UNP Q12BV1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
A	342	SER	-	EXPRESSION TAG	UNP Q12BV1
A	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
A	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
A	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
A	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
A	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
A	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
B	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
B	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
B	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
B	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
B	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
B	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
B	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
B	334	SER	-	EXPRESSION TAG	UNP Q12BV1
B	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
B	342	SER	-	EXPRESSION TAG	UNP Q12BV1
B	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
B	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
B	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
B	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
B	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
B	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
C	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
C	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
C	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
C	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
C	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
C	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
C	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
C	334	SER	-	EXPRESSION TAG	UNP Q12BV1
C	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	337	HIS	-	EXPRESSION TAG	UNP Q12BV1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
C	342	SER	-	EXPRESSION TAG	UNP Q12BV1
C	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
C	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
C	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
C	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
C	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
C	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
D	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
D	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
D	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
D	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
D	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
D	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
D	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
D	334	SER	-	EXPRESSION TAG	UNP Q12BV1
D	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
D	342	SER	-	EXPRESSION TAG	UNP Q12BV1
D	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
D	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
D	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
D	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
D	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
D	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
E	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
E	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
E	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
E	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
E	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
E	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
E	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
E	334	SER	-	EXPRESSION TAG	UNP Q12BV1
E	335	HIS	-	EXPRESSION TAG	UNP Q12BV1

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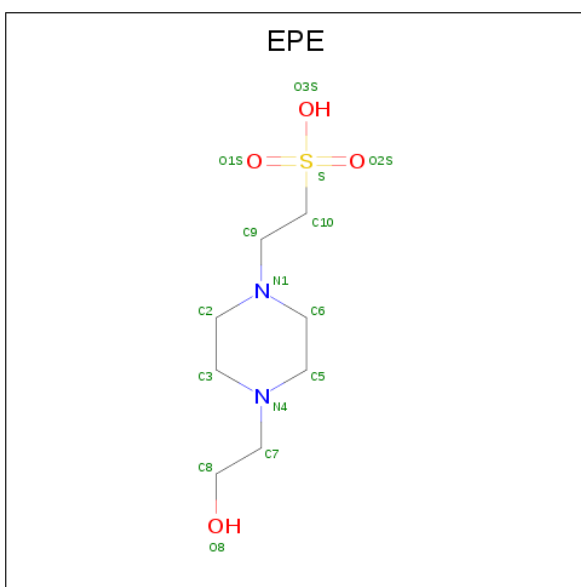
Chain	Residue	Modelled	Actual	Comment	Reference
E	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
E	342	SER	-	EXPRESSION TAG	UNP Q12BV1
E	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
E	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
E	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
E	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
E	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
E	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
F	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
F	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
F	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
F	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
F	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
F	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
F	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
F	334	SER	-	EXPRESSION TAG	UNP Q12BV1
F	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
F	342	SER	-	EXPRESSION TAG	UNP Q12BV1
F	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
F	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
F	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
F	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
F	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
F	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
G	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
G	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
G	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
G	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
G	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
G	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
G	333	GLN	-	EXPRESSION TAG	UNP Q12BV1

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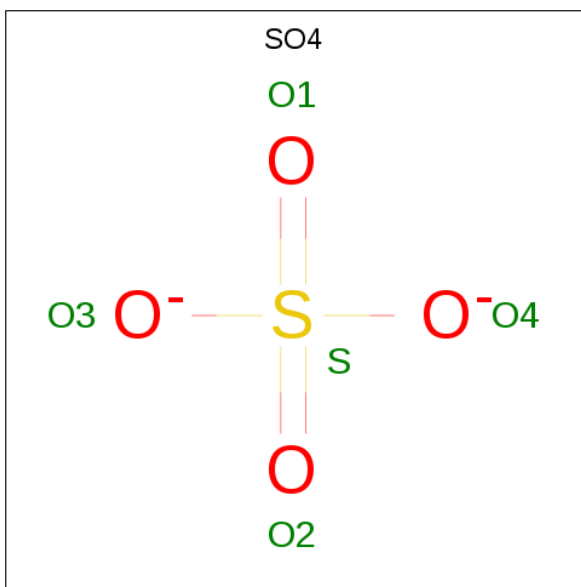
Chain	Residue	Modelled	Actual	Comment	Reference
G	334	SER	-	EXPRESSION TAG	UNP Q12BV1
G	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
G	342	SER	-	EXPRESSION TAG	UNP Q12BV1
G	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
G	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
G	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
G	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
G	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
G	348	LYS	-	EXPRESSION TAG	UNP Q12BV1
H	327	ALA	-	EXPRESSION TAG	UNP Q12BV1
H	328	GLU	-	EXPRESSION TAG	UNP Q12BV1
H	329	ASN	-	EXPRESSION TAG	UNP Q12BV1
H	330	LEU	-	EXPRESSION TAG	UNP Q12BV1
H	331	TYR	-	EXPRESSION TAG	UNP Q12BV1
H	332	PHE	-	EXPRESSION TAG	UNP Q12BV1
H	333	GLN	-	EXPRESSION TAG	UNP Q12BV1
H	334	SER	-	EXPRESSION TAG	UNP Q12BV1
H	335	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	336	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	337	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	338	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	339	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	340	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	341	TRP	-	EXPRESSION TAG	UNP Q12BV1
H	342	SER	-	EXPRESSION TAG	UNP Q12BV1
H	343	HIS	-	EXPRESSION TAG	UNP Q12BV1
H	344	PRO	-	EXPRESSION TAG	UNP Q12BV1
H	345	GLN	-	EXPRESSION TAG	UNP Q12BV1
H	346	PHE	-	EXPRESSION TAG	UNP Q12BV1
H	347	GLU	-	EXPRESSION TAG	UNP Q12BV1
H	348	LYS	-	EXPRESSION TAG	UNP Q12BV1

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	G	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		

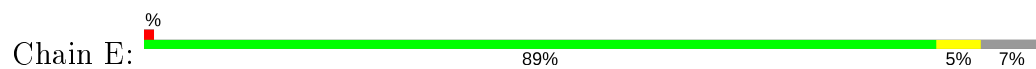
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	211	Total	O	0	0
			211	211		

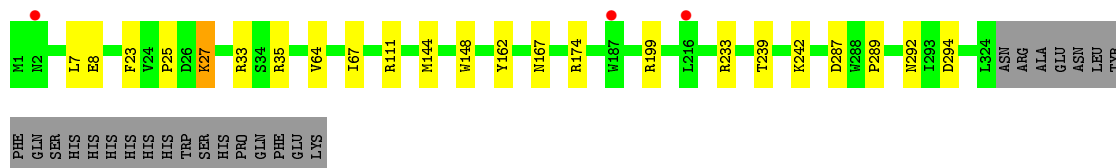
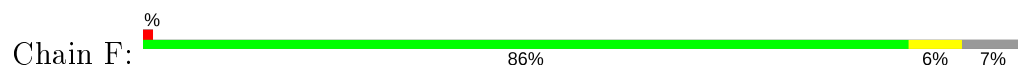
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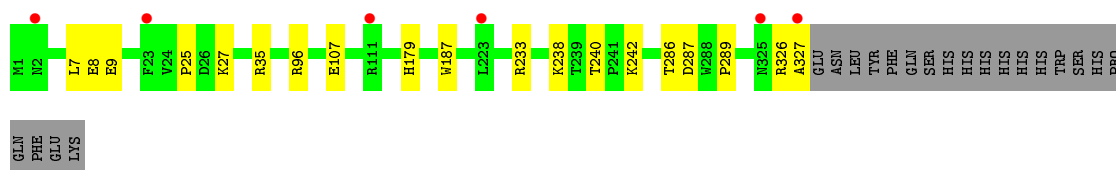
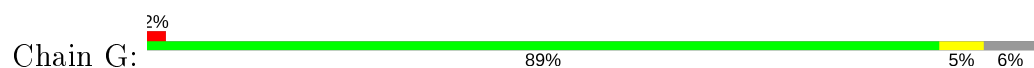
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	163	Total 163	O 163	0	0
7	C	202	Total 202	O 202	0	0
7	D	176	Total 176	O 176	0	0
7	E	209	Total 209	O 209	0	0
7	F	178	Total 178	O 178	0	0
7	G	203	Total 203	O 203	0	0
7	H	171	Total 171	O 171	0	0



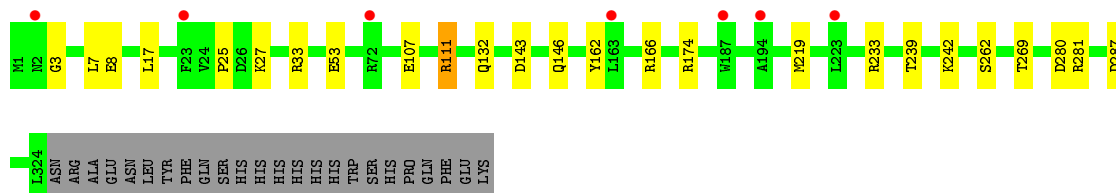
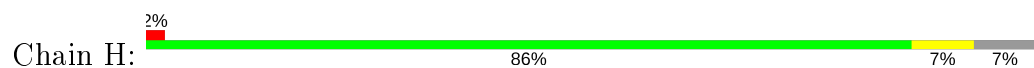
• Molecule 1: Amidohydrolase 2



• Molecule 1: Amidohydrolase 2



• Molecule 1: Amidohydrolase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.02Å 151.24Å 143.41Å 90.00° 91.96° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90 39.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.1 (40.00-1.90) 93.1 (39.16-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.73 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.175 , 0.207 0.190 , 0.220	Depositor DCC
R_{free} test set	12743 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.080 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23306	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6317e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, GOL, ACT, SO4, CL

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	0/2804	0.66	0/3794
1	B	0.64	0/2726	0.64	0/3687
1	C	0.66	0/2748	0.65	0/3716
1	D	0.65	0/2724	0.65	0/3685
1	E	0.83	0/2769	0.72	0/3744
1	F	0.80	2/2709 (0.1%)	0.71	0/3669
1	G	0.84	0/2785	0.70	0/3765
1	H	0.78	0/2715	0.73	2/3673 (0.1%)
All	All	0.74	2/21980 (0.0%)	0.68	2/29733 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	148[A]	TRP	CB-CG	5.42	1.60	1.50
1	F	148[B]	TRP	CB-CG	5.42	1.60	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	280	ASP	CB-CG-OD1	5.13	122.92	118.30
1	H	281	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2737	0	2644	10	0
1	B	2661	0	2586	8	0
1	C	2683	0	2605	9	0
1	D	2658	0	2578	11	0
1	E	2704	0	2619	13	0
1	F	2642	0	2560	16	0
1	G	2720	0	2639	12	0
1	H	2650	0	2574	20	0
2	A	15	0	17	1	0
2	B	15	0	17	3	0
2	D	15	0	17	0	0
2	F	30	0	34	14	0
2	G	30	0	34	12	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
3	C	10	0	0	0	0
3	D	20	0	0	0	0
3	E	20	0	0	2	0
3	F	5	0	0	0	0
3	G	30	0	0	0	0
3	H	25	0	0	1	0
4	A	12	0	9	0	0
4	B	8	0	6	0	0
4	C	8	0	6	0	0
4	D	4	0	3	0	0
4	E	8	0	6	0	0
4	F	8	0	6	0	0
4	G	12	0	9	0	0
4	H	4	0	3	0	0
5	B	1	0	0	0	0
6	C	6	0	8	1	0
6	D	6	0	8	3	0
6	F	6	0	8	5	0
7	A	211	0	0	0	0
7	B	163	0	0	0	0
7	C	202	0	0	0	0
7	D	176	0	0	0	0
7	E	209	0	0	1	0
7	F	178	0	0	0	0
7	G	203	0	0	1	0
7	H	171	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23306	0	20996	100	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 2.

All (100) 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:B:144[B]:MSE:HE2	1:B:144[B]:MSE:HA	1.40	1.04
1:E:23:PHE:HZ	3:E:352:SO4:O4	1.51	0.93
1:H:111[B]:ARG:HD2	1:H:111[B]:ARG:N	1.86	0.86
1:E:23:PHE:CZ	3:E:352:SO4:O4	2.29	0.86
1:F:23:PHE:HZ	6:F:353:GOL:H11	1.41	0.85
1:D:167:ASN:HD22	6:D:354:GOL:H11	1.42	0.84
1:E:27:LYS:HE3	2:F:400:EPE:H31	1.57	0.84
1:B:144[B]:MSE:HA	1:B:144[B]:MSE:CE	2.06	0.84
2:G:349:EPE:H102	1:H:25:PRO:HB3	1.61	0.83
2:G:349:EPE:H31	1:H:27:LYS:HE3	1.62	0.81
1:F:25:PRO:HB3	2:F:349:EPE:H92	1.62	0.79
1:E:110:ALA:O	1:E:114[B]:GLU:HG3	1.95	0.66
1:H:111[A]:ARG:CG	1:H:111[A]:ARG:HH11	2.09	0.65
1:F:167:ASN:HD22	6:F:353:GOL:H32	1.61	0.65
1:H:111[A]:ARG:CB	1:H:111[A]:ARG:HH11	2.11	0.63
1:G:240:THR:H	2:G:349:EPE:H71	1.64	0.62
1:E:27:LYS:CE	2:F:400:EPE:H31	2.28	0.62
1:E:25:PRO:HB3	2:F:400:EPE:H102	1.81	0.61
1:B:25:PRO:HB3	2:B:400:EPE:H91	1.83	0.61
1:D:167:ASN:HD22	6:D:354:GOL:C1	2.14	0.60
1:G:96[A]:ARG:HH21	1:G:327:ALA:HB3	1.65	0.60
1:C:45[B]:ARG:HH11	1:C:45[B]:ARG:HG3	1.67	0.59
1:G:25:PRO:HB3	2:G:400:EPE:H61	1.86	0.58
1:D:167:ASN:ND2	6:D:354:GOL:H11	2.15	0.58
1:F:167:ASN:HD22	6:F:353:GOL:C3	2.17	0.57
1:E:239:THR:OG1	2:F:349:EPE:H32	2.05	0.57
1:E:25:PRO:HB3	2:F:400:EPE:H22	1.86	0.56
1:F:239:THR:OG1	2:F:400:EPE:H32	2.06	0.56
1:G:242:LYS:CE	2:G:349:EPE:H101	2.37	0.55
1:H:111[A]:ARG:HH11	1:H:111[A]:ARG:HG2	1.72	0.54
1:H:132:GLN:NE2	1:H:166:ARG:HH22	2.06	0.54
1:A:239:THR:OG1	2:B:400:EPE:H32	2.10	0.52
1:F:242:LYS:NZ	2:F:400:EPE:H92	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:PHE:CZ	6:F:353:GOL:H11	2.32	0.51
1:C:45[B]:ARG:CG	1:C:45[B]:ARG:HH11	2.23	0.51
1:C:202:GLY:O	1:C:244:PRO:HD2	2.10	0.51
1:F:27:LYS:HE3	2:F:349:EPE:H31	1.91	0.51
1:E:107:GLU:O	1:E:111:ARG:HG2	2.12	0.50
1:F:25:PRO:HB3	2:F:349:EPE:H22	1.94	0.50
1:D:9:GLU:OE2	1:D:286:THR:OG1	2.28	0.49
2:G:400:EPE:H51	1:H:239:THR:OG1	2.11	0.49
1:D:262:SER:HB2	1:D:287:ASP:HB2	1.94	0.49
1:H:111[A]:ARG:HB3	1:H:111[A]:ARG:HH11	1.77	0.48
1:C:179:HIS:NE2	1:D:143:ASP:OD2	2.47	0.48
1:D:219[A]:MSE:HE1	1:D:270:LEU:HD13	1.96	0.48
2:G:400:EPE:H22	7:G:1097:HOH:O	2.13	0.47
1:H:166:ARG:HB2	3:H:353:SO4:O3	2.15	0.47
1:G:242:LYS:HE2	2:G:349:EPE:H101	1.98	0.46
1:D:115:ARG:O	1:D:119:GLU:HB2	2.15	0.46
1:D:119:GLU:HG2	1:G:326:ARG:NH2	2.31	0.46
1:G:9:GLU:OE2	1:G:286:THR:OG1	2.23	0.46
1:H:111[A]:ARG:CG	1:H:111[A]:ARG:NH1	2.76	0.46
1:C:260:THR:HA	1:C:283:LEU:O	2.16	0.46
2:G:400:EPE:H62	1:H:239:THR:OG1	2.14	0.46
1:F:242:LYS:HZ1	2:F:400:EPE:H92	1.81	0.46
1:A:105:ASP:HB3	1:A:108:LEU:HB2	1.98	0.45
1:G:35:ARG:HB3	1:G:289:PRO:HB3	1.98	0.45
1:D:69:ASP:HB3	1:D:72:ARG:HD3	1.97	0.45
1:F:144[B]:MSE:HE2	1:F:199:ARG:HH22	1.81	0.45
2:G:400:EPE:H61	2:G:400:EPE:H102	1.64	0.45
1:B:3:GLY:HA2	1:B:53:GLU:HB2	1.98	0.45
1:F:8:GLU:O	1:F:287:ASP:HA	2.16	0.45
1:B:143:ASP:OD2	1:B:144[B]:MSE:HE3	2.18	0.44
1:A:35:ARG:HB3	1:A:289:PRO:HB3	1.99	0.44
1:C:10:HIS:HA	1:C:58:SER:O	2.18	0.44
1:A:280:ASP:OD1	1:A:312:LYS:NZ	2.51	0.44
1:G:179:HIS:NE2	1:H:143:ASP:OD2	2.48	0.44
1:B:144[B]:MSE:CA	1:B:144[B]:MSE:CE	2.87	0.44
1:A:9:GLU:OE2	1:A:286:THR:OG1	2.29	0.43
1:E:146:GLN:HG2	7:E:1589:HOH:O	2.17	0.43
1:C:8:GLU:O	1:C:287:ASP:HA	2.17	0.43
1:G:8:GLU:O	1:G:287:ASP:HA	2.17	0.43
1:G:326:ARG:HG3	1:G:326:ARG:O	2.18	0.43
2:G:400:EPE:H62	1:H:242:LYS:HZ1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:MSE:HG2	1:A:269:THR:HG22	2.01	0.43
2:F:400:EPE:H22	2:F:400:EPE:H102	1.82	0.43
1:H:111[A]:ARG:NH1	1:H:111[A]:ARG:HG2	2.31	0.43
1:E:9:GLU:OE2	1:E:286:THR:OG1	2.31	0.42
1:A:8:GLU:O	1:A:287:ASP:HA	2.19	0.42
1:H:3:GLY:HA2	1:H:53:GLU:HB2	2.02	0.42
1:C:9:GLU:OE2	1:C:286:THR:OG1	2.34	0.42
1:F:35:ARG:HB3	1:F:289:PRO:HB3	2.01	0.42
1:F:292:ASN:HB3	1:F:294:ASP:OD1	2.20	0.42
2:F:349:EPE:H81	2:F:349:EPE:H52	1.65	0.42
1:A:260:THR:HA	1:A:283:LEU:O	2.19	0.42
1:E:27:LYS:NZ	2:F:400:EPE:H31	2.35	0.42
1:H:262:SER:HB2	1:H:287:ASP:HB2	2.02	0.41
1:B:9:GLU:OE2	1:B:286:THR:OG1	2.35	0.41
1:A:27:LYS:NZ	2:A:400:EPE:H31	2.35	0.41
1:H:219:MSE:HG2	1:H:269:THR:HG22	2.01	0.41
1:D:292:ASN:HB3	1:D:294:ASP:OD1	2.20	0.41
1:A:10:HIS:HA	1:A:58:SER:O	2.20	0.41
1:H:17:LEU:HD21	1:H:33:ARG:HG3	2.03	0.41
1:E:8:GLU:O	1:E:287:ASP:HA	2.21	0.41
1:F:64:VAL:HA	1:F:67:ILE:HD12	2.03	0.41
1:C:180:ALA:HB2	6:C:353:GOL:H2	2.03	0.41
1:H:8:GLU:O	1:H:287:ASP:HA	2.20	0.41
1:F:23:PHE:HZ	6:F:353:GOL:C1	2.23	0.40
1:G:27:LYS:HZ2	2:G:400:EPE:H52	1.86	0.40
1:B:27:LYS:HD3	2:B:400:EPE:H62	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	335/348 (96%)	324 (97%)	11 (3%)	0	100	100
1	B	326/348 (94%)	318 (98%)	8 (2%)	0	100	100
1	C	329/348 (94%)	320 (97%)	8 (2%)	1 (0%)	41	31
1	D	326/348 (94%)	317 (97%)	8 (2%)	1 (0%)	41	31
1	E	331/348 (95%)	321 (97%)	10 (3%)	0	100	100
1	F	324/348 (93%)	315 (97%)	9 (3%)	0	100	100
1	G	333/348 (96%)	324 (97%)	8 (2%)	1 (0%)	41	31
1	H	325/348 (93%)	318 (98%)	7 (2%)	0	100	100
All	All	2629/2784 (94%)	2557 (97%)	69 (3%)	3 (0%)	51	43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	187	TRP
1	D	187	TRP
1	G	187	TRP

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	283/285 (99%)	277 (98%)	6 (2%)	53	48
1	B	275/285 (96%)	272 (99%)	3 (1%)	73	73
1	C	277/285 (97%)	274 (99%)	3 (1%)	73	73
1	D	275/285 (96%)	269 (98%)	6 (2%)	52	47
1	E	280/285 (98%)	275 (98%)	5 (2%)	59	55
1	F	273/285 (96%)	266 (97%)	7 (3%)	46	39
1	G	281/285 (99%)	277 (99%)	4 (1%)	67	65
1	H	274/285 (96%)	265 (97%)	9 (3%)	38	29
All	All	2218/2280 (97%)	2175 (98%)	43 (2%)	57	53

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	23	PHE
1	A	111	ARG
1	A	118	LYS
1	A	162	TYR
1	A	233	ARG
1	B	7	LEU
1	B	162	TYR
1	B	233	ARG
1	C	7	LEU
1	C	233	ARG
1	C	323	LYS
1	D	7	LEU
1	D	107	GLU
1	D	119	GLU
1	D	162	TYR
1	D	233	ARG
1	D	324	LEU
1	E	7	LEU
1	E	107	GLU
1	E	162	TYR
1	E	233	ARG
1	E	325	ASN
1	F	7	LEU
1	F	27	LYS
1	F	33	ARG
1	F	111	ARG
1	F	162	TYR
1	F	174	ARG
1	F	233	ARG
1	G	7	LEU
1	G	107	GLU
1	G	233	ARG
1	G	238	LYS
1	H	7	LEU
1	H	107	GLU
1	H	111[A]	ARG
1	H	111[B]	ARG
1	H	146	GLN
1	H	162	TYR
1	H	174[A]	ARG
1	H	174[B]	ARG

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Mol	Chain	Res	Type
1	H	233	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	A	254	ASN
1	A	329	ASN
1	B	134	ASN
1	B	254	ASN
1	C	134	ASN
1	C	254	ASN
1	D	134	ASN
1	D	254	ASN
1	E	134	ASN
1	E	254	ASN
1	F	134	ASN
1	F	254	ASN
1	G	134	ASN
1	G	254	ASN
1	H	132	GLN
1	H	134	ASN
1	H	254	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 57 ligands modelled in this entry, 1 is monoatomic - leaving 56 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	349	-	4,4,4	0.19	0	6,6,6	0.13	0
3	SO4	A	349	-	4,4,4	0.11	0	6,6,6	0.55	0
3	SO4	G	352	-	4,4,4	0.15	0	6,6,6	0.07	0
4	ACT	F	352	-	1,3,3	1.65	0	0,3,3	0.00	-
3	SO4	E	352	-	4,4,4	0.27	0	6,6,6	1.10	0
4	ACT	E	354	-	1,3,3	1.81	0	0,3,3	0.00	-
4	ACT	F	351	-	1,3,3	2.19	1 (100%)	0,3,3	0.00	-
4	ACT	A	355	-	1,3,3	1.25	0	0,3,3	0.00	-
4	ACT	C	351	-	1,3,3	2.41	1 (100%)	0,3,3	0.00	-
3	SO4	H	349	-	4,4,4	0.22	0	6,6,6	0.58	0
3	SO4	G	350	-	4,4,4	0.14	0	6,6,6	0.69	0
4	ACT	B	353	-	1,3,3	1.71	0	0,3,3	0.00	-
3	SO4	H	351	-	4,4,4	0.14	0	6,6,6	0.12	0
2	EPE	G	349	-	15,15,15	1.01	1 (6%)	18,20,20	2.02	5 (27%)
3	SO4	C	349	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	D	352	-	4,4,4	0.13	0	6,6,6	0.19	0
2	EPE	B	400	-	15,15,15	1.02	1 (6%)	18,20,20	1.94	5 (27%)
4	ACT	G	356	-	1,3,3	3.34	1 (100%)	0,3,3	0.00	-
3	SO4	H	353	-	4,4,4	0.28	0	6,6,6	0.55	0
4	ACT	E	353	-	1,3,3	3.13	1 (100%)	0,3,3	0.00	-
3	SO4	G	353	-	4,4,4	0.16	0	6,6,6	0.54	0
3	SO4	C	350	-	4,4,4	0.10	0	6,6,6	0.54	0
3	SO4	D	351	-	4,4,4	0.14	0	6,6,6	0.21	0
3	SO4	G	355	-	4,4,4	0.14	0	6,6,6	0.42	0
2	EPE	A	400	-	15,15,15	0.98	1 (6%)	18,20,20	2.03	5 (27%)
4	ACT	A	353	-	1,3,3	3.81	1 (100%)	0,3,3	0.00	-
2	EPE	G	400	-	15,15,15	0.95	1 (6%)	18,20,20	2.05	6 (33%)
4	ACT	G	357	-	1,3,3	1.99	0	0,3,3	0.00	-
3	SO4	B	351	-	4,4,4	0.22	0	6,6,6	0.28	0
3	SO4	D	350	-	4,4,4	0.18	0	6,6,6	0.16	0
3	SO4	G	351	-	4,4,4	0.15	0	6,6,6	0.27	0
3	SO4	H	352	-	4,4,4	0.11	0	6,6,6	0.24	0
2	EPE	F	400	-	15,15,15	0.99	1 (6%)	18,20,20	2.22	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	350	-	4,4,4	0.16	0	6,6,6	0.20	0
4	ACT	H	354	-	1,3,3	3.10	1 (100%)	0,3,3	0.00	-
3	SO4	G	354	-	4,4,4	0.15	0	6,6,6	0.26	0
4	ACT	G	358	-	1,3,3	1.42	0	0,3,3	0.00	-
3	SO4	B	349	-	4,4,4	0.19	0	6,6,6	0.22	0
3	SO4	E	349	-	4,4,4	0.15	0	6,6,6	0.19	0
3	SO4	E	351	-	4,4,4	0.15	0	6,6,6	0.49	0
6	GOL	F	353	-	5,5,5	0.62	0	5,5,5	0.87	0
2	EPE	D	400	-	15,15,15	0.89	1 (6%)	18,20,20	1.95	4 (22%)
3	SO4	A	351	-	4,4,4	0.14	0	6,6,6	0.16	0
6	GOL	C	353	-	5,5,5	0.43	0	5,5,5	0.57	0
3	SO4	B	350	-	4,4,4	0.16	0	6,6,6	0.12	0
4	ACT	A	354	-	1,3,3	1.68	0	0,3,3	0.00	-
4	ACT	C	352	-	1,3,3	1.69	0	0,3,3	0.00	-
2	EPE	F	349	-	15,15,15	0.82	1 (6%)	18,20,20	1.74	5 (27%)
3	SO4	A	352	-	4,4,4	0.14	0	6,6,6	0.21	0
3	SO4	H	350	-	4,4,4	0.17	0	6,6,6	0.24	0
3	SO4	F	350	-	4,4,4	0.16	0	6,6,6	0.52	0
4	ACT	D	353	-	1,3,3	1.48	0	0,3,3	0.00	-
3	SO4	E	350	-	4,4,4	0.10	0	6,6,6	0.38	0
6	GOL	D	354	-	5,5,5	0.59	0	5,5,5	0.65	0
3	SO4	B	352	-	4,4,4	0.13	0	6,6,6	0.15	0
4	ACT	B	354	-	1,3,3	1.75	0	0,3,3	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	EPE	A	400	-	-	6/9/19/19	0/1/1/1
6	GOL	C	353	-	-	4/4/4/4	-
2	EPE	G	400	-	-	4/9/19/19	0/1/1/1
2	EPE	D	400	-	-	5/9/19/19	0/1/1/1
2	EPE	B	400	-	-	4/9/19/19	0/1/1/1
2	EPE	F	349	-	-	6/9/19/19	0/1/1/1
6	GOL	F	353	-	-	2/4/4/4	-
2	EPE	F	400	-	-	4/9/19/19	0/1/1/1
6	GOL	D	354	-	-	3/4/4/4	-
2	EPE	G	349	-	-	2/9/19/19	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	353	ACT	CH3-C	3.81	1.53	1.48
2	G	349	EPE	C10-S	3.52	1.82	1.77
2	B	400	EPE	C10-S	3.45	1.82	1.77
2	A	400	EPE	C10-S	3.40	1.82	1.77
2	F	400	EPE	C10-S	3.40	1.82	1.77
4	G	356	ACT	CH3-C	3.34	1.53	1.48
4	E	353	ACT	CH3-C	3.13	1.52	1.48
2	G	400	EPE	C10-S	3.12	1.81	1.77
4	H	354	ACT	CH3-C	3.10	1.52	1.48
2	D	400	EPE	C10-S	3.03	1.81	1.77
2	F	349	EPE	C10-S	2.69	1.81	1.77
4	C	351	ACT	CH3-C	2.41	1.51	1.48
4	F	351	ACT	CH3-C	2.19	1.51	1.48

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	EPE	C5-N4-C3	5.38	120.94	108.83
2	A	400	EPE	C5-N4-C3	5.07	120.24	108.83
2	F	400	EPE	O2S-S-C10	4.73	112.61	106.92
2	G	349	EPE	O1S-S-C10	4.51	112.35	106.92
2	F	400	EPE	C5-N4-C3	4.49	118.93	108.83
2	G	400	EPE	C5-N4-C3	4.45	118.84	108.83
2	B	400	EPE	C5-N4-C3	4.14	118.14	108.83
2	F	400	EPE	C7-N4-C5	3.78	120.90	111.23
2	G	349	EPE	C7-N4-C3	3.77	120.89	111.23
2	G	400	EPE	C7-N4-C3	3.72	120.74	111.23
2	A	400	EPE	C7-N4-C5	3.57	120.36	111.23
2	F	349	EPE	C7-N4-C3	3.55	120.32	111.23
2	B	400	EPE	C7-N4-C5	3.51	120.20	111.23
2	G	400	EPE	C7-N4-C5	3.50	120.18	111.23
2	F	400	EPE	C7-N4-C3	3.49	120.17	111.23
2	G	349	EPE	C5-N4-C3	3.43	116.54	108.83
2	B	400	EPE	O3S-S-C10	3.42	111.30	105.77
2	G	400	EPE	O2S-S-C10	3.42	111.03	106.92
2	G	349	EPE	C7-N4-C5	3.36	119.82	111.23
2	F	349	EPE	C5-N4-C3	3.32	116.29	108.83
2	A	400	EPE	C7-N4-C3	3.05	119.02	111.23
2	D	400	EPE	C7-N4-C3	2.94	118.75	111.23
2	D	400	EPE	C7-N4-C5	2.87	118.57	111.23
2	F	349	EPE	C7-N4-C5	2.85	118.53	111.23
2	D	400	EPE	O3S-S-C10	2.85	110.38	105.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	EPE	C7-N4-C3	2.80	118.39	111.23
2	F	349	EPE	O3S-S-C10	2.79	110.29	105.77
2	G	400	EPE	O3S-S-C10	2.79	110.27	105.77
2	G	349	EPE	O2S-S-C10	2.74	110.22	106.92
2	A	400	EPE	O2S-S-C10	2.67	110.13	106.92
2	F	349	EPE	O2S-S-C10	2.61	110.06	106.92
2	A	400	EPE	O1S-S-C10	2.52	109.95	106.92
2	B	400	EPE	O2S-S-C10	2.36	109.76	106.92
2	F	400	EPE	O3S-S-C10	2.17	109.28	105.77
2	G	400	EPE	C6-N1-C2	2.04	113.41	108.83

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	349	EPE	S-C10-C9-N1
2	B	400	EPE	S-C10-C9-N1
2	A	400	EPE	C10-C9-N1-C6
2	A	400	EPE	C9-C10-S-O2S
2	A	400	EPE	C9-C10-S-O3S
2	G	400	EPE	C10-C9-N1-C6
2	G	400	EPE	S-C10-C9-N1
2	F	400	EPE	C10-C9-N1-C2
6	F	353	GOL	C1-C2-C3-O3
6	F	353	GOL	O2-C2-C3-O3
2	D	400	EPE	C9-C10-S-O1S
2	D	400	EPE	C9-C10-S-O2S
2	D	400	EPE	C9-C10-S-O3S
6	C	353	GOL	O1-C1-C2-C3
6	C	353	GOL	C1-C2-C3-O3
6	C	353	GOL	O2-C2-C3-O3
2	F	349	EPE	C8-C7-N4-C5
2	F	400	EPE	N4-C7-C8-O8
2	D	400	EPE	N4-C7-C8-O8
6	C	353	GOL	O1-C1-C2-O2
2	A	400	EPE	N4-C7-C8-O8
6	D	354	GOL	C1-C2-C3-O3
2	F	349	EPE	N4-C7-C8-O8
2	G	349	EPE	C8-C7-N4-C3
2	F	400	EPE	S-C10-C9-N1
2	F	349	EPE	S-C10-C9-N1
2	A	400	EPE	C10-C9-N1-C2

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Mol	Chain	Res	Type	Atoms
2	G	400	EPE	C10-C9-N1-C2
2	F	349	EPE	C10-C9-N1-C2
2	F	349	EPE	C10-C9-N1-C6
6	D	354	GOL	O2-C2-C3-O3
2	B	400	EPE	C8-C7-N4-C3
2	A	400	EPE	C9-C10-S-O1S
2	F	349	EPE	C8-C7-N4-C3
6	D	354	GOL	O1-C1-C2-C3
2	B	400	EPE	C10-C9-N1-C2
2	B	400	EPE	C10-C9-N1-C6
2	D	400	EPE	C8-C7-N4-C5
2	F	400	EPE	C8-C7-N4-C3
2	G	400	EPE	C8-C7-N4-C3

There are no ring outliers.

11 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	352	SO4	2	0
2	G	349	EPE	5	0
2	B	400	EPE	3	0
3	H	353	SO4	1	0
2	A	400	EPE	1	0
2	G	400	EPE	7	0
2	F	400	EPE	9	0
6	F	353	GOL	5	0
6	C	353	GOL	1	0
2	F	349	EPE	5	0
6	D	354	GOL	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, 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	323/348 (92%)	-0.04	9 (2%)	53	56	17, 25, 38, 47	0
1	B	315/348 (90%)	0.02	7 (2%)	62	64	18, 28, 40, 47	0
1	C	317/348 (91%)	-0.04	8 (2%)	57	60	17, 25, 38, 64	0
1	D	315/348 (90%)	0.04	7 (2%)	62	64	19, 27, 41, 48	0
1	E	316/348 (90%)	-0.12	5 (1%)	72	74	12, 19, 31, 54	0
1	F	315/348 (90%)	-0.09	3 (0%)	82	84	12, 21, 34, 44	0
1	G	318/348 (91%)	-0.11	6 (1%)	66	69	12, 19, 31, 60	0
1	H	315/348 (90%)	-0.06	7 (2%)	62	64	12, 22, 35, 45	0
All	All	2534/2784 (91%)	-0.05	52 (2%)	63	66	12, 23, 38, 64	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	325	ASN	7.3
1	B	2	ASN	5.0
1	C	326	ARG	4.8
1	E	325	ASN	4.4
1	D	23[A]	PHE	4.2
1	D	2	ASN	4.2
1	G	327	ALA	4.2
1	H	2	ASN	4.0
1	H	23	PHE	3.9
1	A	23	PHE	3.8
1	A	2	ASN	3.7
1	F	2	ASN	3.6
1	G	2	ASN	3.6
1	G	325	ASN	3.5
1	C	2	ASN	3.5
1	E	2	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	23	PHE	3.2
1	C	23	PHE	3.2
1	E	23	PHE	2.9
1	G	111[A]	ARG	2.7
1	D	216	LEU	2.6
1	B	23	PHE	2.6
1	G	223	LEU	2.6
1	A	187	TRP	2.6
1	E	223	LEU	2.5
1	B	216	LEU	2.4
1	A	111	ARG	2.4
1	D	163	LEU	2.4
1	H	72	ARG	2.3
1	A	328[A]	GLU	2.3
1	D	194	ALA	2.3
1	D	223	LEU	2.3
1	D	189	PHE	2.3
1	B	195	VAL	2.3
1	C	223	LEU	2.2
1	H	187	TRP	2.2
1	A	331	TYR	2.2
1	H	163	LEU	2.2
1	B	187	TRP	2.1
1	A	223	LEU	2.1
1	E	225	TYR	2.1
1	F	216	LEU	2.1
1	H	194	ALA	2.1
1	B	111[A]	ARG	2.1
1	F	187	TRP	2.1
1	B	163	LEU	2.1
1	H	223	LEU	2.1
1	C	189	PHE	2.0
1	C	187	TRP	2.0
1	C	315	TRP	2.0
1	A	329	ASN	2.0
1	A	190	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
2	EPE	D	400	15/15	0.57	0.29	66,70,72,72	15
2	EPE	A	400	15/15	0.58	0.32	47,53,57,57	15
2	EPE	G	349	15/15	0.59	0.28	40,42,47,49	15
2	EPE	B	400	15/15	0.61	0.30	36,43,45,45	15
6	GOL	C	353	6/6	0.61	0.35	56,60,61,62	0
2	EPE	G	400	15/15	0.66	0.28	44,48,50,50	15
2	EPE	F	400	15/15	0.67	0.27	52,56,59,59	15
2	EPE	F	349	15/15	0.74	0.28	30,33,34,35	15
3	SO4	C	349	5/5	0.75	0.26	108,108,108,108	0
3	SO4	D	352	5/5	0.78	0.26	91,91,92,92	0
3	SO4	E	352	5/5	0.79	0.27	26,33,37,38	5
3	SO4	G	355	5/5	0.80	0.20	48,50,50,51	5
3	SO4	C	350	5/5	0.81	0.22	47,50,51,52	5
3	SO4	G	354	5/5	0.83	0.30	42,42,43,43	5
3	SO4	H	351	5/5	0.83	0.35	89,89,89,90	0
3	SO4	H	352	5/5	0.83	0.16	33,34,36,37	5
3	SO4	G	352	5/5	0.83	0.35	95,95,95,96	0
4	ACT	B	354	4/4	0.83	0.10	53,53,53,53	0
4	ACT	G	357	4/4	0.84	0.13	41,42,42,43	0
3	SO4	A	349	5/5	0.85	0.21	35,40,42,43	5
6	GOL	D	354	6/6	0.86	0.18	33,40,42,44	0
3	SO4	B	352	5/5	0.86	0.25	48,48,49,49	5
4	ACT	F	352	4/4	0.86	0.13	52,53,53,53	0
3	SO4	G	350	5/5	0.87	0.20	25,34,37,37	5
6	GOL	F	353	6/6	0.88	0.19	30,38,38,41	0
4	ACT	A	355	4/4	0.89	0.12	51,51,51,52	0
3	SO4	A	352	5/5	0.90	0.13	52,53,53,54	5
3	SO4	A	351	5/5	0.90	0.31	44,45,45,45	5
3	SO4	B	351	5/5	0.90	0.23	38,41,43,45	5
5	CL	B	355	1/1	0.90	0.18	52,52,52,52	0
4	ACT	G	358	4/4	0.91	0.10	72,72,72,72	0
4	ACT	A	354	4/4	0.91	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ACT	C	352	4/4	0.91	0.11	45,45,45,46	0
3	SO4	H	353	5/5	0.91	0.24	49,50,52,52	5
4	ACT	E	354	4/4	0.92	0.10	43,44,44,44	0
4	ACT	B	353	4/4	0.92	0.14	31,31,31,31	0
3	SO4	E	351	5/5	0.93	0.24	60,60,63,63	0
4	ACT	D	353	4/4	0.93	0.12	30,31,32,32	0
3	SO4	E	350	5/5	0.93	0.17	63,64,64,65	0
3	SO4	G	353	5/5	0.94	0.16	20,22,25,26	5
3	SO4	A	350	5/5	0.94	0.19	65,65,65,65	0
3	SO4	D	351	5/5	0.94	0.17	68,69,70,70	0
4	ACT	A	353	4/4	0.95	0.10	25,25,25,25	0
4	ACT	H	354	4/4	0.95	0.14	20,21,22,22	0
4	ACT	F	351	4/4	0.95	0.15	24,25,25,26	0
3	SO4	B	350	5/5	0.96	0.23	71,71,72,73	0
3	SO4	G	351	5/5	0.96	0.21	61,61,62,62	0
4	ACT	G	356	4/4	0.96	0.09	17,18,19,20	0
4	ACT	E	353	4/4	0.96	0.07	19,20,20,21	0
3	SO4	D	350	5/5	0.96	0.19	60,60,61,61	0
3	SO4	E	349	5/5	0.97	0.22	55,55,56,57	0
4	ACT	C	351	4/4	0.97	0.10	23,25,26,26	0
3	SO4	B	349	5/5	0.98	0.09	39,41,42,43	0
3	SO4	D	349	5/5	0.98	0.09	46,46,47,47	0
3	SO4	H	349	5/5	0.98	0.11	39,40,42,42	0
3	SO4	H	350	5/5	0.98	0.24	57,57,58,59	0
3	SO4	F	350	5/5	0.98	0.08	37,38,39,40	0

6.5 Other polymers

There are no such residues in this entry.