



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 01:07 PM UTC

PDB ID : 8FUM / pdb_00008fum
Title : AibH1H2 metalated with Fe in the presence of Tris
Authors : Powell, M.M.; Rittle, J.
Deposited on : 2023-01-17
Resolution : 1.48 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

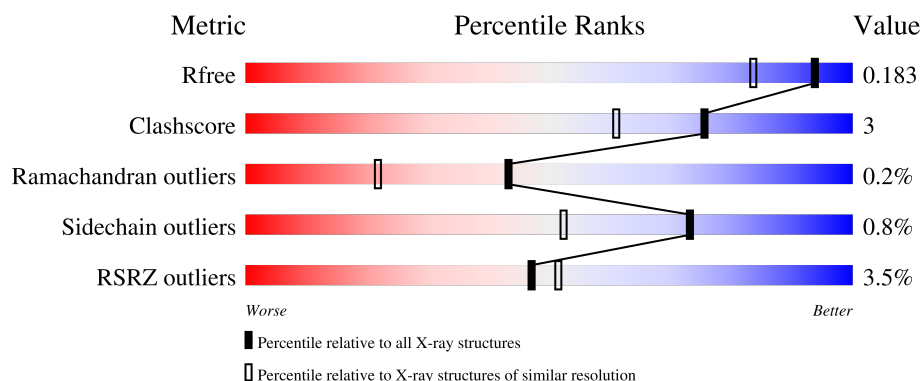
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	392	2% 86% 11%
1	C	392	3% 86% 11%
1	E	392	0% 83% 10%
1	G	392	2% 84% 10%
2	B	378	3% 87% 8%

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Mol	Chain	Length	Quality of chain
2	F	378	
2	H	378	
3	D	378	

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
4	PG4	B	501	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 47082 atoms, of which 21982 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	350	Total	C	H	N	O	S	0	2	0
			5527	1795	2716	491	520	5			
1	C	350	Total	C	H	N	O	S	0	1	0
			5513	1791	2706	491	520	5			
1	E	351	Total	C	H	N	O	S	0	4	0
			5539	1803	2712	495	524	5			
1	G	351	Total	C	H	N	O	S	0	6	0
			5554	1804	2728	495	522	5			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP A0A402C2V4
A	-5	GLY	-	expression tag	UNP A0A402C2V4
A	-4	HIS	-	expression tag	UNP A0A402C2V4
A	-3	HIS	-	expression tag	UNP A0A402C2V4
A	-2	HIS	-	expression tag	UNP A0A402C2V4
A	-1	HIS	-	expression tag	UNP A0A402C2V4
A	0	HIS	-	expression tag	UNP A0A402C2V4
A	1	HIS	-	expression tag	UNP A0A402C2V4
A	2	SER	-	expression tag	UNP A0A402C2V4
A	3	GLY	-	expression tag	UNP A0A402C2V4
A	4	GLU	-	expression tag	UNP A0A402C2V4
A	5	ASN	-	expression tag	UNP A0A402C2V4
A	6	LEU	-	expression tag	UNP A0A402C2V4
A	7	TYR	-	expression tag	UNP A0A402C2V4
A	8	PHE	-	expression tag	UNP A0A402C2V4
A	9	GLN	-	expression tag	UNP A0A402C2V4
A	10	SER	-	expression tag	UNP A0A402C2V4
A	11	GLY	-	expression tag	UNP A0A402C2V4
A	12	GLY	-	expression tag	UNP A0A402C2V4
C	-6	MET	-	expression tag	UNP A0A402C2V4
C	-5	GLY	-	expression tag	UNP A0A402C2V4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP A0A402C2V4
C	-3	HIS	-	expression tag	UNP A0A402C2V4
C	-2	HIS	-	expression tag	UNP A0A402C2V4
C	-1	HIS	-	expression tag	UNP A0A402C2V4
C	0	HIS	-	expression tag	UNP A0A402C2V4
C	1	HIS	-	expression tag	UNP A0A402C2V4
C	2	SER	-	expression tag	UNP A0A402C2V4
C	3	GLY	-	expression tag	UNP A0A402C2V4
C	4	GLU	-	expression tag	UNP A0A402C2V4
C	5	ASN	-	expression tag	UNP A0A402C2V4
C	6	LEU	-	expression tag	UNP A0A402C2V4
C	7	TYR	-	expression tag	UNP A0A402C2V4
C	8	PHE	-	expression tag	UNP A0A402C2V4
C	9	GLN	-	expression tag	UNP A0A402C2V4
C	10	SER	-	expression tag	UNP A0A402C2V4
C	11	GLY	-	expression tag	UNP A0A402C2V4
C	12	GLY	-	expression tag	UNP A0A402C2V4
E	-6	MET	-	expression tag	UNP A0A402C2V4
E	-5	GLY	-	expression tag	UNP A0A402C2V4
E	-4	HIS	-	expression tag	UNP A0A402C2V4
E	-3	HIS	-	expression tag	UNP A0A402C2V4
E	-2	HIS	-	expression tag	UNP A0A402C2V4
E	-1	HIS	-	expression tag	UNP A0A402C2V4
E	0	HIS	-	expression tag	UNP A0A402C2V4
E	1	HIS	-	expression tag	UNP A0A402C2V4
E	2	SER	-	expression tag	UNP A0A402C2V4
E	3	GLY	-	expression tag	UNP A0A402C2V4
E	4	GLU	-	expression tag	UNP A0A402C2V4
E	5	ASN	-	expression tag	UNP A0A402C2V4
E	6	LEU	-	expression tag	UNP A0A402C2V4
E	7	TYR	-	expression tag	UNP A0A402C2V4
E	8	PHE	-	expression tag	UNP A0A402C2V4
E	9	GLN	-	expression tag	UNP A0A402C2V4
E	10	SER	-	expression tag	UNP A0A402C2V4
E	11	GLY	-	expression tag	UNP A0A402C2V4
E	12	GLY	-	expression tag	UNP A0A402C2V4
G	-6	MET	-	expression tag	UNP A0A402C2V4
G	-5	GLY	-	expression tag	UNP A0A402C2V4
G	-4	HIS	-	expression tag	UNP A0A402C2V4
G	-3	HIS	-	expression tag	UNP A0A402C2V4
G	-2	HIS	-	expression tag	UNP A0A402C2V4
G	-1	HIS	-	expression tag	UNP A0A402C2V4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A402C2V4
G	1	HIS	-	expression tag	UNP A0A402C2V4
G	2	SER	-	expression tag	UNP A0A402C2V4
G	3	GLY	-	expression tag	UNP A0A402C2V4
G	4	GLU	-	expression tag	UNP A0A402C2V4
G	5	ASN	-	expression tag	UNP A0A402C2V4
G	6	LEU	-	expression tag	UNP A0A402C2V4
G	7	TYR	-	expression tag	UNP A0A402C2V4
G	8	PHE	-	expression tag	UNP A0A402C2V4
G	9	GLN	-	expression tag	UNP A0A402C2V4
G	10	SER	-	expression tag	UNP A0A402C2V4
G	11	GLY	-	expression tag	UNP A0A402C2V4
G	12	GLY	-	expression tag	UNP A0A402C2V4

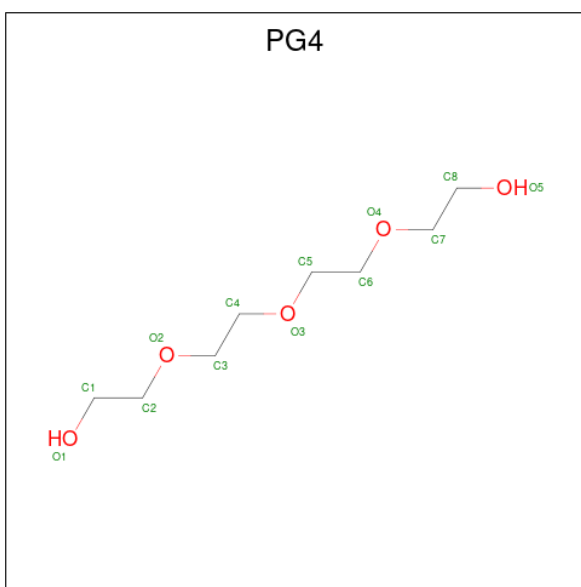
- Molecule 2 is a protein called Amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	363	Total	C	H	N	O	S	0	4	0
			5611	1839	2730	487	546	9			
2	F	362	Total	C	H	N	O	S	0	4	0
			5625	1834	2748	493	541	9			
2	H	364	Total	C	H	N	O	S	0	4	0
			5617	1834	2745	490	539	9			

- Molecule 3 is a protein called Amidohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	D	363	Total	C	H	N	O	S	0	3	0
			5644	1840	2761	493	541	9			

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			31	8	18	5		
4	A	1	Total	C	H	O	0	0
			31	8	18	5		
4	B	1	Total	C	H	O	0	0
			31	8	18	5		
4	C	1	Total	C	H	O	0	0
			31	8	18	5		
4	E	1	Total	C	H	O	0	0
			31	8	18	5		
4	G	1	Total	C	H	O	0	0
			31	8	18	5		
4	G	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Fe	0	0
			1	1		
5	B	2	Total	Fe	0	0
			2	2		
5	C	1	Total	Fe	0	0
			1	1		
5	D	2	Total	Fe	0	0
			2	2		
5	E	1	Total	Fe	0	0
			1	1		

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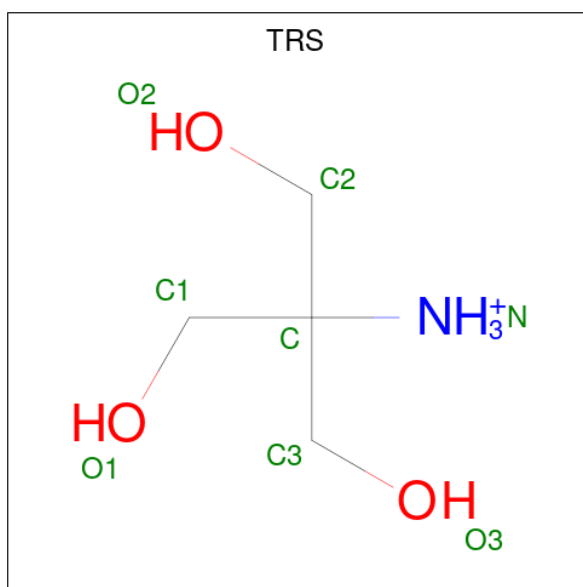
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	2	Total 2	Fe 2	0	0
5	G	1	Total 1	Fe 1	0	0
5	H	2	Total 2	Fe 2	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Mg 2	0	0
6	B	1	Total 1	Mg 1	0	0
6	C	1	Total 1	Mg 1	0	0
6	D	1	Total 1	Mg 1	0	0
6	E	3	Total 3	Mg 3	0	0
6	F	1	Total 1	Mg 1	0	0
6	G	3	Total 3	Mg 3	0	0
6	H	2	Total 2	Mg 2	0	0

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		
7	F	1	Total	C	N	O	0	0
			8	4	1	3		
7	F	1	Total	C	N	O	0	0
			8	4	1	3		
7	F	1	Total	C	N	O	0	0
			8	4	1	3		
7	H	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	E	1	Total	C	H	O	0	0
			17	4	10	3		

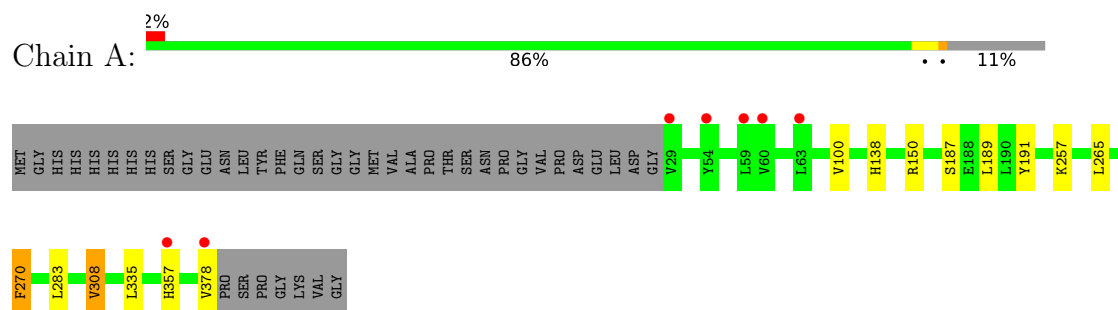
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	272	Total	O	0	0
			272	272		
9	B	277	Total	O	0	0
			277	277		
9	C	243	Total	O	0	0
			243	243		
9	D	288	Total	O	0	0
			288	288		
9	E	292	Total	O	0	0
			292	292		
9	F	260	Total	O	0	0
			260	260		
9	G	268	Total	O	0	0
			268	268		
9	H	236	Total	O	0	0
			236	236		

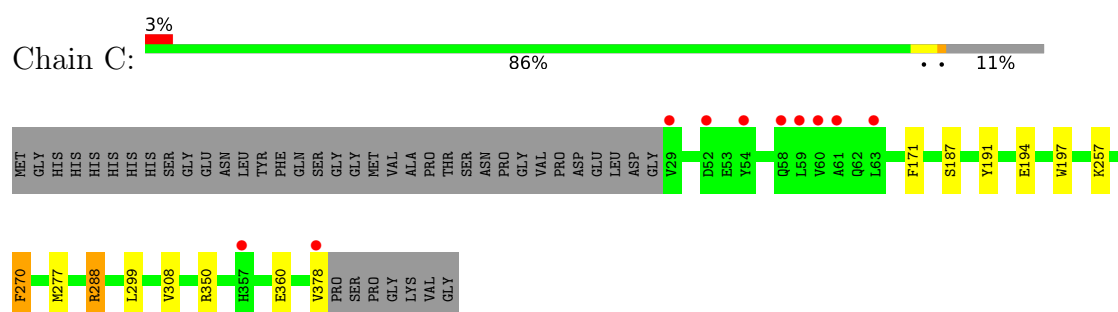
3 Residue-property plots [i](#)

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.

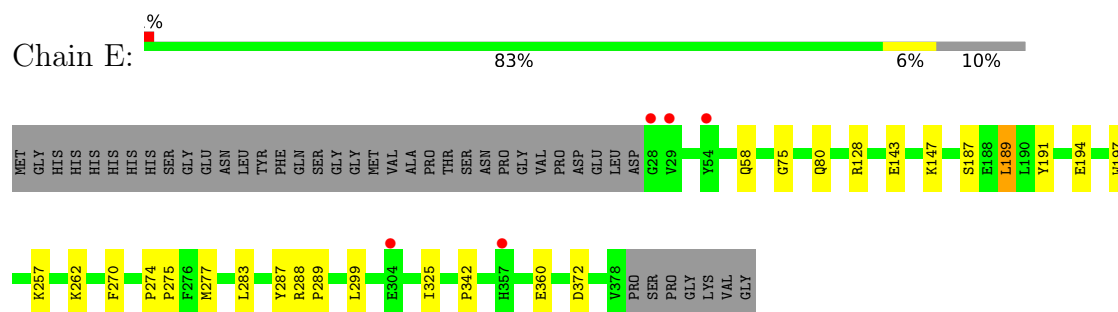
- Molecule 1: Amidohydrolase



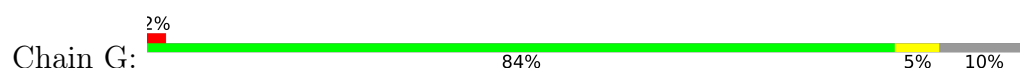
- Molecule 1: Amidohydrolase

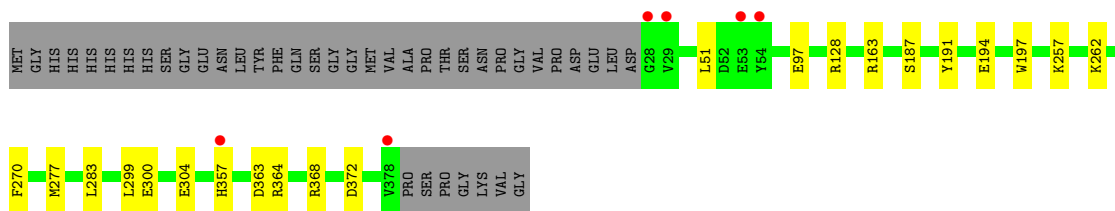


- Molecule 1: Amidohydrolase

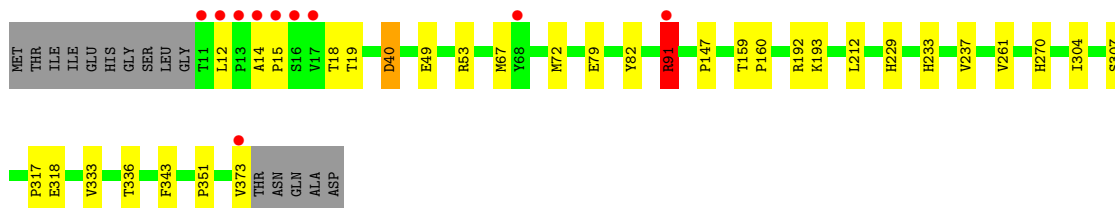
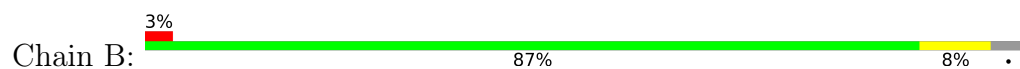


- Molecule 1: Amidohydrolase

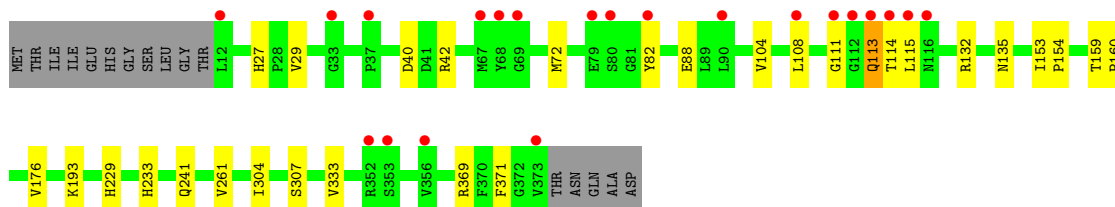
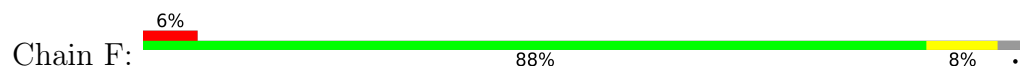




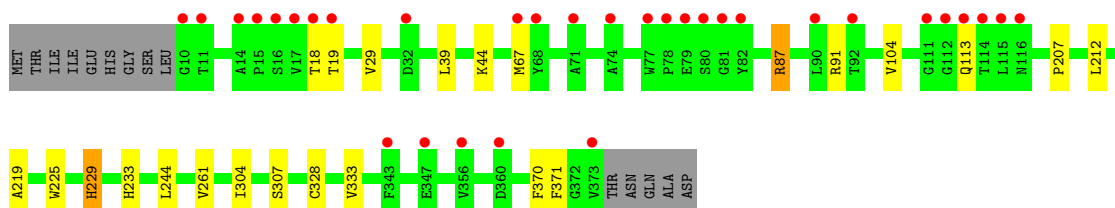
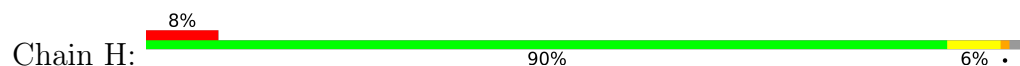
• Molecule 2: Amidohydrolase



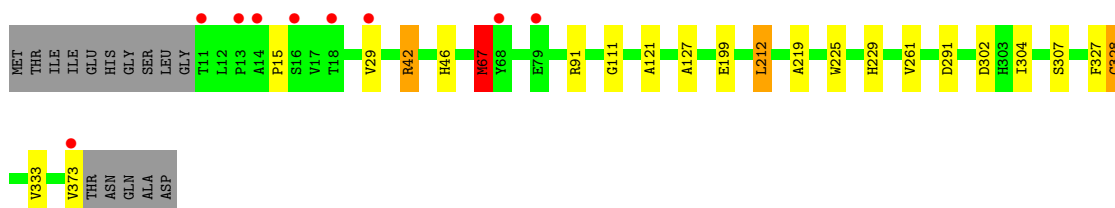
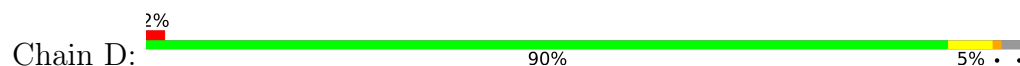
• Molecule 2: Amidohydrolase



• Molecule 2: Amidohydrolase



• Molecule 3: Amidohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.59Å 232.64Å 147.64Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	45.58 – 1.48 45.58 – 1.48	Depositor EDS
% Data completeness (in resolution range)	93.7 (45.58-1.48) 88.7 (45.58-1.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.48Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.159 , 0.184 0.159 , 0.183	Depositor DCC
R_{free} test set	1414 reflections (0.31%)	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.034 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	47082	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, MG, FE, CSO, PEG, PG4

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	0.42	0/2901	0.59	0/3965
1	C	0.38	0/2894	0.60	2/3955 (0.1%)
1	E	0.40	0/2924	0.60	0/3996
1	G	0.42	0/2929	0.58	0/4004
2	B	0.44	2/2971 (0.1%)	0.61	0/4058
2	F	0.37	0/2976	0.59	1/4064 (0.0%)
2	H	0.43	1/2961 (0.0%)	0.58	0/4044
3	D	0.50	6/2978 (0.2%)	0.63	0/4067
All	All	0.42	9/23534 (0.0%)	0.60	3/32153 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	291	ASP	CG-OD2	-7.14	1.11	1.25
3	D	42[A]	ARG	N-CA	7.14	1.54	1.46
3	D	42[B]	ARG	N-CA	7.14	1.54	1.46
2	B	91	ARG	C-O	-6.32	1.16	1.24
3	D	291	ASP	C-O	-5.88	1.16	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	350	ARG	NE-CZ-NH2	8.89	127.20	119.20
1	C	350	ARG	NE-CZ-NH1	-7.76	113.74	121.50
2	F	115	LEU	N-CA-C	6.36	117.81	107.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2811	2716	2714	10	0
1	C	2807	2706	2705	9	0
1	E	2827	2712	2716	22	0
1	G	2826	2728	2720	15	0
2	B	2881	2730	2749	26	0
2	F	2877	2748	2745	29	0
2	H	2872	2745	2749	14	0
3	D	2883	2761	2764	18	0
4	A	26	36	36	2	0
4	B	13	18	17	18	0
4	C	13	18	18	1	0
4	E	13	18	18	3	0
4	G	26	36	36	1	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
5	E	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
6	G	3	0	0	0	0
6	H	2	0	0	0	0
7	B	8	0	10	0	0
7	D	16	0	22	0	0
7	F	24	0	34	3	0
7	H	8	0	11	1	0
8	E	7	10	10	2	0
9	A	272	0	0	0	0
9	B	277	0	0	5	0
9	C	243	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	D	288	0	0	1	0
9	E	292	0	0	0	0
9	F	260	0	0	5	1
9	G	268	0	0	1	1
9	H	236	0	0	2	0
All	All	25100	21982	22074	137	2

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 3.

The worst 5 of 137 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:A:308[B]:VAL:HG23	1:A:335:LEU:HD23	1.54	0.88
2:H:18:THR:HG23	2:H:19:THR:H	1.43	0.84
2:B:91:ARG:HG3	2:B:91:ARG:HH11	1.54	0.73
3:D:42[B]:ARG:HH21	3:D:42[B]:ARG:HG2	1.54	0.71
2:F:40:ASP:HA	7:F:403:TRS:H12	1.73	0.69

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:F:630:HOH:O	9:F:630:HOH:O[2_556]	2.10	0.10
9:G:666:HOH:O	9:G:763:HOH:O[2_556]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	350/392 (89%)	345 (99%)	4 (1%)	1 (0%)	36 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	349/392 (89%)	345 (99%)	3 (1%)	1 (0%)	36	17
1	E	353/392 (90%)	349 (99%)	3 (1%)	1 (0%)	36	17
1	G	355/392 (91%)	349 (98%)	5 (1%)	1 (0%)	36	17
2	B	364/378 (96%)	347 (95%)	16 (4%)	1 (0%)	36	17
2	F	363/378 (96%)	345 (95%)	18 (5%)	0	100	100
2	H	365/378 (97%)	346 (95%)	19 (5%)	0	100	100
3	D	364/378 (96%)	347 (95%)	15 (4%)	2 (0%)	24	8
All	All	2863/3080 (93%)	2773 (97%)	83 (3%)	7 (0%)	43	22

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	328	CYS
1	E	270	PHE
1	A	270	PHE
1	C	270	PHE
3	D	67	MET

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	301/332 (91%)	296 (98%)	5 (2%)	53	24
1	C	300/332 (90%)	297 (99%)	3 (1%)	68	43
1	E	303/332 (91%)	302 (100%)	1 (0%)	86	75
1	G	303/332 (91%)	303 (100%)	0	100	100
2	B	305/317 (96%)	301 (99%)	4 (1%)	61	33
2	F	305/317 (96%)	304 (100%)	1 (0%)	86	75
2	H	302/317 (95%)	298 (99%)	4 (1%)	61	33
3	D	306/318 (96%)	303 (99%)	3 (1%)	68	43
All	All	2425/2597 (93%)	2404 (99%)	21 (1%)	73	48

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	229	HIS
2	H	29	VAL
2	H	229	HIS
2	H	87	ARG
2	F	113	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	124	GLN
2	H	113	GLN
2	F	124	GLN
2	H	98	HIS
1	E	375	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	CSO	B	328	2	3,6,7	0.41	0	1,6,8	1.74	0
2	CSO	F	328	2	3,6,7	0.57	0	1,6,8	0.75	0
2	CSO	H	328	2	3,6,7	0.30	0	1,6,8	2.22	1 (100%)

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	CSO	B	328	2	-	0/1/5/7	-
2	CSO	F	328	2	-	0/1/5/7	-
2	CSO	H	328	2	-	0/1/5/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	328	CSO	CB-CA-C	-2.22	104.78	110.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 41 ligands modelled in this entry, 26 are monoatomic - leaving 15 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	$\# Z > 2$
8	PEG	E	402	-	6,6,6	0.53	0	5,5,5	0.67	0
4	PG4	B	501	-	12,12,12	0.65	0	11,11,11	1.02	1 (9%)
4	PG4	A	402	-	12,12,12	0.45	0	11,11,11	0.85	0
4	PG4	A	401	-	12,12,12	0.47	0	11,11,11	0.61	0
7	TRS	F	402	-	7,7,7	0.27	0	9,9,9	0.91	0
4	PG4	G	402	6	12,12,12	0.41	0	11,11,11	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TRS	F	401	5	7,7,7	0.20	0	9,9,9	0.58	0
7	TRS	D	501	-	7,7,7	0.19	0	9,9,9	0.70	0
4	PG4	G	401	-	12,12,12	0.51	0	11,11,11	0.58	0
7	TRS	D	502	5	7,7,7	0.19	0	9,9,9	0.41	0
7	TRS	F	403	-	7,7,7	0.48	0	9,9,9	1.37	1 (11%)
7	TRS	B	502	5	7,7,7	0.32	0	9,9,9	0.62	0
4	PG4	C	401	-	12,12,12	0.40	0	11,11,11	0.43	0
4	PG4	E	401	-	12,12,12	0.51	0	11,11,11	0.36	0
7	TRS	H	401	5	7,7,7	0.36	0	9,9,9	0.97	0

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
8	PEG	E	402	-	-	2/4/4/4	-
4	PG4	B	501	-	-	7/10/10/10	-
4	PG4	A	402	-	-	6/10/10/10	-
4	PG4	A	401	-	-	6/10/10/10	-
7	TRS	F	402	-	-	3/9/9/9	-
4	PG4	G	402	6	-	7/10/10/10	-
7	TRS	F	401	5	-	3/9/9/9	-
7	TRS	D	501	-	-	8/9/9/9	-
4	PG4	G	401	-	-	5/10/10/10	-
7	TRS	D	502	5	-	3/9/9/9	-
7	TRS	F	403	-	-	6/9/9/9	-
7	TRS	B	502	5	-	3/9/9/9	-
4	PG4	C	401	-	-	6/10/10/10	-
4	PG4	E	401	-	-	2/10/10/10	-
7	TRS	H	401	5	-	0/9/9/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	403	TRS	C2-C-N	3.07	116.00	108.17
4	B	501	PG4	C7-O4-C6	2.33	123.44	113.26

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	501	TRS	C2-C-C1-O1
7	D	501	TRS	C3-C-C1-O1
7	D	501	TRS	N-C-C1-O1
7	F	402	TRS	C1-C-C3-O3
7	F	402	TRS	C2-C-C3-O3

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	402	PEG	2	0
4	B	501	PG4	18	0
4	A	402	PG4	1	0
4	A	401	PG4	1	0
7	F	402	TRS	1	0
4	G	402	PG4	1	0
7	F	403	TRS	2	0
4	C	401	PG4	1	0
4	E	401	PG4	3	0
7	H	401	TRS	1	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	350/392 (89%)	-0.36	7 (2%) 65 69	7, 14, 34, 48	2 (0%)
1	C	350/392 (89%)	-0.08	10 (2%) 53 58	8, 18, 40, 61	1 (0%)
1	E	351/392 (89%)	-0.42	5 (1%) 73 77	6, 14, 30, 69	3 (0%)
1	G	351/392 (89%)	-0.23	6 (1%) 69 73	8, 16, 33, 72	5 (1%)
2	B	362/378 (95%)	-0.22	10 (2%) 55 59	6, 15, 35, 70	4 (1%)
2	F	361/378 (95%)	-0.10	21 (5%) 29 31	7, 16, 44, 72	3 (0%)
2	H	363/378 (96%)	0.18	32 (8%) 15 17	6, 18, 48, 81	4 (1%)
3	D	363/378 (96%)	-0.26	9 (2%) 58 62	6, 15, 35, 67	3 (0%)
All	All	2851/3080 (92%)	-0.19	100 (3%) 47 51	6, 16, 38, 81	25 (0%)

The worst 5 of 100 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	114	THR	7.1
2	H	18	THR	6.2
3	D	373	VAL	5.5
1	E	28	GLY	5.5
3	D	68[A]	TYR	5.2

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

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	CSO	H	328	7/8	0.94	0.08	16,18,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CSO	B	328	7/8	0.97	0.06	12,13,17,25	0
2	CSO	F	328	7/8	0.98	0.05	12,16,21,25	0

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
6	MG	G	406	1/1	0.65	0.17	54,54,54,54	0
7	TRS	F	403	8/8	0.71	0.21	28,36,50,52	0
7	TRS	D	501	8/8	0.74	0.24	19,41,56,59	0
6	MG	A	405	1/1	0.76	0.16	48,48,48,48	0
6	MG	G	405	1/1	0.80	0.21	47,47,47,47	0
4	PG4	A	401	13/13	0.81	0.18	27,38,73,75	0
4	PG4	E	401	13/13	0.82	0.16	29,52,69,70	0
7	TRS	F	402	8/8	0.82	0.19	22,32,49,54	0
4	PG4	A	402	13/13	0.82	0.17	27,38,77,91	0
6	MG	C	403	1/1	0.85	0.14	53,53,53,53	0
4	PG4	G	402	13/13	0.85	0.15	30,41,70,73	0
4	PG4	C	401	13/13	0.86	0.14	30,45,81,88	0
7	TRS	H	401	8/8	0.86	0.18	20,33,56,60	0
4	PG4	G	401	13/13	0.89	0.13	25,42,66,67	0
6	MG	G	404	1/1	0.90	0.17	33,33,33,33	0
8	PEG	E	402	7/7	0.91	0.11	22,32,43,52	0
6	MG	E	405	1/1	0.93	0.13	37,37,37,37	0
7	TRS	F	401	8/8	0.93	0.13	15,26,35,40	0
4	PG4	B	501	13/13	0.94	0.14	8,24,74,78	0
6	MG	E	404	1/1	0.95	0.11	25,25,25,25	1
6	MG	H	404	1/1	0.95	0.07	32,32,32,32	0
7	TRS	B	502	8/8	0.96	0.07	12,15,19,22	0
6	MG	A	404	1/1	0.96	0.11	25,25,25,25	0
7	TRS	D	502	8/8	0.96	0.07	11,16,21,22	0
6	MG	D	505	1/1	0.96	0.10	30,30,30,30	0
6	MG	B	505	1/1	0.97	0.11	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	H	405	1/1	0.97	0.17	26,26,26,26	0
6	MG	F	406	1/1	0.98	0.19	19,19,19,19	0
5	FE	H	403	1/1	0.99	0.07	20,20,20,20	1
6	MG	E	406	1/1	0.99	0.12	15,15,15,15	0
5	FE	B	503	1/1	1.00	0.06	12,12,12,12	0
5	FE	B	504	1/1	1.00	0.02	11,11,11,11	0
5	FE	C	402	1/1	1.00	0.01	11,11,11,11	0
5	FE	D	503	1/1	1.00	0.07	12,12,12,12	0
5	FE	D	504	1/1	1.00	0.03	11,11,11,11	0
5	FE	E	403	1/1	1.00	0.02	9,9,9,9	0
5	FE	F	404	1/1	1.00	0.01	13,13,13,13	0
5	FE	F	405	1/1	1.00	0.05	16,16,16,16	1
5	FE	G	403	1/1	1.00	0.02	10,10,10,10	0
5	FE	H	402	1/1	1.00	0.02	15,15,15,15	0
5	FE	A	403	1/1	1.00	0.02	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.