



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2022 – 12:20 PM EST

PDB ID : 6C4A  
Title : Crystal structure of 3-nitropropionate modified isocitrate lyase from Mycobacterium tuberculosis with pyruvate  
Authors : Kreitler, D.F.; Ray, S.; Murkin, A.S.; Gulick, A.M.  
Deposited on : 2018-01-11  
Resolution : 1.80 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](mailto: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.

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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	:	2.27
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)	:	2.27

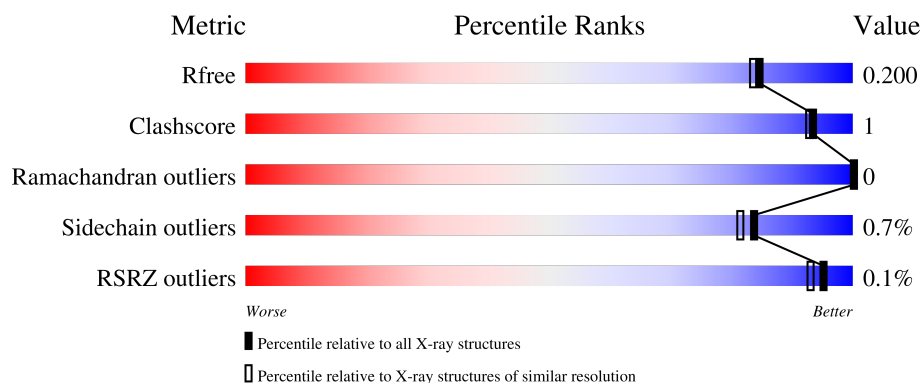
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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.



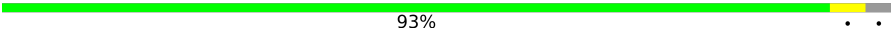
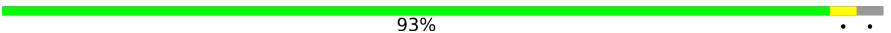
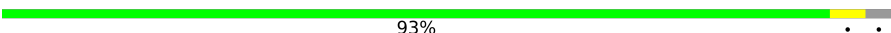
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\geq 3$ , 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	442	93%
1	B	442	93%
1	C	442	93%
1	D	442	94%
1	E	442	92%

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Mol	Chain	Length	Quality of chain
1	F	442	 93% . .
1	G	442	 93% . .
1	H	442	 93% . .

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55149 atoms, of which 25676 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 Isocitrate lyase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	H	N	O	S	0	0	0
			6506	2083	3189	574	650	10			
1	B	428	Total	C	H	N	O	S	0	0	0
			6490	2078	3181	577	645	9			
1	C	428	Total	C	H	N	O	S	0	0	0
			6502	2082	3184	578	649	9			
1	D	428	Total	C	H	N	O	S	0	0	0
			6457	2072	3158	572	646	9			
1	E	428	Total	C	H	N	O	S	0	9	0
			6608	2108	3243	590	658	9			
1	F	428	Total	C	H	N	O	S	0	0	0
			6492	2080	3178	577	648	9			
1	G	427	Total	C	H	N	O	S	0	4	0
			6530	2087	3204	582	648	9			
1	H	428	Total	C	H	N	O	S	0	3	0
			6544	2091	3212	584	648	9			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP H8EVV4
A	-12	HIS	-	expression tag	UNP H8EVV4
A	-11	HIS	-	expression tag	UNP H8EVV4
A	-10	HIS	-	expression tag	UNP H8EVV4
A	-9	HIS	-	expression tag	UNP H8EVV4
A	-8	HIS	-	expression tag	UNP H8EVV4
A	-7	HIS	-	expression tag	UNP H8EVV4
A	-6	LEU	-	expression tag	UNP H8EVV4
A	-5	VAL	-	expression tag	UNP H8EVV4
A	-4	PRO	-	expression tag	UNP H8EVV4
A	-3	ARG	-	expression tag	UNP H8EVV4
A	-2	GLY	-	expression tag	UNP H8EVV4
A	-1	SER	-	expression tag	UNP H8EVV4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP H8EVV4
B	-13	MET	-	initiating methionine	UNP H8EVV4
B	-12	HIS	-	expression tag	UNP H8EVV4
B	-11	HIS	-	expression tag	UNP H8EVV4
B	-10	HIS	-	expression tag	UNP H8EVV4
B	-9	HIS	-	expression tag	UNP H8EVV4
B	-8	HIS	-	expression tag	UNP H8EVV4
B	-7	HIS	-	expression tag	UNP H8EVV4
B	-6	LEU	-	expression tag	UNP H8EVV4
B	-5	VAL	-	expression tag	UNP H8EVV4
B	-4	PRO	-	expression tag	UNP H8EVV4
B	-3	ARG	-	expression tag	UNP H8EVV4
B	-2	GLY	-	expression tag	UNP H8EVV4
B	-1	SER	-	expression tag	UNP H8EVV4
B	0	HIS	-	expression tag	UNP H8EVV4
C	-13	MET	-	initiating methionine	UNP H8EVV4
C	-12	HIS	-	expression tag	UNP H8EVV4
C	-11	HIS	-	expression tag	UNP H8EVV4
C	-10	HIS	-	expression tag	UNP H8EVV4
C	-9	HIS	-	expression tag	UNP H8EVV4
C	-8	HIS	-	expression tag	UNP H8EVV4
C	-7	HIS	-	expression tag	UNP H8EVV4
C	-6	LEU	-	expression tag	UNP H8EVV4
C	-5	VAL	-	expression tag	UNP H8EVV4
C	-4	PRO	-	expression tag	UNP H8EVV4
C	-3	ARG	-	expression tag	UNP H8EVV4
C	-2	GLY	-	expression tag	UNP H8EVV4
C	-1	SER	-	expression tag	UNP H8EVV4
C	0	HIS	-	expression tag	UNP H8EVV4
D	-13	MET	-	initiating methionine	UNP H8EVV4
D	-12	HIS	-	expression tag	UNP H8EVV4
D	-11	HIS	-	expression tag	UNP H8EVV4
D	-10	HIS	-	expression tag	UNP H8EVV4
D	-9	HIS	-	expression tag	UNP H8EVV4
D	-8	HIS	-	expression tag	UNP H8EVV4
D	-7	HIS	-	expression tag	UNP H8EVV4
D	-6	LEU	-	expression tag	UNP H8EVV4
D	-5	VAL	-	expression tag	UNP H8EVV4
D	-4	PRO	-	expression tag	UNP H8EVV4
D	-3	ARG	-	expression tag	UNP H8EVV4
D	-2	GLY	-	expression tag	UNP H8EVV4
D	-1	SER	-	expression tag	UNP H8EVV4

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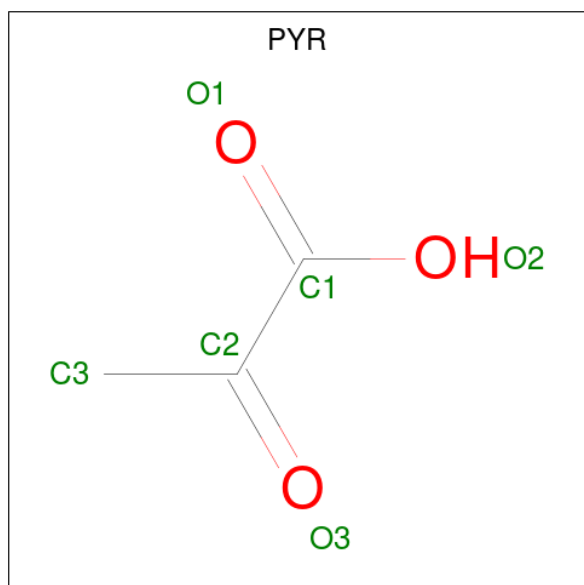
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP H8EVV4
E	-13	MET	-	initiating methionine	UNP H8EVV4
E	-12	HIS	-	expression tag	UNP H8EVV4
E	-11	HIS	-	expression tag	UNP H8EVV4
E	-10	HIS	-	expression tag	UNP H8EVV4
E	-9	HIS	-	expression tag	UNP H8EVV4
E	-8	HIS	-	expression tag	UNP H8EVV4
E	-7	HIS	-	expression tag	UNP H8EVV4
E	-6	LEU	-	expression tag	UNP H8EVV4
E	-5	VAL	-	expression tag	UNP H8EVV4
E	-4	PRO	-	expression tag	UNP H8EVV4
E	-3	ARG	-	expression tag	UNP H8EVV4
E	-2	GLY	-	expression tag	UNP H8EVV4
E	-1	SER	-	expression tag	UNP H8EVV4
E	0	HIS	-	expression tag	UNP H8EVV4
F	-13	MET	-	initiating methionine	UNP H8EVV4
F	-12	HIS	-	expression tag	UNP H8EVV4
F	-11	HIS	-	expression tag	UNP H8EVV4
F	-10	HIS	-	expression tag	UNP H8EVV4
F	-9	HIS	-	expression tag	UNP H8EVV4
F	-8	HIS	-	expression tag	UNP H8EVV4
F	-7	HIS	-	expression tag	UNP H8EVV4
F	-6	LEU	-	expression tag	UNP H8EVV4
F	-5	VAL	-	expression tag	UNP H8EVV4
F	-4	PRO	-	expression tag	UNP H8EVV4
F	-3	ARG	-	expression tag	UNP H8EVV4
F	-2	GLY	-	expression tag	UNP H8EVV4
F	-1	SER	-	expression tag	UNP H8EVV4
F	0	HIS	-	expression tag	UNP H8EVV4
G	-13	MET	-	initiating methionine	UNP H8EVV4
G	-12	HIS	-	expression tag	UNP H8EVV4
G	-11	HIS	-	expression tag	UNP H8EVV4
G	-10	HIS	-	expression tag	UNP H8EVV4
G	-9	HIS	-	expression tag	UNP H8EVV4
G	-8	HIS	-	expression tag	UNP H8EVV4
G	-7	HIS	-	expression tag	UNP H8EVV4
G	-6	LEU	-	expression tag	UNP H8EVV4
G	-5	VAL	-	expression tag	UNP H8EVV4
G	-4	PRO	-	expression tag	UNP H8EVV4
G	-3	ARG	-	expression tag	UNP H8EVV4
G	-2	GLY	-	expression tag	UNP H8EVV4
G	-1	SER	-	expression tag	UNP H8EVV4

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP H8EVV4
H	-13	MET	-	initiating methionine	UNP H8EVV4
H	-12	HIS	-	expression tag	UNP H8EVV4
H	-11	HIS	-	expression tag	UNP H8EVV4
H	-10	HIS	-	expression tag	UNP H8EVV4
H	-9	HIS	-	expression tag	UNP H8EVV4
H	-8	HIS	-	expression tag	UNP H8EVV4
H	-7	HIS	-	expression tag	UNP H8EVV4
H	-6	LEU	-	expression tag	UNP H8EVV4
H	-5	VAL	-	expression tag	UNP H8EVV4
H	-4	PRO	-	expression tag	UNP H8EVV4
H	-3	ARG	-	expression tag	UNP H8EVV4
H	-2	GLY	-	expression tag	UNP H8EVV4
H	-1	SER	-	expression tag	UNP H8EVV4
H	0	HIS	-	expression tag	UNP H8EVV4

- Molecule 2 is PYRUVIC ACID (three-letter code: PYR) (formula:  $C_3H_4O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			9	3	3	3		
2	B	1	Total	C	H	O	0	0
			9	3	3	3		
2	C	1	Total	C	H	O	0	0
			9	3	3	3		
2	D	1	Total	C	H	O	0	0
			9	3	3	3		

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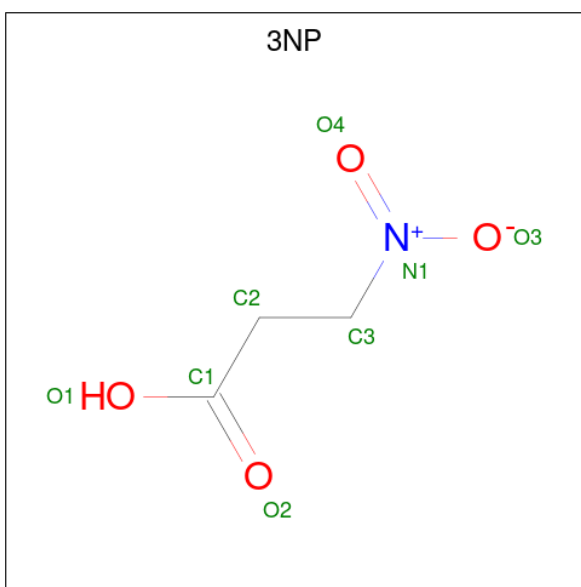
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	H	O	0	0
			9	3	3	3		
2	F	1	Total	C	H	O	0	0
			9	3	3	3		
2	G	1	Total	C	H	O	0	0
			9	3	3	3		
2	H	1	Total	C	H	O	0	0
			9	3	3	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	3	Total	Mg	0	0
			3	3		
3	C	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	E	2	Total	Mg	0	0
			2	2		
3	F	3	Total	Mg	0	0
			3	3		
3	G	3	Total	Mg	0	0
			3	3		
3	H	4	Total	Mg	0	0
			4	4		

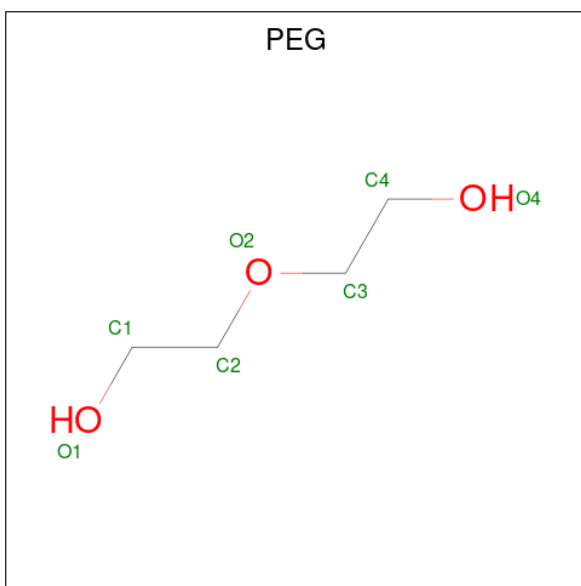
- Molecule 4 is 3-NITROPROPANOIC ACID (three-letter code: 3NP) (formula: C<sub>3</sub>H<sub>5</sub>NO<sub>4</sub>).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	0	1
			24	6	8	2	8		
4	C	1	Total	C	H	N	O	0	1
			24	6	8	2	8		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



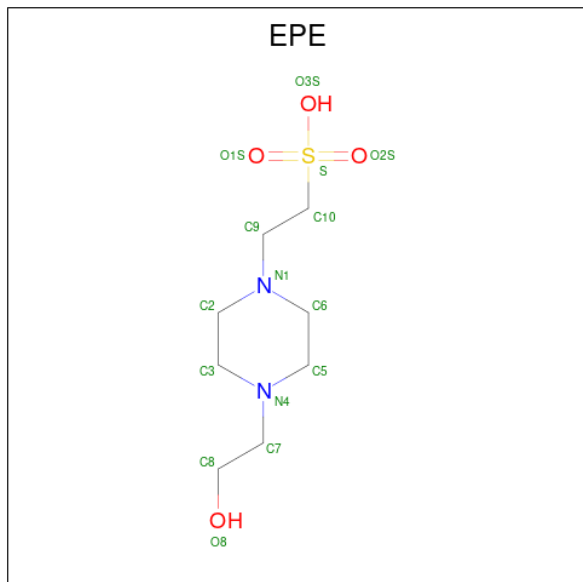
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	E	1	Total	C	H	O	0	0
			17	4	10	3		
5	F	1	Total	C	H	O	0	0
			17	4	10	3		
5	G	1	Total	C	H	O	0	0
			17	4	10	3		
5	H	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	F	1	Total	C	N	O	S	0	0
			7	2	1	3	1		
6	G	1	Total	C	H	N	O	S	0
			32	8	17	2	4	1	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	307	Total	O	0	0
			307	307		
7	B	271	Total	O	0	0
			271	271		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	321	Total 321	O 321	0	0
7	D	304	Total 304	O 304	0	0
7	E	410	Total 410	O 410	0	0
7	F	371	Total 371	O 371	0	0
7	G	389	Total 389	O 389	0	0
7	H	348	Total 348	O 348	0	0

### 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.

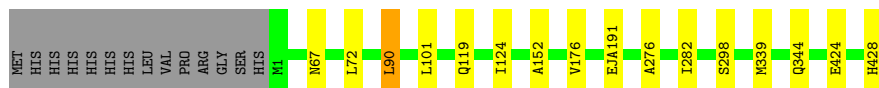
- Molecule 1: Isocitrate lyase 1

Chain A:  93%



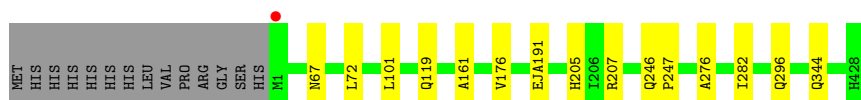
- Molecule 1: Isocitrate lyase 1

Chain B:  93%



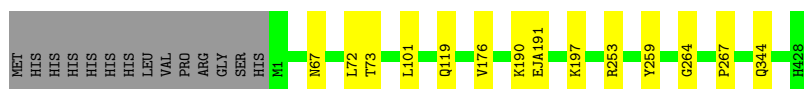
- Molecule 1: Isocitrate lyase 1

Chain C:  93%



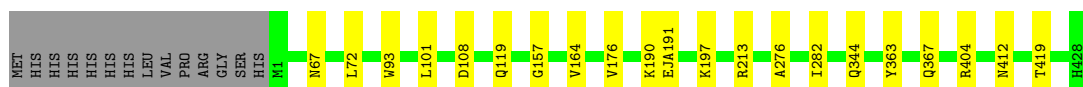
- Molecule 1: Isocitrate lyase 1

Chain D:  94%

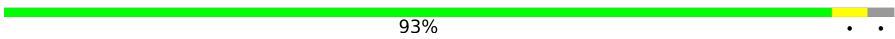


- Molecule 1: Isocitrate lyase 1

Chain E:  92% 5%



- Molecule 1: Isocitrate lyase 1

Chain F:  93% . .



● Molecule 1: Isocitrate lyase 1

Chain G:  93% . .



● Molecule 1: Isocitrate lyase 1

Chain H:  93% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.67Å 84.32Å 156.18Å 90.00° 116.59° 90.00°	Depositor
Resolution (Å)	72.18 – 1.80 72.18 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (72.18-1.80) 87.4 (72.18-1.80)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.40 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.163 , 0.197 0.165 , 0.200	Depositor DCC
$R_{free}$ test set	2000 reflections (0.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 42.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	55149	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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, PYR, 3NP, MG, EJA, PEG

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	0.39	0/3374	0.52	0/4587
1	B	0.38	0/3366	0.52	0/4576
1	C	0.40	0/3376	0.53	0/4590
1	D	0.40	0/3356	0.52	0/4565
1	E	0.45	0/3455	0.56	1/4694 (0.0%)
1	F	0.41	0/3372	0.54	0/4585
1	G	0.42	0/3399	0.55	0/4621
1	H	0.41	0/3400	0.56	0/4620
All	All	0.41	0/27098	0.54	1/36838 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	213	ARG	NE-CZ-NH2	-5.01	117.79	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	3317	3189	3183	8	0
1	B	3309	3181	3175	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3318	3184	3177	8	0
1	D	3299	3158	3151	5	0
1	E	3365	3243	3202	12	0
1	F	3314	3178	3171	10	0
1	G	3326	3204	3181	10	0
1	H	3332	3212	3194	8	0
2	A	6	3	3	0	0
2	B	6	3	3	0	0
2	C	6	3	3	0	0
2	D	6	3	3	0	0
2	E	6	3	3	0	0
2	F	6	3	3	0	0
2	G	6	3	3	0	0
2	H	6	3	3	1	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	4	0	0	0	0
4	B	16	8	8	2	0
4	C	16	8	8	4	0
5	B	7	10	10	0	0
5	C	7	10	10	0	0
5	D	7	10	10	0	0
5	E	7	10	10	0	0
5	F	7	10	10	0	0
5	G	7	10	10	0	0
5	H	7	10	10	0	0
6	F	7	0	4	1	0
6	G	15	17	17	0	0
7	A	307	0	0	5	0
7	B	271	0	0	0	0
7	C	321	0	0	5	0
7	D	304	0	0	2	0
7	E	410	0	0	4	0
7	F	371	0	0	5	0
7	G	389	0	0	6	0
7	H	348	0	0	2	0
All	All	29473	25676	25565	73	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 1.

The worst 5 of 73 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:419:THR:O	7:E:601:HOH:O	2.05	0.74
1:G:25:ASP:OD1	7:G:601:HOH:O	2.04	0.74
1:F:119:GLN:NE2	7:F:603:HOH:O	2.21	0.72
4:C:505[B]:3NP:O3	7:C:601:HOH:O	2.10	0.68
1:C:101:LEU:HD11	1:C:119:GLN:HG3	1.78	0.65

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	425/442 (96%)	418 (98%)	7 (2%)	0	100	100
1	B	425/442 (96%)	418 (98%)	7 (2%)	0	100	100
1	C	425/442 (96%)	417 (98%)	8 (2%)	0	100	100
1	D	425/442 (96%)	420 (99%)	5 (1%)	0	100	100
1	E	434/442 (98%)	425 (98%)	9 (2%)	0	100	100
1	F	425/442 (96%)	419 (99%)	6 (1%)	0	100	100
1	G	428/442 (97%)	421 (98%)	7 (2%)	0	100	100
1	H	428/442 (97%)	423 (99%)	5 (1%)	0	100	100
All	All	3415/3536 (97%)	3361 (98%)	54 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/351 (96%)	332 (99%)	4 (1%)	71	65
1	B	333/351 (95%)	329 (99%)	4 (1%)	71	65
1	C	335/351 (95%)	333 (99%)	2 (1%)	86	84
1	D	331/351 (94%)	328 (99%)	3 (1%)	78	75
1	E	345/351 (98%)	343 (99%)	2 (1%)	86	84
1	F	334/351 (95%)	333 (100%)	1 (0%)	92	91
1	G	338/351 (96%)	336 (99%)	2 (1%)	86	84
1	H	337/351 (96%)	335 (99%)	2 (1%)	86	84
All	All	2689/2808 (96%)	2669 (99%)	20 (1%)	84	81

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	176	VAL
1	G	176	VAL
1	H	176	VAL
1	H	72	LEU
1	B	176	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	367	GLN
1	F	205	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

8 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
1	EJA	E	191	1	6,12,13	1.51	1 (16%)	2,14,16	4.22	1 (50%)
1	EJA	H	191	1	6,12,13	1.38	1 (16%)	2,14,16	3.41	1 (50%)
1	EJA	F	191	1	6,12,13	1.52	1 (16%)	2,14,16	3.76	1 (50%)
1	EJA	G	191	1	6,12,13	2.00	1 (16%)	2,14,16	4.42	1 (50%)
1	EJA	A	191	1	6,12,13	1.54	1 (16%)	2,14,16	3.86	1 (50%)
1	EJA	D	191	1	6,12,13	1.35	1 (16%)	2,14,16	4.07	1 (50%)
1	EJA	C	191	1	6,12,13	1.62	1 (16%)	2,14,16	3.66	1 (50%)
1	EJA	B	191	1	6,12,13	1.03	0	2,14,16	2.82	1 (50%)

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
1	EJA	E	191	1	-	1/4/13/15	-
1	EJA	H	191	1	-	1/4/13/15	-
1	EJA	F	191	1	-	1/4/13/15	-
1	EJA	G	191	1	-	1/4/13/15	-
1	EJA	A	191	1	-	1/4/13/15	-
1	EJA	D	191	1	-	1/4/13/15	-
1	EJA	C	191	1	-	1/4/13/15	-
1	EJA	B	191	1	-	1/4/13/15	-

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	191	EJA	CB-SG	4.61	1.91	1.81
1	C	191	EJA	CB-SG	3.12	1.88	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	EJA	CB-SG	2.98	1.88	1.81
1	E	191	EJA	CB-SG	2.97	1.88	1.81
1	D	191	EJA	CB-SG	2.94	1.88	1.81

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	191	EJA	OZ-NE-CD	6.02	121.09	110.85
1	E	191	EJA	OZ-NE-CD	5.73	120.60	110.85
1	D	191	EJA	OZ-NE-CD	5.53	120.26	110.85
1	A	191	EJA	OZ-NE-CD	5.19	119.68	110.85
1	F	191	EJA	OZ-NE-CD	5.10	119.53	110.85

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	191	EJA	CE-CD-SG-CB
1	B	191	EJA	CE-CD-SG-CB
1	C	191	EJA	CE-CD-SG-CB
1	D	191	EJA	CE-CD-SG-CB
1	E	191	EJA	CE-CD-SG-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 21 are monoatomic - leaving 21 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
5	PEG	C	504	-	6,6,6	0.49	0	5,5,5	0.26	0
5	PEG	B	506	-	6,6,6	0.52	0	5,5,5	0.28	0
4	3NP	B	502[A]	-	2,7,7	0.72	0	1,8,8	0.34	0
2	PYR	G	501	3	2,5,5	1.64	1 (50%)	2,6,6	0.07	0
5	PEG	G	505	-	6,6,6	0.49	0	5,5,5	0.29	0
5	PEG	E	504	-	6,6,6	0.47	0	5,5,5	0.38	0
6	EPE	G	503	-	15,15,15	1.28	1 (6%)	18,20,20	2.18	5 (27%)
2	PYR	E	501	3	2,5,5	1.95	1 (50%)	2,6,6	0.81	0
4	3NP	C	505[A]	-	2,7,7	0.48	0	1,8,8	0.77	0
4	3NP	B	502[B]	-	2,7,7	0.94	0	1,8,8	0.52	0
5	PEG	F	506	-	6,6,6	0.49	0	5,5,5	0.38	0
5	PEG	D	504	-	6,6,6	0.47	0	5,5,5	0.35	0
2	PYR	B	503	3	2,5,5	1.94	1 (50%)	2,6,6	0.37	0
4	3NP	C	505[B]	-	2,7,7	0.40	0	1,8,8	0.05	0
2	PYR	A	501	3	2,5,5	1.81	1 (50%)	2,6,6	0.24	0
5	PEG	H	506	-	6,6,6	0.49	0	5,5,5	0.41	0
6	EPE	F	501	-	6,6,15	1.36	1 (16%)	6,8,20	1.34	1 (16%)
2	PYR	H	502	3	2,5,5	1.62	1 (50%)	2,6,6	0.56	0
2	PYR	C	501	3	2,5,5	1.87	1 (50%)	2,6,6	0.24	0
2	PYR	D	501	3	2,5,5	1.75	1 (50%)	2,6,6	0.29	0
2	PYR	F	502	3	2,5,5	1.64	1 (50%)	2,6,6	0.15	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
5	PEG	C	504	-	-	1/4/4/4	-
5	PEG	B	506	-	-	0/4/4/4	-
4	3NP	B	502[A]	-	-	0/2/5/5	-
2	PYR	G	501	3	-	0/0/4/4	-
5	PEG	G	505	-	-	2/4/4/4	-
5	PEG	E	504	-	-	1/4/4/4	-
6	EPE	G	503	-	-	6/9/19/19	0/1/1/1
2	PYR	E	501	3	-	0/0/4/4	-
4	3NP	C	505[A]	-	-	1/2/5/5	-
4	3NP	B	502[B]	-	-	0/2/5/5	-
5	PEG	F	506	-	-	3/4/4/4	-
5	PEG	D	504	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PYR	B	503	3	-	0/0/4/4	-
4	3NP	C	505[B]	-	-	1/2/5/5	-
2	PYR	A	501	3	-	0/0/4/4	-
5	PEG	H	506	-	-	1/4/4/4	-
6	EPE	F	501	-	-	1/4/4/19	-
2	PYR	H	502	3	-	0/0/4/4	-
2	PYR	C	501	3	-	0/0/4/4	-
2	PYR	D	501	3	-	0/0/4/4	-
2	PYR	F	502	3	-	0/0/4/4	-

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	503	EPE	C10-S	4.65	1.84	1.77
6	F	501	EPE	C10-S	3.14	1.82	1.77
2	E	501	PYR	O3-C2	2.75	1.31	1.22
2	B	503	PYR	O3-C2	2.74	1.31	1.22
2	C	501	PYR	O3-C2	2.63	1.30	1.22

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	503	EPE	O2S-S-C10	5.91	114.03	106.92
6	G	503	EPE	C7-N4-C5	3.42	119.98	111.23
6	G	503	EPE	C5-N4-C3	3.24	116.12	108.83
6	G	503	EPE	O2S-S-O1S	-2.66	104.74	113.95
6	G	503	EPE	C7-N4-C3	2.47	117.55	111.23

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	505[A]	3NP	C1-C2-C3-N1
4	C	505[B]	3NP	C1-C2-C3-N1
6	F	501	EPE	S-C10-C9-N1
6	G	503	EPE	C9-C10-S-O2S
6	G	503	EPE	C8-C7-N4-C5

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	505[A]	3NP	2	0
4	B	502[B]	3NP	2	0
4	C	505[B]	3NP	2	0
6	F	501	EPE	1	0
2	H	502	PYR	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	427/442 (96%)	-0.55	0 100 100	21, 35, 57, 67	0
1	B	427/442 (96%)	-0.48	0 100 100	24, 40, 64, 76	0
1	C	427/442 (96%)	-0.54	1 (0%) 95 93	21, 36, 56, 77	0
1	D	427/442 (96%)	-0.49	0 100 100	22, 37, 58, 76	0
1	E	427/442 (96%)	-0.57	0 100 100	21, 30, 45, 74	0
1	F	427/442 (96%)	-0.60	1 (0%) 95 93	21, 33, 51, 78	0
1	G	426/442 (96%)	-0.59	0 100 100	21, 31, 47, 64	0
1	H	427/442 (96%)	-0.59	0 100 100	21, 32, 51, 62	0
All	All	3415/3536 (96%)	-0.55	2 (0%) 95 93	21, 34, 55, 78	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	5.4
1	F	1	MET	2.7

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	EJA	D	191	13/14	0.95	0.10	40,46,55,56	0
1	EJA	A	191	13/14	0.96	0.09	29,35,48,48	0
1	EJA	H	191	13/14	0.96	0.07	27,34,48,48	0
1	EJA	E	191	13/14	0.97	0.08	19,26,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	EJA	F	191	13/14	0.97	0.07	26,31,39,43	0
1	EJA	G	191	13/14	0.97	0.09	25,30,40,42	0
1	EJA	B	191	13/14	0.97	0.08	30,36,50,51	0
1	EJA	C	191	13/14	0.98	0.08	22,34,42,50	0

### 6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
3	MG	B	501	1/1	0.57	0.33	79,79,79,79	0
3	MG	G	506	1/1	0.64	0.09	78,78,78,78	0
5	PEG	B	506	7/7	0.64	0.30	65,78,85,85	0
5	PEG	D	504	7/7	0.72	0.21	70,85,93,94	0
5	PEG	E	504	7/7	0.76	0.13	60,72,82,82	0
4	3NP	B	502[B]	8/8	0.77	0.25	56,63,72,72	12
4	3NP	B	502[A]	8/8	0.77	0.25	56,63,72,72	12
5	PEG	F	506	7/7	0.77	0.18	72,87,94,94	0
5	PEG	G	505	7/7	0.79	0.15	63,79,95,97	0
4	3NP	C	505[B]	8/8	0.81	0.25	77,78,92,92	12
4	3NP	C	505[A]	8/8	0.81	0.25	77,78,92,92	12
5	PEG	H	506	7/7	0.81	0.13	58,69,79,84	0
5	PEG	C	504	7/7	0.82	0.13	55,69,84,84	0
3	MG	H	504	1/1	0.92	0.03	49,49,49,49	0
2	PYR	C	501	6/6	0.93	0.08	29,32,40,40	0
3	MG	D	503	1/1	0.93	0.07	38,38,38,38	0
2	PYR	D	501	6/6	0.93	0.11	33,37,46,46	0
3	MG	C	503	1/1	0.94	0.07	35,35,35,35	0
2	PYR	A	501	6/6	0.95	0.10	30,34,40,40	0
3	MG	H	505	1/1	0.96	0.05	32,32,32,32	0
2	PYR	B	503	6/6	0.96	0.09	28,30,38,38	0
3	MG	B	505	1/1	0.96	0.06	46,46,46,46	0
6	EPE	F	501	7/15	0.96	0.11	44,47,55,56	0
6	EPE	G	503	15/15	0.96	0.14	44,73,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PYR	F	502	6/6	0.97	0.09	26,28,37,37	0
3	MG	F	505	1/1	0.97	0.07	41,41,41,41	0
2	PYR	G	501	6/6	0.97	0.07	25,30,37,37	0
3	MG	C	502	1/1	0.97	0.04	26,26,26,26	0
2	PYR	H	502	6/6	0.97	0.07	25,30,36,36	0
3	MG	D	502	1/1	0.97	0.03	31,31,31,31	0
3	MG	F	503	1/1	0.98	0.03	23,23,23,23	0
3	MG	F	504	1/1	0.98	0.04	41,41,41,41	0
2	PYR	E	501	6/6	0.98	0.08	22,26,29,29	0
3	MG	G	502	1/1	0.98	0.05	19,19,19,19	0
3	MG	A	502	1/1	0.98	0.03	27,27,27,27	0
3	MG	H	501	1/1	0.98	0.06	37,37,37,37	0
3	MG	A	503	1/1	0.98	0.06	41,41,41,41	0
3	MG	B	504	1/1	0.99	0.02	30,30,30,30	0
3	MG	G	504	1/1	0.99	0.04	30,30,30,30	0
3	MG	E	502	1/1	0.99	0.12	26,26,26,26	0
3	MG	E	503	1/1	0.99	0.07	30,30,30,30	0
3	MG	H	503	1/1	0.99	0.05	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.