Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:30 PM GMT

PDB ID	:	4IHC
Title	:	Crystal structure of probable mannonate dehydratase Dd703_0947 (target EFI-502222) from Dickeya dadantii Ech703
Authors	:	Patskovsky, Y.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Al Obaidi, N.F.; Stead, M.; Love, J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on	:	2012-12-18
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

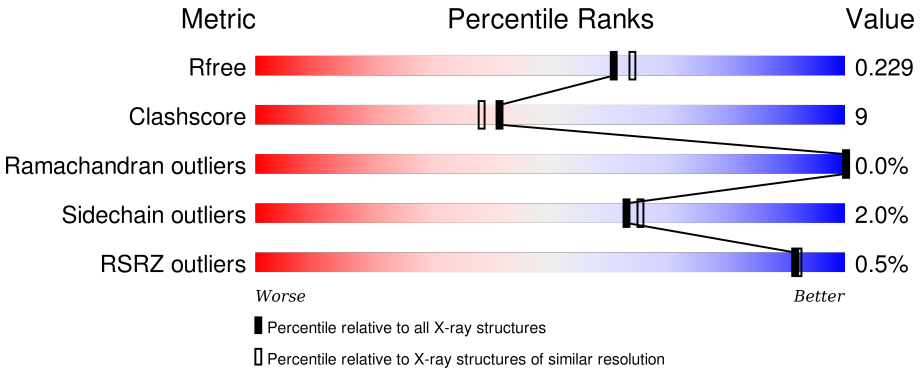
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	440	77% 11% • 10%
1	B	440	% 73% 16% • 10%
1	C	440	% 74% 14% • 10%
1	D	440	74% 15% 10%
1	E	440	% 73% 16% • 10%

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Mol	Chain	Length	Quality of chain
1	F	440	
1	G	440	
1	H	440	

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	GOL	A	505	-	-	-	X
3	GOL	B	502	-	-	-	X
3	GOL	C	507	-	-	-	X
3	GOL	E	502	-	-	-	X
3	GOL	F	502	-	-	-	X
3	GOL	G	502	-	-	-	X
3	GOL	H	504	-	-	-	X
4	FMT	B	505	-	-	X	-
4	FMT	E	505	-	-	-	X
4	FMT	F	503	-	-	-	X
4	FMT	F	506	-	-	-	X
4	FMT	G	505	-	-	X	-
5	IOD	A	506	-	-	X	-
5	IOD	C	506	-	-	X	-
5	IOD	E	508	-	-	X	-
5	IOD	F	509	-	-	X	-
6	CL	G	504	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26763 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 Mandelate racemase/muconate lactonizing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	0	0
			3084	1964	522	577	21			
1	B	395	Total	C	N	O	S	0	2	0
			3086	1967	521	576	22			
1	C	395	Total	C	N	O	S	0	2	0
			3072	1958	520	573	21			
1	D	395	Total	C	N	O	S	0	1	0
			3077	1960	520	576	21			
1	E	395	Total	C	N	O	S	0	1	0
			3081	1963	521	576	21			
1	F	395	Total	C	N	O	S	0	2	0
			3083	1964	520	578	21			
1	G	396	Total	C	N	O	S	0	1	0
			3079	1962	518	577	22			
1	H	395	Total	C	N	O	S	0	0	0
			3075	1959	520	575	21			

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP C6CBG9
A	-21	HIS	-	EXPRESSION TAG	UNP C6CBG9
A	-20	HIS	-	EXPRESSION TAG	UNP C6CBG9
A	-19	HIS	-	EXPRESSION TAG	UNP C6CBG9
A	-18	HIS	-	EXPRESSION TAG	UNP C6CBG9
A	-17	HIS	-	EXPRESSION TAG	UNP C6CBG9
A	-16	HIS	-	EXPRESSION TAG	UNP C6CBG9
A	-15	SER	-	EXPRESSION TAG	UNP C6CBG9
A	-14	SER	-	EXPRESSION TAG	UNP C6CBG9
A	-13	GLY	-	EXPRESSION TAG	UNP C6CBG9
A	-12	VAL	-	EXPRESSION TAG	UNP C6CBG9
A	-11	ASP	-	EXPRESSION TAG	UNP C6CBG9
A	-10	LEU	-	EXPRESSION TAG	UNP C6CBG9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	EXPRESSION TAG	UNP C6CBG9
A	-8	THR	-	EXPRESSION TAG	UNP C6CBG9
A	-7	GLU	-	EXPRESSION TAG	UNP C6CBG9
A	-6	ASN	-	EXPRESSION TAG	UNP C6CBG9
A	-5	LEU	-	EXPRESSION TAG	UNP C6CBG9
A	-4	TYR	-	EXPRESSION TAG	UNP C6CBG9
A	-3	PHE	-	EXPRESSION TAG	UNP C6CBG9
A	-2	GLN	-	EXPRESSION TAG	UNP C6CBG9
A	-1	SER	-	EXPRESSION TAG	UNP C6CBG9
A	0	MET	-	EXPRESSION TAG	UNP C6CBG9
B	-22	MET	-	EXPRESSION TAG	UNP C6CBG9
B	-21	HIS	-	EXPRESSION TAG	UNP C6CBG9
B	-20	HIS	-	EXPRESSION TAG	UNP C6CBG9
B	-19	HIS	-	EXPRESSION TAG	UNP C6CBG9
B	-18	HIS	-	EXPRESSION TAG	UNP C6CBG9
B	-17	HIS	-	EXPRESSION TAG	UNP C6CBG9
B	-16	HIS	-	EXPRESSION TAG	UNP C6CBG9
B	-15	SER	-	EXPRESSION TAG	UNP C6CBG9
B	-14	SER	-	EXPRESSION TAG	UNP C6CBG9
B	-13	GLY	-	EXPRESSION TAG	UNP C6CBG9
B	-12	VAL	-	EXPRESSION TAG	UNP C6CBG9
B	-11	ASP	-	EXPRESSION TAG	UNP C6CBG9
B	-10	LEU	-	EXPRESSION TAG	UNP C6CBG9
B	-9	GLY	-	EXPRESSION TAG	UNP C6CBG9
B	-8	THR	-	EXPRESSION TAG	UNP C6CBG9
B	-7	GLU	-	EXPRESSION TAG	UNP C6CBG9
B	-6	ASN	-	EXPRESSION TAG	UNP C6CBG9
B	-5	LEU	-	EXPRESSION TAG	UNP C6CBG9
B	-4	TYR	-	EXPRESSION TAG	UNP C6CBG9
B	-3	PHE	-	EXPRESSION TAG	UNP C6CBG9
B	-2	GLN	-	EXPRESSION TAG	UNP C6CBG9
B	-1	SER	-	EXPRESSION TAG	UNP C6CBG9
B	0	MET	-	EXPRESSION TAG	UNP C6CBG9
C	-22	MET	-	EXPRESSION TAG	UNP C6CBG9
C	-21	HIS	-	EXPRESSION TAG	UNP C6CBG9
C	-20	HIS	-	EXPRESSION TAG	UNP C6CBG9
C	-19	HIS	-	EXPRESSION TAG	UNP C6CBG9
C	-18	HIS	-	EXPRESSION TAG	UNP C6CBG9
C	-17	HIS	-	EXPRESSION TAG	UNP C6CBG9
C	-16	HIS	-	EXPRESSION TAG	UNP C6CBG9
C	-15	SER	-	EXPRESSION TAG	UNP C6CBG9
C	-14	SER	-	EXPRESSION TAG	UNP C6CBG9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	GLY	-	EXPRESSION TAG	UNP C6CBG9
C	-12	VAL	-	EXPRESSION TAG	UNP C6CBG9
C	-11	ASP	-	EXPRESSION TAG	UNP C6CBG9
C	-10	LEU	-	EXPRESSION TAG	UNP C6CBG9
C	-9	GLY	-	EXPRESSION TAG	UNP C6CBG9
C	-8	THR	-	EXPRESSION TAG	UNP C6CBG9
C	-7	GLU	-	EXPRESSION TAG	UNP C6CBG9
C	-6	ASN	-	EXPRESSION TAG	UNP C6CBG9
C	-5	LEU	-	EXPRESSION TAG	UNP C6CBG9
C	-4	TYR	-	EXPRESSION TAG	UNP C6CBG9
C	-3	PHE	-	EXPRESSION TAG	UNP C6CBG9
C	-2	GLN	-	EXPRESSION TAG	UNP C6CBG9
C	-1	SER	-	EXPRESSION TAG	UNP C6CBG9
C	0	MET	-	EXPRESSION TAG	UNP C6CBG9
D	-22	MET	-	EXPRESSION TAG	UNP C6CBG9
D	-21	HIS	-	EXPRESSION TAG	UNP C6CBG9
D	-20	HIS	-	EXPRESSION TAG	UNP C6CBG9
D	-19	HIS	-	EXPRESSION TAG	UNP C6CBG9
D	-18	HIS	-	EXPRESSION TAG	UNP C6CBG9
D	-17	HIS	-	EXPRESSION TAG	UNP C6CBG9
D	-16	HIS	-	EXPRESSION TAG	UNP C6CBG9
D	-15	SER	-	EXPRESSION TAG	UNP C6CBG9
D	-14	SER	-	EXPRESSION TAG	UNP C6CBG9
D	-13	GLY	-	EXPRESSION TAG	UNP C6CBG9
D	-12	VAL	-	EXPRESSION TAG	UNP C6CBG9
D	-11	ASP	-	EXPRESSION TAG	UNP C6CBG9
D	-10	LEU	-	EXPRESSION TAG	UNP C6CBG9
D	-9	GLY	-	EXPRESSION TAG	UNP C6CBG9
D	-8	THR	-	EXPRESSION TAG	UNP C6CBG9
D	-7	GLU	-	EXPRESSION TAG	UNP C6CBG9
D	-6	ASN	-	EXPRESSION TAG	UNP C6CBG9
D	-5	LEU	-	EXPRESSION TAG	UNP C6CBG9
D	-4	TYR	-	EXPRESSION TAG	UNP C6CBG9
D	-3	PHE	-	EXPRESSION TAG	UNP C6CBG9
D	-2	GLN	-	EXPRESSION TAG	UNP C6CBG9
D	-1	SER	-	EXPRESSION TAG	UNP C6CBG9
D	0	MET	-	EXPRESSION TAG	UNP C6CBG9
E	-22	MET	-	EXPRESSION TAG	UNP C6CBG9
E	-21	HIS	-	EXPRESSION TAG	UNP C6CBG9
E	-20	HIS	-	EXPRESSION TAG	UNP C6CBG9
E	-19	HIS	-	EXPRESSION TAG	UNP C6CBG9
E	-18	HIS	-	EXPRESSION TAG	UNP C6CBG9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-17	HIS	-	EXPRESSION TAG	UNP C6CBG9
E	-16	HIS	-	EXPRESSION TAG	UNP C6CBG9
E	-15	SER	-	EXPRESSION TAG	UNP C6CBG9
E	-14	SER	-	EXPRESSION TAG	UNP C6CBG9
E	-13	GLY	-	EXPRESSION TAG	UNP C6CBG9
E	-12	VAL	-	EXPRESSION TAG	UNP C6CBG9
E	-11	ASP	-	EXPRESSION TAG	UNP C6CBG9
E	-10	LEU	-	EXPRESSION TAG	UNP C6CBG9
E	-9	GLY	-	EXPRESSION TAG	UNP C6CBG9
E	-8	THR	-	EXPRESSION TAG	UNP C6CBG9
E	-7	GLU	-	EXPRESSION TAG	UNP C6CBG9
E	-6	ASN	-	EXPRESSION TAG	UNP C6CBG9
E	-5	LEU	-	EXPRESSION TAG	UNP C6CBG9
E	-4	TYR	-	EXPRESSION TAG	UNP C6CBG9
E	-3	PHE	-	EXPRESSION TAG	UNP C6CBG9
E	-2	GLN	-	EXPRESSION TAG	UNP C6CBG9
E	-1	SER	-	EXPRESSION TAG	UNP C6CBG9
E	0	MET	-	EXPRESSION TAG	UNP C6CBG9
F	-22	MET	-	EXPRESSION TAG	UNP C6CBG9
F	-21	HIS	-	EXPRESSION TAG	UNP C6CBG9
F	-20	HIS	-	EXPRESSION TAG	UNP C6CBG9
F	-19	HIS	-	EXPRESSION TAG	UNP C6CBG9
F	-18	HIS	-	EXPRESSION TAG	UNP C6CBG9
F	-17	HIS	-	EXPRESSION TAG	UNP C6CBG9
F	-16	HIS	-	EXPRESSION TAG	UNP C6CBG9
F	-15	SER	-	EXPRESSION TAG	UNP C6CBG9
F	-14	SER	-	EXPRESSION TAG	UNP C6CBG9
F	-13	GLY	-	EXPRESSION TAG	UNP C6CBG9
F	-12	VAL	-	EXPRESSION TAG	UNP C6CBG9
F	-11	ASP	-	EXPRESSION TAG	UNP C6CBG9
F	-10	LEU	-	EXPRESSION TAG	UNP C6CBG9
F	-9	GLY	-	EXPRESSION TAG	UNP C6CBG9
F	-8	THR	-	EXPRESSION TAG	UNP C6CBG9
F	-7	GLU	-	EXPRESSION TAG	UNP C6CBG9
F	-6	ASN	-	EXPRESSION TAG	UNP C6CBG9
F	-5	LEU	-	EXPRESSION TAG	UNP C6CBG9
F	-4	TYR	-	EXPRESSION TAG	UNP C6CBG9
F	-3	PHE	-	EXPRESSION TAG	UNP C6CBG9
F	-2	GLN	-	EXPRESSION TAG	UNP C6CBG9
F	-1	SER	-	EXPRESSION TAG	UNP C6CBG9
F	0	MET	-	EXPRESSION TAG	UNP C6CBG9
G	-22	MET	-	EXPRESSION TAG	UNP C6CBG9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	HIS	-	EXPRESSION TAG	UNP C6CBG9
G	-20	HIS	-	EXPRESSION TAG	UNP C6CBG9
G	-19	HIS	-	EXPRESSION TAG	UNP C6CBG9
G	-18	HIS	-	EXPRESSION TAG	UNP C6CBG9
G	-17	HIS	-	EXPRESSION TAG	UNP C6CBG9
G	-16	HIS	-	EXPRESSION TAG	UNP C6CBG9
G	-15	SER	-	EXPRESSION TAG	UNP C6CBG9
G	-14	SER	-	EXPRESSION TAG	UNP C6CBG9
G	-13	GLY	-	EXPRESSION TAG	UNP C6CBG9
G	-12	VAL	-	EXPRESSION TAG	UNP C6CBG9
G	-11	ASP	-	EXPRESSION TAG	UNP C6CBG9
G	-10	LEU	-	EXPRESSION TAG	UNP C6CBG9
G	-9	GLY	-	EXPRESSION TAG	UNP C6CBG9
G	-8	THR	-	EXPRESSION TAG	UNP C6CBG9
G	-7	GLU	-	EXPRESSION TAG	UNP C6CBG9
G	-6	ASN	-	EXPRESSION TAG	UNP C6CBG9
G	-5	LEU	-	EXPRESSION TAG	UNP C6CBG9
G	-4	TYR	-	EXPRESSION TAG	UNP C6CBG9
G	-3	PHE	-	EXPRESSION TAG	UNP C6CBG9
G	-2	GLN	-	EXPRESSION TAG	UNP C6CBG9
G	-1	SER	-	EXPRESSION TAG	UNP C6CBG9
G	0	MET	-	EXPRESSION TAG	UNP C6CBG9
H	-22	MET	-	EXPRESSION TAG	UNP C6CBG9
H	-21	HIS	-	EXPRESSION TAG	UNP C6CBG9
H	-20	HIS	-	EXPRESSION TAG	UNP C6CBG9
H	-19	HIS	-	EXPRESSION TAG	UNP C6CBG9
H	-18	HIS	-	EXPRESSION TAG	UNP C6CBG9
H	-17	HIS	-	EXPRESSION TAG	UNP C6CBG9
H	-16	HIS	-	EXPRESSION TAG	UNP C6CBG9
H	-15	SER	-	EXPRESSION TAG	UNP C6CBG9
H	-14	SER	-	EXPRESSION TAG	UNP C6CBG9
H	-13	GLY	-	EXPRESSION TAG	UNP C6CBG9
H	-12	VAL	-	EXPRESSION TAG	UNP C6CBG9
H	-11	ASP	-	EXPRESSION TAG	UNP C6CBG9
H	-10	LEU	-	EXPRESSION TAG	UNP C6CBG9
H	-9	GLY	-	EXPRESSION TAG	UNP C6CBG9
H	-8	THR	-	EXPRESSION TAG	UNP C6CBG9
H	-7	GLU	-	EXPRESSION TAG	UNP C6CBG9
H	-6	ASN	-	EXPRESSION TAG	UNP C6CBG9
H	-5	LEU	-	EXPRESSION TAG	UNP C6CBG9
H	-4	TYR	-	EXPRESSION TAG	UNP C6CBG9
H	-3	PHE	-	EXPRESSION TAG	UNP C6CBG9

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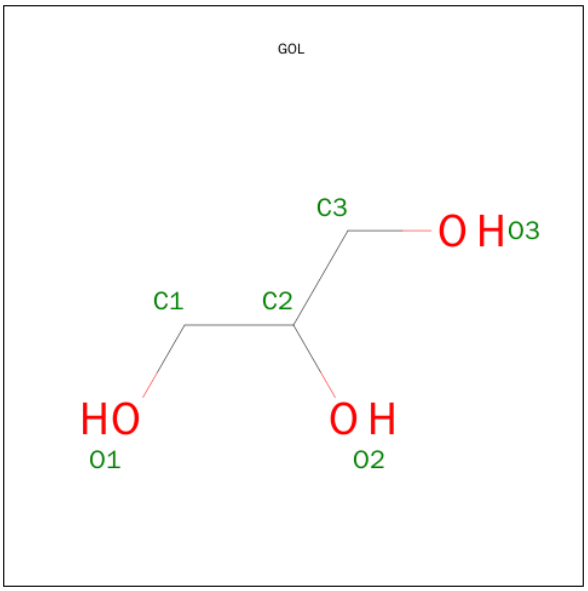
Chain	Residue	Modelled	Actual	Comment	Reference
H	-2	GLN	-	EXPRESSION TAG	UNP C6CBG9
H	-1	SER	-	EXPRESSION TAG	UNP C6CBG9
H	0	MET	-	EXPRESSION TAG	UNP C6CBG9

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

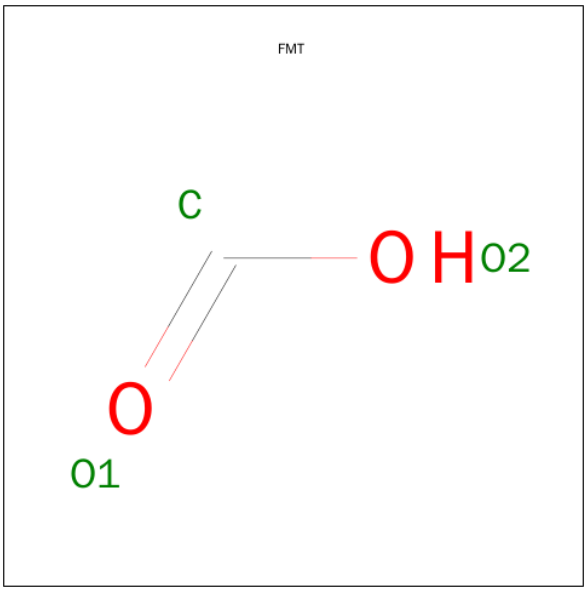
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



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

- Molecule 5 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	3	Total I 3 3	0	0
5	E	3	Total I 3 3	0	0
5	H	2	Total I 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total I 3 3	0	0
5	C	3	Total I 3 3	0	0
5	A	2	Total I 2 2	0	0
5	F	3	Total I 3 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	244	Total O 244 244	0	0
7	B	255	Total O 255 255	0	0
7	C	237	Total O 237 237	0	0
7	D	237	Total O 237 237	0	0
7	E	275	Total O 276 276	0	1
7	F	239	Total O 239 239	0	0

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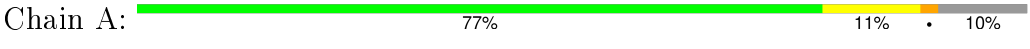
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	234	Total O 234 234	0	0
7	H	257	Total O 257 257	0	0

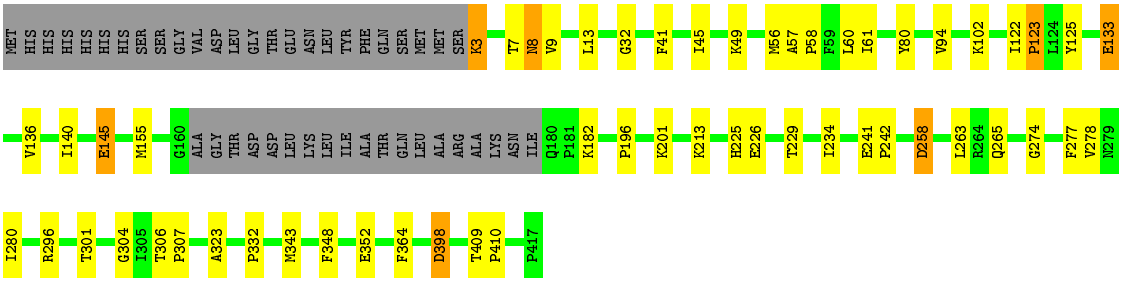
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Mandelate racemase/muconate lactonizing protein

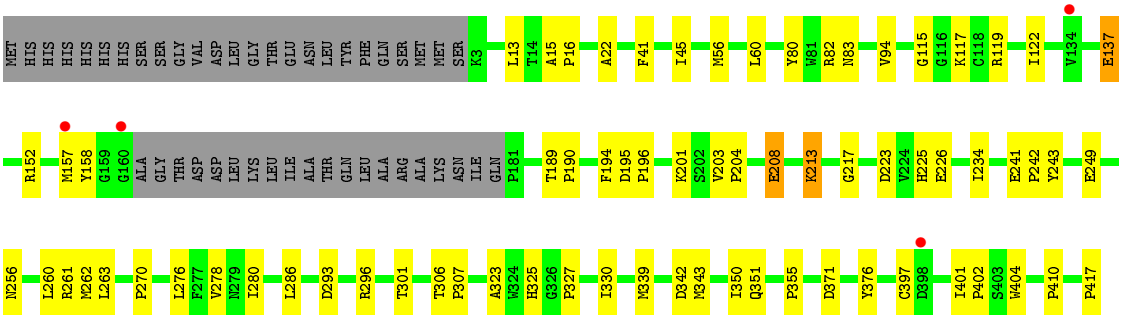
Chain A:





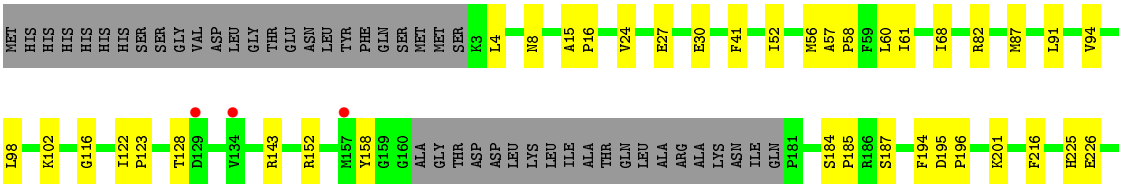
- Molecule 1: Mandelate racemase/muconate lactonizing protein

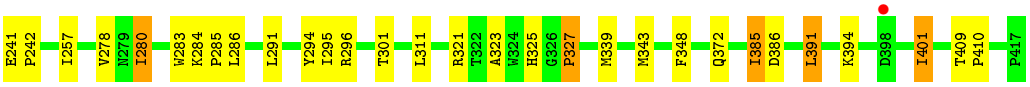
Chain B:



- Molecule 1: Mandelate racemase/muconate lactonizing protein

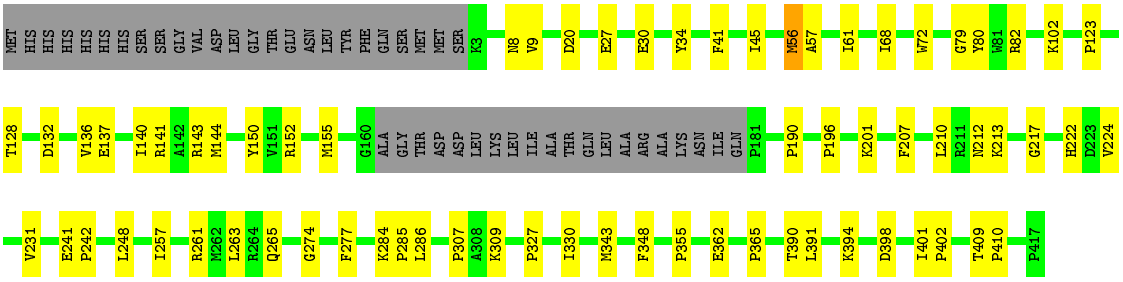
Chain C:





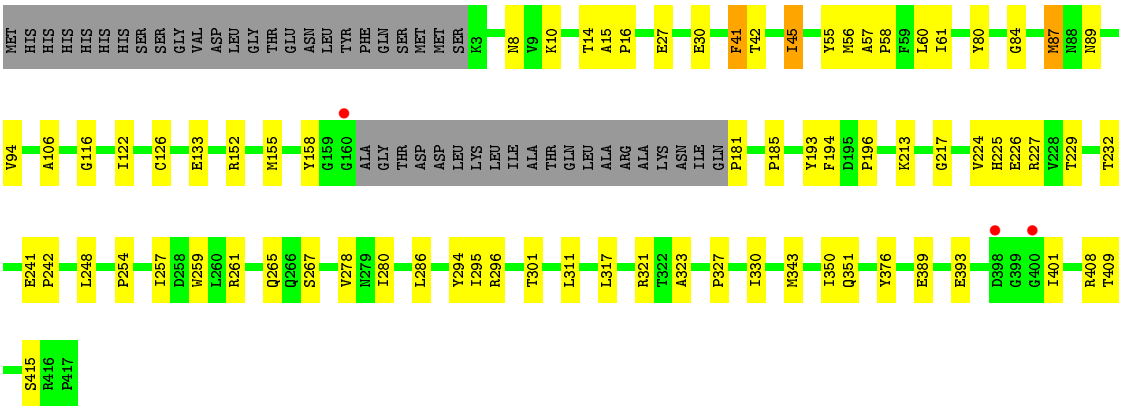
• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain D:



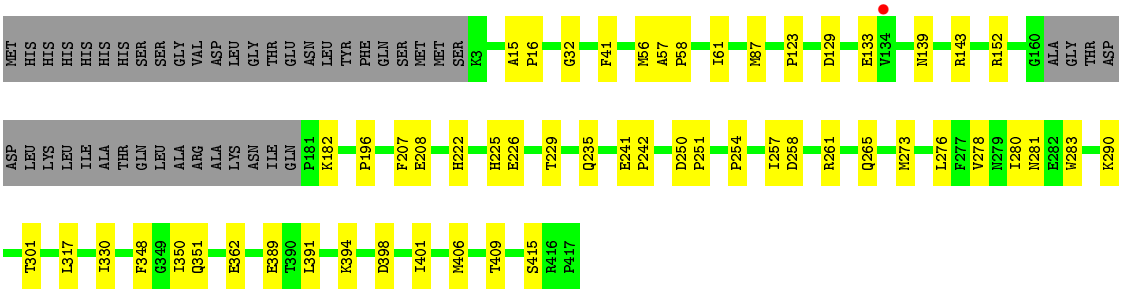
• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain E:



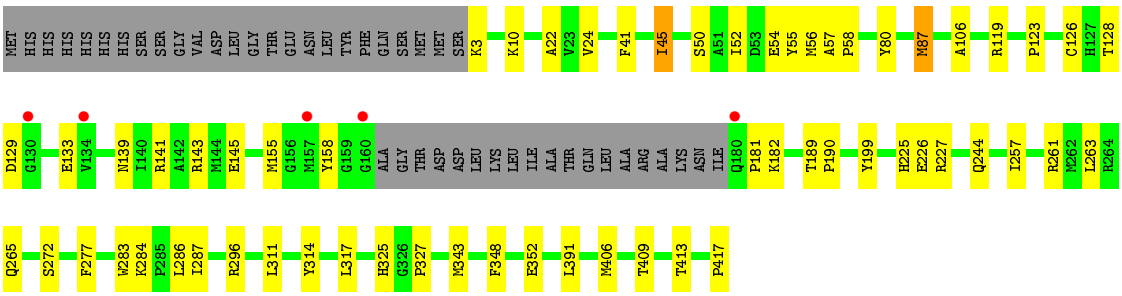
• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain F:



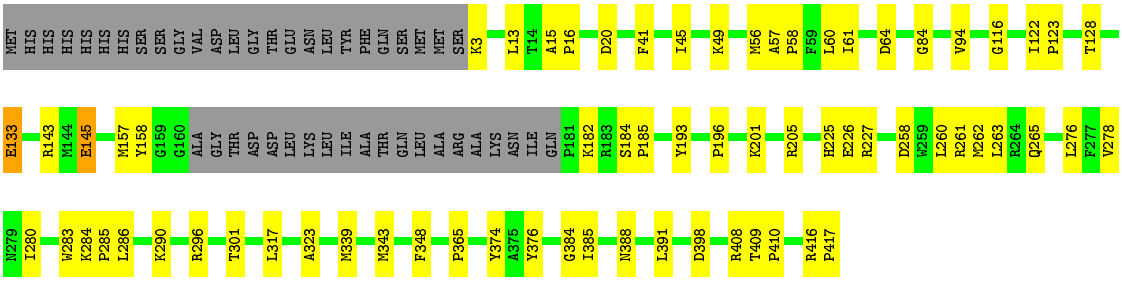
• Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain G:



- Molecule 1: Mandelate racemase/muconate lactonizing protein

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	224.33Å 224.35Å 87.08Å 90.00° 97.96° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 47.02 – 1.94	Depositor EDS
% Data completeness (in resolution range)	88.0 (40.00-2.00) 87.3 (47.02-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.7.0025	Depositor
R, R_{free}	0.173 , 0.228 0.175 , 0.229	Depositor DCC
R_{free} test set	7664 reflections (3.14%)	DCC
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 274398 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	26763	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, IOD, FMT, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.52	0/3162	0.67	0/4296
1	B	0.52	0/3170	0.69	0/4305
1	C	0.51	0/3156	0.70	1/4289 (0.0%)
1	D	0.54	0/3158	0.69	0/4291
1	E	0.54	0/3162	0.71	1/4295 (0.0%)
1	F	0.52	0/3167	0.69	0/4303
1	G	0.53	0/3160	0.71	1/4295 (0.0%)
1	H	0.52	0/3153	0.71	1/4283 (0.0%)
All	All	0.53	0/25288	0.70	4/34357 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	87	MET	CG-SD-CE	5.98	109.77	100.20
1	C	91	LEU	CA-CB-CG	5.65	128.30	115.30
1	H	64	ASP	CB-CG-OD1	5.42	123.18	118.30
1	G	227	ARG	NE-CZ-NH1	-5.07	117.76	120.30

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	3084	0	3036	50	0
1	B	3086	0	3046	59	0
1	C	3072	0	3023	67	0
1	D	3077	0	3026	58	0
1	E	3081	0	3037	61	0
1	F	3083	0	3032	40	0
1	G	3079	0	3023	47	0
1	H	3075	0	3029	54	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	12	0	16	3	0
3	B	12	0	16	1	0
3	C	12	0	16	1	0
3	D	12	0	16	2	0
3	E	6	0	8	0	0
3	F	12	0	16	2	0
3	G	6	0	8	0	0
3	H	12	0	16	1	0
4	A	3	0	1	1	0
4	B	3	0	1	3	0
4	C	3	0	1	0	0
4	D	3	0	1	0	0
4	E	3	0	1	0	0
4	F	6	0	2	1	0
4	G	3	0	1	2	0
4	H	3	0	1	1	0
5	A	2	0	0	2	0
5	B	3	0	0	1	0
5	C	3	0	0	4	0
5	D	3	0	0	2	0
5	E	3	0	0	3	0
5	F	3	0	0	4	0
5	H	2	0	0	1	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1	0	0	0	0
6	G	2	0	0	0	0
6	H	1	0	0	0	0
7	A	244	0	0	6	0
7	B	255	0	0	11	0
7	C	237	0	0	4	0
7	D	237	0	0	10	0
7	E	276	0	0	13	0
7	F	239	0	0	8	0
7	G	234	0	0	7	0
7	H	257	0	0	9	0
All	All	26763	0	24373	419	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 9.

All (419) 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:122:ILE:HD11	1:E:343:MET:HE2	1.23	1.11
1:E:122:ILE:HD11	1:E:343:MET:CE	1.83	1.07
7:E:874:HOH:O	1:F:257:ILE:HD11	1.63	0.98
1:C:280:ILE:O	1:C:280:ILE:HD13	1.67	0.94
1:H:416:ARG:HD2	7:H:846:HOH:O	1.66	0.94
1:D:201:LYS:HE2	7:F:828:HOH:O	1.69	0.92
1:E:126:CYS:HB2	7:E:744:HOH:O	1.69	0.92
1:A:145:GLU:HA	1:A:145:GLU:OE1	1.77	0.84
1:A:8:ASN:HA	1:A:61:ILE:HD11	1.61	0.83
1:H:57:ALA:HB3	1:H:58:PRO:HD3	1.61	0.83
1:C:187:SER:HB2	7:E:852:HOH:O	1.80	0.82
1:B:325:HIS:CD2	4:B:505:FMT:H	2.16	0.80
1:A:182:LYS:HE2	1:D:150:TYR:CZ	2.17	0.79
1:G:352:GLU:OE2	4:G:505:FMT:H	1.83	0.79
7:A:752:HOH:O	5:C:506:IOD:I	2.71	0.79
1:C:280:ILE:HD11	1:C:284:LYS:HD3	1.65	0.78
1:D:137:GLU:HB3	1:D:141:ARG:NH2	2.00	0.76
1:G:181:PRO:HB2	7:G:765:HOH:O	1.84	0.76
1:A:13:LEU:HD11	1:A:49:LYS:HD3	1.68	0.75
1:F:182:LYS:HE3	7:G:766:HOH:O	1.86	0.75
1:E:122:ILE:CD1	1:E:343:MET:CE	2.65	0.74
1:H:196:PRO:HD2	7:H:805:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:HIS:NE2	4:B:505:FMT:H	2.03	0.74
7:A:620:HOH:O	1:C:284:LYS:HE3	1.89	0.73
7:A:794:HOH:O	1:B:401:ILE:HD13	1.88	0.73
1:H:388:ASN:CG	1:H:391:LEU:HD12	2.09	0.72
1:F:57:ALA:O	1:F:61:ILE:HG12	1.89	0.71
1:G:24:VAL:CG2	1:G:52:ILE:HD13	2.21	0.71
1:E:229:THR:HG23	5:E:508:IOD:I	2.59	0.71
1:E:232:THR:HG23	7:E:864:HOH:O	1.92	0.70
1:C:4:LEU:HD13	1:C:30:GLU:HG3	1.74	0.70
1:D:56:MET:HE3	1:D:56:MET:HA	1.74	0.70
1:H:145:GLU:HG2	7:H:699:HOH:O	1.91	0.70
1:H:196:PRO:HB2	5:H:507:IOD:I	2.61	0.69
1:C:280:ILE:CD1	1:C:284:LYS:HB2	2.23	0.69
1:G:391:LEU:HD11	7:G:825:HOH:O	1.92	0.69
1:E:57:ALA:O	1:E:61:ILE:HG12	1.92	0.69
1:D:391:LEU:HD12	1:D:394:LYS:HE2	1.75	0.68
1:B:152:ARG:HD2	7:B:710:HOH:O	1.94	0.67
1:A:57:ALA:HB3	1:A:58:PRO:HD3	1.77	0.67
1:B:119:ARG:O	1:B:343[B]:MET:HE1	1.95	0.66
1:F:196:PRO:HB2	5:F:509:IOD:I	2.66	0.66
1:C:280:ILE:C	1:C:280:ILE:HD13	2.16	0.66
1:H:56:MET:HA	1:H:56:MET:HE3	1.77	0.66
1:A:32:GLY:H	3:A:505:GOL:H2	1.60	0.66
1:A:122:ILE:HD11	1:A:343:MET:HG2	1.77	0.65
1:C:280:ILE:HD11	1:C:284:LYS:HB2	1.77	0.65
1:E:122:ILE:CD1	1:E:343:MET:HE2	2.15	0.64
1:B:117:LYS:HG2	1:B:343[A]:MET:SD	2.37	0.64
1:A:234:ILE:HG12	1:A:263:LEU:HB2	1.80	0.64
1:A:8:ASN:HD22	1:A:9:VAL:H	1.44	0.64
1:C:184:SER:HB3	1:C:185:PRO:HD2	1.80	0.63
1:D:391:LEU:CD1	1:D:394:LYS:HE2	2.29	0.63
1:E:278:VAL:HG12	1:E:301:THR:HG22	1.79	0.63
1:D:137:GLU:HB3	1:D:141:ARG:HH21	1.64	0.62
1:A:196:PRO:HB2	5:A:506:IOD:I	2.70	0.62
1:E:122:ILE:HD11	1:E:343:MET:HE1	1.80	0.62
1:F:278:VAL:HG12	1:F:301:THR:HG22	1.82	0.62
1:H:145:GLU:CG	7:H:699:HOH:O	2.48	0.62
1:F:251:PRO:HD2	1:F:273:MET:SD	2.40	0.62
1:A:258:ASP:HB2	7:A:773:HOH:O	1.98	0.61
1:A:7:THR:O	1:A:61:ILE:HD12	2.00	0.61
1:C:391:LEU:HD13	1:C:394:LYS:HD3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:MET:HA	1:F:56:MET:HE3	1.84	0.60
1:H:388:ASN:CB	1:H:391:LEU:HD12	2.31	0.60
1:A:182:LYS:HE2	1:D:150:TYR:OH	2.00	0.60
1:A:225:HIS:O	1:A:226:GLU:HG2	2.01	0.60
1:A:145:GLU:CA	1:A:145:GLU:OE1	2.46	0.60
1:D:401:ILE:HD12	7:H:849:HOH:O	2.02	0.60
1:G:56:MET:HE3	1:G:56:MET:HA	1.83	0.59
1:C:284:LYS:N	1:C:285:PRO:HD2	2.17	0.59
7:A:801:HOH:O	1:G:182:LYS:HE3	2.02	0.59
1:B:152:ARG:NH2	7:B:613:HOH:O	2.34	0.59
1:G:24:VAL:HG22	1:G:52:ILE:HD13	1.83	0.58
1:D:190:PRO:HA	7:D:738:HOH:O	2.03	0.58
1:C:391:LEU:CD1	1:C:394:LYS:HD3	2.34	0.58
1:H:263:LEU:HD23	1:H:263:LEU:C	2.23	0.58
1:C:82:ARG:HA	1:C:87:MET:CE	2.32	0.58
1:D:132:ASP:O	1:D:136:VAL:HG23	2.03	0.58
1:B:261:ARG:HD2	7:B:769:HOH:O	2.04	0.57
1:E:122:ILE:CD1	1:E:343:MET:HE1	2.32	0.57
1:E:389:GLU:O	1:E:393:GLU:HG3	2.05	0.57
1:F:152:ARG:HD3	7:F:822:HOH:O	2.05	0.57
1:D:327:PRO:O	1:D:330:ILE:HG22	2.04	0.57
1:E:152:ARG:HD3	7:E:667:HOH:O	2.05	0.56
1:F:406:MET:O	1:F:406:MET:HG3	2.03	0.56
1:A:7:THR:C	1:A:61:ILE:HD12	2.25	0.56
1:G:257:ILE:HB	1:G:286:LEU:HD21	1.86	0.56
1:C:4:LEU:HD13	1:C:30:GLU:CG	2.35	0.56
1:C:60:LEU:HD11	1:C:94:VAL:HG21	1.88	0.56
1:D:152:ARG:HD3	7:D:798:HOH:O	2.04	0.56
1:A:123:PRO:HD2	1:A:348:PHE:CE2	2.40	0.56
1:C:391:LEU:O	1:C:391:LEU:HD12	2.05	0.56
1:E:261:ARG:O	1:E:265[B]:GLN:HG3	2.05	0.56
1:B:343[B]:MET:HE3	1:B:343[B]:MET:HA	1.87	0.56
1:C:401:ILE:N	1:C:401:ILE:HD13	2.21	0.56
1:E:181:PRO:HB2	7:E:771:HOH:O	2.07	0.55
1:C:278:VAL:HG12	1:C:301:THR:HG22	1.88	0.55
1:C:122:ILE:HD11	1:C:343:MET:HG2	1.88	0.55
1:B:196:PRO:HB2	5:B:508:IOD:I	2.77	0.55
1:D:274:GLY:HA2	1:D:277:PHE:CD2	2.42	0.55
1:G:119:ARG:O	1:G:343[A]:MET:HE1	2.07	0.55
1:A:133:GLU:OE1	1:A:155:MET:SD	2.65	0.55
1:B:225:HIS:ND1	1:B:417:PRO:OXT	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ILE:HD12	1:D:102:LYS:HE3	1.89	0.55
1:D:284:LYS:HB3	1:D:285:PRO:HD3	1.89	0.54
1:E:196:PRO:HB2	5:E:508:IOD:I	2.76	0.54
1:G:158:TYR:HD1	1:G:199:TYR:CE1	2.26	0.54
1:A:398:ASP:HB2	7:A:756:HOH:O	2.07	0.54
1:A:136:VAL:O	1:A:140:ILE:HG13	2.07	0.54
1:E:295:ILE:HG12	1:E:311:LEU:HD21	1.89	0.54
1:C:201:LYS:HE2	7:E:861:HOH:O	2.07	0.54
1:B:208:GLU:HG3	1:B:243:TYR:OH	2.08	0.54
1:D:231:VAL:HG12	7:D:696:HOH:O	2.08	0.54
1:A:60:LEU:HD11	1:A:94:VAL:HG21	1.90	0.54
1:D:241:GLU:N	1:D:242:PRO:CD	2.70	0.54
1:D:20:ASP:HB3	1:D:45:ILE:HD13	1.89	0.54
1:E:57:ALA:HB3	1:E:58:PRO:HD3	1.90	0.54
1:F:15:ALA:N	1:F:16:PRO:HD3	2.23	0.54
1:G:141:ARG:O	1:G:145:GLU:HG2	2.08	0.53
1:G:284:LYS:NZ	7:G:688:HOH:O	2.40	0.53
5:D:505:IOD:I	1:H:84:GLY:HA3	2.79	0.53
1:B:137:GLU:CD	1:B:213:LYS:HE2	2.28	0.53
1:C:196:PRO:HB2	5:C:508:IOD:I	2.78	0.53
1:H:365:PRO:O	1:H:385:ILE:HD12	2.08	0.53
1:B:278:VAL:HG12	1:B:301:THR:HG22	1.90	0.53
1:A:7:THR:C	1:A:61:ILE:CD1	2.77	0.53
1:H:13:LEU:HD11	1:H:49:LYS:HD2	1.90	0.53
1:E:280:ILE:HG22	7:E:831:HOH:O	2.09	0.53
1:C:301:THR:O	1:C:301:THR:HG22	2.09	0.53
1:C:68:ILE:HD11	1:C:102:LYS:HE2	1.90	0.53
1:B:325:HIS:NE2	4:B:505:FMT:C	2.70	0.53
1:B:15:ALA:N	1:B:16:PRO:HD3	2.24	0.53
1:F:235:GLN:CD	7:F:756:HOH:O	2.47	0.53
1:E:8:ASN:OD1	1:E:27:GLU:OE1	2.27	0.53
1:E:317:LEU:HD13	1:G:283:TRP:HH2	1.73	0.52
1:C:257:ILE:HB	1:C:286:LEU:HD21	1.90	0.52
1:A:56:MET:HA	1:A:56:MET:HE3	1.90	0.52
1:B:122:ILE:HD13	1:B:339:MET:HG2	1.91	0.52
1:C:325:HIS:CE1	1:C:327:PRO:HG3	2.45	0.52
1:A:409:THR:HB	1:A:410:PRO:CD	2.40	0.52
1:E:327:PRO:O	1:E:330:ILE:HG22	2.09	0.52
1:F:317:LEU:HD13	1:H:283:TRP:HH2	1.75	0.52
5:F:507:IOD:I	1:H:116:GLY:HA2	2.80	0.52
1:F:229:THR:HG23	5:F:509:IOD:I	2.81	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:106:ALA:HB1	1:G:106:ALA:HB1	1.91	0.51
3:A:502:GOL:H12	1:B:80:TYR:CD2	2.45	0.51
1:C:123:PRO:HG2	1:C:348:PHE:HE2	1.76	0.51
1:H:260:LEU:HD12	1:H:286:LEU:HD21	1.91	0.51
1:C:184:SER:HB3	1:C:185:PRO:CD	2.40	0.51
1:G:406:MET:HG3	1:G:406:MET:O	2.11	0.51
1:C:280:ILE:CD1	1:C:284:LYS:HD3	2.39	0.51
1:A:125:TYR:CZ	1:A:352:GLU:HB2	2.45	0.51
1:E:133:GLU:HG3	1:E:155:MET:SD	2.50	0.51
1:C:82:ARG:HA	1:C:87:MET:HE2	1.93	0.51
1:A:265:GLN:HE22	1:D:265[B]:GLN:HG2	1.75	0.51
1:H:20:ASP:HB3	1:H:45:ILE:HD13	1.92	0.51
1:E:224:VAL:HG23	1:E:248:LEU:HD11	1.92	0.51
1:A:3:LYS:O	1:A:3:LYS:HG3	2.09	0.51
1:G:284:LYS:HE2	1:G:314:TYR:OH	2.11	0.51
1:A:241:GLU:N	1:A:242:PRO:CD	2.73	0.51
1:D:224:VAL:HG23	1:D:248:LEU:HD11	1.93	0.51
1:A:409:THR:HB	1:A:410:PRO:HD2	1.92	0.50
1:F:57:ALA:HB3	1:F:58:PRO:HD3	1.94	0.50
1:D:355:PRO:HD2	7:D:757:HOH:O	2.11	0.50
1:A:32:GLY:N	3:A:505:GOL:H2	2.26	0.50
1:E:15:ALA:N	1:E:16:PRO:HD3	2.26	0.50
1:C:158:TYR:O	1:C:194:PHE:HB2	2.12	0.50
1:D:140:ILE:O	1:D:144:MET:HG3	2.11	0.50
1:G:87:MET:HE2	7:G:603:HOH:O	2.12	0.50
1:A:296:ARG:HD2	1:A:323:ALA:O	2.11	0.50
1:C:152:ARG:HD3	7:C:687:HOH:O	2.12	0.50
1:E:217:GLY:N	7:E:773:HOH:O	2.44	0.50
1:F:362[A]:GLU:HG3	7:F:675:HOH:O	2.11	0.50
1:B:201:LYS:HE2	1:C:216:PHE:O	2.12	0.50
1:H:123:PRO:HG2	1:H:348:PHE:HE2	1.77	0.50
1:F:290:LYS:NZ	7:F:677:HOH:O	2.45	0.50
1:C:280:ILE:HD11	1:C:284:LYS:CD	2.37	0.49
1:G:123:PRO:HG2	1:G:348:PHE:HE2	1.76	0.49
1:H:388:ASN:HB3	1:H:391:LEU:HD12	1.94	0.49
1:D:68:ILE:CD1	1:D:102:LYS:HE3	2.41	0.49
1:D:241:GLU:N	1:D:242:PRO:HD2	2.27	0.49
1:C:295:ILE:HG12	1:C:311:LEU:HD21	1.95	0.49
1:A:304:GLY:O	1:A:307:PRO:HD2	2.11	0.49
1:D:30:GLU:HA	1:D:30:GLU:OE1	2.12	0.49
1:H:133:GLU:OE1	1:H:133:GLU:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:PHE:CZ	1:D:222:HIS:HB2	2.48	0.49
1:F:283:TRP:HH2	1:H:317:LEU:HD13	1.77	0.49
1:C:15:ALA:N	1:C:16:PRO:HD3	2.28	0.49
1:B:22:ALA:HB2	1:B:45:ILE:HD11	1.95	0.49
1:E:259:TRP:CE2	1:H:290:LYS:HD2	2.47	0.49
1:C:116:GLY:HA2	5:C:506:IOD:I	2.83	0.49
1:C:123:PRO:HG2	1:C:348:PHE:CE2	2.48	0.48
1:E:241:GLU:N	1:E:242:PRO:CD	2.76	0.48
1:G:133:GLU:HG3	1:G:155:MET:SD	2.53	0.48
1:D:137:GLU:HG3	1:D:210:LEU:CD2	2.44	0.48
1:H:384:GLY:HA2	7:H:736:HOH:O	2.12	0.48
1:H:343:MET:HE2	1:H:343:MET:HB3	1.73	0.48
1:E:224:VAL:CG2	1:E:248:LEU:HD11	2.44	0.48
1:A:278:VAL:HG12	1:A:301:THR:HG22	1.95	0.48
1:F:250:ASP:HA	1:F:273:MET:SD	2.53	0.48
1:E:257:ILE:HD11	1:F:281:ASN:OD1	2.14	0.48
1:D:390:THR:HB	7:D:828:HOH:O	2.13	0.48
1:B:137:GLU:OE2	1:B:213:LYS:HE2	2.12	0.48
1:G:277:PHE:CD2	1:G:283:TRP:HB3	2.49	0.48
1:C:280:ILE:CD1	1:C:280:ILE:C	2.82	0.48
1:E:257:ILE:HB	1:E:286:LEU:HD21	1.95	0.48
1:G:158:TYR:CD1	1:G:199:TYR:CE1	3.02	0.48
1:C:68:ILE:CD1	1:C:102:LYS:HE2	2.44	0.48
1:C:280:ILE:HD13	1:C:284:LYS:HB2	1.92	0.48
1:G:189:THR:CG2	1:G:190:PRO:HD2	2.43	0.48
1:E:350:ILE:HG13	1:E:351:GLN:N	2.29	0.48
1:B:217:GLY:N	7:B:821:HOH:O	2.38	0.48
1:B:241:GLU:N	1:B:242:PRO:HD2	2.29	0.47
1:B:201:LYS:HE2	7:C:764:HOH:O	2.14	0.47
1:E:376:TYR:HA	7:E:823:HOH:O	2.14	0.47
1:D:132:ASP:HA	1:D:155:MET:SD	2.54	0.47
1:E:60:LEU:HD11	1:E:94:VAL:HG21	1.96	0.47
1:G:55:TYR:C	1:G:58:PRO:HD2	2.35	0.47
1:B:234:ILE:HG12	1:B:263:LEU:HB2	1.95	0.47
1:D:8:ASN:ND2	1:D:9:VAL:H	2.12	0.47
1:E:294:TYR:HA	1:E:321:ARG:O	2.15	0.47
1:B:13:LEU:HB3	1:B:397:CYS:SG	2.54	0.47
1:H:388:ASN:CG	1:H:391:LEU:CD1	2.80	0.47
1:E:254:PRO:HD3	7:E:637:HOH:O	2.15	0.47
1:G:272:SER:HB2	1:G:296:ARG:CG	2.45	0.47
1:F:207:PHE:CZ	1:F:222:HIS:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:TYR:HB3	3:D:503:GOL:H31	1.97	0.47
1:H:128:THR:CG2	1:H:143:ARG:HG3	2.45	0.47
1:A:332:PRO:HG2	1:A:364:PHE:CD2	2.49	0.47
1:D:402:PRO:HD3	7:D:660:HOH:O	2.14	0.47
1:B:350:ILE:HG13	1:B:351:GLN:N	2.29	0.47
1:H:284:LYS:HB3	1:H:285:PRO:HD3	1.97	0.47
1:G:283:TRP:CE3	1:G:287:ILE:HD12	2.50	0.47
1:E:42:THR:HA	1:E:45:ILE:HG23	1.95	0.47
1:C:4:LEU:CD1	1:C:30:GLU:CG	2.93	0.46
1:H:128:THR:HG22	1:H:143:ARG:HG3	1.97	0.46
1:E:261:ARG:O	1:E:265[A]:GLN:HG3	2.14	0.46
1:D:261:ARG:O	1:D:265[A]:GLN:HG3	2.15	0.46
1:E:55:TYR:O	1:F:401:ILE:HD11	2.14	0.46
1:D:196:PRO:HB2	5:D:508:IOD:I	2.84	0.46
1:C:401:ILE:H	1:C:401:ILE:HD13	1.79	0.46
1:A:296:ARG:NH2	4:A:503:FMT:H	2.31	0.46
1:F:32:GLY:H	3:F:508:GOL:H2	1.79	0.46
1:E:56:MET:CG	1:E:94:VAL:HG21	2.44	0.46
1:B:158:TYR:O	1:B:194:PHE:HB2	2.15	0.46
1:A:265:GLN:HE22	1:D:265[A]:GLN:HG2	1.80	0.46
1:G:189:THR:HG23	1:G:190:PRO:HD2	1.97	0.46
1:E:80:TYR:CZ	1:F:276:LEU:HD21	2.50	0.46
1:F:389:GLU:HG3	7:F:779:HOH:O	2.14	0.46
1:F:254:PRO:O	1:F:257:ILE:HG23	2.16	0.46
1:H:260:LEU:HD12	1:H:286:LEU:CD2	2.46	0.46
1:F:261:ARG:O	1:F:265[B]:GLN:HG3	2.16	0.46
1:H:193:TYR:HA	1:H:408:ARG:O	2.15	0.46
1:B:226:GLU:OE1	1:B:417:PRO:O	2.34	0.46
1:B:355:PRO:HD2	7:B:712:HOH:O	2.16	0.46
1:B:260:LEU:HD12	1:B:286:LEU:CD2	2.46	0.46
1:C:225:HIS:CD2	7:C:724:HOH:O	2.68	0.46
1:D:123:PRO:HG2	1:D:348:PHE:HE2	1.80	0.46
1:A:8:ASN:ND2	1:A:9:VAL:H	2.13	0.45
1:B:339:MET:HA	1:B:342:ASP:HB2	1.97	0.45
1:E:193:TYR:HA	1:E:408:ARG:O	2.16	0.45
1:C:82:ARG:HA	1:C:87:MET:HE3	1.97	0.45
1:D:261:ARG:O	1:D:265[B]:GLN:HG3	2.14	0.45
1:G:409:THR:OG1	1:G:413:THR:HB	2.15	0.45
1:A:8:ASN:CA	1:A:61:ILE:HD11	2.37	0.45
1:G:352:GLU:OE2	4:G:505:FMT:C	2.58	0.45
1:G:126:CYS:SG	1:G:143:ARG:HD3	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:ALA:CB	1:H:58:PRO:HD3	2.41	0.45
1:B:152:ARG:NH1	7:B:748:HOH:O	2.49	0.45
1:B:223:ASP:HA	1:B:249:GLU:HB3	1.99	0.45
1:H:409:THR:HB	1:H:410:PRO:CD	2.47	0.45
1:G:139:ASN:O	1:G:143:ARG:HG2	2.16	0.45
1:D:72:TRP:CZ2	1:D:307:PRO:HG3	2.52	0.45
1:H:278:VAL:HG12	1:H:301:THR:HG22	1.98	0.45
1:E:225:HIS:O	1:E:226:GLU:HG3	2.17	0.45
1:C:225:HIS:O	1:C:226:GLU:HG2	2.15	0.45
1:A:8:ASN:HD22	1:A:9:VAL:N	2.13	0.45
1:C:4:LEU:CD1	1:C:30:GLU:HG2	2.46	0.45
1:E:10:LYS:HB2	1:E:10:LYS:HE3	1.70	0.45
1:E:226:GLU:HA	7:E:838:HOH:O	2.17	0.45
1:B:280:ILE:O	1:B:280:ILE:HG12	2.16	0.45
1:B:82:ARG:O	1:B:83:ASN:HB2	2.16	0.45
1:F:350:ILE:HG13	1:F:351:GLN:N	2.32	0.45
1:H:122:ILE:HD13	1:H:339:MET:HG2	1.99	0.45
1:A:229:THR:HG23	5:A:506:IOD:I	2.87	0.45
1:D:224:VAL:CG2	1:D:248:LEU:HD11	2.46	0.45
1:F:261:ARG:O	1:F:265[A]:GLN:HG3	2.17	0.45
1:C:225:HIS:O	1:C:226:GLU:CG	2.64	0.45
7:B:822:HOH:O	1:H:201:LYS:HE2	2.16	0.45
1:H:158:TYR:CD1	1:H:227:ARG:HG3	2.51	0.45
1:H:226:GLU:OE1	1:H:417:PRO:O	2.35	0.45
1:A:13:LEU:HD11	1:A:49:LYS:CD	2.42	0.44
1:C:409:THR:HB	1:C:410:PRO:HD2	1.99	0.44
1:B:189:THR:HG23	1:B:190:PRO:HD2	1.98	0.44
1:E:196:PRO:HD2	7:E:862:HOH:O	2.16	0.44
1:B:261:ARG:HB3	1:B:261:ARG:CZ	2.47	0.44
1:D:257:ILE:HB	1:D:286:LEU:HD21	2.00	0.44
1:F:258:ASP:HB3	7:G:802:HOH:O	2.17	0.44
1:C:280:ILE:HG12	1:C:283:TRP:CZ2	2.52	0.44
1:C:128:THR:HG22	1:C:143:ARG:HG3	1.98	0.44
1:B:371:ASP:HB3	1:B:376:TYR:HE2	1.82	0.44
1:D:82:ARG:HD2	3:H:504:GOL:H31	1.99	0.44
1:B:225:HIS:O	1:B:226:GLU:HG2	2.17	0.44
1:B:115:GLY:HA2	7:B:798:HOH:O	2.17	0.44
1:C:385:ILE:HG13	1:C:386:ASP:N	2.32	0.44
1:F:362[B]:GLU:HG2	1:F:391:LEU:CD1	2.47	0.44
1:G:22:ALA:HB2	1:G:45:ILE:HG22	1.99	0.44
1:C:296:ARG:HD2	1:C:323:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:LEU:HD12	1:B:286:LEU:HD21	1.98	0.44
1:D:80:TYR:CZ	1:H:276:LEU:HD21	2.52	0.44
1:D:217:GLY:N	7:D:762:HOH:O	2.47	0.44
1:H:280:ILE:HG22	7:H:718:HOH:O	2.17	0.44
1:A:213:LYS:HA	1:A:213:LYS:HD3	1.89	0.44
1:G:50:SER:O	1:G:54:GLU:HB2	2.18	0.44
1:B:296:ARG:HD2	1:B:323:ALA:O	2.18	0.43
1:B:261:ARG:CB	1:B:261:ARG:CZ	2.95	0.43
1:E:14:THR:C	1:E:16:PRO:HD3	2.38	0.43
1:B:194:PHE:O	1:B:410:PRO:HD3	2.18	0.43
1:B:56:MET:HA	1:B:56:MET:HE3	2.00	0.43
1:G:244:GLN:HA	7:G:801:HOH:O	2.17	0.43
1:G:128:THR:HG22	1:G:143:ARG:HG3	2.00	0.43
1:H:258:ASP:OD1	1:H:261:ARG:HD3	2.18	0.43
1:H:60:LEU:HD11	1:H:94:VAL:HG11	2.00	0.43
1:D:409:THR:HB	1:D:410:PRO:CD	2.48	0.43
1:C:24:VAL:HG22	1:C:52:ILE:HD13	1.99	0.43
1:G:263:LEU:HD23	1:G:263:LEU:C	2.38	0.43
1:H:57:ALA:HB3	1:H:58:PRO:CD	2.42	0.43
1:H:15:ALA:N	1:H:16:PRO:HD3	2.33	0.43
1:E:84:GLY:HA3	5:F:505:IOD:I	2.89	0.43
1:C:294:TYR:HA	1:C:321:ARG:O	2.18	0.43
1:D:362:GLU:O	1:D:365:PRO:HD3	2.19	0.43
1:A:304:GLY:C	1:A:307:PRO:HD2	2.39	0.43
1:G:261:ARG:O	1:G:265:GLN:HG3	2.19	0.43
1:E:158:TYR:O	1:E:194:PHE:HB2	2.19	0.43
1:B:261:ARG:HB3	1:B:261:ARG:NH2	2.34	0.43
1:H:409:THR:HB	1:H:410:PRO:HD2	2.01	0.43
1:H:184:SER:HB3	1:H:185:PRO:HD2	2.01	0.43
1:F:409:THR:HG23	1:F:415:SER:OG	2.19	0.43
1:C:241:GLU:N	1:C:242:PRO:CD	2.82	0.43
1:D:343:MET:CE	7:D:780:HOH:O	2.67	0.43
1:G:225:HIS:O	1:G:226:GLU:HG3	2.19	0.43
1:C:57:ALA:O	1:C:61:ILE:HG12	2.19	0.43
1:B:306:THR:HB	1:B:307:PRO:CD	2.49	0.43
1:B:83:ASN:OD1	3:B:504:GOL:H11	2.19	0.42
1:C:57:ALA:HB3	1:C:58:PRO:HD3	2.01	0.42
1:B:256:ASN:ND2	7:B:639:HOH:O	2.30	0.42
1:E:241:GLU:N	1:E:242:PRO:HD2	2.34	0.42
1:D:343:MET:HE1	7:D:780:HOH:O	2.19	0.42
1:G:317:LEU:HD23	1:G:317:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:PRO:HG3	1:H:374:TYR:CE1	2.54	0.42
1:E:41:PHE:HB2	1:E:89:ASN:ND2	2.35	0.42
1:E:116:GLY:HA2	5:E:506:IOD:I	2.89	0.42
1:B:203:VAL:HB	1:B:204:PRO:HD3	2.01	0.42
1:F:241:GLU:N	1:F:242:PRO:CD	2.82	0.42
1:D:309:LYS:HB3	7:D:827:HOH:O	2.18	0.42
1:E:296:ARG:HD2	1:E:323:ALA:O	2.20	0.42
1:E:409:THR:HG23	1:E:415:SER:OG	2.19	0.42
1:A:102:LYS:HB2	1:A:102:LYS:HE3	1.91	0.42
1:E:56:MET:HG2	1:E:94:VAL:HG21	2.02	0.42
1:D:79:GLY:O	1:D:80:TYR:HB3	2.20	0.42
1:G:225:HIS:ND1	1:G:417:PRO:OXT	2.51	0.42
1:C:280:ILE:CD1	1:C:284:LYS:CB	2.93	0.42
1:H:60:LEU:HD11	1:H:94:VAL:HG21	2.02	0.42
1:A:263:LEU:C	1:A:263:LEU:HD23	2.40	0.41
1:G:55:TYR:O	1:G:58:PRO:HD2	2.19	0.41
1:G:325:HIS:CE1	1:G:327:PRO:HG3	2.55	0.41
1:C:8:ASN:ND2	1:C:27:GLU:OE1	2.45	0.41
1:D:263:LEU:C	1:D:263:LEU:HD23	2.40	0.41
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.85	0.41
1:G:283:TRP:CE2	1:G:311:LEU:HD13	2.55	0.41
4:F:506:FMT:H	7:F:800:HOH:O	2.18	0.41
1:B:195:ASP:HA	1:B:196:PRO:HD3	1.84	0.41
1:D:27:GLU:HB3	3:D:503:GOL:H32	2.01	0.41
1:C:94:VAL:O	1:C:98:LEU:HG	2.21	0.41
1:E:80:TYR:CE1	1:F:276:LEU:HD21	2.54	0.41
1:B:115:GLY:CA	7:B:798:HOH:O	2.69	0.41
1:A:265:GLN:NE2	1:D:265[B]:GLN:HG2	2.35	0.41
1:F:265[B]:GLN:NE2	1:G:265:GLN:HA	2.35	0.41
1:H:376:TYR:HA	7:H:754:HOH:O	2.20	0.41
1:B:402:PRO:HB2	1:B:404:TRP:CD1	2.56	0.41
1:H:13:LEU:CD1	1:H:49:LYS:HD2	2.50	0.41
1:D:409:THR:HB	1:D:410:PRO:HD2	2.01	0.41
1:B:262:MET:HB2	7:B:763:HOH:O	2.19	0.41
1:F:139:ASN:O	1:F:143:ARG:HG2	2.21	0.41
1:F:330:ILE:O	1:F:330:ILE:HG23	2.21	0.41
1:D:137:GLU:HG3	1:D:210:LEU:HD23	2.03	0.41
1:G:57:ALA:HB3	1:G:58:PRO:HD3	2.02	0.41
1:E:80:TYR:CD2	3:F:502:GOL:H12	2.56	0.41
3:C:502:GOL:H12	1:G:80:TYR:CD2	2.56	0.41
1:C:56:MET:CG	1:C:94:VAL:HG21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ILE:HA	1:C:123:PRO:HD2	1.90	0.41
1:B:327:PRO:O	1:B:330:ILE:HG22	2.21	0.41
1:E:227:ARG:HD3	1:E:227:ARG:HA	1.94	0.41
1:D:57:ALA:O	1:D:61:ILE:HG12	2.20	0.41
1:F:123:PRO:HG2	1:F:348:PHE:HE2	1.86	0.41
1:H:57:ALA:O	1:H:61:ILE:HG12	2.21	0.41
1:C:123:PRO:CG	1:C:348:PHE:HE2	2.34	0.41
1:D:274:GLY:HA2	1:D:277:PHE:CE2	2.56	0.41
1:A:274:GLY:HA2	1:A:277:PHE:CD2	2.57	0.41
1:C:122:ILE:HD13	1:C:339:MET:HG2	2.03	0.40
1:F:225:HIS:O	1:F:226:GLU:CG	2.69	0.40
1:F:394:LYS:HB2	1:F:394:LYS:HE3	1.81	0.40
1:H:262:MET:HA	1:H:265:GLN:HE21	1.85	0.40
1:A:280:ILE:HD13	7:C:613:HOH:O	2.20	0.40
1:A:80:TYR:CZ	1:B:276:LEU:HD21	2.56	0.40
1:H:296:ARG:HD2	1:H:323:ALA:O	2.21	0.40
1:H:296:ARG:NH2	4:H:505:FMT:H	2.36	0.40
1:C:87:MET:HG2	5:C:505:IOD:I	2.91	0.40
1:F:280:ILE:HD13	7:H:673:HOH:O	2.21	0.40
1:B:60:LEU:HD11	1:B:94:VAL:HG11	2.02	0.40
1:G:343[A]:MET:HE3	1:G:343[A]:MET:HA	2.02	0.40
1:C:195:ASP:HA	1:C:196:PRO:HD2	1.95	0.40
1:A:306:THR:HB	1:A:307:PRO:HD3	2.04	0.40
1:G:272:SER:HB2	1:G:296:ARG:HG2	2.02	0.40
1:E:401:ILE:HD13	7:F:821:HOH:O	2.20	0.40
1:H:158:TYR:OH	1:H:225:HIS:HB2	2.21	0.40
1:D:128:THR:HG22	1:D:143:ARG:HG3	2.04	0.40
1:B:270:PRO:HA	1:B:293:ASP:OD2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/440 (89%)	384 (98%)	8 (2%)	0	100	100
1	B	393/440 (89%)	379 (96%)	14 (4%)	0	100	100
1	C	393/440 (89%)	382 (97%)	10 (2%)	1 (0%)	46	41
1	D	392/440 (89%)	380 (97%)	12 (3%)	0	100	100
1	E	392/440 (89%)	380 (97%)	12 (3%)	0	100	100
1	F	393/440 (89%)	378 (96%)	15 (4%)	0	100	100
1	G	393/440 (89%)	383 (98%)	10 (2%)	0	100	100
1	H	391/440 (89%)	381 (97%)	10 (3%)	0	100	100
All	All	3139/3520 (89%)	3047 (97%)	91 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	PRO

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	331/369 (90%)	321 (97%)	10 (3%)	48	47
1	B	332/369 (90%)	327 (98%)	5 (2%)	72	75
1	C	329/369 (89%)	323 (98%)	6 (2%)	66	69
1	D	330/369 (89%)	325 (98%)	5 (2%)	72	75
1	E	331/369 (90%)	325 (98%)	6 (2%)	66	69
1	F	331/369 (90%)	325 (98%)	6 (2%)	66	69
1	G	330/369 (89%)	324 (98%)	6 (2%)	66	69
1	H	330/369 (89%)	322 (98%)	8 (2%)	57	58
All	All	2644/2952 (90%)	2592 (98%)	52 (2%)	63	65

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	8	ASN
1	A	41	PHE
1	A	45	ILE
1	A	123	PRO
1	A	133	GLU
1	A	145	GLU
1	A	201	LYS
1	A	258	ASP
1	A	398	ASP
1	B	41	PHE
1	B	137	GLU
1	B	157	MET
1	B	208	GLU
1	B	213	LYS
1	C	41	PHE
1	C	280	ILE
1	C	372	GLN
1	C	385	ILE
1	C	391	LEU
1	C	401	ILE
1	D	41	PHE
1	D	56	MET
1	D	212	ASN
1	D	213	LYS
1	D	398	ASP
1	E	30	GLU
1	E	41	PHE
1	E	45	ILE
1	E	87	MET
1	E	213	LYS
1	E	267	SER
1	F	41	PHE
1	F	87	MET
1	F	129	ASP
1	F	133	GLU
1	F	208	GLU
1	F	398	ASP
1	G	3	LYS
1	G	10	LYS
1	G	41	PHE
1	G	45	ILE
1	G	87	MET

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Mol	Chain	Res	Type
1	G	129	ASP
1	H	3	LYS
1	H	41	PHE
1	H	133	GLU
1	H	145	GLU
1	H	157	MET
1	H	182	LYS
1	H	205	ARG
1	H	398	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	256	ASN
1	A	265	GLN
1	B	8	ASN
1	B	212	ASN
1	C	209	HIS
1	C	244	GLN
1	C	256	ASN
1	C	265	GLN
1	C	372	GLN
1	D	8	ASN
1	D	244	GLN
1	E	8	ASN
1	E	212	ASN
1	E	244	GLN
1	E	256	ASN
1	F	8	ASN
1	F	256	ASN
1	G	8	ASN
1	G	212	ASN
1	H	244	GLN
1	H	256	ASN
1	H	265	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 59 ligands modelled in this entry, 36 are monoatomic - leaving 23 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	GOL	A	502	-	5,5,5	0.33	0	5,5,5	0.32	0
4	FMT	A	503	2	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	A	505	-	5,5,5	0.21	0	5,5,5	0.45	0
3	GOL	B	502	-	5,5,5	0.52	0	5,5,5	0.32	0
3	GOL	B	504	-	5,5,5	0.35	0	5,5,5	0.36	0
4	FMT	B	505	2	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	C	502	-	5,5,5	0.41	0	5,5,5	0.31	0
4	FMT	C	503	2	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	C	507	-	5,5,5	0.24	0	5,5,5	0.48	0
3	GOL	D	502	-	5,5,5	0.49	0	5,5,5	0.41	0
3	GOL	D	503	-	5,5,5	0.19	0	5,5,5	0.51	0
4	FMT	D	506	2	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	E	502	-	5,5,5	0.34	0	5,5,5	0.71	0
4	FMT	E	505	2	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	F	502	-	5,5,5	0.46	0	5,5,5	0.48	0
4	FMT	F	503	2	0,2,2	0.00	-	0,1,1	0.00	-
4	FMT	F	506	-	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	F	508	-	5,5,5	0.16	0	5,5,5	0.52	0
3	GOL	G	502	-	5,5,5	0.35	0	5,5,5	0.19	0
4	FMT	G	505	2	0,2,2	0.00	-	0,1,1	0.00	-
3	GOL	H	502	-	5,5,5	0.35	0	5,5,5	0.54	0
3	GOL	H	504	-	5,5,5	0.23	0	5,5,5	0.47	0
4	FMT	H	505	2	0,2,2	0.00	-	0,1,1	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	502	-	-	0/4/4/4	0/0/0/0
4	FMT	A	503	2	-	0/0/0/0	0/0/0/0
3	GOL	A	505	-	-	0/4/4/4	0/0/0/0
3	GOL	B	502	-	-	0/4/4/4	0/0/0/0
3	GOL	B	504	-	-	0/4/4/4	0/0/0/0
4	FMT	B	505	2	-	0/0/0/0	0/0/0/0
3	GOL	C	502	-	-	0/4/4/4	0/0/0/0
4	FMT	C	503	2	-	0/0/0/0	0/0/0/0
3	GOL	C	507	-	-	0/4/4/4	0/0/0/0
3	GOL	D	502	-	-	0/4/4/4	0/0/0/0
3	GOL	D	503	-	-	0/4/4/4	0/0/0/0
4	FMT	D	506	2	-	0/0/0/0	0/0/0/0
3	GOL	E	502	-	-	0/4/4/4	0/0/0/0
4	FMT	E	505	2	-	0/0/0/0	0/0/0/0
3	GOL	F	502	-	-	0/4/4/4	0/0/0/0
4	FMT	F	503	2	-	0/0/0/0	0/0/0/0
4	FMT	F	506	-	-	0/0/0/0	0/0/0/0
3	GOL	F	508	-	-	0/4/4/4	0/0/0/0
3	GOL	G	502	-	-	0/4/4/4	0/0/0/0
4	FMT	G	505	2	-	0/0/0/0	0/0/0/0
3	GOL	H	502	-	-	0/4/4/4	0/0/0/0
3	GOL	H	504	-	-	0/4/4/4	0/0/0/0
4	FMT	H	505	2	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	GOL	1	0
4	A	503	FMT	1	0
3	A	505	GOL	2	0
3	B	504	GOL	1	0
4	B	505	FMT	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	GOL	1	0
3	D	503	GOL	2	0
3	F	502	GOL	1	0
4	F	506	FMT	1	0
3	F	508	GOL	1	0
4	G	505	FMT	2	0
3	H	504	GOL	1	0
4	H	505	FMT	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	396/440 (90%)	-0.73	0 100 100	8, 17, 40, 69	0
1	B	395/440 (89%)	-0.68	4 (1%) 84 84	7, 16, 45, 89	0
1	C	395/440 (89%)	-0.64	4 (1%) 84 84	7, 16, 40, 75	0
1	D	395/440 (89%)	-0.72	0 100 100	7, 16, 41, 65	0
1	E	395/440 (89%)	-0.76	3 (0%) 87 88	6, 15, 39, 77	0
1	F	395/440 (89%)	-0.66	1 (0%) 94 94	7, 17, 43, 85	0
1	G	396/440 (90%)	-0.69	5 (1%) 79 80	7, 17, 47, 100	0
1	H	395/440 (89%)	-0.75	0 100 100	7, 15, 39, 70	0
All	All	3162/3520 (89%)	-0.70	17 (0%) 91 92	6, 16, 42, 100	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	160	GLY	3.5
1	G	130	GLY	3.2
1	B	134	VAL	3.0
1	B	398	ASP	2.8
1	C	129	ASP	2.8
1	B	157	MET	2.6
1	C	157	MET	2.5
1	C	398	ASP	2.5
1	C	134	VAL	2.5
1	G	134	VAL	2.5
1	E	400	GLY	2.3
1	B	160	GLY	2.2
1	G	157	MET	2.2
1	F	134	VAL	2.2
1	G	160	GLY	2.2
1	E	398	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	180	GLN	2.1

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^{th} 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^2)	Q<0.9
4	FMT	F	506	3/3	0.90	0.16	6.49	30,30,31,46	0
3	GOL	F	502	6/6	0.94	0.10	5.50	17,23,29,30	0
3	GOL	B	502	6/6	0.93	0.11	5.32	17,22,37,39	0
4	FMT	E	505	3/3	0.94	0.10	2.72	23,23,29,36	0
3	GOL	A	505	6/6	0.94	0.22	2.67	31,43,56,56	0
3	GOL	H	504	6/6	0.94	0.15	2.44	20,31,39,41	0
4	FMT	F	503	3/3	0.93	0.09	2.40	26,26,31,31	0
3	GOL	E	502	6/6	0.93	0.09	2.33	19,23,25,46	0
3	GOL	G	502	6/6	0.95	0.09	2.32	16,19,27,38	0
3	GOL	C	507	6/6	0.96	0.13	2.20	26,27,33,43	0
6	CL	G	504	1/1	0.98	0.11	2.11	35,35,35,35	0
3	GOL	C	502	6/6	0.95	0.10	1.93	17,22,31,40	0
3	GOL	H	502	6/6	0.95	0.09	1.93	9,19,25,34	0
4	FMT	B	505	3/3	0.95	0.09	1.68	28,28,29,49	0
3	GOL	B	504	6/6	0.95	0.13	1.53	24,40,40,46	0
3	GOL	D	503	6/6	0.91	0.14	1.36	33,34,41,47	0
3	GOL	A	502	6/6	0.95	0.10	1.24	13,22,29,44	0
3	GOL	D	502	6/6	0.96	0.10	1.13	12,22,26,28	0
4	FMT	A	503	3/3	0.96	0.08	1.07	30,30,32,42	0
3	GOL	F	508	6/6	0.94	0.14	0.77	26,29,55,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	CL	F	504	1/1	0.97	0.09	0.69	34,34,34,34	0
4	FMT	D	506	3/3	0.96	0.08	0.69	28,28,43,53	0
4	FMT	G	505	3/3	0.97	0.07	0.10	19,19,28,37	0
6	CL	C	504	1/1	0.96	0.08	0.06	38,38,38,38	0
6	CL	H	503	1/1	0.98	0.08	-0.24	37,37,37,37	0
6	CL	B	503	1/1	0.97	0.06	-0.57	33,33,33,33	0
6	CL	D	504	1/1	0.97	0.07	-0.64	27,27,27,27	0
4	FMT	H	505	3/3	0.97	0.06	-0.75	17,17,25,29	0
5	IOD	B	507	1/1	0.98	0.06	-0.95	32,32,32,32	1
5	IOD	A	504	1/1	0.92	0.05	-1.14	38,38,38,38	1
6	CL	E	503	1/1	0.98	0.06	-1.15	33,33,33,33	0
6	CL	G	503	1/1	0.96	0.05	-1.18	30,30,30,30	0
5	IOD	E	507	1/1	0.98	0.06	-1.29	31,31,31,31	1
5	IOD	E	506	1/1	0.95	0.06	-1.33	34,34,34,34	1
5	IOD	B	508	1/1	0.98	0.04	-1.95	33,33,33,33	1
4	FMT	C	503	3/3	0.98	0.04	-2.30	26,26,27,35	0
2	MG	B	501	1/1	0.98	0.04	-2.37	14,14,14,14	0
5	IOD	H	506	1/1	0.98	0.05	-2.44	30,30,30,30	1
5	IOD	C	505	1/1	1.00	0.05	-2.46	15,15,15,15	0
5	IOD	F	505	1/1	1.00	0.05	-2.62	15,15,15,15	0
5	IOD	F	507	1/1	0.97	0.05	-2.72	35,35,35,35	1
5	IOD	D	507	1/1	0.97	0.04	-2.96	33,33,33,33	1
2	MG	F	501	1/1	0.98	0.05	-3.03	20,20,20,20	0
2	MG	E	501	1/1	0.99	0.03	-3.17	17,17,17,17	0
2	MG	G	501	1/1	0.99	0.03	-3.25	15,15,15,15	0
5	IOD	D	505	1/1	0.99	0.06	-3.42	14,14,14,14	0
2	MG	C	501	1/1	1.00	0.04	-3.45	16,16,16,16	0
2	MG	D	501	1/1	0.99	0.03	-3.83	14,14,14,14	0
2	MG	H	501	1/1	0.99	0.02	-4.47	14,14,14,14	0
5	IOD	C	506	1/1	0.98	0.04	-4.83	33,33,33,33	1
2	MG	A	501	1/1	0.99	0.03	-5.37	11,11,11,11	0
5	IOD	B	506	1/1	1.00	0.05	-6.87	15,15,15,15	0
6	CL	E	504	1/1	0.98	0.05	-	35,35,35,35	0
5	IOD	D	508	1/1	0.99	0.04	-	38,38,38,38	1
5	IOD	C	508	1/1	0.99	0.03	-	33,33,33,33	1
5	IOD	H	507	1/1	0.99	0.02	-	30,30,30,30	1
5	IOD	A	506	1/1	0.99	0.03	-	31,31,31,31	1
5	IOD	F	509	1/1	0.99	0.03	-	35,35,35,35	1
5	IOD	E	508	1/1	0.98	0.04	-	32,32,32,32	1

6.5 Other polymers (i)

There are no such residues in this entry.