Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:36 PM GMT

PDB ID	:	4UB9
Title	:	Structural and catalytic characterization of molinate hydrolase
Authors	:	Leite, J.P.; Duarte, M.; Paiva, A.; Ferreira-da-Silva, F.; Matias, P.M.; Nunes, O.; Gales, L.
Deposited on	:	2014-08-12
Resolution	:	2.27 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:

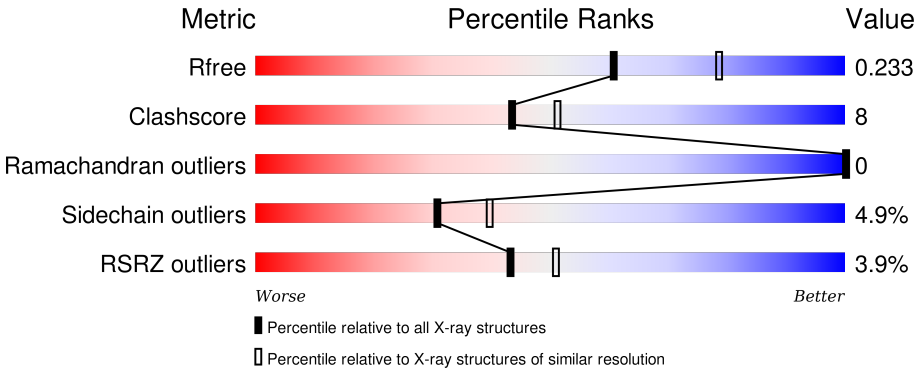
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.27 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	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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	496	81% 11% • 6%
1	B	496	4% 82% 10% • 6%
1	C	496	3% 82% 9% • 6%
1	D	496	2% 83% 9% • 6%
1	E	496	81% 11% • 6%

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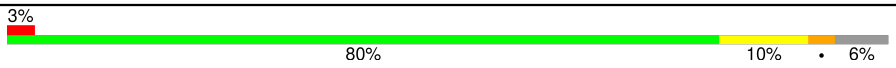
Mol	Chain	Length	Quality of chain
1	F	496	
1	G	496	
1	H	496	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29391 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 Molinate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3597	2276	619	680	22			
1	B	467	Total	C	N	O	S	0	1	0
			3602	2279	619	682	22			
1	C	467	Total	C	N	O	S	0	0	0
			3597	2276	619	680	22			
1	D	467	Total	C	N	O	S	0	0	0
			3597	2276	619	680	22			
1	E	467	Total	C	N	O	S	0	0	0
			3597	2276	619	680	22			
1	F	467	Total	C	N	O	S	0	0	0
			3597	2276	619	680	22			
1	G	467	Total	C	N	O	S	0	1	0
			3597	2276	619	680	22			
1	H	467	Total	C	N	O	S	0	0	0
			3597	2276	619	680	22			

There are 256 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP G2XLB0
A	2	ALA	-	expression tag	UNP G2XLB0
A	3	SER	-	expression tag	UNP G2XLB0
A	4	TRP	-	expression tag	UNP G2XLB0
A	5	SER	-	expression tag	UNP G2XLB0
A	6	HIS	-	expression tag	UNP G2XLB0
A	7	PRO	-	expression tag	UNP G2XLB0
A	8	GLN	-	expression tag	UNP G2XLB0
A	9	PHE	-	expression tag	UNP G2XLB0
A	10	GLU	-	expression tag	UNP G2XLB0
A	11	LYS	-	expression tag	UNP G2XLB0
A	12	ILE	-	expression tag	UNP G2XLB0
A	13	GLU	-	expression tag	UNP G2XLB0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	14	GLY	-	expression tag	UNP G2XLB0
A	15	ARG	-	expression tag	UNP G2XLB0
A	16	ARG	-	expression tag	UNP G2XLB0
A	17	ASP	-	expression tag	UNP G2XLB0
A	18	ARG	-	expression tag	UNP G2XLB0
A	19	GLY	-	expression tag	UNP G2XLB0
A	20	PRO	-	expression tag	UNP G2XLB0
A	21	GLU	-	expression tag	UNP G2XLB0
A	22	PHE	-	expression tag	UNP G2XLB0
A	23	GLU	-	expression tag	UNP G2XLB0
A	24	LEU	-	expression tag	UNP G2XLB0
A	25	GLY	-	expression tag	UNP G2XLB0
A	26	THR	-	expression tag	UNP G2XLB0
A	27	GLU	-	expression tag	UNP G2XLB0
A	28	ASN	-	expression tag	UNP G2XLB0
A	29	LEU	-	expression tag	UNP G2XLB0
A	30	PHE	-	expression tag	UNP G2XLB0
A	31	PHE	-	expression tag	UNP G2XLB0
A	32	GLU	-	expression tag	UNP G2XLB0
B	1	MET	-	initiating methionine	UNP G2XLB0
B	2	ALA	-	expression tag	UNP G2XLB0
B	3	SER	-	expression tag	UNP G2XLB0
B	4	TRP	-	expression tag	UNP G2XLB0
B	5	SER	-	expression tag	UNP G2XLB0
B	6	HIS	-	expression tag	UNP G2XLB0
B	7	PRO	-	expression tag	UNP G2XLB0
B	8	GLN	-	expression tag	UNP G2XLB0
B	9	PHE	-	expression tag	UNP G2XLB0
B	10	GLU	-	expression tag	UNP G2XLB0
B	11	LYS	-	expression tag	UNP G2XLB0
B	12	ILE	-	expression tag	UNP G2XLB0
B	13	GLU	-	expression tag	UNP G2XLB0
B	14	GLY	-	expression tag	UNP G2XLB0
B	15	ARG	-	expression tag	UNP G2XLB0
B	16	ARG	-	expression tag	UNP G2XLB0
B	17	ASP	-	expression tag	UNP G2XLB0
B	18	ARG	-	expression tag	UNP G2XLB0
B	19	GLY	-	expression tag	UNP G2XLB0
B	20	PRO	-	expression tag	UNP G2XLB0
B	21	GLU	-	expression tag	UNP G2XLB0
B	22	PHE	-	expression tag	UNP G2XLB0
B	23	GLU	-	expression tag	UNP G2XLB0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	24	LEU	-	expression tag	UNP G2XLB0
B	25	GLY	-	expression tag	UNP G2XLB0
B	26	THR	-	expression tag	UNP G2XLB0
B	27	GLU	-	expression tag	UNP G2XLB0
B	28	ASN	-	expression tag	UNP G2XLB0
B	29	LEU	-	expression tag	UNP G2XLB0
B	30	PHE	-	expression tag	UNP G2XLB0
B	31	PHE	-	expression tag	UNP G2XLB0
B	32	GLU	-	expression tag	UNP G2XLB0
C	1	MET	-	initiating methionine	UNP G2XLB0
C	2	ALA	-	expression tag	UNP G2XLB0
C	3	SER	-	expression tag	UNP G2XLB0
C	4	TRP	-	expression tag	UNP G2XLB0
C	5	SER	-	expression tag	UNP G2XLB0
C	6	HIS	-	expression tag	UNP G2XLB0
C	7	PRO	-	expression tag	UNP G2XLB0
C	8	GLN	-	expression tag	UNP G2XLB0
C	9	PHE	-	expression tag	UNP G2XLB0
C	10	GLU	-	expression tag	UNP G2XLB0
C	11	LYS	-	expression tag	UNP G2XLB0
C	12	ILE	-	expression tag	UNP G2XLB0
C	13	GLU	-	expression tag	UNP G2XLB0
C	14	GLY	-	expression tag	UNP G2XLB0
C	15	ARG	-	expression tag	UNP G2XLB0
C	16	ARG	-	expression tag	UNP G2XLB0
C	17	ASP	-	expression tag	UNP G2XLB0
C	18	ARG	-	expression tag	UNP G2XLB0
C	19	GLY	-	expression tag	UNP G2XLB0
C	20	PRO	-	expression tag	UNP G2XLB0
C	21	GLU	-	expression tag	UNP G2XLB0
C	22	PHE	-	expression tag	UNP G2XLB0
C	23	GLU	-	expression tag	UNP G2XLB0
C	24	LEU	-	expression tag	UNP G2XLB0
C	25	GLY	-	expression tag	UNP G2XLB0
C	26	THR	-	expression tag	UNP G2XLB0
C	27	GLU	-	expression tag	UNP G2XLB0
C	28	ASN	-	expression tag	UNP G2XLB0
C	29	LEU	-	expression tag	UNP G2XLB0
C	30	PHE	-	expression tag	UNP G2XLB0
C	31	PHE	-	expression tag	UNP G2XLB0
C	32	GLU	-	expression tag	UNP G2XLB0
D	1	MET	-	initiating methionine	UNP G2XLB0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	2	ALA	-	expression tag	UNP G2XLB0
D	3	SER	-	expression tag	UNP G2XLB0
D	4	TRP	-	expression tag	UNP G2XLB0
D	5	SER	-	expression tag	UNP G2XLB0
D	6	HIS	-	expression tag	UNP G2XLB0
D	7	PRO	-	expression tag	UNP G2XLB0
D	8	GLN	-	expression tag	UNP G2XLB0
D	9	PHE	-	expression tag	UNP G2XLB0
D	10	GLU	-	expression tag	UNP G2XLB0
D	11	LYS	-	expression tag	UNP G2XLB0
D	12	ILE	-	expression tag	UNP G2XLB0
D	13	GLU	-	expression tag	UNP G2XLB0
D	14	GLY	-	expression tag	UNP G2XLB0
D	15	ARG	-	expression tag	UNP G2XLB0
D	16	ARG	-	expression tag	UNP G2XLB0
D	17	ASP	-	expression tag	UNP G2XLB0
D	18	ARG	-	expression tag	UNP G2XLB0
D	19	GLY	-	expression tag	UNP G2XLB0
D	20	PRO	-	expression tag	UNP G2XLB0
D	21	GLU	-	expression tag	UNP G2XLB0
D	22	PHE	-	expression tag	UNP G2XLB0
D	23	GLU	-	expression tag	UNP G2XLB0
D	24	LEU	-	expression tag	UNP G2XLB0
D	25	GLY	-	expression tag	UNP G2XLB0
D	26	THR	-	expression tag	UNP G2XLB0
D	27	GLU	-	expression tag	UNP G2XLB0
D	28	ASN	-	expression tag	UNP G2XLB0
D	29	LEU	-	expression tag	UNP G2XLB0
D	30	PHE	-	expression tag	UNP G2XLB0
D	31	PHE	-	expression tag	UNP G2XLB0
D	32	GLU	-	expression tag	UNP G2XLB0
E	1	MET	-	initiating methionine	UNP G2XLB0
E	2	ALA	-	expression tag	UNP G2XLB0
E	3	SER	-	expression tag	UNP G2XLB0
E	4	TRP	-	expression tag	UNP G2XLB0
E	5	SER	-	expression tag	UNP G2XLB0
E	6	HIS	-	expression tag	UNP G2XLB0
E	7	PRO	-	expression tag	UNP G2XLB0
E	8	GLN	-	expression tag	UNP G2XLB0
E	9	PHE	-	expression tag	UNP G2XLB0
E	10	GLU	-	expression tag	UNP G2XLB0
E	11	LYS	-	expression tag	UNP G2XLB0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	12	ILE	-	expression tag	UNP G2XLB0
E	13	GLU	-	expression tag	UNP G2XLB0
E	14	GLY	-	expression tag	UNP G2XLB0
E	15	ARG	-	expression tag	UNP G2XLB0
E	16	ARG	-	expression tag	UNP G2XLB0
E	17	ASP	-	expression tag	UNP G2XLB0
E	18	ARG	-	expression tag	UNP G2XLB0
E	19	GLY	-	expression tag	UNP G2XLB0
E	20	PRO	-	expression tag	UNP G2XLB0
E	21	GLU	-	expression tag	UNP G2XLB0
E	22	PHE	-	expression tag	UNP G2XLB0
E	23	GLU	-	expression tag	UNP G2XLB0
E	24	LEU	-	expression tag	UNP G2XLB0
E	25	GLY	-	expression tag	UNP G2XLB0
E	26	THR	-	expression tag	UNP G2XLB0
E	27	GLU	-	expression tag	UNP G2XLB0
E	28	ASN	-	expression tag	UNP G2XLB0
E	29	LEU	-	expression tag	UNP G2XLB0
E	30	PHE	-	expression tag	UNP G2XLB0
E	31	PHE	-	expression tag	UNP G2XLB0
E	32	GLU	-	expression tag	UNP G2XLB0
F	1	MET	-	initiating methionine	UNP G2XLB0
F	2	ALA	-	expression tag	UNP G2XLB0
F	3	SER	-	expression tag	UNP G2XLB0
F	4	TRP	-	expression tag	UNP G2XLB0
F	5	SER	-	expression tag	UNP G2XLB0
F	6	HIS	-	expression tag	UNP G2XLB0
F	7	PRO	-	expression tag	UNP G2XLB0
F	8	GLN	-	expression tag	UNP G2XLB0
F	9	PHE	-	expression tag	UNP G2XLB0
F	10	GLU	-	expression tag	UNP G2XLB0
F	11	LYS	-	expression tag	UNP G2XLB0
F	12	ILE	-	expression tag	UNP G2XLB0
F	13	GLU	-	expression tag	UNP G2XLB0
F	14	GLY	-	expression tag	UNP G2XLB0
F	15	ARG	-	expression tag	UNP G2XLB0
F	16	ARG	-	expression tag	UNP G2XLB0
F	17	ASP	-	expression tag	UNP G2XLB0
F	18	ARG	-	expression tag	UNP G2XLB0
F	19	GLY	-	expression tag	UNP G2XLB0
F	20	PRO	-	expression tag	UNP G2XLB0
F	21	GLU	-	expression tag	UNP G2XLB0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	22	PHE	-	expression tag	UNP G2XLB0
F	23	GLU	-	expression tag	UNP G2XLB0
F	24	LEU	-	expression tag	UNP G2XLB0
F	25	GLY	-	expression tag	UNP G2XLB0
F	26	THR	-	expression tag	UNP G2XLB0
F	27	GLU	-	expression tag	UNP G2XLB0
F	28	ASN	-	expression tag	UNP G2XLB0
F	29	LEU	-	expression tag	UNP G2XLB0
F	30	PHE	-	expression tag	UNP G2XLB0
F	31	PHE	-	expression tag	UNP G2XLB0
F	32	GLU	-	expression tag	UNP G2XLB0
G	1	MET	-	initiating methionine	UNP G2XLB0
G	2	ALA	-	expression tag	UNP G2XLB0
G	3	SER	-	expression tag	UNP G2XLB0
G	4	TRP	-	expression tag	UNP G2XLB0
G	5	SER	-	expression tag	UNP G2XLB0
G	6	HIS	-	expression tag	UNP G2XLB0
G	7	PRO	-	expression tag	UNP G2XLB0
G	8	GLN	-	expression tag	UNP G2XLB0
G	9	PHE	-	expression tag	UNP G2XLB0
G	10	GLU	-	expression tag	UNP G2XLB0
G	11	LYS	-	expression tag	UNP G2XLB0
G	12	ILE	-	expression tag	UNP G2XLB0
G	13	GLU	-	expression tag	UNP G2XLB0
G	14	GLY	-	expression tag	UNP G2XLB0
G	15	ARG	-	expression tag	UNP G2XLB0
G	16	ARG	-	expression tag	UNP G2XLB0
G	17	ASP	-	expression tag	UNP G2XLB0
G	18	ARG	-	expression tag	UNP G2XLB0
G	19	GLY	-	expression tag	UNP G2XLB0
G	20	PRO	-	expression tag	UNP G2XLB0
G	21	GLU	-	expression tag	UNP G2XLB0
G	22	PHE	-	expression tag	UNP G2XLB0
G	23	GLU	-	expression tag	UNP G2XLB0
G	24	LEU	-	expression tag	UNP G2XLB0
G	25	GLY	-	expression tag	UNP G2XLB0
G	26	THR	-	expression tag	UNP G2XLB0
G	27	GLU	-	expression tag	UNP G2XLB0
G	28	ASN	-	expression tag	UNP G2XLB0
G	29	LEU	-	expression tag	UNP G2XLB0
G	30	PHE	-	expression tag	UNP G2XLB0
G	31	PHE	-	expression tag	UNP G2XLB0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	32	GLU	-	expression tag	UNP G2XLB0
H	1	MET	-	initiating methionine	UNP G2XLB0
H	2	ALA	-	expression tag	UNP G2XLB0
H	3	SER	-	expression tag	UNP G2XLB0
H	4	TRP	-	expression tag	UNP G2XLB0
H	5	SER	-	expression tag	UNP G2XLB0
H	6	HIS	-	expression tag	UNP G2XLB0
H	7	PRO	-	expression tag	UNP G2XLB0
H	8	GLN	-	expression tag	UNP G2XLB0
H	9	PHE	-	expression tag	UNP G2XLB0
H	10	GLU	-	expression tag	UNP G2XLB0
H	11	LYS	-	expression tag	UNP G2XLB0
H	12	ILE	-	expression tag	UNP G2XLB0
H	13	GLU	-	expression tag	UNP G2XLB0
H	14	GLY	-	expression tag	UNP G2XLB0
H	15	ARG	-	expression tag	UNP G2XLB0
H	16	ARG	-	expression tag	UNP G2XLB0
H	17	ASP	-	expression tag	UNP G2XLB0
H	18	ARG	-	expression tag	UNP G2XLB0
H	19	GLY	-	expression tag	UNP G2XLB0
H	20	PRO	-	expression tag	UNP G2XLB0
H	21	GLU	-	expression tag	UNP G2XLB0
H	22	PHE	-	expression tag	UNP G2XLB0
H	23	GLU	-	expression tag	UNP G2XLB0
H	24	LEU	-	expression tag	UNP G2XLB0
H	25	GLY	-	expression tag	UNP G2XLB0
H	26	THR	-	expression tag	UNP G2XLB0
H	27	GLU	-	expression tag	UNP G2XLB0
H	28	ASN	-	expression tag	UNP G2XLB0
H	29	LEU	-	expression tag	UNP G2XLB0
H	30	PHE	-	expression tag	UNP G2XLB0
H	31	PHE	-	expression tag	UNP G2XLB0
H	32	GLU	-	expression tag	UNP G2XLB0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0

- Molecule 3 is water.

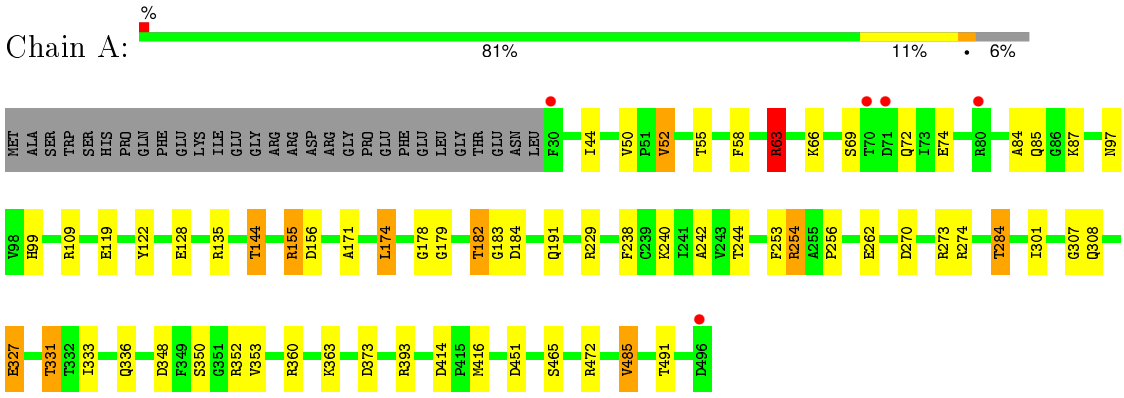
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	116	Total O 116 116	0	0
3	B	112	Total O 112 112	0	0
3	C	67	Total O 67 67	0	0
3	D	83	Total O 83 83	0	0
3	E	75	Total O 75 75	0	0
3	F	50	Total O 50 50	0	0
3	G	54	Total O 54 54	0	0
3	H	45	Total O 45 45	0	0

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.

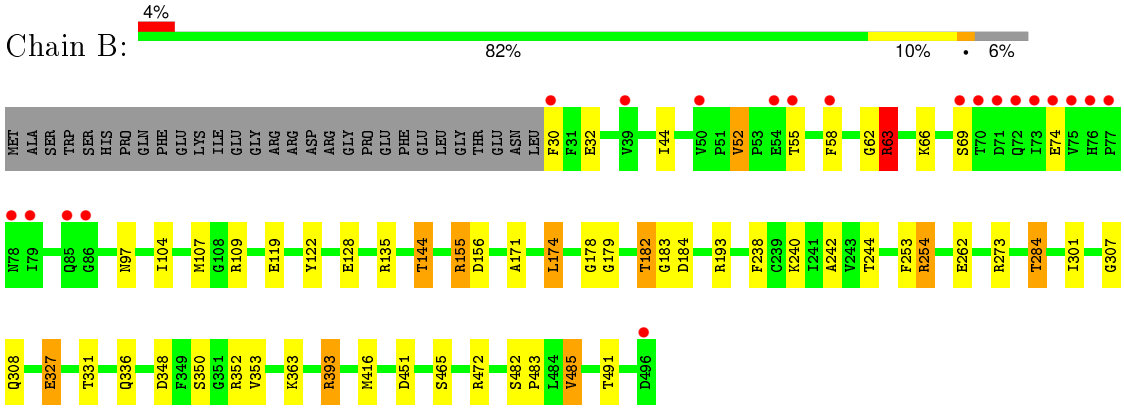
- Molecule 1: Molinate hydrolase

Chain A:



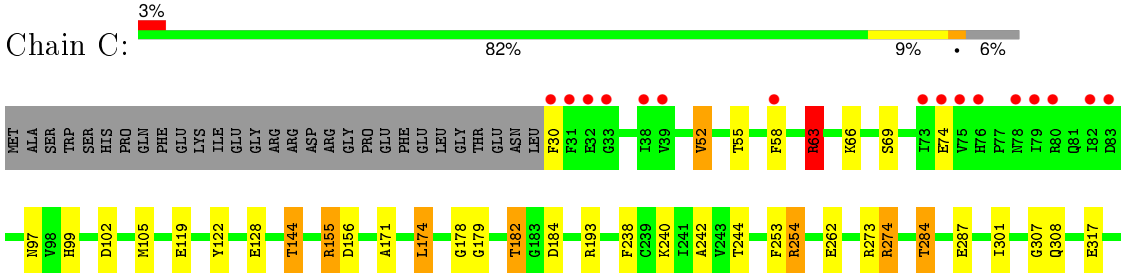
- Molecule 1: Molinate hydrolase

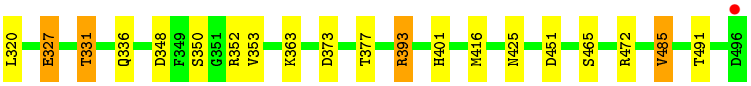
Chain B:



- Molecule 1: Molinate hydrolase

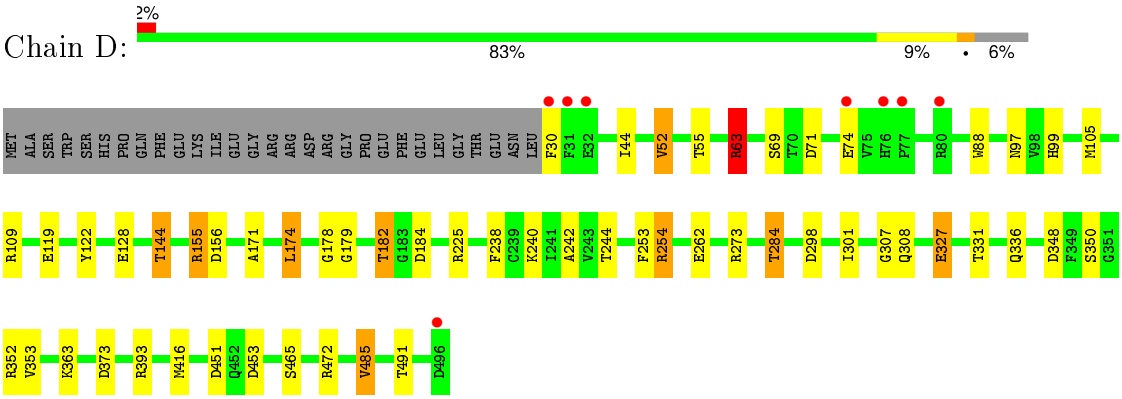
Chain C:





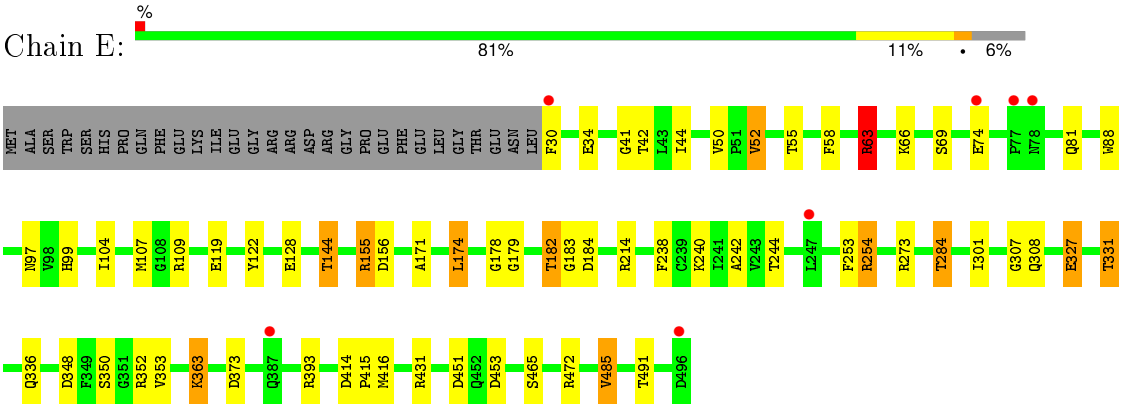
- Molecule 1: Molinate hydrolase

Chain D:



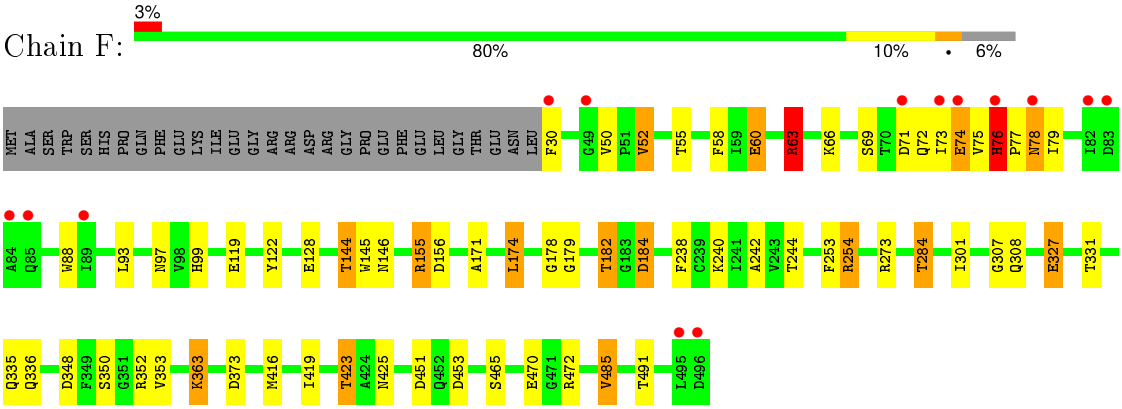
- Molecule 1: Molinate hydrolase

Chain E:



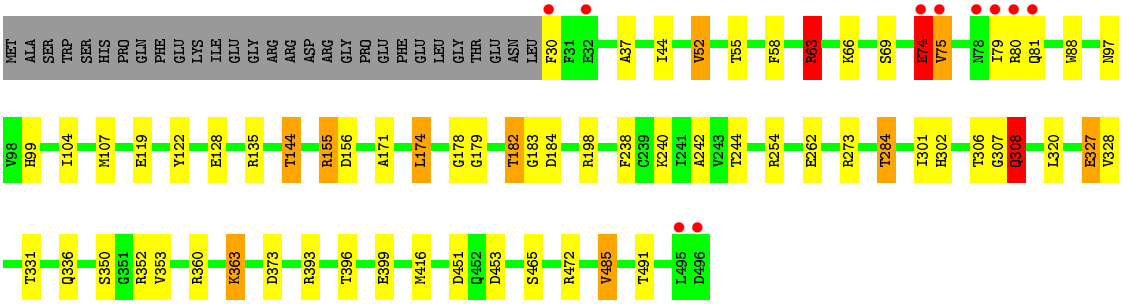
- Molecule 1: Molinate hydrolase

Chain F:

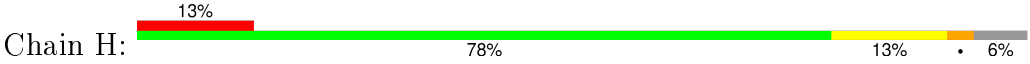


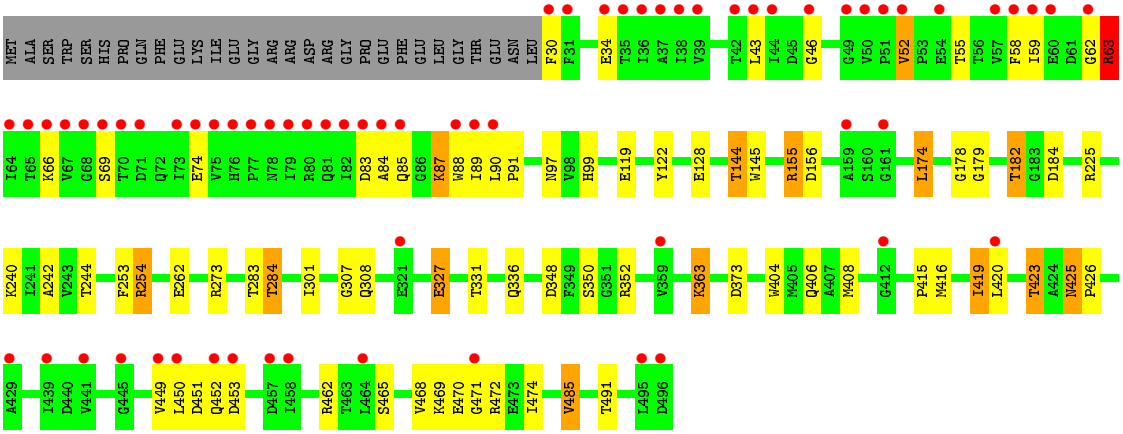
- Molecule 1: Molinate hydrolase

Chain G:



- Molecule 1: Molinate hydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	367.70Å 99.08Å 131.34Å 90.00° 109.61° 90.00°	Depositor
Resolution (Å)	123.72 – 2.27 49.54 – 2.27	Depositor EDS
% Data completeness (in resolution range)	94.5 (123.72-2.27) 94.5 (49.54-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.48 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.201 , 0.229 0.207 , 0.233	Depositor DCC
R_{free} test set	9639 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 27.0	EDS
Estimated twinning fraction	0.018 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 192685 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	29391	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ZN

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	0.72	0/3673	0.84	5/4989 (0.1%)
1	B	0.72	1/3681 (0.0%)	0.84	3/5000 (0.1%)
1	C	0.69	0/3673	0.84	5/4989 (0.1%)
1	D	0.69	0/3673	0.86	4/4989 (0.1%)
1	E	0.66	0/3673	0.82	4/4989 (0.1%)
1	F	0.65	0/3673	0.83	3/4989 (0.1%)
1	G	0.68	2/3673 (0.1%)	0.86	9/4989 (0.2%)
1	H	0.64	0/3673	0.82	1/4989 (0.0%)
All	All	0.68	3/29392 (0.0%)	0.84	34/39923 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	32	GLU	CD-OE2	-5.45	1.19	1.25
1	G	307	GLY	N-CA	-5.09	1.38	1.46
1	G	307	GLY	C-O	-5.06	1.15	1.23

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	71	ASP	CB-CG-OD2	-11.29	108.14	118.30
1	D	71	ASP	CB-CG-OD1	9.91	127.22	118.30
1	H	63	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	F	63	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	G	308	GLN	N-CA-CB	-7.57	96.98	110.60
1	C	63	ARG	NE-CZ-NH1	7.53	124.07	120.30
1	C	274	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	D	63	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	G	63	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	G	307	GLY	N-CA-C	7.11	130.87	113.10
1	B	63	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	E	63	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	A	63	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	F	76	HIS	C-N-CD	6.08	141.18	128.40
1	A	270	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	C	274	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	G	307	GLY	C-N-CA	5.97	136.64	121.70
1	A	72	GLN	CA-CB-CG	5.69	125.92	113.40
1	C	317	GLU	CA-CB-CG	-5.60	101.08	113.40
1	C	393	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	G	360	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	G	198	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	G	135	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	393	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	360	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	298	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	109	ARG	CG-CD-NE	-5.17	100.95	111.80
1	E	109	ARG	CG-CD-NE	-5.14	101.00	111.80
1	E	431	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	G	74	GLU	CB-CA-C	5.09	120.59	110.40
1	A	393	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	E	393	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	F	60	GLU	CG-CD-OE2	5.03	128.36	118.30
1	G	306	THR	C-N-CA	-5.02	111.77	122.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	77	PRO	Peptide
1	G	74	GLU	Peptide

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	3597	0	3555	54	0
1	B	3602	0	3559	47	0
1	C	3597	0	3555	51	0
1	D	3597	0	3555	49	0
1	E	3597	0	3555	52	0
1	F	3597	0	3555	64	1
1	G	3597	0	3545	64	1
1	H	3597	0	3555	91	1
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	116	0	0	12	0
3	B	112	0	0	10	0
3	C	67	0	0	11	0
3	D	83	0	0	12	0
3	E	75	0	0	11	2
3	F	50	0	0	12	1
3	G	54	0	0	15	1
3	H	45	0	0	21	0
All	All	29391	0	28434	461	4

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 8.

All (461) 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:H:59:ILE:HG22	3:H:641:HOH:O	1.26	1.30
1:H:88:TRP:CZ2	1:H:453:ASP:HB2	1.67	1.30
1:F:331:THR:HG22	3:F:646:HOH:O	1.34	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:PHE:CE1	1:F:75:VAL:HG11	1.79	1.16
1:G:331:THR:HG21	1:G:336:GLN:HE21	1.12	1.15
1:H:415:PRO:O	3:H:637:HOH:O	1.66	1.12
1:H:331:THR:HG21	1:H:336:GLN:HE21	1.11	1.12
1:E:331:THR:HG21	1:E:336:GLN:HE21	1.12	1.12
1:H:34:GLU:HG3	1:H:471:GLY:O	1.46	1.11
1:H:59:ILE:CG2	3:H:641:HOH:O	1.83	1.11
1:E:34:GLU:HG2	3:E:662:HOH:O	1.50	1.10
1:C:331:THR:HG21	1:C:336:GLN:HE21	1.13	1.09
1:D:331:THR:HG21	1:D:336:GLN:HE21	1.11	1.09
1:D:105:MET:HG2	3:D:662:HOH:O	1.53	1.09
1:G:37:ALA:HB3	1:G:81:GLN:OE1	1.52	1.08
1:F:331:THR:HG21	1:F:336:GLN:HE21	1.15	1.07
1:B:331:THR:HG21	1:B:336:GLN:HE21	1.10	1.07
1:F:71:ASP:OD1	1:F:72:GLN:NE2	1.88	1.07
1:A:331:THR:HG21	1:A:336:GLN:HE21	1.13	1.04
1:D:52:VAL:HG21	3:D:671:HOH:O	1.58	1.03
1:G:302:HIS:HA	3:G:654:HOH:O	1.57	1.02
1:D:52:VAL:CG2	3:D:671:HOH:O	2.08	1.02
1:H:34:GLU:CD	1:H:472:ARG:HA	1.81	0.99
1:H:34:GLU:OE2	1:H:472:ARG:HA	1.60	0.99
1:H:472:ARG:NH2	1:H:474:ILE:CD1	2.27	0.98
1:A:284:THR:HG21	3:A:660:HOH:O	1.64	0.97
1:F:331:THR:CG2	3:F:646:HOH:O	2.00	0.96
1:F:58:PHE:HE1	1:F:75:VAL:HG11	1.25	0.94
1:H:88:TRP:CE2	1:H:453:ASP:HB2	2.05	0.92
1:H:34:GLU:CG	1:H:471:GLY:O	2.19	0.90
1:G:331:THR:HG22	3:G:644:HOH:O	1.71	0.90
1:F:145:TRP:O	3:F:644:HOH:O	1.89	0.88
1:B:135:ARG:HD2	3:B:712:HOH:O	1.72	0.88
1:D:331:THR:HG21	1:D:336:GLN:NE2	1.91	0.86
1:B:331:THR:HG21	1:B:336:GLN:NE2	1.90	0.85
1:E:331:THR:HG21	1:E:336:GLN:NE2	1.92	0.85
1:H:83:ASP:OD1	3:H:622:HOH:O	1.95	0.84
1:H:89:ILE:O	1:H:90:LEU:HD12	1.76	0.84
1:H:89:ILE:C	1:H:90:LEU:HD12	1.98	0.84
1:C:274:ARG:CD	3:C:602:HOH:O	2.26	0.84
1:B:416:MET:CE	3:B:629:HOH:O	2.24	0.83
1:G:331:THR:HG21	1:G:336:GLN:NE2	1.92	0.83
1:A:331:THR:HG21	1:A:336:GLN:NE2	1.93	0.83
1:A:416:MET:CE	3:A:629:HOH:O	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:PHE:CE1	1:F:75:VAL:CG1	2.62	0.82
1:C:331:THR:HG21	1:C:336:GLN:NE2	1.93	0.82
1:G:75:VAL:HG21	1:G:81:GLN:NE2	1.94	0.82
1:F:331:THR:HG21	1:F:336:GLN:NE2	1.94	0.82
1:H:419:ILE:O	1:H:423:THR:OG1	1.98	0.81
1:H:331:THR:HG21	1:H:336:GLN:NE2	1.92	0.81
1:D:105:MET:HE2	3:D:662:HOH:O	1.79	0.81
1:C:274:ARG:HD3	3:C:602:HOH:O	1.80	0.80
1:H:88:TRP:CZ2	1:H:453:ASP:CB	2.61	0.80
1:G:178:GLY:HA3	1:G:182:THR:HG21	1.64	0.79
1:E:179:GLY:O	1:E:182:THR:HB	1.81	0.79
1:A:179:GLY:O	1:A:182:THR:HB	1.82	0.79
1:H:284:THR:HG21	3:H:645:HOH:O	1.83	0.79
1:C:179:GLY:O	1:C:182:THR:HB	1.83	0.79
1:A:50:VAL:HG12	1:E:414:ASP:OD1	1.82	0.79
1:D:179:GLY:O	1:D:182:THR:HB	1.82	0.78
1:D:178:GLY:HA3	1:D:182:THR:HG21	1.65	0.78
1:H:449:VAL:HG12	3:H:602:HOH:O	1.82	0.78
1:F:179:GLY:O	1:F:182:THR:HB	1.83	0.78
1:H:179:GLY:O	1:H:182:THR:HB	1.83	0.78
1:B:179:GLY:O	1:B:182:THR:HB	1.83	0.78
1:H:88:TRP:CE2	1:H:453:ASP:CB	2.66	0.78
1:G:179:GLY:O	1:G:182:THR:HB	1.84	0.78
1:H:468:VAL:HA	1:H:472:ARG:O	1.85	0.77
1:H:178:GLY:HA3	1:H:182:THR:HG21	1.66	0.77
1:H:472:ARG:NH2	1:H:474:ILE:HD12	1.98	0.77
1:A:178:GLY:HA3	1:A:182:THR:HG21	1.66	0.77
1:C:105:MET:SD	3:C:657:HOH:O	2.41	0.77
1:G:399:GLU:HB2	3:G:635:HOH:O	1.83	0.76
1:F:76:HIS:CD2	1:F:78:ASN:HD21	2.03	0.76
1:E:178:GLY:HA3	1:E:182:THR:HG21	1.67	0.76
1:A:262:GLU:HG3	1:B:262:GLU:HG3	1.65	0.76
1:F:284:THR:HG21	3:F:635:HOH:O	1.86	0.75
1:F:71:ASP:OD1	1:F:72:GLN:N	2.20	0.75
1:C:178:GLY:HA3	1:C:182:THR:HG21	1.67	0.75
1:H:415:PRO:O	1:H:419:ILE:HG12	1.82	0.75
1:F:178:GLY:HA3	1:F:182:THR:HG21	1.68	0.75
1:B:178:GLY:HA3	1:B:182:THR:HG21	1.68	0.74
1:B:393:ARG:HD2	3:B:711:HOH:O	1.86	0.74
1:E:416:MET:CE	3:E:625:HOH:O	2.35	0.74
1:G:416:MET:CE	3:G:612:HOH:O	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:MET:CE	3:D:625:HOH:O	2.35	0.74
1:C:262:GLU:HG3	1:D:262:GLU:HG3	1.69	0.73
1:F:419:ILE:O	1:F:423:THR:OG1	2.07	0.72
1:D:105:MET:CE	3:D:662:HOH:O	2.37	0.72
1:H:283:THR:OG1	3:H:615:HOH:O	2.06	0.72
1:H:89:ILE:HG13	3:H:636:HOH:O	1.90	0.71
1:D:225:ARG:HD2	1:G:320:LEU:HD13	1.74	0.70
1:E:284:THR:CG2	3:E:661:HOH:O	2.40	0.70
1:F:244:THR:OG1	1:F:284:THR:HB	1.92	0.70
1:F:146:ASN:HA	3:F:644:HOH:O	1.91	0.69
1:A:333:ILE:O	3:A:706:HOH:O	2.10	0.69
1:H:87:LYS:HD3	1:H:451:ASP:HA	1.74	0.69
1:G:75:VAL:HG21	1:G:81:GLN:HE22	1.54	0.69
1:D:244:THR:OG1	1:D:284:THR:HB	1.92	0.69
1:G:244:THR:OG1	1:G:284:THR:HB	1.93	0.69
1:H:244:THR:OG1	1:H:284:THR:HB	1.93	0.69
1:E:416:MET:HE1	3:E:625:HOH:O	1.93	0.69
1:H:174:LEU:HD23	1:H:242:ALA:HB2	1.74	0.69
1:G:393:ARG:HD2	3:G:646:HOH:O	1.92	0.68
1:D:174:LEU:HD23	1:D:242:ALA:HB2	1.76	0.68
1:F:174:LEU:HD23	1:F:242:ALA:HB2	1.75	0.68
1:F:76:HIS:O	1:F:79:ILE:HG12	1.94	0.68
1:F:416:MET:CE	3:F:616:HOH:O	2.41	0.68
1:H:99:HIS:HE1	1:H:373:ASP:OD1	1.77	0.68
1:E:244:THR:OG1	1:E:284:THR:HB	1.94	0.67
1:B:244:THR:OG1	1:B:284:THR:HB	1.94	0.67
1:C:244:THR:OG1	1:C:284:THR:HB	1.94	0.67
1:F:63:ARG:HH11	1:F:63:ARG:HG3	1.59	0.67
1:G:75:VAL:CG2	1:G:81:GLN:NE2	2.57	0.67
1:D:52:VAL:HG22	3:D:671:HOH:O	1.85	0.67
1:E:284:THR:HG21	3:E:661:HOH:O	1.95	0.67
1:C:451:ASP:OD1	1:C:465:SER:OG	2.13	0.67
1:G:284:THR:HG21	3:G:621:HOH:O	1.95	0.67
1:B:174:LEU:HD23	1:B:242:ALA:HB2	1.75	0.67
1:G:262:GLU:HG3	1:H:262:GLU:HG3	1.77	0.67
1:H:451:ASP:OD1	1:H:465:SER:OG	2.13	0.67
1:A:174:LEU:HD23	1:A:242:ALA:HB2	1.76	0.67
1:A:451:ASP:OD1	1:A:465:SER:OG	2.13	0.66
1:D:174:LEU:HD11	1:D:240:LYS:HE3	1.78	0.66
1:E:451:ASP:OD1	1:E:465:SER:OG	2.13	0.66
1:G:174:LEU:HD23	1:G:242:ALA:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LEU:HD23	1:E:242:ALA:HB2	1.76	0.66
1:F:451:ASP:OD1	1:F:465:SER:OG	2.13	0.66
1:G:174:LEU:HD11	1:G:240:LYS:HE3	1.77	0.66
1:B:451:ASP:OD1	1:B:465:SER:OG	2.14	0.66
1:D:99:HIS:HE1	1:D:373:ASP:OD1	1.79	0.66
1:D:451:ASP:OD1	1:D:465:SER:OG	2.14	0.65
1:E:174:LEU:HD11	1:E:240:LYS:HE3	1.78	0.65
1:H:85:GLN:HB2	3:H:622:HOH:O	1.96	0.65
1:F:174:LEU:HD11	1:F:240:LYS:HE3	1.78	0.65
1:B:174:LEU:HD11	1:B:240:LYS:HE3	1.78	0.65
1:G:451:ASP:OD1	1:G:465:SER:OG	2.13	0.65
1:A:99:HIS:HE1	1:A:373:ASP:OD1	1.78	0.65
1:F:416:MET:HE1	3:F:616:HOH:O	1.95	0.65
1:F:99:HIS:HE1	1:F:373:ASP:OD1	1.80	0.65
1:G:63:ARG:HG3	1:G:63:ARG:HH11	1.62	0.65
1:H:87:LYS:HB3	1:H:450:LEU:O	1.96	0.65
1:B:63:ARG:HG3	1:B:63:ARG:HH11	1.62	0.65
1:E:63:ARG:HG3	1:E:63:ARG:HH11	1.62	0.65
1:A:63:ARG:HH11	1:A:63:ARG:HG3	1.60	0.65
1:G:99:HIS:HE1	1:G:373:ASP:OD1	1.80	0.65
1:H:34:GLU:O	3:H:641:HOH:O	2.15	0.64
1:C:99:HIS:HE1	1:C:373:ASP:OD1	1.80	0.64
1:H:63:ARG:HH11	1:H:63:ARG:HG3	1.61	0.64
1:C:63:ARG:HG3	1:C:63:ARG:HH11	1.61	0.64
1:B:135:ARG:HB3	3:B:712:HOH:O	1.96	0.64
1:D:63:ARG:HG3	1:D:63:ARG:HH11	1.62	0.64
1:C:174:LEU:HD11	1:C:240:LYS:HE3	1.80	0.64
1:C:174:LEU:HD23	1:C:242:ALA:HB2	1.77	0.64
1:H:406:GLN:OE1	3:H:601:HOH:O	2.15	0.64
1:E:99:HIS:HE1	1:E:373:ASP:OD1	1.81	0.64
1:H:425:ASN:HD22	1:H:425:ASN:N	1.95	0.64
1:H:34:GLU:CD	1:H:472:ARG:CA	2.58	0.64
1:C:274:ARG:HD2	3:C:602:HOH:O	1.91	0.64
1:A:174:LEU:HD11	1:A:240:LYS:HE3	1.79	0.63
1:H:174:LEU:HD11	1:H:240:LYS:HE3	1.80	0.63
1:H:472:ARG:NH2	1:H:474:ILE:HD13	2.13	0.63
1:C:320:LEU:HD13	1:H:225:ARG:CD	2.28	0.63
1:H:450:LEU:C	3:H:602:HOH:O	2.36	0.62
1:F:335:GLN:NE2	3:F:645:HOH:O	2.32	0.62
1:H:91:PRO:HG2	1:H:423:THR:HG21	1.79	0.62
1:H:182:THR:HG22	1:H:184:ASP:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:TRP:O	3:H:643:HOH:O	2.16	0.62
1:B:193:ARG:O	1:D:109:ARG:NH1	2.34	0.61
1:G:182:THR:HG22	1:G:184:ASP:H	1.65	0.61
1:F:470:GLU:HB2	3:F:642:HOH:O	1.99	0.61
1:F:78:ASN:HD22	1:F:78:ASN:C	2.03	0.61
1:F:58:PHE:CE2	1:F:60:GLU:HG2	2.36	0.61
1:C:102:ASP:HB3	3:C:657:HOH:O	2.02	0.60
1:A:284:THR:HG23	3:A:678:HOH:O	2.00	0.60
1:G:396:THR:CG2	3:G:635:HOH:O	2.50	0.60
1:F:75:VAL:HG22	1:F:76:HIS:N	2.17	0.60
1:C:416:MET:CE	3:C:618:HOH:O	2.48	0.59
1:F:146:ASN:CA	3:F:644:HOH:O	2.49	0.59
1:H:88:TRP:NE1	1:H:453:ASP:CG	2.56	0.59
1:A:301:ILE:HA	1:A:327:GLU:HG3	1.85	0.59
1:A:109:ARG:NH1	1:C:193:ARG:O	2.34	0.58
1:E:182:THR:HG22	1:E:184:ASP:H	1.68	0.58
1:H:284:THR:CG2	3:H:645:HOH:O	2.46	0.58
1:B:182:THR:HG22	1:B:184:ASP:H	1.67	0.58
1:A:244:THR:OG1	1:A:284:THR:HB	2.03	0.58
1:E:81:GLN:OE1	3:E:663:HOH:O	2.17	0.57
1:H:301:ILE:HA	1:H:327:GLU:HG3	1.85	0.57
1:H:88:TRP:CZ3	1:H:452:GLN:HA	2.39	0.57
1:A:182:THR:HG22	1:A:184:ASP:H	1.69	0.57
1:C:182:THR:HG22	1:C:184:ASP:H	1.70	0.57
1:F:301:ILE:HA	1:F:327:GLU:HG3	1.86	0.57
1:H:88:TRP:NE1	1:H:453:ASP:OD1	2.37	0.57
1:G:37:ALA:HB3	1:G:81:GLN:CD	2.24	0.57
1:C:393:ARG:HG3	3:C:650:HOH:O	2.05	0.57
1:B:301:ILE:HA	1:B:327:GLU:HG3	1.87	0.57
1:E:128:GLU:OE1	1:E:485:VAL:HG13	2.05	0.57
1:B:331:THR:HG23	1:B:336:GLN:HB2	1.86	0.57
1:G:301:ILE:HA	1:G:327:GLU:HG3	1.87	0.57
1:H:43:LEU:CA	3:H:623:HOH:O	2.53	0.56
1:H:331:THR:HG23	1:H:336:GLN:HB2	1.87	0.56
1:B:416:MET:HE1	3:B:629:HOH:O	1.94	0.56
1:F:76:HIS:CD2	1:F:78:ASN:ND2	2.73	0.56
1:E:331:THR:HG23	1:E:336:GLN:HB2	1.88	0.56
1:H:46:GLY:O	1:H:420:LEU:CD2	2.54	0.56
1:C:331:THR:HG23	1:C:336:GLN:HB2	1.87	0.56
1:A:331:THR:HG23	1:A:336:GLN:HB2	1.88	0.56
1:D:182:THR:HG22	1:D:184:ASP:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:ILE:HA	1:E:327:GLU:HG3	1.88	0.56
1:H:472:ARG:HH22	1:H:474:ILE:HD12	1.69	0.55
1:H:144:THR:HG23	1:H:240:LYS:HE2	1.87	0.55
1:G:331:THR:CG2	3:G:644:HOH:O	2.41	0.55
1:D:225:ARG:CD	1:G:320:LEU:HD13	2.36	0.55
1:D:144:THR:HG23	1:D:240:LYS:HE2	1.87	0.55
1:A:144:THR:HG23	1:A:240:LYS:HE2	1.87	0.55
1:H:52:VAL:HG22	1:H:55:THR:OG1	2.07	0.55
1:H:43:LEU:N	3:H:623:HOH:O	2.38	0.55
1:G:128:GLU:OE1	1:G:485:VAL:HG13	2.06	0.55
1:F:331:THR:HG23	1:F:336:GLN:HB2	1.89	0.55
1:D:105:MET:CG	3:D:662:HOH:O	2.28	0.55
1:A:128:GLU:OE1	1:A:485:VAL:HG13	2.07	0.55
1:A:416:MET:HE3	3:A:629:HOH:O	2.01	0.55
1:C:144:THR:HG23	1:C:240:LYS:HE2	1.88	0.55
1:E:144:THR:HG23	1:E:240:LYS:HE2	1.90	0.55
1:B:144:THR:HG23	1:B:240:LYS:HE2	1.89	0.54
1:F:128:GLU:OE1	1:F:485:VAL:HG13	2.07	0.54
1:C:301:ILE:HA	1:C:327:GLU:HG3	1.90	0.54
1:H:128:GLU:OE1	1:H:485:VAL:HG13	2.07	0.54
1:G:80:ARG:C	1:G:81:GLN:HG2	2.27	0.54
1:G:396:THR:HG22	3:G:635:HOH:O	2.06	0.54
1:D:174:LEU:CD1	1:D:240:LYS:HE3	2.37	0.54
1:G:174:LEU:CD1	1:G:240:LYS:HE3	2.37	0.54
1:D:128:GLU:OE1	1:D:485:VAL:HG13	2.07	0.54
1:F:93:LEU:HB3	3:F:643:HOH:O	2.06	0.54
1:E:174:LEU:CD1	1:E:240:LYS:HE3	2.38	0.54
1:H:144:THR:HG23	1:H:240:LYS:CE	2.38	0.54
1:F:52:VAL:HG22	1:F:55:THR:OG1	2.07	0.54
1:C:52:VAL:HG22	1:C:55:THR:OG1	2.08	0.54
1:D:52:VAL:HG22	1:D:55:THR:OG1	2.07	0.54
1:F:182:THR:HG22	1:F:184:ASP:H	1.71	0.54
1:H:174:LEU:CD1	1:H:240:LYS:HE3	2.38	0.54
1:A:52:VAL:HG22	1:A:55:THR:OG1	2.08	0.54
1:B:97:ASN:OD1	1:B:144:THR:HB	2.09	0.53
1:C:144:THR:HG23	1:C:240:LYS:CE	2.39	0.53
1:G:52:VAL:HG22	1:G:55:THR:OG1	2.08	0.53
1:D:331:THR:HG23	1:D:336:GLN:HB2	1.90	0.53
1:F:174:LEU:CD1	1:F:240:LYS:HE3	2.38	0.53
1:C:287:GLU:HB2	3:D:666:HOH:O	2.08	0.53
1:B:62:GLY:HA3	3:B:688:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:THR:HG23	1:G:336:GLN:HB2	1.89	0.53
1:C:174:LEU:CD1	1:C:240:LYS:HE3	2.39	0.53
1:D:301:ILE:HA	1:D:327:GLU:HG3	1.90	0.53
1:B:128:GLU:OE1	1:B:485:VAL:HG13	2.08	0.53
1:E:34:GLU:CG	3:E:662:HOH:O	2.29	0.53
1:B:144:THR:HG23	1:B:240:LYS:CE	2.38	0.53
1:A:174:LEU:CD1	1:A:240:LYS:HE3	2.38	0.53
1:C:128:GLU:OE1	1:C:485:VAL:HG13	2.09	0.53
1:D:144:THR:HG23	1:D:240:LYS:CE	2.39	0.53
1:F:97:ASN:OD1	1:F:144:THR:HB	2.08	0.53
1:A:63:ARG:CG	1:A:63:ARG:HH11	2.22	0.52
1:F:144:THR:HG23	1:F:240:LYS:HE2	1.90	0.52
1:B:63:ARG:CG	1:B:63:ARG:HH11	2.23	0.52
1:H:63:ARG:HH11	1:H:63:ARG:CG	2.22	0.52
1:F:58:PHE:CZ	1:F:75:VAL:HG11	2.37	0.52
1:B:174:LEU:CD1	1:B:240:LYS:HE3	2.39	0.52
1:F:63:ARG:CG	1:F:63:ARG:HH11	2.21	0.52
1:A:144:THR:HG23	1:A:240:LYS:CE	2.39	0.52
1:F:155:ARG:HG3	1:F:156:ASP:N	2.25	0.52
1:E:171:ALA:HB2	1:E:238:PHE:CE1	2.45	0.52
1:E:52:VAL:HG22	1:E:55:THR:OG1	2.09	0.52
1:C:63:ARG:HH11	1:C:63:ARG:CG	2.23	0.52
1:G:75:VAL:CG2	1:G:81:GLN:HE22	2.19	0.52
1:B:52:VAL:HG22	1:B:55:THR:OG1	2.08	0.52
1:B:155:ARG:HG3	1:B:156:ASP:N	2.25	0.51
1:C:401:HIS:CE1	3:C:658:HOH:O	2.63	0.51
1:G:144:THR:HG23	1:G:240:LYS:HE2	1.91	0.51
1:D:155:ARG:HG3	1:D:156:ASP:N	2.25	0.51
1:A:256:PRO:HB3	1:A:284:THR:HG22	1.92	0.51
1:E:144:THR:HG23	1:E:240:LYS:CE	2.41	0.51
1:G:63:ARG:HH11	1:G:63:ARG:CG	2.23	0.51
1:D:63:ARG:HH11	1:D:63:ARG:CG	2.24	0.51
1:A:135:ARG:HD2	3:A:693:HOH:O	2.10	0.51
1:A:135:ARG:HB3	3:A:693:HOH:O	2.09	0.51
1:D:416:MET:HE1	3:D:625:HOH:O	2.06	0.51
1:H:469:LYS:O	1:H:472:ARG:HB2	2.11	0.51
1:C:416:MET:HE1	3:C:618:HOH:O	2.11	0.51
1:H:88:TRP:CD2	1:H:453:ASP:HA	2.46	0.50
1:E:63:ARG:CG	1:E:63:ARG:HH11	2.24	0.50
1:D:393:ARG:HG3	3:D:646:HOH:O	2.10	0.50
1:G:144:THR:HG23	1:G:240:LYS:CE	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:ASN:CB	3:F:644:HOH:O	2.60	0.50
1:H:84:ALA:HB1	3:H:636:HOH:O	2.11	0.50
1:F:144:THR:HG23	1:F:240:LYS:CE	2.41	0.50
1:G:97:ASN:OD1	1:G:144:THR:HB	2.11	0.50
1:C:97:ASN:OD1	1:C:144:THR:HB	2.11	0.50
1:F:119:GLU:HA	1:F:122:TYR:CZ	2.47	0.50
1:H:43:LEU:HB2	3:H:623:HOH:O	2.11	0.50
1:F:308:GLN:HE22	1:F:353:VAL:H	1.58	0.50
1:A:171:ALA:HB2	1:A:238:PHE:CE1	2.47	0.50
1:G:174:LEU:HD11	1:G:240:LYS:CE	2.42	0.50
1:E:42:THR:N	3:E:664:HOH:O	2.45	0.49
1:H:331:THR:CG2	1:H:336:GLN:HB2	2.43	0.49
1:C:102:ASP:CB	3:C:657:HOH:O	2.59	0.49
1:A:99:HIS:CE1	1:A:373:ASP:OD1	2.64	0.49
1:E:214:ARG:HD3	3:E:602:HOH:O	2.12	0.49
1:H:155:ARG:HG3	1:H:156:ASP:N	2.28	0.49
1:B:240:LYS:NZ	3:B:656:HOH:O	2.23	0.49
1:E:97:ASN:OD1	1:E:144:THR:HB	2.11	0.49
1:C:425:ASN:HD22	1:C:425:ASN:N	2.08	0.49
1:G:416:MET:HE1	3:G:612:HOH:O	2.04	0.49
1:H:97:ASN:OD1	1:H:144:THR:HB	2.13	0.49
1:D:416:MET:HE3	3:D:625:HOH:O	2.07	0.49
1:A:97:ASN:OD1	1:A:144:THR:HB	2.12	0.49
1:E:331:THR:CG2	1:E:336:GLN:HB2	2.43	0.48
1:G:155:ARG:HG3	1:G:156:ASP:N	2.28	0.48
1:G:302:HIS:CB	3:G:654:HOH:O	2.61	0.48
1:G:119:GLU:HA	1:G:122:TYR:CZ	2.49	0.48
1:C:331:THR:CG2	1:C:336:GLN:HB2	2.44	0.48
1:E:174:LEU:HD11	1:E:240:LYS:CE	2.43	0.48
1:A:191:GLN:NE2	3:A:697:HOH:O	2.28	0.48
1:D:308:GLN:HE22	1:D:353:VAL:H	1.62	0.48
1:G:331:THR:CG2	1:G:336:GLN:HB2	2.44	0.48
1:B:284:THR:HG21	3:B:653:HOH:O	2.14	0.48
1:H:425:ASN:ND2	1:H:425:ASN:N	2.60	0.47
1:F:254:ARG:NH1	1:F:348:ASP:OD2	2.44	0.47
1:G:79:ILE:HG22	1:G:81:GLN:NE2	2.30	0.47
1:D:99:HIS:CE1	1:D:373:ASP:OD1	2.65	0.47
1:A:44:ILE:HG23	1:A:416:MET:HE1	1.94	0.47
1:E:99:HIS:CE1	1:E:373:ASP:OD1	2.66	0.47
1:E:253:PHE:O	1:E:307:GLY:HA2	2.15	0.47
1:C:352:ARG:N	1:C:352:ARG:HD2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:416:MET:HA	3:H:637:HOH:O	2.14	0.47
1:F:174:LEU:HD11	1:F:240:LYS:CE	2.43	0.47
1:G:308:GLN:HE22	1:G:353:VAL:H	1.63	0.47
1:C:99:HIS:CE1	1:C:373:ASP:OD1	2.64	0.47
1:C:308:GLN:HE22	1:C:353:VAL:H	1.63	0.47
1:A:416:MET:HE1	3:A:629:HOH:O	2.03	0.47
1:D:97:ASN:OD1	1:D:144:THR:HB	2.14	0.46
1:C:254:ARG:NH1	1:C:348:ASP:OD2	2.46	0.46
1:G:284:THR:CG2	3:G:621:HOH:O	2.60	0.46
1:A:184:ASP:CG	3:A:696:HOH:O	2.53	0.46
1:B:331:THR:CG2	1:B:336:GLN:HB2	2.44	0.46
1:E:44:ILE:HG23	1:E:416:MET:HE1	1.98	0.46
1:D:174:LEU:HD11	1:D:240:LYS:CE	2.44	0.46
1:H:119:GLU:HA	1:H:122:TYR:CZ	2.51	0.46
1:C:119:GLU:HA	1:C:122:TYR:CZ	2.51	0.46
1:A:331:THR:CG2	1:A:336:GLN:HB2	2.45	0.46
1:A:174:LEU:HD11	1:A:240:LYS:CE	2.45	0.46
1:C:155:ARG:HG3	1:C:156:ASP:N	2.30	0.46
1:B:308:GLN:HE22	1:B:353:VAL:H	1.63	0.46
1:H:88:TRP:CE2	1:H:453:ASP:CA	2.99	0.45
1:G:328:VAL:HA	3:G:654:HOH:O	2.15	0.45
1:H:419:ILE:H	1:H:419:ILE:HG12	1.58	0.45
1:A:119:GLU:HA	1:A:122:TYR:CZ	2.52	0.45
1:G:99:HIS:CE1	1:G:373:ASP:OD1	2.65	0.45
1:A:229:ARG:NH1	3:A:656:HOH:O	2.45	0.45
1:D:119:GLU:HA	1:D:122:TYR:CZ	2.52	0.45
1:B:174:LEU:HD11	1:B:240:LYS:CE	2.45	0.45
1:E:308:GLN:HE22	1:E:353:VAL:H	1.65	0.45
1:H:46:GLY:O	1:H:420:LEU:HD21	2.17	0.45
1:D:331:THR:CG2	1:D:336:GLN:HB2	2.46	0.45
1:B:416:MET:HE3	3:B:629:HOH:O	2.03	0.45
1:H:174:LEU:HD11	1:H:240:LYS:CE	2.45	0.45
1:F:253:PHE:O	1:F:307:GLY:HA2	2.17	0.45
1:H:62:GLY:N	3:H:641:HOH:O	2.49	0.45
1:B:352:ARG:HD2	1:B:352:ARG:N	2.32	0.45
1:B:119:GLU:HA	1:B:122:TYR:CZ	2.52	0.45
1:H:99:HIS:CE1	1:H:373:ASP:OD1	2.63	0.45
1:F:331:THR:HB	1:F:350:SER:HB2	1.98	0.44
1:F:75:VAL:HG22	1:F:76:HIS:H	1.81	0.44
1:F:75:VAL:CG2	1:F:76:HIS:N	2.80	0.44
1:D:44:ILE:HG23	1:D:416:MET:HE1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:THR:HG23	3:E:661:HOH:O	2.11	0.44
1:E:254:ARG:NH1	1:E:348:ASP:OD2	2.47	0.44
1:C:174:LEU:HD11	1:C:240:LYS:CE	2.46	0.44
1:F:331:THR:CG2	1:F:336:GLN:HB2	2.46	0.44
1:B:44:ILE:HG23	1:B:416:MET:HE1	2.00	0.44
1:A:308:GLN:HE22	1:A:353:VAL:H	1.65	0.44
1:A:50:VAL:CG1	1:E:415:PRO:HD2	2.47	0.44
1:B:393:ARG:HG3	3:B:611:HOH:O	2.17	0.44
1:F:425:ASN:HD22	1:F:425:ASN:N	2.14	0.44
1:D:331:THR:HB	1:D:350:SER:HB2	1.99	0.44
1:D:253:PHE:O	1:D:307:GLY:HA2	2.18	0.44
1:H:468:VAL:HG13	1:H:472:ARG:N	2.32	0.44
1:H:331:THR:HB	1:H:350:SER:HB2	1.99	0.44
1:C:171:ALA:HB2	1:C:238:PHE:CE2	2.53	0.44
1:H:253:PHE:O	1:H:307:GLY:HA2	2.17	0.44
1:E:58:PHE:HB3	1:E:66:LYS:HB2	2.00	0.44
1:E:119:GLU:HA	1:E:122:TYR:CZ	2.52	0.43
1:E:331:THR:HB	1:E:350:SER:HB2	2.00	0.43
1:G:182:THR:CG2	1:G:184:ASP:H	2.30	0.43
1:C:253:PHE:O	1:C:307:GLY:HA2	2.17	0.43
1:B:58:PHE:HB3	1:B:66:LYS:HB2	2.01	0.43
1:H:416:MET:CA	3:H:637:HOH:O	2.66	0.43
1:B:331:THR:HB	1:B:350:SER:HB2	2.00	0.43
1:F:171:ALA:HB2	1:F:238:PHE:CE2	2.54	0.43
1:A:155:ARG:HG3	1:A:156:ASP:N	2.32	0.43
1:A:254:ARG:NH1	1:A:348:ASP:OD2	2.46	0.43
1:F:76:HIS:HD2	1:F:78:ASN:ND2	2.17	0.43
1:C:331:THR:HB	1:C:350:SER:HB2	2.01	0.43
1:A:331:THR:HB	1:A:350:SER:HB2	2.00	0.43
1:G:393:ARG:HG3	3:G:634:HOH:O	2.18	0.43
1:E:155:ARG:HG3	1:E:156:ASP:N	2.33	0.43
1:B:104:ILE:HD13	1:B:107:MET:HE1	2.00	0.43
1:D:254:ARG:NH1	1:D:348:ASP:OD2	2.46	0.43
1:B:182:THR:CG2	1:B:184:ASP:H	2.32	0.42
1:F:352:ARG:N	1:F:352:ARG:HD2	2.34	0.42
1:C:377:THR:OG1	1:C:393:ARG:NH2	2.53	0.42
1:C:240:LYS:NZ	3:C:645:HOH:O	2.34	0.42
1:C:58:PHE:HB3	1:C:66:LYS:HB2	2.01	0.42
1:G:88:TRP:CZ2	1:G:453:ASP:HB2	2.54	0.42
1:B:253:PHE:O	1:B:307:GLY:HA2	2.20	0.42
1:A:253:PHE:O	1:A:307:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:THR:HB	1:G:350:SER:HB2	2.02	0.42
1:D:88:TRP:CZ2	1:D:453:ASP:HB2	2.55	0.42
1:G:302:HIS:CA	3:G:654:HOH:O	2.36	0.42
1:H:182:THR:CG2	1:H:184:ASP:H	2.30	0.42
1:F:99:HIS:CE1	1:F:373:ASP:OD1	2.66	0.42
1:D:171:ALA:HB2	1:D:238:PHE:CE2	2.55	0.42
1:G:182:THR:CG2	1:G:183:GLY:N	2.83	0.41
1:E:182:THR:CG2	1:E:183:GLY:N	2.81	0.41
1:B:254:ARG:NH1	1:B:348:ASP:OD2	2.46	0.41
1:F:73:ILE:HG22	1:F:74:GLU:N	2.35	0.41
1:H:308:GLN:HE22	1:H:352:ARG:HB2	1.84	0.41
1:G:171:ALA:HB2	1:G:238:PHE:CE2	2.55	0.41
1:B:182:THR:CG2	1:B:183:GLY:N	2.83	0.41
1:E:88:TRP:CZ2	1:E:453:ASP:HB2	2.56	0.41
1:H:88:TRP:CE2	1:H:453:ASP:HA	2.55	0.41
1:A:414:ASP:OD1	1:E:50:VAL:HG12	2.20	0.41
1:D:352:ARG:N	1:D:352:ARG:HD2	2.34	0.41
1:G:182:THR:HG22	1:G:184:ASP:N	2.34	0.41
1:A:182:THR:CG2	1:A:183:GLY:N	2.84	0.41
1:E:308:GLN:HE22	1:E:352:ARG:HB2	1.85	0.41
1:D:182:THR:CG2	1:D:184:ASP:H	2.34	0.41
1:E:41:GLY:C	3:E:664:HOH:O	2.59	0.41
1:B:171:ALA:HB2	1:B:238:PHE:CE2	2.55	0.41
1:H:363:LYS:HA	1:H:363:LYS:HD2	1.93	0.41
1:A:84:ALA:O	1:A:87:LYS:HB2	2.21	0.41
1:F:58:PHE:HB3	1:F:66:LYS:HB2	2.02	0.41
1:C:182:THR:CG2	1:C:184:ASP:H	2.34	0.41
1:H:254:ARG:NH1	1:H:348:ASP:OD2	2.46	0.41
1:G:363:LYS:HA	1:G:363:LYS:HD2	1.94	0.41
1:G:104:ILE:HD13	1:G:107:MET:HE1	2.02	0.41
1:G:79:ILE:O	1:G:81:GLN:HG2	2.21	0.41
1:A:182:THR:CG2	1:A:184:ASP:H	2.32	0.41
1:A:352:ARG:HD2	1:A:352:ARG:N	2.36	0.41
1:E:182:THR:HG23	1:E:183:GLY:N	2.36	0.41
1:G:58:PHE:HB3	1:G:66:LYS:HB2	2.02	0.41
1:F:363:LYS:HA	1:F:363:LYS:HD2	1.93	0.41
1:C:425:ASN:ND2	1:C:425:ASN:N	2.69	0.40
1:H:58:PHE:HB3	1:H:66:LYS:HB2	2.03	0.40
1:H:404:TRP:CH2	1:H:408:MET:HG3	2.56	0.40
1:E:363:LYS:HA	1:E:363:LYS:HD2	1.91	0.40
1:G:44:ILE:HG23	1:G:416:MET:HE1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:308:GLN:HE22	1:G:352:ARG:HB2	1.86	0.40
1:A:155:ARG:HD2	3:A:695:HOH:O	2.20	0.40
1:F:88:TRP:CZ2	1:F:453:ASP:HB2	2.56	0.40
1:H:425:ASN:HB2	1:H:426:PRO:HD3	2.03	0.40
1:E:104:ILE:HD13	1:E:107:MET:HE1	2.03	0.40
1:B:482:SER:O	1:B:483:PRO:C	2.58	0.40
1:A:58:PHE:HB3	1:A:66:LYS:HB2	2.03	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:611:HOH:O	3:G:601:HOH:O[3_455]	1.49	0.71
3:E:602:HOH:O	3:F:603:HOH:O[4_558]	1.53	0.67
1:H:452:GLN:NE2	1:H:462:ARG:O[2_657]	1.87	0.33
1:F:74:GLU:O	1:G:74:GLU:OE2[1_565]	2.09	0.11

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	465/496 (94%)	454 (98%)	11 (2%)	0	100	100
1	B	466/496 (94%)	453 (97%)	13 (3%)	0	100	100
1	C	465/496 (94%)	452 (97%)	13 (3%)	0	100	100
1	D	465/496 (94%)	453 (97%)	12 (3%)	0	100	100
1	E	465/496 (94%)	451 (97%)	14 (3%)	0	100	100
1	F	465/496 (94%)	451 (97%)	14 (3%)	0	100	100
1	G	465/496 (94%)	449 (97%)	16 (3%)	0	100	100
1	H	465/496 (94%)	450 (97%)	15 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3721/3968 (94%)	3613 (97%)	108 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	382/407 (94%)	363 (95%)	19 (5%)	30 39
1	B	383/407 (94%)	366 (96%)	17 (4%)	35 45
1	C	382/407 (94%)	364 (95%)	18 (5%)	32 42
1	D	382/407 (94%)	365 (96%)	17 (4%)	34 44
1	E	382/407 (94%)	364 (95%)	18 (5%)	32 42
1	F	382/407 (94%)	360 (94%)	22 (6%)	25 31
1	G	382/407 (94%)	363 (95%)	19 (5%)	30 39
1	H	382/407 (94%)	361 (94%)	21 (6%)	27 34
All	All	3057/3256 (94%)	2906 (95%)	151 (5%)	31 40

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	63	ARG
1	A	69	SER
1	A	74	GLU
1	A	85	GLN
1	A	144	THR
1	A	155	ARG
1	A	174	LEU
1	A	182	THR
1	A	254	ARG
1	A	273	ARG
1	A	274	ARG

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Mol	Chain	Res	Type
1	A	284	THR
1	A	327	GLU
1	A	331	THR
1	A	363	LYS
1	A	472	ARG
1	A	485	VAL
1	A	491	THR
1	B	30	PHE
1	B	52	VAL
1	B	63	ARG
1	B	69	SER
1	B	74	GLU
1	B	144	THR
1	B	155	ARG
1	B	174	LEU
1	B	182	THR
1	B	254	ARG
1	B	273	ARG
1	B	284	THR
1	B	327	GLU
1	B	363	LYS
1	B	472	ARG
1	B	485	VAL
1	B	491	THR
1	C	30	PHE
1	C	52	VAL
1	C	63	ARG
1	C	69	SER
1	C	74	GLU
1	C	144	THR
1	C	155	ARG
1	C	174	LEU
1	C	182	THR
1	C	254	ARG
1	C	273	ARG
1	C	284	THR
1	C	327	GLU
1	C	331	THR
1	C	363	LYS
1	C	472	ARG
1	C	485	VAL
1	C	491	THR

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Mol	Chain	Res	Type
1	D	30	PHE
1	D	52	VAL
1	D	63	ARG
1	D	69	SER
1	D	74	GLU
1	D	144	THR
1	D	155	ARG
1	D	174	LEU
1	D	182	THR
1	D	254	ARG
1	D	273	ARG
1	D	284	THR
1	D	327	GLU
1	D	363	LYS
1	D	472	ARG
1	D	485	VAL
1	D	491	THR
1	E	30	PHE
1	E	52	VAL
1	E	63	ARG
1	E	69	SER
1	E	74	GLU
1	E	144	THR
1	E	155	ARG
1	E	174	LEU
1	E	182	THR
1	E	254	ARG
1	E	273	ARG
1	E	284	THR
1	E	327	GLU
1	E	331	THR
1	E	363	LYS
1	E	472	ARG
1	E	485	VAL
1	E	491	THR
1	F	30	PHE
1	F	50	VAL
1	F	52	VAL
1	F	63	ARG
1	F	69	SER
1	F	74	GLU
1	F	76	HIS

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Mol	Chain	Res	Type
1	F	78	ASN
1	F	144	THR
1	F	155	ARG
1	F	174	LEU
1	F	182	THR
1	F	184	ASP
1	F	254	ARG
1	F	273	ARG
1	F	284	THR
1	F	327	GLU
1	F	363	LYS
1	F	423	THR
1	F	472	ARG
1	F	485	VAL
1	F	491	THR
1	G	30	PHE
1	G	52	VAL
1	G	63	ARG
1	G	69	SER
1	G	74	GLU
1	G	75	VAL
1	G	144	THR
1	G	155	ARG
1	G	174	LEU
1	G	182	THR
1	G	254	ARG
1	G	273	ARG
1	G	284	THR
1	G	308	GLN
1	G	327	GLU
1	G	363	LYS
1	G	472	ARG
1	G	485	VAL
1	G	491	THR
1	H	30	PHE
1	H	52	VAL
1	H	63	ARG
1	H	69	SER
1	H	74	GLU
1	H	87	LYS
1	H	144	THR
1	H	155	ARG

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Mol	Chain	Res	Type
1	H	174	LEU
1	H	182	THR
1	H	254	ARG
1	H	273	ARG
1	H	284	THR
1	H	327	GLU
1	H	363	LYS
1	H	419	ILE
1	H	423	THR
1	H	425	ASN
1	H	470	GLU
1	H	485	VAL
1	H	491	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	78	ASN
1	A	99	HIS
1	A	191	GLN
1	A	308	GLN
1	A	323	GLN
1	A	329	GLN
1	A	336	GLN
1	A	425	ASN
1	B	47	ASN
1	B	78	ASN
1	B	191	GLN
1	B	308	GLN
1	B	323	GLN
1	B	329	GLN
1	B	335	GLN
1	B	336	GLN
1	B	425	ASN
1	C	47	ASN
1	C	78	ASN
1	C	99	HIS
1	C	191	GLN
1	C	308	GLN
1	C	323	GLN
1	C	329	GLN

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Mol	Chain	Res	Type
1	C	335	GLN
1	C	336	GLN
1	C	425	ASN
1	D	47	ASN
1	D	78	ASN
1	D	99	HIS
1	D	191	GLN
1	D	308	GLN
1	D	323	GLN
1	D	329	GLN
1	D	335	GLN
1	D	336	GLN
1	D	425	ASN
1	E	47	ASN
1	E	78	ASN
1	E	99	HIS
1	E	191	GLN
1	E	308	GLN
1	E	323	GLN
1	E	329	GLN
1	E	336	GLN
1	E	425	ASN
1	F	47	ASN
1	F	76	HIS
1	F	78	ASN
1	F	99	HIS
1	F	191	GLN
1	F	308	GLN
1	F	323	GLN
1	F	329	GLN
1	F	335	GLN
1	F	336	GLN
1	F	425	ASN
1	G	47	ASN
1	G	78	ASN
1	G	99	HIS
1	G	191	GLN
1	G	308	GLN
1	G	323	GLN
1	G	329	GLN
1	G	335	GLN
1	G	336	GLN

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Mol	Chain	Res	Type
1	G	425	ASN
1	H	47	ASN
1	H	78	ASN
1	H	99	HIS
1	H	191	GLN
1	H	308	GLN
1	H	323	GLN
1	H	329	GLN
1	H	335	GLN
1	H	336	GLN
1	H	406	GLN
1	H	425	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	467/496 (94%)	-0.15	5 (1%) 82 86	27, 37, 62, 122	0
1	B	467/496 (94%)	0.01	20 (4%) 39 47	27, 39, 60, 105	0
1	C	467/496 (94%)	0.05	17 (3%) 46 54	28, 42, 70, 104	0
1	D	467/496 (94%)	-0.10	8 (1%) 73 79	27, 43, 65, 98	0
1	E	467/496 (94%)	0.06	7 (1%) 76 81	32, 42, 67, 105	0
1	F	467/496 (94%)	0.11	14 (2%) 54 62	32, 53, 80, 126	0
1	G	467/496 (94%)	0.10	10 (2%) 67 73	34, 49, 81, 133	0
1	H	467/496 (94%)	0.80	66 (14%) 4 5	32, 60, 108, 153	0
All	All	3736/3968 (94%)	0.11	147 (3%) 43 51	27, 45, 82, 153	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	68	GLY	9.6
1	H	30	PHE	7.7
1	H	67	VAL	6.1
1	A	70	THR	6.0
1	D	30	PHE	6.0
1	H	77	PRO	6.0
1	C	496	ASP	5.9
1	F	496	ASP	5.7
1	H	79	ILE	5.6
1	H	75	VAL	5.5
1	B	496	ASP	5.5
1	H	43	LEU	5.4
1	E	30	PHE	5.1
1	H	52	VAL	5.0
1	G	496	ASP	4.9
1	D	496	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
1	H	49	GLY	4.8
1	H	439	ILE	4.8
1	H	58	PHE	4.7
1	H	70	THR	4.6
1	H	42	THR	4.6
1	H	38	ILE	4.5
1	G	81	GLN	4.5
1	H	76	HIS	4.5
1	H	496	ASP	4.4
1	B	77	PRO	4.4
1	H	36	ILE	4.4
1	H	73	ILE	4.3
1	H	441	VAL	4.3
1	B	73	ILE	4.2
1	G	30	PHE	4.2
1	H	34	GLU	4.2
1	C	79	ILE	4.2
1	C	30	PHE	4.1
1	H	50	VAL	4.1
1	H	65	THR	4.1
1	A	71	ASP	4.0
1	H	57	VAL	4.0
1	C	32	GLU	3.8
1	E	496	ASP	3.8
1	C	78	ASN	3.7
1	H	64	ILE	3.6
1	H	80	ARG	3.6
1	A	496	ASP	3.6
1	H	66	LYS	3.6
1	B	75	VAL	3.6
1	B	71	ASP	3.5
1	H	71	ASP	3.5
1	H	89	ILE	3.5
1	H	159	ALA	3.5
1	H	44	ILE	3.4
1	H	450	LEU	3.4
1	C	80	ARG	3.4
1	B	76	HIS	3.4
1	D	77	PRO	3.4
1	H	35	THR	3.3
1	B	72	GLN	3.3
1	H	54	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	78	ASN	3.2
1	B	74	GLU	3.2
1	H	74	GLU	3.2
1	F	78	ASN	3.1
1	B	79	ILE	3.1
1	G	75	VAL	3.1
1	G	80	ARG	3.1
1	H	83	ASP	3.1
1	H	429	ALA	3.0
1	H	81	GLN	3.0
1	H	445	GLY	3.0
1	B	70	THR	3.0
1	F	30	PHE	2.9
1	G	74	GLU	2.9
1	H	69	SER	2.9
1	B	85	GLN	2.8
1	D	76	HIS	2.8
1	F	495	LEU	2.8
1	C	39	VAL	2.8
1	H	412	GLY	2.8
1	H	39	VAL	2.8
1	D	31	PHE	2.7
1	B	39	VAL	2.7
1	B	54	GLU	2.7
1	B	30	PHE	2.7
1	C	76	HIS	2.7
1	H	60	GLU	2.7
1	G	78	ASN	2.7
1	H	90	LEU	2.7
1	H	495	LEU	2.7
1	A	80	ARG	2.6
1	F	73	ILE	2.6
1	D	32	GLU	2.6
1	C	31	PHE	2.6
1	E	74	GLU	2.6
1	F	82	ILE	2.6
1	H	458	ILE	2.6
1	D	74	GLU	2.6
1	H	51	PRO	2.5
1	F	71	ASP	2.5
1	H	449	VAL	2.5
1	F	76	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	78	ASN	2.5
1	E	77	PRO	2.5
1	H	46	GLY	2.4
1	C	73	ILE	2.4
1	H	59	ILE	2.4
1	H	82	ILE	2.4
1	F	74	GLU	2.4
1	C	33	GLY	2.4
1	H	84	ALA	2.4
1	H	31	PHE	2.4
1	H	452	GLN	2.4
1	B	50	VAL	2.4
1	C	58	PHE	2.4
1	H	471	GLY	2.4
1	C	75	VAL	2.4
1	B	69	SER	2.4
1	C	38	ILE	2.3
1	C	82	ILE	2.3
1	H	85	GLN	2.3
1	G	495	LEU	2.3
1	F	83	ASP	2.3
1	B	78	ASN	2.3
1	H	464	LEU	2.3
1	B	58	PHE	2.2
1	C	74	GLU	2.2
1	F	84	ALA	2.2
1	H	62	GLY	2.2
1	C	83	ASP	2.2
1	F	49	GLY	2.2
1	E	247	LEU	2.2
1	G	79	ILE	2.2
1	G	32	GLU	2.2
1	A	30	PHE	2.2
1	F	85	GLN	2.2
1	E	387	GLN	2.1
1	H	359	VAL	2.1
1	H	161	GLY	2.1
1	H	453	ASP	2.1
1	H	457	ASP	2.1
1	B	55	THR	2.1
1	F	89	ILE	2.1
1	H	321	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	86	GLY	2.1
1	H	88	TRP	2.0
1	H	37	ALA	2.0
1	D	80	ARG	2.0
1	H	420	LEU	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^{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
2	ZN	D	501	1/1	0.76	0.12	-0.07	56,56,56,56	1
2	ZN	B	501	1/1	0.89	0.08	-2.09	55,55,55,55	1
2	ZN	C	501	1/1	0.85	0.11	-2.79	65,65,65,65	1
2	ZN	H	501	1/1	0.87	0.07	-4.94	67,67,67,67	1
2	ZN	G	501	1/1	0.92	0.10	-	55,55,55,55	1
2	ZN	E	501	1/1	0.90	0.08	-	60,60,60,60	1
2	ZN	F	501	1/1	0.91	0.08	-	63,63,63,63	1
2	ZN	A	501	1/1	0.94	0.10	-	48,48,48,48	1

6.5 Other polymers (i)

There are no such residues in this entry.