



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:05 am GMT

PDB ID : 4E6M  
Title : Crystal structure of Putative dehydratase protein from Salmonella enterica subsp. enterica serovar Typhimurium (Salmonella typhimurium)  
Authors : Malashkevich, V.N.; Bhosle, R.; Toro, R.; Hillerich, B.; Gizzi, A.; Garforth, S.; Kar, A.; Chan, M.K.; Laffuer, J.; Patel, H.; Matikainen, B.; Chamala, S.; Lim, S.; Celikgil, A.; Villegas, G.; Evans, B.; Zenchek, W.; Love, J.; Fiser, A.; Khafizov, K.; Seidel, R.; Bonanno, J.B.; Almo, S.C.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2012-03-15  
Resolution : 1.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

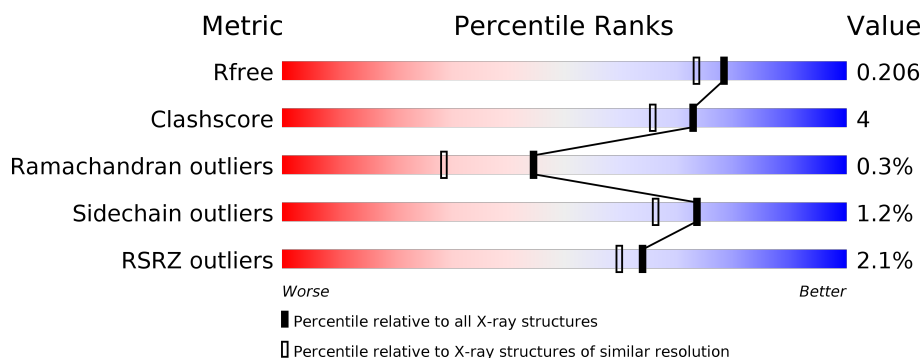
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	423	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>5%</div> </div> </div>
1	B	423	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>5%</div> </div> </div>
1	C	423	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> </div>
1	D	423	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>7%</div> <div>5%</div> </div> </div>
1	E	423	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>5%</div> </div> </div>
1	F	423	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>6%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	423	
1	H	423	

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
3	MPD	A	502	-	-	-	X
3	MPD	A	503	-	-	-	X
3	MPD	B	701	-	-	-	X
3	MPD	C	502	-	-	-	X
3	MPD	D	502	-	-	-	X
3	MPD	G	502	-	-	-	X
3	MPD	H	501	-	-	-	X
3	MPD	H	503	-	-	-	X
4	EPE	B	702	-	-	-	X
4	EPE	B	703	-	-	-	X
4	EPE	C	503	-	-	-	X
4	EPE	D	503	-	-	-	X
4	EPE	E	503	-	-	-	X
4	EPE	E	504	-	-	-	X
4	EPE	G	503	-	-	-	X
4	EPE	H	504	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27937 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 Putative dehydratase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	9	0
			3184	2029	534	602	19			
1	B	401	Total	C	N	O	S	0	8	0
			3178	2022	536	601	19			
1	C	401	Total	C	N	O	S	0	7	0
			3169	2013	535	603	18			
1	D	401	Total	C	N	O	S	0	6	0
			3171	2016	536	601	18			
1	E	401	Total	C	N	O	S	0	8	0
			3179	2022	535	604	18			
1	F	401	Total	C	N	O	S	0	5	0
			3157	2005	532	602	18			
1	G	401	Total	C	N	O	S	0	6	0
			3163	2011	531	603	18			
1	H	401	Total	C	N	O	S	0	8	0
			3177	2020	535	604	18			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q8ZNH1
A	-21	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
A	-20	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
A	-19	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
A	-18	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
A	-17	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
A	-16	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
A	-15	SER	-	EXPRESSION TAG	UNP Q8ZNH1
A	-14	SER	-	EXPRESSION TAG	UNP Q8ZNH1
A	-13	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
A	-12	VAL	-	EXPRESSION TAG	UNP Q8ZNH1
A	-11	ASP	-	EXPRESSION TAG	UNP Q8ZNH1
A	-10	LEU	-	EXPRESSION TAG	UNP Q8ZNH1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
A	-8	THR	-	EXPRESSION TAG	UNP Q8ZNH1
A	-7	GLU	-	EXPRESSION TAG	UNP Q8ZNH1
A	-6	ASN	-	EXPRESSION TAG	UNP Q8ZNH1
A	-5	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
A	-4	TYR	-	EXPRESSION TAG	UNP Q8ZNH1
A	-3	PHE	-	EXPRESSION TAG	UNP Q8ZNH1
A	-2	GLN	-	EXPRESSION TAG	UNP Q8ZNH1
A	-1	SER	-	EXPRESSION TAG	UNP Q8ZNH1
A	0	MET	-	EXPRESSION TAG	UNP Q8ZNH1
B	-22	MET	-	EXPRESSION TAG	UNP Q8ZNH1
B	-21	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
B	-20	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
B	-19	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
B	-18	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
B	-17	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
B	-16	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
B	-15	SER	-	EXPRESSION TAG	UNP Q8ZNH1
B	-14	SER	-	EXPRESSION TAG	UNP Q8ZNH1
B	-13	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
B	-12	VAL	-	EXPRESSION TAG	UNP Q8ZNH1
B	-11	ASP	-	EXPRESSION TAG	UNP Q8ZNH1
B	-10	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
B	-9	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
B	-8	THR	-	EXPRESSION TAG	UNP Q8ZNH1
B	-7	GLU	-	EXPRESSION TAG	UNP Q8ZNH1
B	-6	ASN	-	EXPRESSION TAG	UNP Q8ZNH1
B	-5	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
B	-4	TYR	-	EXPRESSION TAG	UNP Q8ZNH1
B	-3	PHE	-	EXPRESSION TAG	UNP Q8ZNH1
B	-2	GLN	-	EXPRESSION TAG	UNP Q8ZNH1
B	-1	SER	-	EXPRESSION TAG	UNP Q8ZNH1
B	0	MET	-	EXPRESSION TAG	UNP Q8ZNH1
C	-22	MET	-	EXPRESSION TAG	UNP Q8ZNH1
C	-21	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
C	-20	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
C	-19	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
C	-18	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
C	-17	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
C	-16	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
C	-15	SER	-	EXPRESSION TAG	UNP Q8ZNH1
C	-14	SER	-	EXPRESSION TAG	UNP Q8ZNH1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
C	-12	VAL	-	EXPRESSION TAG	UNP Q8ZNH1
C	-11	ASP	-	EXPRESSION TAG	UNP Q8ZNH1
C	-10	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
C	-9	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
C	-8	THR	-	EXPRESSION TAG	UNP Q8ZNH1
C	-7	GLU	-	EXPRESSION TAG	UNP Q8ZNH1
C	-6	ASN	-	EXPRESSION TAG	UNP Q8ZNH1
C	-5	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
C	-4	TYR	-	EXPRESSION TAG	UNP Q8ZNH1
C	-3	PHE	-	EXPRESSION TAG	UNP Q8ZNH1
C	-2	GLN	-	EXPRESSION TAG	UNP Q8ZNH1
C	-1	SER	-	EXPRESSION TAG	UNP Q8ZNH1
C	0	MET	-	EXPRESSION TAG	UNP Q8ZNH1
D	-22	MET	-	EXPRESSION TAG	UNP Q8ZNH1
D	-21	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
D	-20	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
D	-19	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
D	-18	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
D	-17	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
D	-16	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
D	-15	SER	-	EXPRESSION TAG	UNP Q8ZNH1
D	-14	SER	-	EXPRESSION TAG	UNP Q8ZNH1
D	-13	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
D	-12	VAL	-	EXPRESSION TAG	UNP Q8ZNH1
D	-11	ASP	-	EXPRESSION TAG	UNP Q8ZNH1
D	-10	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
D	-9	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
D	-8	THR	-	EXPRESSION TAG	UNP Q8ZNH1
D	-7	GLU	-	EXPRESSION TAG	UNP Q8ZNH1
D	-6	ASN	-	EXPRESSION TAG	UNP Q8ZNH1
D	-5	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
D	-4	TYR	-	EXPRESSION TAG	UNP Q8ZNH1
D	-3	PHE	-	EXPRESSION TAG	UNP Q8ZNH1
D	-2	GLN	-	EXPRESSION TAG	UNP Q8ZNH1
D	-1	SER	-	EXPRESSION TAG	UNP Q8ZNH1
D	0	MET	-	EXPRESSION TAG	UNP Q8ZNH1
E	-22	MET	-	EXPRESSION TAG	UNP Q8ZNH1
E	-21	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
E	-20	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
E	-19	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
E	-18	HIS	-	EXPRESSION TAG	UNP Q8ZNH1

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
E	-16	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
E	-15	SER	-	EXPRESSION TAG	UNP Q8ZNH1
E	-14	SER	-	EXPRESSION TAG	UNP Q8ZNH1
E	-13	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
E	-12	VAL	-	EXPRESSION TAG	UNP Q8ZNH1
E	-11	ASP	-	EXPRESSION TAG	UNP Q8ZNH1
E	-10	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
E	-9	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
E	-8	THR	-	EXPRESSION TAG	UNP Q8ZNH1
E	-7	GLU	-	EXPRESSION TAG	UNP Q8ZNH1
E	-6	ASN	-	EXPRESSION TAG	UNP Q8ZNH1
E	-5	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
E	-4	TYR	-	EXPRESSION TAG	UNP Q8ZNH1
E	-3	PHE	-	EXPRESSION TAG	UNP Q8ZNH1
E	-2	GLN	-	EXPRESSION TAG	UNP Q8ZNH1
E	-1	SER	-	EXPRESSION TAG	UNP Q8ZNH1
E	0	MET	-	EXPRESSION TAG	UNP Q8ZNH1
F	-22	MET	-	EXPRESSION TAG	UNP Q8ZNH1
F	-21	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
F	-20	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
F	-19	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
F	-18	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
F	-17	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
F	-16	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
F	-15	SER	-	EXPRESSION TAG	UNP Q8ZNH1
F	-14	SER	-	EXPRESSION TAG	UNP Q8ZNH1
F	-13	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
F	-12	VAL	-	EXPRESSION TAG	UNP Q8ZNH1
F	-11	ASP	-	EXPRESSION TAG	UNP Q8ZNH1
F	-10	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
F	-9	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
F	-8	THR	-	EXPRESSION TAG	UNP Q8ZNH1
F	-7	GLU	-	EXPRESSION TAG	UNP Q8ZNH1
F	-6	ASN	-	EXPRESSION TAG	UNP Q8ZNH1
F	-5	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
F	-4	TYR	-	EXPRESSION TAG	UNP Q8ZNH1
F	-3	PHE	-	EXPRESSION TAG	UNP Q8ZNH1
F	-2	GLN	-	EXPRESSION TAG	UNP Q8ZNH1
F	-1	SER	-	EXPRESSION TAG	UNP Q8ZNH1
F	0	MET	-	EXPRESSION TAG	UNP Q8ZNH1
G	-22	MET	-	EXPRESSION TAG	UNP Q8ZNH1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
G	-20	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
G	-19	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
G	-18	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
G	-17	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
G	-16	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
G	-15	SER	-	EXPRESSION TAG	UNP Q8ZNH1
G	-14	SER	-	EXPRESSION TAG	UNP Q8ZNH1
G	-13	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
G	-12	VAL	-	EXPRESSION TAG	UNP Q8ZNH1
G	-11	ASP	-	EXPRESSION TAG	UNP Q8ZNH1
G	-10	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
G	-9	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
G	-8	THR	-	EXPRESSION TAG	UNP Q8ZNH1
G	-7	GLU	-	EXPRESSION TAG	UNP Q8ZNH1
G	-6	ASN	-	EXPRESSION TAG	UNP Q8ZNH1
G	-5	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
G	-4	TYR	-	EXPRESSION TAG	UNP Q8ZNH1
G	-3	PHE	-	EXPRESSION TAG	UNP Q8ZNH1
G	-2	GLN	-	EXPRESSION TAG	UNP Q8ZNH1
G	-1	SER	-	EXPRESSION TAG	UNP Q8ZNH1
G	0	MET	-	EXPRESSION TAG	UNP Q8ZNH1
H	-22	MET	-	EXPRESSION TAG	UNP Q8ZNH1
H	-21	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
H	-20	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
H	-19	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
H	-18	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
H	-17	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
H	-16	HIS	-	EXPRESSION TAG	UNP Q8ZNH1
H	-15	SER	-	EXPRESSION TAG	UNP Q8ZNH1
H	-14	SER	-	EXPRESSION TAG	UNP Q8ZNH1
H	-13	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
H	-12	VAL	-	EXPRESSION TAG	UNP Q8ZNH1
H	-11	ASP	-	EXPRESSION TAG	UNP Q8ZNH1
H	-10	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
H	-9	GLY	-	EXPRESSION TAG	UNP Q8ZNH1
H	-8	THR	-	EXPRESSION TAG	UNP Q8ZNH1
H	-7	GLU	-	EXPRESSION TAG	UNP Q8ZNH1
H	-6	ASN	-	EXPRESSION TAG	UNP Q8ZNH1
H	-5	LEU	-	EXPRESSION TAG	UNP Q8ZNH1
H	-4	TYR	-	EXPRESSION TAG	UNP Q8ZNH1
H	-3	PHE	-	EXPRESSION TAG	UNP Q8ZNH1

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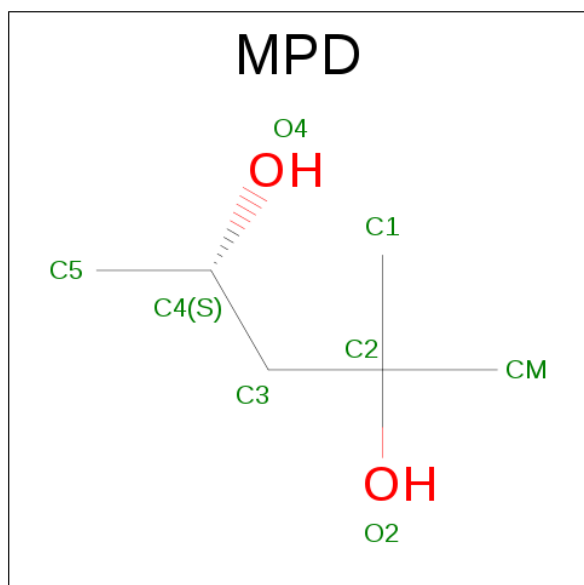
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	GLN	-	EXPRESSION TAG	UNP Q8ZNH1
H	-1	SER	-	EXPRESSION TAG	UNP Q8ZNH1
H	0	MET	-	EXPRESSION TAG	UNP Q8ZNH1

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

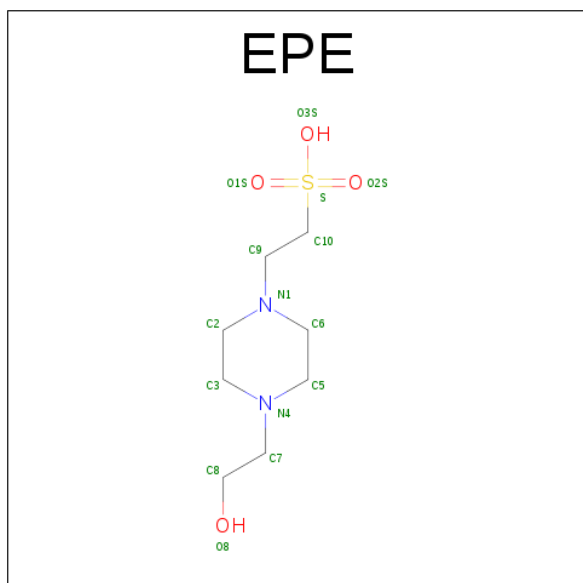
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	G	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		
3	H	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 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
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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

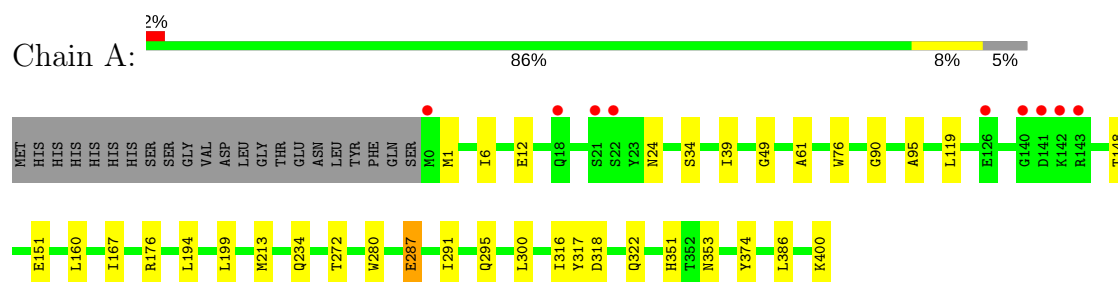
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	282	Total	O	0	0
			282	282		
5	B	294	Total	O	0	0
			294	294		
5	C	281	Total	O	0	0
			281	281		
5	D	301	Total	O	0	0
			301	301		
5	E	287	Total	O	0	0
			287	287		
5	F	312	Total	O	0	0
			312	312		
5	G	301	Total	O	0	0
			301	301		
5	H	293	Total	O	0	0
			293	293		

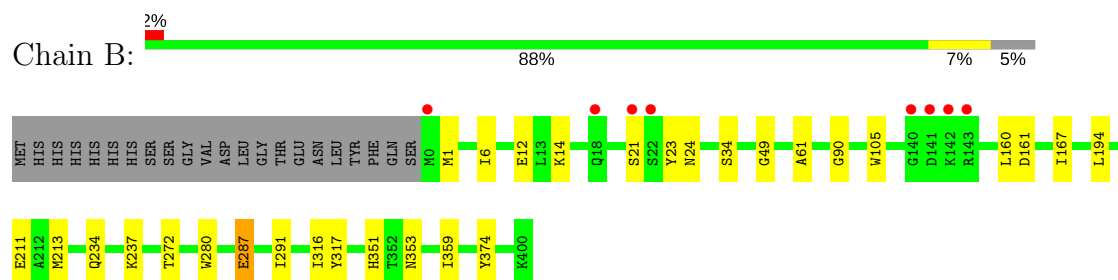
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

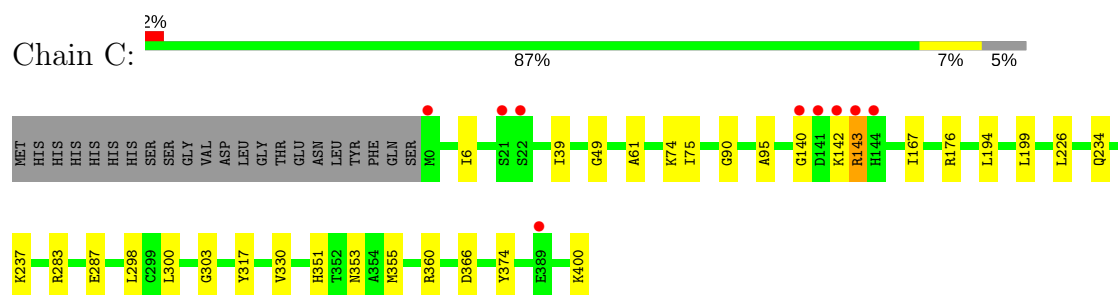
#### • Molecule 1: Putative dehydratase protein



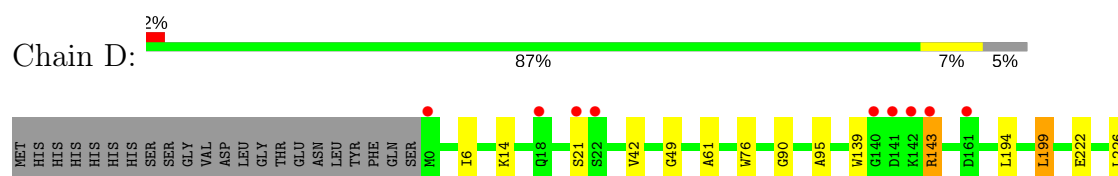
#### • Molecule 1: Putative dehydratase protein



#### • Molecule 1: Putative dehydratase protein

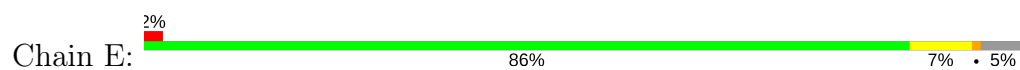


#### • Molecule 1: Putative dehydratase protein

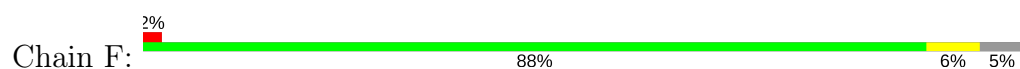




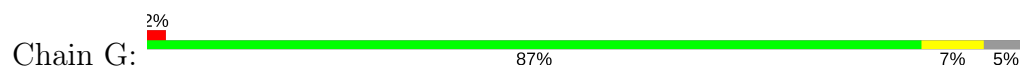
• Molecule 1: Putative dehydratase protein



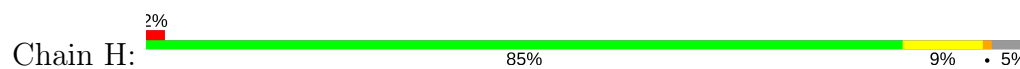
• Molecule 1: Putative dehydratase protein



• Molecule 1: Putative dehydratase protein



• Molecule 1: Putative dehydratase protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.13Å 87.14Å 200.59Å 90.00° 91.39° 90.00°	Depositor
Resolution (Å)	19.96 – 1.80 19.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (19.96-1.80) 91.9 (19.96-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.173 , 0.206 0.173 , 0.206	Depositor DCC
$R_{free}$ test set	16680 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.5	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	27937	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EPE, MPD

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	0.64	3/3278 (0.1%)	0.68	1/4436 (0.0%)
1	B	0.62	3/3268 (0.1%)	0.67	0/4421
1	C	0.60	0/3256	0.65	1/4408 (0.0%)
1	D	0.58	3/3252 (0.1%)	0.66	1/4400 (0.0%)
1	E	0.63	3/3270 (0.1%)	0.68	3/4428 (0.1%)
1	F	0.62	2/3237 (0.1%)	0.67	1/4382 (0.0%)
1	G	0.61	1/3246 (0.0%)	0.68	1/4394 (0.0%)
1	H	0.60	1/3267 (0.0%)	0.67	1/4421 (0.0%)
All	All	0.61	16/26074 (0.1%)	0.67	9/35290 (0.0%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	287	GLU	CD-OE1	-6.37	1.18	1.25
1	B	287	GLU	CD-OE1	-5.61	1.19	1.25
1	A	76	TRP	CD2-CE2	5.55	1.48	1.41
1	E	287	GLU	CD-OE1	-5.42	1.19	1.25
1	A	280	TRP	CD2-CE2	5.39	1.47	1.41
1	B	280	TRP	CD2-CE2	5.39	1.47	1.41
1	H	76	TRP	CD2-CE2	5.33	1.47	1.41
1	E	280	TRP	CD2-CE2	5.31	1.47	1.41
1	D	76	TRP	CD2-CE2	5.28	1.47	1.41
1	E	287	GLU	CD-OE2	-5.23	1.19	1.25
1	D	280	TRP	CD2-CE2	5.16	1.47	1.41
1	B	105	TRP	CD2-CE2	5.12	1.47	1.41
1	D	139	TRP	CD2-CE2	5.12	1.47	1.41
1	G	76	TRP	CD2-CE2	5.09	1.47	1.41
1	A	287	GLU	CD-OE1	-5.01	1.20	1.25
1	F	280	TRP	CD2-CE2	5.01	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	199	LEU	CA-CB-CG	7.89	133.45	115.30
1	D	199	LEU	CA-CB-CG	7.53	132.62	115.30
1	E	199	LEU	CA-CB-CG	6.65	130.60	115.30
1	A	199	LEU	CA-CB-CG	5.88	128.82	115.30
1	F	199	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	199	LEU	CA-CB-CG	5.37	127.64	115.30
1	E	175	ASP	CB-CG-OD1	5.36	123.13	118.30
1	G	199	LEU	CA-CB-CG	5.33	127.56	115.30
1	E	165	ASP	CB-CG-OD1	5.28	123.06	118.30

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	3184	0	3168	25	0
1	B	3178	0	3162	26	0
1	C	3169	0	3138	27	0
1	D	3171	0	3146	26	0
1	E	3179	0	3149	26	0
1	F	3157	0	3125	27	0
1	G	3163	0	3136	31	0
1	H	3177	0	3153	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	16	0	28	3	0
3	B	8	0	14	2	0
3	C	8	0	14	1	0
3	D	8	0	14	5	0
3	E	8	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	8	0	14	0	0
3	G	8	0	14	0	0
3	H	16	0	28	2	0
4	B	30	0	36	0	0
4	C	15	0	18	2	0
4	D	15	0	18	1	0
4	E	30	0	36	3	0
4	G	15	0	18	4	0
4	H	15	0	18	0	0
5	A	282	0	0	0	0
5	B	294	0	0	2	0
5	C	281	0	0	2	0
5	D	301	0	0	3	0
5	E	287	0	0	5	0
5	F	312	0	0	4	0
5	G	301	0	0	1	0
5	H	293	0	0	3	0
All	All	27937	0	25461	201	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 4.

All (201) 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:161:ASP:HB3	5:B:958:HOH:O	1.56	1.03
1:H:18[A]:GLN:HA	1:H:18[A]:GLN:HE21	1.23	1.00
1:H:18[A]:GLN:HE21	1:H:18[A]:GLN:CA	1.76	0.96
1:H:18[A]:GLN:HA	1:H:18[A]:GLN:NE2	1.81	0.91
1:G:143:ARG:HH21	1:G:143:ARG:HG3	1.35	0.90
1:A:194:LEU:H	1:A:234:GLN:HE22	1.14	0.89
1:A:351:HIS:HD2	1:A:353:ASN:H	1.20	0.86
3:A:503:MPD:H53	5:F:829:HOH:O	1.74	0.86
1:B:194:LEU:H	1:B:234:GLN:HE22	1.21	0.86
1:H:194:LEU:H	1:H:234:GLN:HE22	1.21	0.85
1:A:160:LEU:HD13	1:A:213[B]:MET:SD	2.18	0.84
1:E:74:LYS:HD3	4:E:503:EPE:H82	1.60	0.84
1:G:283:ARG:O	1:G:287:GLU:HG3	1.77	0.83
1:F:194:LEU:H	1:F:234:GLN:HE22	1.21	0.83
1:B:351:HIS:HD2	1:B:353:ASN:H	1.26	0.82
1:E:194:LEU:H	1:E:234:GLN:HE22	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:LEU:H	1:D:234:GLN:HE22	1.25	0.81
1:E:351:HIS:HD2	1:E:353:ASN:H	1.27	0.81
1:C:194:LEU:H	1:C:234:GLN:HE22	1.29	0.81
1:C:90:GLY:HA3	1:D:90:GLY:HA3	1.62	0.81
1:G:194:LEU:H	1:G:234:GLN:HE22	1.26	0.80
1:D:351:HIS:HD2	1:D:353:ASN:H	1.29	0.79
1:C:351:HIS:HD2	1:C:353[B]:ASN:H	1.30	0.78
1:C:351:HIS:HD2	1:C:353[A]:ASN:H	1.31	0.77
1:A:90:GLY:HA3	1:B:90:GLY:HA3	1.67	0.76
1:D:393:GLU:HG2	5:D:829:HOH:O	1.86	0.75
1:B:160:LEU:HD13	1:B:213[B]:MET:SD	2.27	0.75
1:C:140:GLY:HA3	1:C:143:ARG:HE	1.52	0.74
1:G:90:GLY:HA3	1:H:90:GLY:HA3	1.68	0.74
1:A:351:HIS:CD2	1:A:353:ASN:H	2.07	0.71
1:G:67:GLU:HB3	4:G:503:EPE:H81	1.72	0.70
1:E:237:LYS:CE	5:E:764:HOH:O	2.40	0.70
1:H:15:LYS:HD2	5:H:772:HOH:O	1.92	0.70
3:D:502:MPD:HM1	3:D:502:MPD:H52	1.72	0.70
1:F:351:HIS:HD2	1:F:353[A]:ASN:H	1.41	0.69
1:G:143:ARG:CG	1:G:143:ARG:HH21	2.02	0.68
1:A:194:LEU:H	1:A:234:GLN:NE2	1.91	0.67
1:F:351:HIS:HD2	1:F:353[B]:ASN:H	1.41	0.67
1:D:351:HIS:CD2	1:D:353:ASN:H	2.11	0.67
1:E:90:GLY:HA3	1:F:90:GLY:HA3	1.76	0.67
1:H:224:HIS:NE2	3:H:503:MPD:HM3	2.10	0.66
1:D:351:HIS:HE1	3:D:502:MPD:H53	1.60	0.65
1:B:351:HIS:CD2	1:B:353:ASN:H	2.13	0.65
1:G:140:GLY:O	1:G:143:ARG:NH2	2.30	0.65
1:A:160:LEU:CD1	1:A:213[B]:MET:SD	2.86	0.64
3:A:503:MPD:H52	5:F:913:HOH:O	1.98	0.64
1:D:351:HIS:HE1	3:D:502:MPD:C5	2.11	0.64
1:G:194:LEU:H	1:G:234:GLN:NE2	1.95	0.63
1:F:194:LEU:H	1:F:234:GLN:NE2	1.95	0.63
1:H:355:MET:HE2	1:H:360:ARG:HD3	1.81	0.63
1:H:351:HIS:HD2	1:H:353:ASN:H	1.46	0.63
1:G:143:ARG:HG3	1:G:143:ARG:NH2	2.11	0.62
1:H:18[A]:GLN:NE2	1:H:18[A]:GLN:CA	2.48	0.62
1:H:194:LEU:H	1:H:234:GLN:NE2	1.97	0.61
1:B:194:LEU:H	1:B:234:GLN:NE2	1.97	0.60
1:C:140:GLY:HA3	1:C:143:ARG:NE	2.16	0.60
1:G:21:SER:OG	1:G:22:SER:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:143:ARG:CG	1:G:143:ARG:NH2	2.61	0.59
1:G:351:HIS:HD2	1:G:353:ASN:HB2	1.67	0.59
1:F:1:MET:HG2	1:F:34:SER:HB3	1.84	0.59
1:B:237:LYS:NZ	5:B:957:HOH:O	2.35	0.58
1:A:119:LEU:O	3:A:503:MPD:H13	2.03	0.58
1:C:287:GLU:OE2	1:H:317[A]:TYR:OH	2.23	0.57
1:E:22:SER:HA	5:E:872:HOH:O	2.05	0.57
1:C:75:ILE:HG13	4:C:503:EPE:H81	1.86	0.56
1:F:12:GLU:HG2	1:F:24:ASN:HD21	1.71	0.56
1:C:143:ARG:HB2	5:C:858:HOH:O	2.06	0.56
4:E:504:EPE:H81	1:F:74:LYS:HD3	1.88	0.56
1:B:167:ILE:HG23	1:B:213[B]:MET:HE1	1.88	0.56
1:G:284:GLU:OE1	1:G:288:LYS:NZ	2.39	0.56
1:F:194:LEU:N	1:F:234:GLN:HE22	2.00	0.55
1:G:12:GLU:HG2	1:G:24:ASN:HD21	1.70	0.55
1:A:194:LEU:N	1:A:234:GLN:HE22	1.96	0.55
1:C:351:HIS:CD2	1:C:353[B]:ASN:H	2.20	0.55
1:G:194:LEU:N	1:G:234:GLN:HE22	2.01	0.54
1:C:351:HIS:CD2	1:C:353[A]:ASN:H	2.20	0.54
1:H:14:LYS:HB3	1:H:21:SER:HA	1.88	0.54
1:G:75:ILE:HG13	4:G:503:EPE:H82	1.89	0.54
1:G:272:THR:HG22	1:G:291:ILE:HG21	1.90	0.54
1:B:287:GLU:OE2	1:G:317[A]:TYR:OH	2.23	0.53
1:B:1:MET:HG2	1:B:34:SER:HB3	1.90	0.53
1:H:1:MET:HG2	1:H:34:SER:HB3	1.91	0.53
3:B:701:MPD:C1	3:B:701:MPD:H53	2.39	0.53
1:H:18[B]:GLN:NE2	5:H:808:HOH:O	2.41	0.53
1:B:160:LEU:CD1	1:B:213[B]:MET:SD	2.95	0.53
1:D:194:LEU:H	1:D:234:GLN:NE2	2.00	0.53
1:F:351:HIS:CD2	1:F:353[B]:ASN:H	2.25	0.53
1:F:351:HIS:CD2	1:F:353[A]:ASN:H	2.25	0.53
1:H:256:SER:OG	1:H:288:LYS:NZ	2.42	0.52
1:E:194:LEU:H	1:E:234:GLN:NE2	2.03	0.52
1:D:143:ARG:HG2	1:D:143:ARG:O	2.10	0.52
1:H:150:GLU:H	1:H:150:GLU:CD	2.13	0.52
1:H:24:ASN:HD21	1:H:51:LYS:HZ3	1.57	0.52
1:D:351:HIS:CE1	3:D:502:MPD:C5	2.93	0.52
1:D:287:GLU:OE2	1:E:317[A]:TYR:OH	2.22	0.52
1:E:15:LYS:HE3	5:E:768:HOH:O	2.09	0.52
1:G:67:GLU:OE1	4:G:503:EPE:H32	2.09	0.52
1:A:287:GLU:OE2	1:F:317[A]:TYR:OH	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LYS:HE3	1:E:267:THR:CG2	2.40	0.51
1:C:283:ARG:O	1:C:287:GLU:HG3	2.10	0.51
1:D:317[A]:TYR:OH	1:E:287:GLU:OE2	2.25	0.51
1:B:317[A]:TYR:OH	1:G:287:GLU:OE2	2.26	0.51
1:A:287:GLU:OE2	1:F:317[B]:TYR:OH	2.22	0.51
1:C:194:LEU:H	1:C:234:GLN:NE2	2.04	0.50
1:B:317[B]:TYR:OH	1:G:287:GLU:OE2	2.21	0.50
1:C:226:LEU:HD12	5:C:650:HOH:O	2.11	0.50
1:D:14:LYS:HB3	1:D:21:SER:HA	1.93	0.49
1:E:351:HIS:CD2	1:E:353:ASN:H	2.17	0.49
1:A:148:THR:OG1	1:A:151:GLU:HG3	2.12	0.49
1:B:237:LYS:HE3	1:F:267:THR:HG22	1.95	0.49
1:G:75:ILE:CG1	4:G:503:EPE:H82	2.43	0.49
1:B:12:GLU:HG2	1:B:24:ASN:ND2	2.28	0.49
1:B:316:ILE:HG21	1:G:279:ARG:HB3	1.94	0.49
1:F:23:TYR:CE2	1:F:359:ILE:HD11	2.48	0.48
1:B:287:GLU:OE2	1:G:317[B]:TYR:OH	2.22	0.48
1:B:6:ILE:HD13	1:B:61:ALA:HB1	1.95	0.48
1:B:351:HIS:HE1	3:B:701:MPD:H32	1.79	0.48
1:A:317[A]:TYR:OH	1:F:287:GLU:OE2	2.22	0.48
1:A:12:GLU:HG2	1:A:24:ASN:HD21	1.79	0.48
1:A:6:ILE:HD13	1:A:61:ALA:HB1	1.94	0.48
1:C:167:ILE:C	1:C:167:ILE:HD12	2.34	0.48
1:C:298:LEU:O	1:C:303:GLY:HA2	2.14	0.48
1:D:42:VAL:HG13	1:D:95:ALA:HB1	1.96	0.48
1:C:237:LYS:HE3	1:E:267:THR:HG22	1.96	0.48
1:H:140:GLY:O	1:H:143:ARG:HD3	2.14	0.47
1:B:14:LYS:HB3	1:B:21:SER:HA	1.95	0.47
1:E:272:THR:HG22	1:E:291:ILE:HG21	1.96	0.47
1:A:1:MET:HG2	1:A:34:SER:HB3	1.96	0.47
1:B:12:GLU:HG2	1:B:24:ASN:HD21	1.79	0.47
1:F:12:GLU:HG2	1:F:24:ASN:ND2	2.28	0.47
1:F:231:SER:HA	1:F:234:GLN:HE21	1.80	0.47
1:D:226:LEU:HD12	5:D:710:HOH:O	2.15	0.47
1:D:295:GLN:HA	1:D:322:GLN:O	2.15	0.47
1:A:95:ALA:HB2	1:A:300:LEU:HD23	1.97	0.46
1:D:272:THR:HG22	1:D:291:ILE:HG21	1.95	0.46
1:E:24:ASN:HD21	1:E:51:LYS:NZ	2.13	0.46
1:G:351:HIS:CD2	1:G:353:ASN:H	2.32	0.46
1:C:6:ILE:HD13	1:C:61:ALA:HB1	1.97	0.46
1:C:74:LYS:HD3	4:C:503:EPE:H82	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:HG2	1:A:24:ASN:ND2	2.30	0.46
1:H:194:LEU:N	1:H:234:GLN:HE22	2.00	0.46
1:H:308:LYS:HG3	3:H:501:MPD:H53	1.97	0.46
1:A:272:THR:HG22	1:A:291:ILE:HG21	1.97	0.46
1:B:237:LYS:HE3	1:F:267:THR:CG2	2.46	0.46
1:D:351:HIS:CD2	1:D:353:ASN:HB2	2.51	0.46
1:E:256:SER:OG	1:E:288:LYS:NZ	2.48	0.46
1:E:75:ILE:HG13	4:E:503:EPE:H81	1.97	0.45
1:G:39:ILE:HG21	1:G:386:LEU:HG	1.99	0.45
1:C:317[A]:TYR:OH	1:H:287:GLU:OE2	2.24	0.45
4:D:503:EPE:H102	4:D:503:EPE:H21	1.81	0.45
1:H:351:HIS:CD2	1:H:353:ASN:H	2.30	0.45
1:A:39:ILE:HG21	1:A:386:LEU:HG	1.98	0.45
1:C:95:ALA:HB2	1:C:300:LEU:HD23	1.99	0.45
1:C:143:ARG:HA	1:C:143:ARG:HD3	1.46	0.45
1:D:351:HIS:CE1	3:D:502:MPD:H51	2.52	0.45
1:C:360:ARG:HD2	1:C:366:ASP:OD2	2.16	0.44
1:E:295:GLN:HA	1:E:322:GLN:O	2.17	0.44
1:A:317[B]:TYR:OH	1:F:287:GLU:OE2	2.23	0.44
1:B:194:LEU:N	1:B:234:GLN:HE22	2.02	0.44
1:D:351:HIS:HD2	1:D:353:ASN:HB2	1.83	0.44
1:F:95:ALA:HB2	1:F:300:LEU:HD23	2.00	0.44
1:C:39:ILE:HD12	1:C:330:VAL:HG22	1.99	0.44
1:D:285:LEU:HG	5:D:726:HOH:O	2.17	0.44
1:A:167:ILE:HG23	1:A:213[B]:MET:HE1	1.99	0.43
1:A:316[A]:ILE:HG21	1:F:279:ARG:HB3	1.99	0.43
1:E:194:LEU:N	1:E:234:GLN:HE22	2.06	0.43
1:H:355:MET:CE	1:H:360:ARG:HD3	2.47	0.43
1:D:231:SER:HA	1:D:234:GLN:HE21	1.83	0.43
1:A:295:GLN:HA	1:A:322:GLN:O	2.18	0.43
1:F:237:LYS:NZ	5:F:1103:HOH:O	2.50	0.43
1:G:377:PRO:HB2	5:G:605:HOH:O	2.18	0.43
1:B:23:TYR:CE2	1:B:359:ILE:HD11	2.54	0.43
1:H:6:ILE:HD13	1:H:61:ALA:HB1	2.00	0.43
1:G:284:GLU:CD	1:G:288:LYS:HZ1	2.20	0.42
1:E:237:LYS:HE3	5:E:764:HOH:O	2.15	0.42
1:D:6:ILE:HD13	1:D:61:ALA:HB1	2.01	0.42
1:C:351:HIS:HE1	3:C:502:MPD:O4	2.03	0.42
1:C:194:LEU:N	1:C:234:GLN:HE22	2.08	0.42
1:H:100:ILE:O	1:H:104:LEU:HG	2.19	0.42
1:F:298:LEU:O	1:F:303:GLY:HA2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:ILE:C	1:H:167:ILE:HD12	2.39	0.42
1:G:95:ALA:HB2	1:G:300:LEU:HD23	2.02	0.42
1:E:140:GLY:HA2	5:E:879:HOH:O	2.20	0.42
1:H:13:LEU:HD11	1:H:359:ILE:HD13	2.02	0.42
1:H:272:THR:HG22	1:H:291:ILE:HG21	2.01	0.41
1:F:226:LEU:HD12	5:F:872:HOH:O	2.21	0.41
1:E:140:GLY:O	1:E:143:ARG:NH2	2.43	0.41
1:G:12:GLU:HG2	1:G:24:ASN:ND2	2.36	0.41
1:D:316:ILE:HG21	1:E:279:ARG:HB3	2.02	0.41
1:E:43:GLY:O	1:E:300:LEU:HD21	2.21	0.41
1:B:272:THR:HG22	1:B:291:ILE:HG21	2.02	0.41
1:D:287:GLU:OE2	1:E:317[B]:TYR:OH	2.23	0.40
1:H:223:ILE:O	1:H:223:ILE:HG22	2.21	0.40
1:H:365:HIS:HD2	5:H:739:HOH:O	2.03	0.40
1:D:222:GLU:HA	1:D:248:GLU:HB3	2.04	0.40
1:E:133:SER:HB3	1:E:351:HIS:HA	2.03	0.40
1:G:298:LEU:O	1:G:303:GLY:HA2	2.20	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	408/423 (96%)	397 (97%)	10 (2%)	1 (0%)	51	35
1	B	407/423 (96%)	395 (97%)	11 (3%)	1 (0%)	51	35
1	C	406/423 (96%)	391 (96%)	14 (3%)	1 (0%)	51	35
1	D	405/423 (96%)	393 (97%)	11 (3%)	1 (0%)	51	35
1	E	407/423 (96%)	393 (97%)	13 (3%)	1 (0%)	51	35
1	F	404/423 (96%)	391 (97%)	12 (3%)	1 (0%)	51	35
1	G	405/423 (96%)	390 (96%)	14 (4%)	1 (0%)	51	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	407/423 (96%)	391 (96%)	14 (3%)	2 (0%)	32	17
All	All	3249/3384 (96%)	3141 (97%)	99 (3%)	9 (0%)	44	29

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	49	GLY
1	A	49	GLY
1	D	49	GLY
1	H	49	GLY
1	B	49	GLY
1	F	49	GLY
1	H	140	GLY
1	E	49	GLY
1	G	49	GLY

### 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	339/350 (97%)	336 (99%)	3 (1%)	82	78
1	B	338/350 (97%)	336 (99%)	2 (1%)	89	87
1	C	337/350 (96%)	331 (98%)	6 (2%)	64	53
1	D	336/350 (96%)	333 (99%)	3 (1%)	82	78
1	E	338/350 (97%)	330 (98%)	8 (2%)	54	40
1	F	335/350 (96%)	333 (99%)	2 (1%)	89	87
1	G	336/350 (96%)	332 (99%)	4 (1%)	75	69
1	H	338/350 (97%)	332 (98%)	6 (2%)	64	53
All	All	2697/2800 (96%)	2663 (99%)	34 (1%)	73	66

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	ARG
1	A	374	TYR
1	A	400	LYS
1	B	211	GLU
1	B	374	TYR
1	C	142	LYS
1	C	143	ARG
1	C	176	ARG
1	C	355	MET
1	C	374	TYR
1	C	400	LYS
1	D	143	ARG
1	D	199	LEU
1	D	374	TYR
1	E	22	SER
1	E	143	ARG
1	E	188	ARG
1	E	199	LEU
1	E	211	GLU
1	E	322	GLN
1	E	370	GLU
1	E	374	TYR
1	F	22	SER
1	F	374	TYR
1	G	18	GLN
1	G	22	SER
1	G	143	ARG
1	G	374	TYR
1	H	18[A]	GLN
1	H	18[B]	GLN
1	H	199	LEU
1	H	316	ILE
1	H	355	MET
1	H	374	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	234	GLN
1	A	351	HIS
1	B	24	ASN
1	B	118	GLN

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Mol	Chain	Res	Type
1	B	234	GLN
1	B	351	HIS
1	C	24	ASN
1	C	234	GLN
1	C	351	HIS
1	D	24	ASN
1	D	118	GLN
1	D	144	HIS
1	D	234	GLN
1	D	351	HIS
1	E	24	ASN
1	E	144	HIS
1	E	234	GLN
1	E	351	HIS
1	F	24	ASN
1	F	234	GLN
1	F	351	HIS
1	F	365	HIS
1	G	18	GLN
1	G	24	ASN
1	G	118	GLN
1	G	234	GLN
1	G	350	HIS
1	G	351	HIS
1	G	365	HIS
1	H	24	ASN
1	H	118	GLN
1	H	234	GLN
1	H	351	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 8 are monoatomic - leaving 18 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	MPD	A	502	-	7,7,7	0.29	0	9,10,10	0.51	0
3	MPD	A	503	-	7,7,7	0.41	0	9,10,10	0.61	0
3	MPD	B	701	-	7,7,7	0.34	0	9,10,10	0.64	0
4	EPE	B	702	-	15,15,15	2.27	2 (13%)	18,20,20	1.88	6 (33%)
4	EPE	B	703	-	15,15,15	1.99	2 (13%)	18,20,20	2.53	8 (44%)
3	MPD	C	502	-	7,7,7	0.25	0	9,10,10	0.44	0
4	EPE	C	503	-	15,15,15	2.04	2 (13%)	18,20,20	1.91	4 (22%)
3	MPD	D	502	-	7,7,7	0.27	0	9,10,10	0.55	0
4	EPE	D	503	-	15,15,15	2.10	2 (13%)	18,20,20	1.86	4 (22%)
3	MPD	E	502	-	7,7,7	0.27	0	9,10,10	0.31	0
4	EPE	E	503	-	15,15,15	2.09	2 (13%)	18,20,20	1.67	3 (16%)
4	EPE	E	504	-	15,15,15	1.94	2 (13%)	18,20,20	1.96	4 (22%)
3	MPD	F	701	-	7,7,7	0.19	0	9,10,10	0.35	0
3	MPD	G	502	-	7,7,7	0.28	0	9,10,10	0.25	0
4	EPE	G	503	-	15,15,15	2.04	2 (13%)	18,20,20	2.27	5 (27%)
3	MPD	H	501	-	7,7,7	0.33	0	9,10,10	0.57	0
3	MPD	H	503	-	7,7,7	0.28	0	9,10,10	0.54	0
4	EPE	H	504	-	15,15,15	2.02	2 (13%)	18,20,20	1.85	4 (22%)

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
3	MPD	A	502	-	-	0/5/5/5	0/0/0/0
3	MPD	A	503	-	-	0/5/5/5	0/0/0/0
3	MPD	B	701	-	-	0/5/5/5	0/0/0/0
4	EPE	B	702	-	-	0/9/19/19	0/1/1/1
4	EPE	B	703	-	-	0/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	C	502	-	-	0/5/5/5	0/0/0/0
4	EPE	C	503	-	-	0/9/19/19	0/1/1/1
3	MPD	D	502	-	-	0/5/5/5	0/0/0/0
4	EPE	D	503	-	-	0/9/19/19	0/1/1/1
3	MPD	E	502	-	-	0/5/5/5	0/0/0/0
4	EPE	E	503	-	-	0/9/19/19	0/1/1/1
4	EPE	E	504	-	-	0/9/19/19	0/1/1/1
3	MPD	F	701	-	-	0/5/5/5	0/0/0/0
3	MPD	G	502	-	-	0/5/5/5	0/0/0/0
4	EPE	G	503	-	-	0/9/19/19	0/1/1/1
3	MPD	H	501	-	-	0/5/5/5	0/0/0/0
3	MPD	H	503	-	-	0/5/5/5	0/0/0/0
4	EPE	H	504	-	-	0/9/19/19	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	EPE	C10-S	-7.16	1.66	1.77
4	E	503	EPE	C10-S	-6.07	1.68	1.77
4	C	503	EPE	C10-S	-5.95	1.68	1.77
4	D	503	EPE	C10-S	-5.92	1.68	1.77
4	H	504	EPE	C10-S	-5.89	1.68	1.77
4	G	503	EPE	C10-S	-5.67	1.69	1.77
4	B	703	EPE	C10-S	-5.32	1.69	1.77
4	E	504	EPE	C10-S	-5.19	1.69	1.77
4	H	504	EPE	O3S-S	4.86	1.63	1.47
4	E	504	EPE	O3S-S	4.89	1.63	1.47
4	C	503	EPE	O3S-S	4.93	1.64	1.47
4	G	503	EPE	O3S-S	4.96	1.64	1.47
4	E	503	EPE	O3S-S	4.96	1.64	1.47
4	B	702	EPE	O3S-S	4.97	1.64	1.47
4	B	703	EPE	O3S-S	4.98	1.64	1.47
4	D	503	EPE	O3S-S	5.07	1.64	1.47

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	504	EPE	C5-N4-C3	-2.50	103.21	108.87
4	B	703	EPE	C5-N4-C3	-2.21	103.87	108.87
4	B	703	EPE	C2-C3-N4	-2.12	106.35	110.63
4	B	702	EPE	C5-C6-N1	-2.08	106.43	110.63
4	D	503	EPE	C2-C3-N4	-2.04	106.51	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	EPE	C9-N1-C2	-2.02	106.08	111.26
4	B	703	EPE	O3S-S-O2S	-2.02	106.75	111.37
4	H	504	EPE	C3-C2-N1	2.15	114.98	110.63
4	E	504	EPE	C3-C2-N1	2.21	115.10	110.63
4	C	503	EPE	O3S-S-C10	2.35	108.94	106.06
4	B	702	EPE	O3S-S-C10	2.41	109.02	106.06
4	B	702	EPE	C2-C3-N4	2.52	115.73	110.63
4	E	504	EPE	C2-C3-N4	2.60	115.90	110.63
4	E	503	EPE	O1S-S-C10	2.74	109.15	106.79
4	B	702	EPE	C5-N4-C3	2.75	115.09	108.87
4	B	703	EPE	C6-N1-C2	2.75	115.09	108.87
4	B	703	EPE	C5-C6-N1	2.75	116.20	110.63
4	B	702	EPE	O2S-S-C10	2.96	109.34	106.79
4	E	503	EPE	O3S-S-C10	2.98	109.72	106.06
4	C	503	EPE	C2-C3-N4	3.20	117.11	110.63
4	D	503	EPE	O1S-S-C10	3.34	109.66	106.79
4	B	703	EPE	O3S-S-C10	3.39	110.23	106.06
4	G	503	EPE	O2S-S-C10	3.56	109.85	106.79
4	G	503	EPE	O3S-S-C10	3.63	110.53	106.06
4	H	504	EPE	O3S-S-C10	3.75	110.67	106.06
4	D	503	EPE	O3S-S-C10	3.82	110.76	106.06
4	D	503	EPE	O2S-S-C10	3.91	110.15	106.79
4	G	503	EPE	C3-C2-N1	3.97	118.67	110.63
4	H	504	EPE	O2S-S-C10	4.04	110.27	106.79
4	B	702	EPE	O1S-S-C10	4.06	110.28	106.79
4	G	503	EPE	C2-C3-N4	4.07	118.87	110.63
4	G	503	EPE	O1S-S-C10	4.10	110.32	106.79
4	C	503	EPE	O1S-S-C10	4.17	110.37	106.79
4	C	503	EPE	O2S-S-C10	4.31	110.50	106.79
4	E	504	EPE	O1S-S-C10	4.67	110.80	106.79
4	E	504	EPE	O3S-S-C10	4.72	111.86	106.06
4	E	503	EPE	O2S-S-C10	4.85	110.96	106.79
4	B	703	EPE	O2S-S-C10	7.63	113.35	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	MPD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	MPD	2	0
3	C	502	MPD	1	0
4	C	503	EPE	2	0
3	D	502	MPD	5	0
4	D	503	EPE	1	0
4	E	503	EPE	2	0
4	E	504	EPE	1	0
4	G	503	EPE	4	0
3	H	501	MPD	1	0
3	H	503	MPD	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, 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	401/423 (94%)	-0.42	9 (2%) 62 58	16, 23, 42, 82	0
1	B	401/423 (94%)	-0.43	8 (1%) 65 61	16, 23, 43, 78	0
1	C	401/423 (94%)	-0.40	9 (2%) 62 58	16, 25, 45, 87	0
1	D	401/423 (94%)	-0.42	9 (2%) 62 58	16, 25, 44, 88	0
1	E	401/423 (94%)	-0.42	9 (2%) 62 58	17, 24, 42, 87	0
1	F	401/423 (94%)	-0.45	8 (1%) 65 61	16, 24, 42, 69	0
1	G	401/423 (94%)	-0.45	7 (1%) 70 67	16, 24, 42, 77	0
1	H	401/423 (94%)	-0.40	8 (1%) 65 61	17, 24, 42, 80	0
All	All	3208/3384 (94%)	-0.42	67 (2%) 64 60	16, 24, 43, 88	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	142	LYS	8.0
1	C	141	ASP	7.8
1	E	142	LYS	7.3
1	D	142	LYS	6.5
1	H	141	ASP	6.0
1	A	141	ASP	6.0
1	E	141	ASP	6.0
1	A	142	LYS	5.8
1	D	141	ASP	5.6
1	C	142	LYS	5.2
1	E	143	ARG	5.0
1	G	141	ASP	4.9
1	C	0	MET	4.7
1	H	0	MET	4.7
1	B	141	ASP	4.6
1	E	140	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	0	MET	4.5
1	B	142	LYS	4.3
1	H	22	SER	4.3
1	B	22	SER	4.3
1	F	0	MET	4.2
1	F	141	ASP	4.1
1	F	18	GLN	4.0
1	E	0	MET	3.9
1	D	0	MET	3.9
1	B	140	GLY	3.7
1	G	143	ARG	3.7
1	G	0	MET	3.6
1	A	140	GLY	3.5
1	H	143	ARG	3.5
1	C	143	ARG	3.4
1	B	0	MET	3.4
1	D	18	GLN	3.3
1	D	143	ARG	3.2
1	A	18	GLN	3.2
1	G	18	GLN	3.2
1	A	22	SER	3.2
1	D	140	GLY	3.1
1	H	140	GLY	3.1
1	B	18	GLN	3.0
1	G	140	GLY	3.0
1	F	143	ARG	3.0
1	E	144	HIS	3.0
1	A	143	ARG	2.9
1	F	22	SER	2.9
1	D	22[A]	SER	2.8
1	C	144	HIS	2.8
1	H	21	SER	2.6
1	D	21	SER	2.5
1	E	22	SER	2.5
1	F	140	GLY	2.5
1	A	21	SER	2.4
1	F	389	GLU	2.4
1	C	140	GLY	2.3
1	F	21	SER	2.3
1	E	355	MET	2.3
1	B	21	SER	2.3
1	G	389	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	22	SER	2.2
1	D	161	ASP	2.2
1	G	142	LYS	2.1
1	A	126	GLU	2.1
1	C	389	GLU	2.1
1	B	143	ARG	2.1
1	E	371[A]	ASN	2.1
1	H	144	HIS	2.0
1	C	21	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MPD	H	501	8/8	0.69	0.32	34.05	25,34,36,39	8
4	EPE	H	504	15/15	0.38	0.51	18.24	28,38,48,51	15
4	EPE	B	703	15/15	0.59	0.30	13.64	30,45,57,63	14
4	EPE	E	504	15/15	0.55	0.38	13.36	24,36,42,43	15
3	MPD	A	503	8/8	0.70	0.25	12.74	28,37,40,43	0
4	EPE	C	503	15/15	0.55	0.36	10.81	23,32,43,45	15
4	EPE	E	503	15/15	0.57	0.36	10.47	26,36,42,42	15
4	EPE	G	503	15/15	0.66	0.27	9.36	30,53,79,82	0
4	EPE	D	503	15/15	0.56	0.32	7.97	32,48,59,61	15
3	MPD	B	701	8/8	0.77	0.28	7.15	44,51,55,59	0
3	MPD	C	502	8/8	0.92	0.20	4.80	32,34,38,40	8
3	MPD	G	502	8/8	0.85	0.21	3.50	29,32,38,38	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MPD	H	503	8/8	0.81	0.20	3.24	38,41,45,46	8
4	EPE	B	702	15/15	0.81	0.23	2.81	51,59,99,101	0
3	MPD	D	502	8/8	0.86	0.16	2.49	37,42,47,51	0
3	MPD	A	502	8/8	0.87	0.16	2.32	39,41,46,48	0
3	MPD	E	502	8/8	0.91	0.16	1.69	38,46,48,48	0
3	MPD	F	701	8/8	0.93	0.15	1.59	32,36,37,37	8
2	MG	C	501	1/1	0.99	0.09	0.61	29,29,29,29	0
2	MG	A	501	1/1	0.98	0.08	-0.10	31,31,31,31	0
2	MG	H	502	1/1	0.98	0.05	-0.94	28,28,28,28	0
2	MG	D	501	1/1	0.99	0.06	-1.11	29,29,29,29	0
2	MG	E	501	1/1	0.97	0.04	-1.58	30,30,30,30	0
2	MG	B	700	1/1	0.99	0.06	-1.70	27,27,27,27	0
2	MG	F	700	1/1	0.98	0.04	-2.43	29,29,29,29	0
2	MG	G	501	1/1	0.99	0.03	-4.56	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.