Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:39 AM GMT

PDB ID	:	2DUT
Title	:	Crystal structure of a M-loop deletion variant of MENT in the native conformation
Authors	:	Whisstock, J.C.; Buckle, A.M.; McGowan, S.; Irving, J.A.
Deposited on	:	2006-07-26
Resolution	:	3.00 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 ⓘ symbol.

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

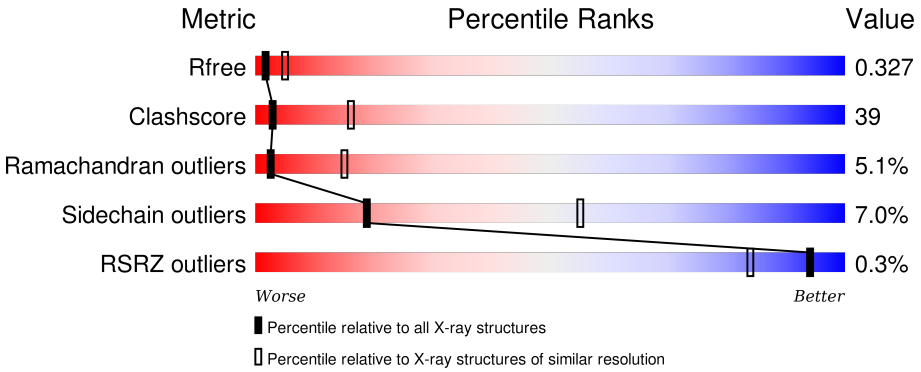
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	423	39% 41% 6% 13%
1	B	423	39% 42% 6% 13%
1	C	423	39% 42% 6% 13%
1	D	423	38% 42% 6% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11020 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 Heterochromatin-associated protein MENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2721	1753	441	512	15			
1	B	366	Total	C	N	O	S	0	0	0
			2721	1753	441	512	15			
1	C	366	Total	C	N	O	S	0	0	0
			2721	1753	441	512	15			
1	D	366	Total	C	N	O	S	0	0	0
			2721	1753	441	512	15			

There are 276 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	CLONING ARTIFACT	UNP O73790
A	-39	GLY	-	CLONING ARTIFACT	UNP O73790
A	-38	GLY	-	CLONING ARTIFACT	UNP O73790
A	-37	SER	-	CLONING ARTIFACT	UNP O73790
A	-36	HIS	-	CLONING ARTIFACT	UNP O73790
A	-35	HIS	-	CLONING ARTIFACT	UNP O73790
A	-34	HIS	-	CLONING ARTIFACT	UNP O73790
A	-33	HIS	-	CLONING ARTIFACT	UNP O73790
A	-32	HIS	-	CLONING ARTIFACT	UNP O73790
A	-31	HIS	-	CLONING ARTIFACT	UNP O73790
A	-30	GLY	-	CLONING ARTIFACT	UNP O73790
A	-29	MET	-	CLONING ARTIFACT	UNP O73790
A	-28	ALA	-	CLONING ARTIFACT	UNP O73790
A	-27	SER	-	CLONING ARTIFACT	UNP O73790
A	-26	MET	-	CLONING ARTIFACT	UNP O73790
A	-25	THR	-	CLONING ARTIFACT	UNP O73790
A	-24	GLY	-	CLONING ARTIFACT	UNP O73790
A	-23	GLY	-	CLONING ARTIFACT	UNP O73790
A	-22	GLN	-	CLONING ARTIFACT	UNP O73790
A	-21	GLN	-	CLONING ARTIFACT	UNP O73790
A	-20	MET	-	CLONING ARTIFACT	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	CLONING ARTIFACT	UNP O73790
A	-18	ARG	-	CLONING ARTIFACT	UNP O73790
A	-17	ASP	-	CLONING ARTIFACT	UNP O73790
A	-16	LEU	-	CLONING ARTIFACT	UNP O73790
A	-15	TYR	-	CLONING ARTIFACT	UNP O73790
A	-14	ASP	-	CLONING ARTIFACT	UNP O73790
A	-13	ASP	-	CLONING ARTIFACT	UNP O73790
A	-12	ASP	-	CLONING ARTIFACT	UNP O73790
A	-11	ASP	-	CLONING ARTIFACT	UNP O73790
A	-10	LYS	-	CLONING ARTIFACT	UNP O73790
A	-9	ASP	-	CLONING ARTIFACT	UNP O73790
A	-8	ARG	-	CLONING ARTIFACT	UNP O73790
A	-7	TRP	-	CLONING ARTIFACT	UNP O73790
A	-6	GLY	-	CLONING ARTIFACT	UNP O73790
A	-5	SER	-	CLONING ARTIFACT	UNP O73790
A	-4	GLU	-	CLONING ARTIFACT	UNP O73790
A	-3	LEU	-	CLONING ARTIFACT	UNP O73790
A	-2	GLU	-	CLONING ARTIFACT	UNP O73790
A	-1	ILE	-	CLONING ARTIFACT	UNP O73790
A	0	SER	-	CLONING ARTIFACT	UNP O73790
A	?	-	THR	DELETION	UNP O73790
A	?	-	GLU	DELETION	UNP O73790
A	?	-	ALA	DELETION	UNP O73790
A	?	-	VAL	DELETION	UNP O73790
A	?	-	ARG	DELETION	UNP O73790
A	?	-	ALA	DELETION	UNP O73790
A	?	-	GLU	DELETION	UNP O73790
A	?	-	SER	DELETION	UNP O73790
A	?	-	SER	DELETION	UNP O73790
A	?	-	SER	DELETION	UNP O73790
A	?	-	VAL	DELETION	UNP O73790
A	?	-	ALA	DELETION	UNP O73790
A	?	-	ARG	DELETION	UNP O73790
A	?	-	PRO	DELETION	UNP O73790
A	?	-	SER	DELETION	UNP O73790
A	?	-	ARG	DELETION	UNP O73790
A	?	-	GLY	DELETION	UNP O73790
A	?	-	ARG	DELETION	UNP O73790
A	?	-	PRO	DELETION	UNP O73790
A	?	-	LYS	DELETION	UNP O73790
A	?	-	ARG	DELETION	UNP O73790
A	?	-	ARG	DELETION	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	DELETION	UNP O73790
A	?	-	MET	DELETION	UNP O73790
A	?	-	ASP	DELETION	UNP O73790
A	?	-	PRO	DELETION	UNP O73790
A	?	-	GLU	DELETION	UNP O73790
A	?	-	HIS	DELETION	UNP O73790
B	-40	MET	-	CLONING ARTIFACT	UNP O73790
B	-39	GLY	-	CLONING ARTIFACT	UNP O73790
B	-38	GLY	-	CLONING ARTIFACT	UNP O73790
B	-37	SER	-	CLONING ARTIFACT	UNP O73790
B	-36	HIS	-	CLONING ARTIFACT	UNP O73790
B	-35	HIS	-	CLONING ARTIFACT	UNP O73790
B	-34	HIS	-	CLONING ARTIFACT	UNP O73790
B	-33	HIS	-	CLONING ARTIFACT	UNP O73790
B	-32	HIS	-	CLONING ARTIFACT	UNP O73790
B	-31	HIS	-	CLONING ARTIFACT	UNP O73790
B	-30	GLY	-	CLONING ARTIFACT	UNP O73790
B	-29	MET	-	CLONING ARTIFACT	UNP O73790
B	-28	ALA	-	CLONING ARTIFACT	UNP O73790
B	-27	SER	-	CLONING ARTIFACT	UNP O73790
B	-26	MET	-	CLONING ARTIFACT	UNP O73790
B	-25	THR	-	CLONING ARTIFACT	UNP O73790
B	-24	GLY	-	CLONING ARTIFACT	UNP O73790
B	-23	GLY	-	CLONING ARTIFACT	UNP O73790
B	-22	GLN	-	CLONING ARTIFACT	UNP O73790
B	-21	GLN	-	CLONING ARTIFACT	UNP O73790
B	-20	MET	-	CLONING ARTIFACT	UNP O73790
B	-19	GLY	-	CLONING ARTIFACT	UNP O73790
B	-18	ARG	-	CLONING ARTIFACT	UNP O73790
B	-17	ASP	-	CLONING ARTIFACT	UNP O73790
B	-16	LEU	-	CLONING ARTIFACT	UNP O73790
B	-15	TYR	-	CLONING ARTIFACT	UNP O73790
B	-14	ASP	-	CLONING ARTIFACT	UNP O73790
B	-13	ASP	-	CLONING ARTIFACT	UNP O73790
B	-12	ASP	-	CLONING ARTIFACT	UNP O73790
B	-11	ASP	-	CLONING ARTIFACT	UNP O73790
B	-10	LYS	-	CLONING ARTIFACT	UNP O73790
B	-9	ASP	-	CLONING ARTIFACT	UNP O73790
B	-8	ARG	-	CLONING ARTIFACT	UNP O73790
B	-7	TRP	-	CLONING ARTIFACT	UNP O73790
B	-6	GLY	-	CLONING ARTIFACT	UNP O73790
B	-5	SER	-	CLONING ARTIFACT	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLU	-	CLONING ARTIFACT	UNP O73790
B	-3	LEU	-	CLONING ARTIFACT	UNP O73790
B	-2	GLU	-	CLONING ARTIFACT	UNP O73790
B	-1	ILE	-	CLONING ARTIFACT	UNP O73790
B	0	SER	-	CLONING ARTIFACT	UNP O73790
B	?	-	THR	DELETION	UNP O73790
B	?	-	GLU	DELETION	UNP O73790
B	?	-	ALA	DELETION	UNP O73790
B	?	-	VAL	DELETION	UNP O73790
B	?	-	ARG	DELETION	UNP O73790
B	?	-	ALA	DELETION	UNP O73790
B	?	-	GLU	DELETION	UNP O73790
B	?	-	SER	DELETION	UNP O73790
B	?	-	SER	DELETION	UNP O73790
B	?	-	SER	DELETION	UNP O73790
B	?	-	VAL	DELETION	UNP O73790
B	?	-	ALA	DELETION	UNP O73790
B	?	-	ARG	DELETION	UNP O73790
B	?	-	PRO	DELETION	UNP O73790
B	?	-	SER	DELETION	UNP O73790
B	?	-	ARG	DELETION	UNP O73790
B	?	-	GLY	DELETION	UNP O73790
B	?	-	ARG	DELETION	UNP O73790
B	?	-	PRO	DELETION	UNP O73790
B	?	-	LYS	DELETION	UNP O73790
B	?	-	ARG	DELETION	UNP O73790
B	?	-	ARG	DELETION	UNP O73790
B	?	-	ARG	DELETION	UNP O73790
B	?	-	MET	DELETION	UNP O73790
B	?	-	ASP	DELETION	UNP O73790
B	?	-	PRO	DELETION	UNP O73790
B	?	-	GLU	DELETION	UNP O73790
B	?	-	HIS	DELETION	UNP O73790
C	-40	MET	-	CLONING ARTIFACT	UNP O73790
C	-39	GLY	-	CLONING ARTIFACT	UNP O73790
C	-38	GLY	-	CLONING ARTIFACT	UNP O73790
C	-37	SER	-	CLONING ARTIFACT	UNP O73790
C	-36	HIS	-	CLONING ARTIFACT	UNP O73790
C	-35	HIS	-	CLONING ARTIFACT	UNP O73790
C	-34	HIS	-	CLONING ARTIFACT	UNP O73790
C	-33	HIS	-	CLONING ARTIFACT	UNP O73790
C	-32	HIS	-	CLONING ARTIFACT	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-31	HIS	-	CLONING ARTIFACT	UNP O73790
C	-30	GLY	-	CLONING ARTIFACT	UNP O73790
C	-29	MET	-	CLONING ARTIFACT	UNP O73790
C	-28	ALA	-	CLONING ARTIFACT	UNP O73790
C	-27	SER	-	CLONING ARTIFACT	UNP O73790
C	-26	MET	-	CLONING ARTIFACT	UNP O73790
C	-25	THR	-	CLONING ARTIFACT	UNP O73790
C	-24	GLY	-	CLONING ARTIFACT	UNP O73790
C	-23	GLY	-	CLONING ARTIFACT	UNP O73790
C	-22	GLN	-	CLONING ARTIFACT	UNP O73790
C	-21	GLN	-	CLONING ARTIFACT	UNP O73790
C	-20	MET	-	CLONING ARTIFACT	UNP O73790
C	-19	GLY	-	CLONING ARTIFACT	UNP O73790
C	-18	ARG	-	CLONING ARTIFACT	UNP O73790
C	-17	ASP	-	CLONING ARTIFACT	UNP O73790
C	-16	LEU	-	CLONING ARTIFACT	UNP O73790
C	-15	TYR	-	CLONING ARTIFACT	UNP O73790
C	-14	ASP	-	CLONING ARTIFACT	UNP O73790
C	-13	ASP	-	CLONING ARTIFACT	UNP O73790
C	-12	ASP	-	CLONING ARTIFACT	UNP O73790
C	-11	ASP	-	CLONING ARTIFACT	UNP O73790
C	-10	LYS	-	CLONING ARTIFACT	UNP O73790
C	-9	ASP	-	CLONING ARTIFACT	UNP O73790
C	-8	ARG	-	CLONING ARTIFACT	UNP O73790
C	-7	TRP	-	CLONING ARTIFACT	UNP O73790
C	-6	GLY	-	CLONING ARTIFACT	UNP O73790
C	-5	SER	-	CLONING ARTIFACT	UNP O73790
C	-4	GLU	-	CLONING ARTIFACT	UNP O73790
C	-3	LEU	-	CLONING ARTIFACT	UNP O73790
C	-2	GLU	-	CLONING ARTIFACT	UNP O73790
C	-1	ILE	-	CLONING ARTIFACT	UNP O73790
C	0	SER	-	CLONING ARTIFACT	UNP O73790
C	?	-	THR	DELETION	UNP O73790
C	?	-	GLU	DELETION	UNP O73790
C	?	-	ALA	DELETION	UNP O73790
C	?	-	VAL	DELETION	UNP O73790
C	?	-	ARG	DELETION	UNP O73790
C	?	-	ALA	DELETION	UNP O73790
C	?	-	GLU	DELETION	UNP O73790
C	?	-	SER	DELETION	UNP O73790
C	?	-	SER	DELETION	UNP O73790
C	?	-	SER	DELETION	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	VAL	DELETION	UNP O73790
C	?	-	ALA	DELETION	UNP O73790
C	?	-	ARG	DELETION	UNP O73790
C	?	-	PRO	DELETION	UNP O73790
C	?	-	SER	DELETION	UNP O73790
C	?	-	ARG	DELETION	UNP O73790
C	?	-	GLY	DELETION	UNP O73790
C	?	-	ARG	DELETION	UNP O73790
C	?	-	PRO	DELETION	UNP O73790
C	?	-	LYS	DELETION	UNP O73790
C	?	-	ARG	DELETION	UNP O73790
C	?	-	ARG	DELETION	UNP O73790
C	?	-	ARG	DELETION	UNP O73790
C	?	-	MET	DELETION	UNP O73790
C	?	-	ASP	DELETION	UNP O73790
C	?	-	PRO	DELETION	UNP O73790
C	?	-	GLU	DELETION	UNP O73790
C	?	-	HIS	DELETION	UNP O73790
D	-40	MET	-	CLONING ARTIFACT	UNP O73790
D	-39	GLY	-	CLONING ARTIFACT	UNP O73790
D	-38	GLY	-	CLONING ARTIFACT	UNP O73790
D	-37	SER	-	CLONING ARTIFACT	UNP O73790
D	-36	HIS	-	CLONING ARTIFACT	UNP O73790
D	-35	HIS	-	CLONING ARTIFACT	UNP O73790
D	-34	HIS	-	CLONING ARTIFACT	UNP O73790
D	-33	HIS	-	CLONING ARTIFACT	UNP O73790
D	-32	HIS	-	CLONING ARTIFACT	UNP O73790
D	-31	HIS	-	CLONING ARTIFACT	UNP O73790
D	-30	GLY	-	CLONING ARTIFACT	UNP O73790
D	-29	MET	-	CLONING ARTIFACT	UNP O73790
D	-28	ALA	-	CLONING ARTIFACT	UNP O73790
D	-27	SER	-	CLONING ARTIFACT	UNP O73790
D	-26	MET	-	CLONING ARTIFACT	UNP O73790
D	-25	THR	-	CLONING ARTIFACT	UNP O73790
D	-24	GLY	-	CLONING ARTIFACT	UNP O73790
D	-23	GLY	-	CLONING ARTIFACT	UNP O73790
D	-22	GLN	-	CLONING ARTIFACT	UNP O73790
D	-21	GLN	-	CLONING ARTIFACT	UNP O73790
D	-20	MET	-	CLONING ARTIFACT	UNP O73790
D	-19	GLY	-	CLONING ARTIFACT	UNP O73790
D	-18	ARG	-	CLONING ARTIFACT	UNP O73790
D	-17	ASP	-	CLONING ARTIFACT	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	LEU	-	CLONING ARTIFACT	UNP O73790
D	-15	TYR	-	CLONING ARTIFACT	UNP O73790
D	-14	ASP	-	CLONING ARTIFACT	UNP O73790
D	-13	ASP	-	CLONING ARTIFACT	UNP O73790
D	-12	ASP	-	CLONING ARTIFACT	UNP O73790
D	-11	ASP	-	CLONING ARTIFACT	UNP O73790
D	-10	LYS	-	CLONING ARTIFACT	UNP O73790
D	-9	ASP	-	CLONING ARTIFACT	UNP O73790
D	-8	ARG	-	CLONING ARTIFACT	UNP O73790
D	-7	TRP	-	CLONING ARTIFACT	UNP O73790
D	-6	GLY	-	CLONING ARTIFACT	UNP O73790
D	-5	SER	-	CLONING ARTIFACT	UNP O73790
D	-4	GLU	-	CLONING ARTIFACT	UNP O73790
D	-3	LEU	-	CLONING ARTIFACT	UNP O73790
D	-2	GLU	-	CLONING ARTIFACT	UNP O73790
D	-1	ILE	-	CLONING ARTIFACT	UNP O73790
D	0	SER	-	CLONING ARTIFACT	UNP O73790
D	?	-	THR	DELETION	UNP O73790
D	?	-	GLU	DELETION	UNP O73790
D	?	-	ALA	DELETION	UNP O73790
D	?	-	VAL	DELETION	UNP O73790
D	?	-	ARG	DELETION	UNP O73790
D	?	-	ALA	DELETION	UNP O73790
D	?	-	GLU	DELETION	UNP O73790
D	?	-	SER	DELETION	UNP O73790
D	?	-	SER	DELETION	UNP O73790
D	?	-	SER	DELETION	UNP O73790
D	?	-	VAL	DELETION	UNP O73790
D	?	-	ALA	DELETION	UNP O73790
D	?	-	ARG	DELETION	UNP O73790
D	?	-	PRO	DELETION	UNP O73790
D	?	-	SER	DELETION	UNP O73790
D	?	-	ARG	DELETION	UNP O73790
D	?	-	GLY	DELETION	UNP O73790
D	?	-	ARG	DELETION	UNP O73790
D	?	-	PRO	DELETION	UNP O73790
D	?	-	LYS	DELETION	UNP O73790
D	?	-	ARG	DELETION	UNP O73790
D	?	-	ARG	DELETION	UNP O73790
D	?	-	ARG	DELETION	UNP O73790
D	?	-	MET	DELETION	UNP O73790
D	?	-	ASP	DELETION	UNP O73790

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP O73790
D	?	-	GLU	DELETION	UNP O73790
D	?	-	HIS	DELETION	UNP O73790

- Molecule 2 is water.

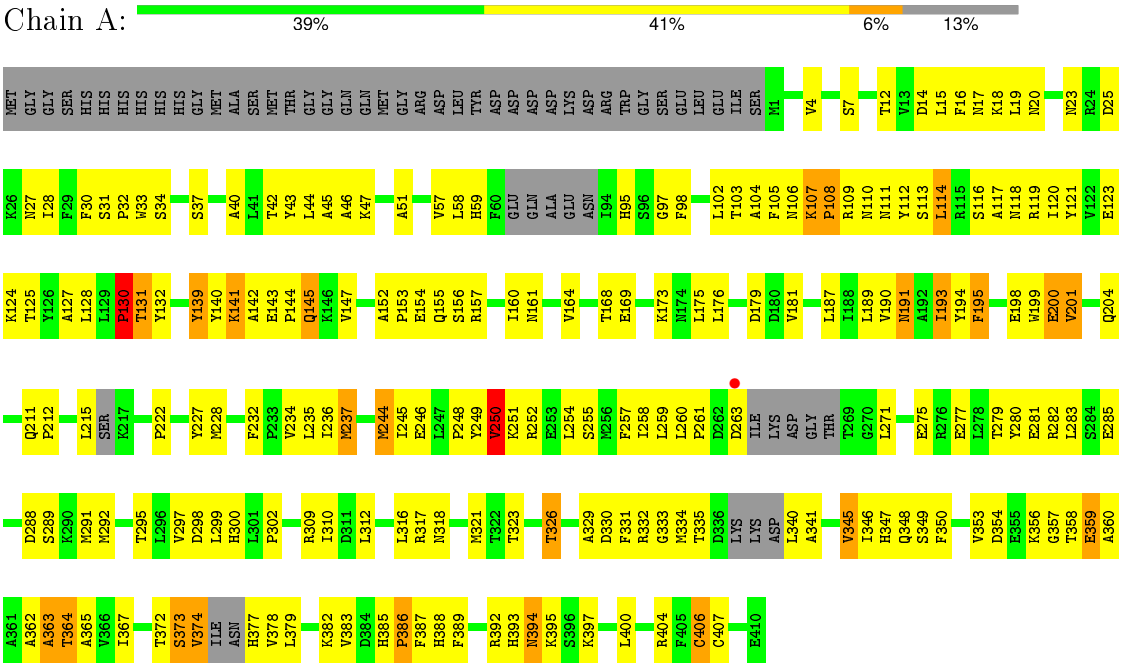
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	34	Total O 34 34	0	0
2	B	34	Total O 34 34	0	0
2	C	33	Total O 33 33	0	0
2	D	35	Total O 35 35	0	0

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.

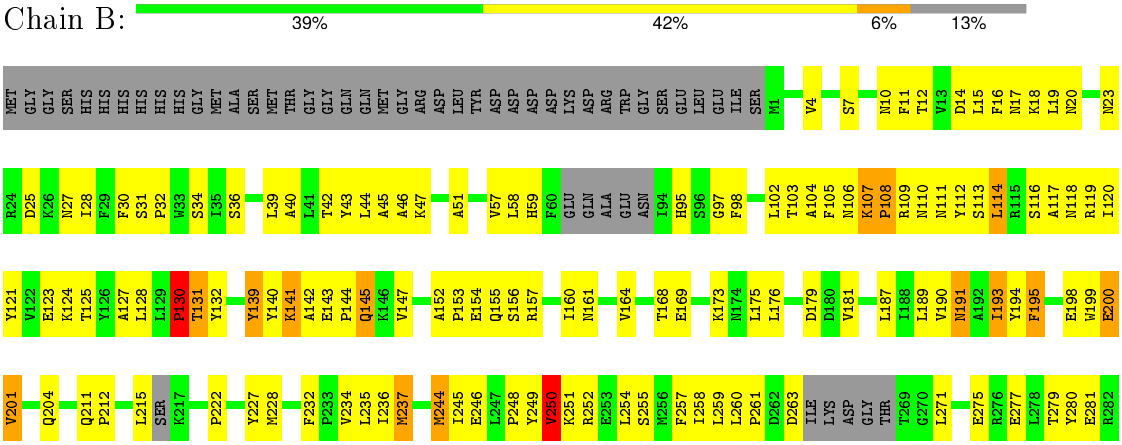
- Molecule 1: Heterochromatin-associated protein MENT

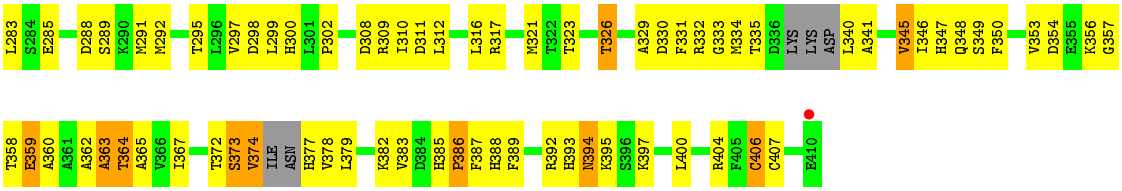
Chain A:



- Molecule 1: Heterochromatin-associated protein MENT

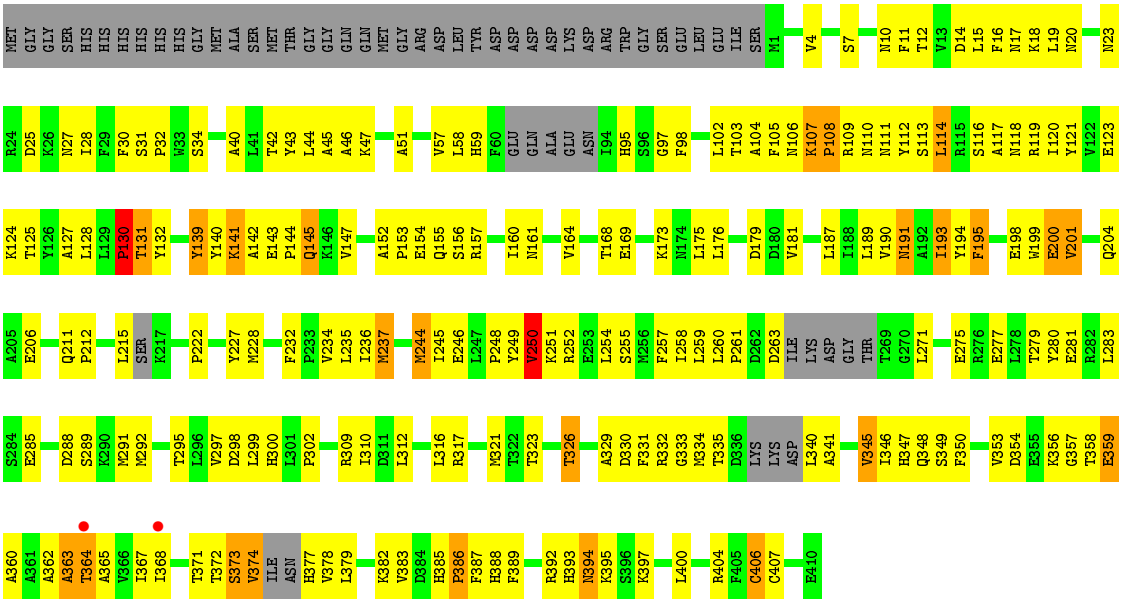
Chain B:





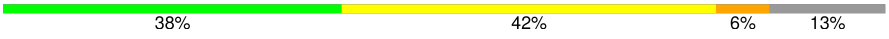
• Molecule 1: Heterochromatin-associated protein MENT

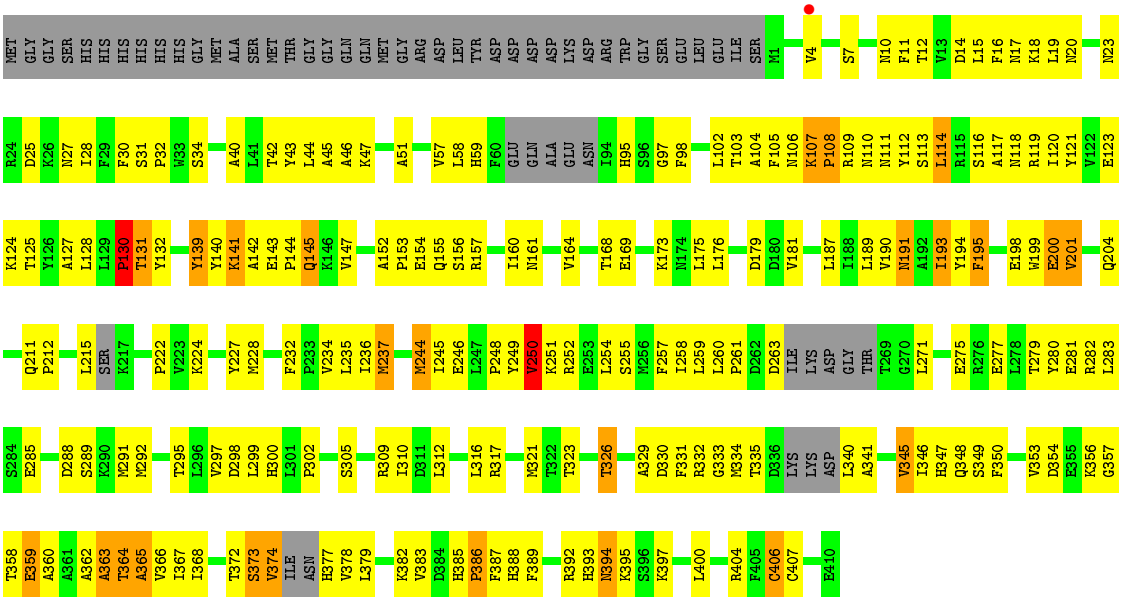
Chain C:



• Molecule 1: Heterochromatin-associated protein MENT

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	182.56Å 182.56Å 96.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-3.00) 95.6 (19.97-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.02 (at 2.98Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.278 , 0.293 0.293 , 0.327	Depositor DCC
R_{free} test set	3090 reflections (4.70%)	DCC
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 65.1	EDS
Estimated twinning fraction	0.073 for -h,-k,l 0.073 for h,-h-k,-l 0.499 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 68817 reflections	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	11020	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.75% 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

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	0.50	0/2780	0.81	4/3785 (0.1%)
1	B	0.50	0/2780	0.81	4/3785 (0.1%)
1	C	0.50	0/2780	0.81	4/3785 (0.1%)
1	D	0.50	0/2780	0.81	4/3785 (0.1%)
All	All	0.50	0/11120	0.81	16/15140 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	373	SER	N-CA-C	9.84	137.58	111.00
1	D	373	SER	N-CA-C	9.84	137.57	111.00
1	C	373	SER	N-CA-C	9.83	137.54	111.00
1	A	373	SER	N-CA-C	9.82	137.53	111.00
1	D	200	GLU	N-CA-C	-6.20	94.25	111.00
1	C	200	GLU	N-CA-C	-6.19	94.30	111.00
1	A	200	GLU	N-CA-C	-6.17	94.33	111.00
1	B	200	GLU	N-CA-C	-6.17	94.35	111.00
1	A	377	HIS	N-CA-C	-5.46	96.26	111.00
1	B	377	HIS	N-CA-C	-5.46	96.27	111.00
1	C	377	HIS	N-CA-C	-5.45	96.27	111.00
1	D	377	HIS	N-CA-C	-5.44	96.30	111.00
1	A	374	VAL	N-CA-C	5.37	125.50	111.00
1	B	374	VAL	N-CA-C	5.37	125.50	111.00
1	C	374	VAL	N-CA-C	5.37	125.49	111.00
1	D	374	VAL	N-CA-C	5.35	125.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2721	0	2497	206	0
1	B	2721	0	2497	210	0
1	C	2721	0	2497	202	0
1	D	2721	0	2497	227	0
2	A	34	0	0	2	0
2	B	34	0	0	2	0
2	C	33	0	0	2	0
2	D	35	0	0	3	0
All	All	11020	0	9988	821	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 39.

All (821) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ASP:HB2	1:D:368:ILE:HG12	1.37	1.06
1:A:317:ARG:HA	1:A:321:MET:O	1.55	1.06
1:B:317:ARG:HA	1:B:321:MET:O	1.55	1.05
1:C:317:ARG:HA	1:C:321:MET:O	1.55	1.05
1:D:317:ARG:HA	1:D:321:MET:O	1.55	1.04
1:C:279:THR:HG22	1:C:281:GLU:H	1.22	1.00
1:D:279:THR:HG22	1:D:281:GLU:H	1.22	1.00
1:A:279:THR:HG22	1:A:281:GLU:H	1.22	1.00
1:B:279:THR:HG22	1:B:281:GLU:H	1.22	1.00
1:B:308:ASP:CB	1:D:368:ILE:HG12	1.98	0.94
1:B:4:VAL:HG21	1:B:97:GLY:HA3	1.58	0.86
1:A:4:VAL:HG21	1:A:97:GLY:HA3	1.57	0.85
1:D:4:VAL:HG21	1:D:97:GLY:HA3	1.57	0.85
1:C:4:VAL:HG21	1:C:97:GLY:HA3	1.57	0.84
1:C:191:ASN:HD22	1:C:191:ASN:N	1.77	0.81
1:B:191:ASN:HD22	1:B:191:ASN:N	1.77	0.79
1:C:46:ALA:O	1:C:51:ALA:HB2	1.82	0.79
1:B:46:ALA:O	1:B:51:ALA:HB2	1.82	0.79
1:D:46:ALA:O	1:D:51:ALA:HB2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:MET:HG3	1:C:259:LEU:HG	1.65	0.79
1:D:191:ASN:N	1:D:191:ASN:HD22	1.77	0.79
1:A:191:ASN:N	1:A:191:ASN:HD22	1.77	0.79
1:A:244:MET:HG3	1:A:259:LEU:HG	1.65	0.78
1:B:244:MET:HG3	1:B:259:LEU:HG	1.65	0.78
1:A:46:ALA:O	1:A:51:ALA:HB2	1.82	0.78
1:D:244:MET:HG3	1:D:259:LEU:HG	1.65	0.78
1:A:392:ARG:HD2	1:A:397:LYS:HA	1.68	0.76
1:B:392:ARG:HD2	1:B:397:LYS:HA	1.68	0.75
1:C:392:ARG:HD2	1:C:397:LYS:HA	1.68	0.75
1:D:259:LEU:N	1:D:259:LEU:HD12	2.02	0.74
1:D:392:ARG:HD2	1:D:397:LYS:HA	1.68	0.74
1:B:259:LEU:HD12	1:B:259:LEU:N	2.03	0.73
1:A:45:ALA:HB2	1:A:132:TYR:CE1	2.24	0.73
1:C:45:ALA:HB2	1:C:132:TYR:CE1	2.24	0.73
1:D:45:ALA:HB2	1:D:132:TYR:CE1	2.24	0.73
1:A:259:LEU:HD12	1:A:259:LEU:N	2.02	0.73
1:B:45:ALA:HB2	1:B:132:TYR:CE1	2.24	0.73
1:C:259:LEU:HD12	1:C:259:LEU:N	2.02	0.72
1:D:95:HIS:CD2	1:D:140:TYR:HH	2.08	0.72
1:B:95:HIS:CD2	1:B:140:TYR:HH	2.08	0.72
1:B:191:ASN:HD22	1:B:191:ASN:H	1.35	0.72
1:D:191:ASN:HD22	1:D:191:ASN:H	1.35	0.72
1:A:191:ASN:HD22	1:A:191:ASN:H	1.35	0.71
1:C:364:THR:OG1	1:C:367:ILE:HD11	1.90	0.71
1:D:364:THR:OG1	1:D:367:ILE:HD11	1.90	0.71
1:A:95:HIS:CD2	1:A:140:TYR:HH	2.08	0.71
1:C:44:LEU:HB2	1:C:95:HIS:HE1	1.56	0.71
1:C:191:ASN:HD22	1:C:191:ASN:H	1.35	0.70
1:C:95:HIS:CD2	1:C:140:TYR:HH	2.08	0.70
1:C:187:LEU:HB2	1:C:340:LEU:HD21	1.74	0.70
1:D:44:LEU:HB2	1:D:95:HIS:HE1	1.56	0.70
1:B:244:MET:CE	1:B:257:PHE:HD2	2.04	0.70
1:B:121:TYR:HE2	1:B:160:ILE:HG23	1.57	0.70
1:A:246:GLU:O	1:A:248:PRO:HD3	1.92	0.70
1:C:244:MET:CE	1:C:257:PHE:HD2	2.04	0.70
1:A:244:MET:CE	1:A:257:PHE:HD2	2.04	0.70
1:A:44:LEU:HB2	1:A:95:HIS:HE1	1.56	0.70
1:B:246:GLU:O	1:B:248:PRO:HD3	1.92	0.70
1:B:364:THR:OG1	1:B:367:ILE:HD11	1.90	0.69
1:B:44:LEU:HB2	1:B:95:HIS:HE1	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:THR:OG1	1:A:367:ILE:HD11	1.90	0.69
1:A:121:TYR:HE2	1:A:160:ILE:HG23	1.57	0.69
1:C:246:GLU:O	1:C:248:PRO:HD3	1.92	0.69
1:D:244:MET:CE	1:D:257:PHE:HD2	2.04	0.69
1:D:246:GLU:O	1:D:248:PRO:HD3	1.92	0.69
1:A:187:LEU:HB2	1:A:340:LEU:HD21	1.74	0.69
1:A:393:HIS:CE1	1:A:395:LYS:HB3	2.28	0.69
1:D:275:GLU:HG2	1:D:388:HIS:NE2	2.08	0.69
1:C:393:HIS:CE1	1:C:395:LYS:HB3	2.28	0.69
1:B:275:GLU:HG2	1:B:388:HIS:NE2	2.08	0.69
1:C:275:GLU:HG2	1:C:388:HIS:NE2	2.08	0.69
1:D:393:HIS:CE1	1:D:395:LYS:HB3	2.28	0.69
1:C:12:THR:HG23	1:C:32:PRO:HB3	1.75	0.69
1:B:187:LEU:HB2	1:B:340:LEU:HD21	1.74	0.68
1:C:279:THR:HG22	1:C:281:GLU:N	2.04	0.68
1:C:121:TYR:HE2	1:C:160:ILE:HG23	1.57	0.68
1:C:121:TYR:CE2	1:C:160:ILE:HG23	2.29	0.68
1:A:275:GLU:HG2	1:A:388:HIS:NE2	2.08	0.68
1:D:12:THR:HG23	1:D:32:PRO:HB3	1.75	0.68
1:D:187:LEU:HB2	1:D:340:LEU:HD21	1.74	0.68
1:C:45:ALA:CB	1:C:334:MET:HE2	2.23	0.68
1:A:121:TYR:CE2	1:A:160:ILE:HG23	2.29	0.68
1:D:279:THR:HG22	1:D:281:GLU:N	2.04	0.68
1:B:393:HIS:CE1	1:B:395:LYS:HB3	2.28	0.68
1:B:120:ILE:HG23	1:B:187:LEU:HD11	1.76	0.68
1:D:121:TYR:HE2	1:D:160:ILE:HG23	1.57	0.68
1:B:311:ASP:HB3	1:D:365:ALA:HA	1.76	0.68
1:A:120:ILE:HG23	1:A:187:LEU:HD11	1.76	0.67
1:B:117:ALA:C	1:B:118:ASN:HD22	1.98	0.67
1:B:121:TYR:CE2	1:B:160:ILE:HG23	2.29	0.67
1:D:120:ILE:HG23	1:D:187:LEU:HD11	1.76	0.67
1:C:120:ILE:HG23	1:C:187:LEU:HD11	1.75	0.67
1:A:12:THR:HG23	1:A:32:PRO:HB3	1.75	0.67
1:D:121:TYR:CE2	1:D:160:ILE:HG23	2.29	0.67
1:D:45:ALA:CB	1:D:334:MET:HE2	2.24	0.67
1:B:45:ALA:CB	1:B:334:MET:HE2	2.24	0.66
1:D:117:ALA:C	1:D:118:ASN:HD22	1.98	0.66
1:A:117:ALA:C	1:A:118:ASN:HD22	1.98	0.66
1:B:12:THR:HG23	1:B:32:PRO:HB3	1.75	0.66
1:A:279:THR:HG22	1:A:281:GLU:N	2.04	0.66
1:A:347:HIS:HE1	1:A:349:SER:OG	1.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ALA:CB	1:A:334:MET:HE2	2.26	0.66
1:C:140:TYR:O	1:C:141:LYS:C	2.34	0.66
1:B:347:HIS:HE1	1:B:349:SER:OG	1.79	0.66
1:B:140:TYR:O	1:B:141:LYS:C	2.34	0.66
1:C:117:ALA:C	1:C:118:ASN:HD22	1.98	0.66
1:C:347:HIS:HE1	1:C:349:SER:OG	1.79	0.66
1:A:140:TYR:O	1:A:141:LYS:C	2.34	0.66
1:D:140:TYR:O	1:D:141:LYS:C	2.34	0.65
1:D:347:HIS:HE1	1:D:349:SER:OG	1.79	0.65
1:C:28:ILE:N	1:C:28:ILE:HD12	2.12	0.65
1:B:279:THR:HG22	1:B:281:GLU:N	2.04	0.65
1:B:191:ASN:O	1:B:347:HIS:HA	1.97	0.64
1:A:28:ILE:N	1:A:28:ILE:HD12	2.12	0.64
1:A:297:VAL:HG13	1:A:379:LEU:O	1.98	0.64
1:D:28:ILE:N	1:D:28:ILE:HD12	2.12	0.64
1:C:191:ASN:O	1:C:347:HIS:HA	1.97	0.64
1:B:297:VAL:HG13	1:B:379:LEU:O	1.98	0.64
1:D:191:ASN:O	1:D:347:HIS:HA	1.97	0.64
1:C:123:GLU:HA	1:C:147:VAL:O	1.97	0.64
1:A:191:ASN:O	1:A:347:HIS:HA	1.97	0.64
1:B:28:ILE:HD12	1:B:28:ILE:N	2.12	0.64
1:B:17:ASN:O	1:B:20:ASN:HB3	1.99	0.63
1:D:297:VAL:HG13	1:D:379:LEU:O	1.98	0.63
1:B:353:VAL:HA	1:B:357:GLY:O	1.99	0.63
1:D:153:PRO:HG2	1:D:154:GLU:H	1.64	0.63
1:A:282:ARG:HH21	1:D:317:ARG:NH2	1.97	0.63
1:C:40:ALA:O	1:C:43:TYR:HB3	1.98	0.63
1:D:123:GLU:HA	1:D:147:VAL:O	1.98	0.63
1:C:17:ASN:O	1:C:20:ASN:HB3	1.99	0.63
1:A:353:VAL:HA	1:A:357:GLY:O	1.99	0.63
1:A:153:PRO:HG2	1:A:154:GLU:H	1.64	0.63
1:B:132:TYR:HE2	1:B:144:PRO:HG2	1.64	0.63
1:B:40:ALA:O	1:B:43:TYR:HB3	1.98	0.63
1:C:153:PRO:HG2	1:C:154:GLU:H	1.64	0.63
1:A:40:ALA:O	1:A:43:TYR:HB3	1.98	0.63
1:C:297:VAL:HG13	1:C:379:LEU:O	1.98	0.63
1:C:132:TYR:HE2	1:C:144:PRO:HG2	1.64	0.63
1:D:40:ALA:O	1:D:43:TYR:HB3	1.98	0.63
1:A:358:THR:O	1:A:360:ALA:N	2.32	0.62
1:D:358:THR:O	1:D:360:ALA:N	2.33	0.62
1:B:358:THR:O	1:B:360:ALA:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:THR:HG22	1:D:280:TYR:N	2.14	0.62
1:D:132:TYR:HE2	1:D:144:PRO:HG2	1.64	0.62
1:B:153:PRO:HG2	1:B:154:GLU:H	1.64	0.62
1:B:123:GLU:HA	1:B:147:VAL:O	1.98	0.62
1:A:279:THR:HG22	1:A:280:TYR:N	2.14	0.62
1:C:353:VAL:HA	1:C:357:GLY:O	1.99	0.62
1:C:358:THR:O	1:C:360:ALA:N	2.33	0.62
1:A:123:GLU:HA	1:A:147:VAL:O	1.98	0.62
1:B:279:THR:HG22	1:B:280:TYR:N	2.14	0.62
1:A:17:ASN:O	1:A:20:ASN:HB3	1.99	0.62
1:B:258:ILE:HG23	1:B:387:PHE:CD2	2.35	0.62
1:A:132:TYR:HE2	1:A:144:PRO:HG2	1.64	0.62
1:D:17:ASN:O	1:D:20:ASN:HB3	1.99	0.62
1:C:279:THR:HG22	1:C:280:TYR:N	2.14	0.61
1:D:191:ASN:N	1:D:191:ASN:ND2	2.48	0.61
1:C:258:ILE:HG23	1:C:387:PHE:CD2	2.35	0.61
1:D:258:ILE:HG23	1:D:387:PHE:CD2	2.35	0.61
1:B:309:ARG:HB3	1:D:367:ILE:HB	1.82	0.61
1:D:353:VAL:HA	1:D:357:GLY:O	1.99	0.61
1:A:258:ILE:HG23	1:A:387:PHE:CD2	2.35	0.61
1:A:191:ASN:N	1:A:191:ASN:ND2	2.48	0.61
1:B:346:ILE:N	1:B:346:ILE:HD12	2.16	0.61
1:A:346:ILE:HD12	1:A:346:ILE:N	2.16	0.60
1:C:346:ILE:N	1:C:346:ILE:HD12	2.16	0.60
1:D:346:ILE:HD12	1:D:346:ILE:N	2.16	0.60
1:A:248:PRO:HB3	1:A:252:ARG:HG3	1.83	0.60
1:B:120:ILE:HG23	1:B:187:LEU:CD1	2.32	0.60
1:C:98:PHE:O	1:C:102:LEU:HB2	2.01	0.60
1:B:191:ASN:ND2	1:B:191:ASN:N	2.48	0.60
1:A:120:ILE:HG23	1:A:187:LEU:CD1	2.32	0.60
1:D:248:PRO:HB3	1:D:252:ARG:HG3	1.83	0.60
1:D:98:PHE:O	1:D:102:LEU:HB2	2.02	0.59
1:C:120:ILE:HG23	1:C:187:LEU:CD1	2.32	0.59
1:A:98:PHE:O	1:A:102:LEU:HB2	2.01	0.59
1:D:120:ILE:HG23	1:D:187:LEU:CD1	2.32	0.59
1:D:285:GLU:O	1:D:289:SER:HB2	2.03	0.59
1:B:248:PRO:HB3	1:B:252:ARG:HG3	1.83	0.59
1:B:98:PHE:O	1:B:102:LEU:HB2	2.01	0.59
1:D:309:ARG:HG2	1:D:309:ARG:HH11	1.68	0.59
1:D:44:LEU:HB2	1:D:95:HIS:CE1	2.38	0.59
1:D:127:ALA:O	1:D:335:THR:HA	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ARG:HH11	1:C:309:ARG:HG2	1.68	0.58
1:C:248:PRO:HB3	1:C:252:ARG:HG3	1.83	0.58
1:B:127:ALA:O	1:B:335:THR:HA	2.03	0.58
1:B:44:LEU:HB2	1:B:95:HIS:CE1	2.38	0.58
1:C:285:GLU:O	1:C:289:SER:HB2	2.03	0.58
1:B:309:ARG:HH11	1:B:309:ARG:HG2	1.68	0.58
1:B:323:THR:HA	1:B:326:THR:HG23	1.86	0.58
1:D:323:THR:HA	1:D:326:THR:HG23	1.86	0.58
1:A:277:GLU:HG3	2:A:428:HOH:O	2.04	0.58
1:D:277:GLU:HG3	2:D:429:HOH:O	2.04	0.58
1:A:309:ARG:HG2	1:A:309:ARG:HH11	1.68	0.58
1:A:285:GLU:O	1:A:289:SER:HB2	2.03	0.58
1:B:340:LEU:HD22	1:B:341:ALA:N	2.19	0.58
1:B:277:GLU:HG3	2:B:428:HOH:O	2.04	0.58
1:A:259:LEU:N	1:A:259:LEU:CD1	2.67	0.57
1:A:340:LEU:HD22	1:A:341:ALA:N	2.19	0.57
1:A:127:ALA:O	1:A:335:THR:HA	2.03	0.57
1:C:259:LEU:N	1:C:259:LEU:CD1	2.67	0.57
1:C:277:GLU:HG3	2:C:427:HOH:O	2.03	0.57
1:A:323:THR:HA	1:A:326:THR:HG23	1.86	0.57
1:B:285:GLU:O	1:B:289:SER:HB2	2.03	0.57
1:A:44:LEU:HB2	1:A:95:HIS:CE1	2.38	0.57
1:C:323:THR:HA	1:C:326:THR:HG23	1.86	0.57
1:B:108:PRO:O	1:B:109:ARG:C	2.43	0.57
1:A:108:PRO:O	1:A:109:ARG:C	2.43	0.57
1:A:128:LEU:O	1:A:130:PRO:HD3	2.05	0.57
1:C:108:PRO:O	1:C:109:ARG:C	2.43	0.57
1:D:340:LEU:HD22	1:D:341:ALA:N	2.19	0.57
1:B:259:LEU:CD1	1:B:259:LEU:N	2.67	0.57
1:C:44:LEU:HB2	1:C:95:HIS:CE1	2.38	0.57
1:A:161:ASN:HD21	1:A:176:LEU:HB2	1.70	0.57
1:D:373:SER:C	1:D:374:VAL:HG23	2.25	0.57
1:C:340:LEU:HD22	1:C:341:ALA:N	2.19	0.57
1:C:128:LEU:O	1:C:130:PRO:HD3	2.05	0.57
1:D:108:PRO:O	1:D:109:ARG:C	2.43	0.57
1:D:140:TYR:O	1:D:142:ALA:N	2.38	0.57
1:B:161:ASN:HD21	1:B:176:LEU:HB2	1.69	0.57
1:A:110:ASN:O	1:A:111:ASN:HB2	2.05	0.57
1:B:27:ASN:O	1:D:368:ILE:HG21	2.04	0.57
1:A:317:ARG:CZ	1:D:282:ARG:HH21	2.18	0.57
1:B:110:ASN:O	1:B:111:ASN:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:NH2	1:D:282:ARG:HH21	2.03	0.57
1:D:161:ASN:HD21	1:D:176:LEU:HB2	1.70	0.57
1:B:168:THR:O	1:B:169:GLU:HB2	2.05	0.57
1:B:308:ASP:HB2	1:D:368:ILE:CG1	2.24	0.56
1:A:140:TYR:O	1:A:142:ALA:N	2.38	0.56
1:B:140:TYR:O	1:B:142:ALA:N	2.38	0.56
1:C:161:ASN:HD21	1:C:176:LEU:HB2	1.70	0.56
1:C:127:ALA:O	1:C:335:THR:HA	2.03	0.56
1:C:140:TYR:O	1:C:142:ALA:N	2.38	0.56
1:B:385:HIS:HB2	1:B:386:PRO:HD2	1.88	0.56
1:A:385:HIS:HB2	1:A:386:PRO:HD2	1.88	0.56
1:D:168:THR:O	1:D:169:GLU:HB2	2.05	0.56
1:D:128:LEU:O	1:D:130:PRO:HD3	2.05	0.56
1:B:128:LEU:O	1:B:130:PRO:HD3	2.05	0.56
1:C:110:ASN:O	1:C:111:ASN:HB2	2.05	0.56
1:C:374:VAL:HG21	1:D:224:LYS:HE3	1.87	0.56
1:C:373:SER:C	1:C:374:VAL:HG23	2.25	0.56
1:D:249:TYR:HB2	1:D:254:LEU:O	2.06	0.56
1:B:58:LEU:O	1:B:59:HIS:HB2	2.06	0.56
1:B:244:MET:CG	1:B:259:LEU:HG	2.36	0.56
1:A:103:THR:O	1:A:104:ALA:C	2.44	0.56
1:B:118:ASN:N	1:B:118:ASN:HD22	2.03	0.56
1:A:106:ASN:O	1:A:107:LYS:O	2.24	0.56
1:B:103:THR:O	1:B:104:ALA:C	2.45	0.56
1:B:249:TYR:HB2	1:B:254:LEU:O	2.06	0.56
1:D:118:ASN:N	1:D:118:ASN:HD22	2.03	0.56
1:C:45:ALA:HB1	1:C:334:MET:HG2	1.88	0.56
1:C:385:HIS:HB2	1:C:386:PRO:HD2	1.88	0.56
1:C:168:THR:O	1:C:169:GLU:HB2	2.05	0.56
1:C:118:ASN:HD22	1:C:118:ASN:N	2.03	0.55
1:B:106:ASN:O	1:B:107:LYS:O	2.24	0.55
1:B:373:SER:C	1:B:374:VAL:HG23	2.25	0.55
1:A:45:ALA:HB1	1:A:334:MET:HG2	1.88	0.55
1:C:103:THR:O	1:C:104:ALA:C	2.45	0.55
1:A:244:MET:CG	1:A:259:LEU:HG	2.36	0.55
1:A:249:TYR:HB2	1:A:254:LEU:O	2.06	0.55
1:C:106:ASN:O	1:C:107:LYS:O	2.24	0.55
1:A:373:SER:C	1:A:374:VAL:HG23	2.25	0.55
1:C:58:LEU:O	1:C:59:HIS:HB2	2.06	0.55
1:D:110:ASN:O	1:D:111:ASN:HB2	2.05	0.55
1:C:191:ASN:ND2	1:C:191:ASN:N	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:TYR:C	1:B:45:ALA:H	2.10	0.55
1:A:309:ARG:HD2	1:A:348:GLN:OE1	2.07	0.55
1:A:43:TYR:C	1:A:45:ALA:H	2.10	0.55
1:C:43:TYR:C	1:C:45:ALA:H	2.10	0.55
1:D:385:HIS:HB2	1:D:386:PRO:HD2	1.88	0.55
1:D:309:ARG:HD2	1:D:348:GLN:OE1	2.07	0.55
1:C:249:TYR:HB2	1:C:254:LEU:O	2.06	0.55
1:A:168:THR:O	1:A:169:GLU:HB2	2.05	0.55
1:D:259:LEU:N	1:D:259:LEU:CD1	2.67	0.55
1:C:132:TYR:CE2	1:C:144:PRO:HG2	2.41	0.55
1:D:58:LEU:O	1:D:59:HIS:HB2	2.06	0.55
1:A:132:TYR:CE2	1:A:144:PRO:HG2	2.41	0.54
1:B:309:ARG:HD2	1:B:348:GLN:OE1	2.07	0.54
1:C:244:MET:CG	1:C:259:LEU:HG	2.36	0.54
1:D:103:THR:O	1:D:104:ALA:C	2.44	0.54
1:B:45:ALA:HB1	1:B:334:MET:HG2	1.88	0.54
1:D:43:TYR:C	1:D:45:ALA:H	2.10	0.54
1:D:45:ALA:HB1	1:D:334:MET:HG2	1.88	0.54
1:D:127:ALA:O	1:D:335:THR:HG22	2.08	0.54
1:B:132:TYR:CE2	1:B:144:PRO:HG2	2.41	0.54
1:C:121:TYR:HE1	1:C:145:GLN:CG	2.21	0.54
1:D:106:ASN:O	1:D:107:LYS:O	2.24	0.54
1:D:119:ARG:O	1:D:189:LEU:HD12	2.08	0.54
1:B:358:THR:O	1:B:359:GLU:C	2.46	0.54
1:A:119:ARG:O	1:A:189:LEU:HD12	2.08	0.54
1:C:309:ARG:HD2	1:C:348:GLN:OE1	2.07	0.54
1:A:44:LEU:HG	1:A:44:LEU:O	2.08	0.54
1:C:329:ALA:HB3	1:C:340:LEU:O	2.08	0.54
1:A:358:THR:O	1:A:359:GLU:C	2.46	0.54
1:A:58:LEU:O	1:A:59:HIS:HB2	2.06	0.54
1:A:118:ASN:N	1:A:118:ASN:HD22	2.03	0.54
1:A:110:ASN:O	1:A:111:ASN:CB	2.56	0.54
1:D:44:LEU:HG	1:D:44:LEU:O	2.08	0.54
1:D:121:TYR:HE1	1:D:145:GLN:CG	2.21	0.54
1:D:244:MET:CG	1:D:259:LEU:HG	2.36	0.53
1:C:44:LEU:O	1:C:44:LEU:HG	2.08	0.53
1:A:121:TYR:HE1	1:A:145:GLN:CG	2.21	0.53
1:C:20:ASN:HD21	1:C:404:ARG:HH12	1.55	0.53
1:A:124:LYS:N	1:A:147:VAL:O	2.42	0.53
1:C:119:ARG:O	1:C:189:LEU:HD12	2.08	0.53
1:A:282:ARG:HH21	1:D:317:ARG:CZ	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ALA:HB3	1:A:340:LEU:O	2.08	0.53
1:D:132:TYR:CE2	1:D:144:PRO:HG2	2.41	0.53
1:B:121:TYR:HE1	1:B:145:GLN:CG	2.21	0.53
1:B:329:ALA:HB3	1:B:340:LEU:O	2.08	0.53
1:C:358:THR:O	1:C:359:GLU:C	2.46	0.53
1:B:127:ALA:O	1:B:335:THR:HG22	2.08	0.53
1:C:127:ALA:O	1:C:335:THR:HG22	2.08	0.53
1:C:105:PHE:HA	1:C:112:TYR:OH	2.08	0.53
1:D:105:PHE:HA	1:D:112:TYR:OH	2.08	0.53
1:A:295:THR:O	1:A:297:VAL:HG23	2.08	0.53
1:B:124:LYS:N	1:B:147:VAL:O	2.42	0.53
1:C:295:THR:O	1:C:297:VAL:HG23	2.08	0.53
1:B:119:ARG:O	1:B:189:LEU:HD12	2.08	0.53
1:C:124:LYS:N	1:C:147:VAL:O	2.42	0.53
1:B:105:PHE:HA	1:B:112:TYR:OH	2.08	0.53
1:B:44:LEU:O	1:B:44:LEU:HG	2.08	0.53
1:B:110:ASN:O	1:B:111:ASN:CB	2.56	0.53
1:A:105:PHE:HA	1:A:112:TYR:OH	2.08	0.53
1:D:329:ALA:HB3	1:D:340:LEU:O	2.08	0.53
1:B:295:THR:O	1:B:297:VAL:HG23	2.08	0.53
1:C:110:ASN:O	1:C:111:ASN:CB	2.56	0.53
1:D:124:LYS:N	1:D:147:VAL:O	2.41	0.53
1:D:358:THR:O	1:D:359:GLU:C	2.46	0.53
1:C:350:PHE:CD1	1:C:350:PHE:C	2.82	0.53
1:A:127:ALA:O	1:A:335:THR:HG22	2.08	0.52
1:B:308:ASP:HB3	1:D:368:ILE:HG12	1.87	0.52
1:A:317:ARG:NE	1:D:282:ARG:HH21	2.07	0.52
1:B:244:MET:HE1	1:B:257:PHE:HD2	1.74	0.52
1:A:20:ASN:HD21	1:A:404:ARG:HH12	1.55	0.52
1:B:20:ASN:HD21	1:B:404:ARG:HH12	1.55	0.52
1:D:350:PHE:C	1:D:350:PHE:CD1	2.83	0.52
1:A:318:ASN:OD1	1:D:282:ARG:NH1	2.38	0.52
1:D:20:ASN:HD21	1:D:404:ARG:HH12	1.55	0.52
1:D:295:THR:O	1:D:297:VAL:HG23	2.08	0.52
1:D:110:ASN:O	1:D:111:ASN:CB	2.56	0.52
1:D:211:GLN:HB3	1:D:212:PRO:HD2	1.92	0.52
1:C:121:TYR:CD2	1:C:160:ILE:HG12	2.45	0.52
1:B:121:TYR:CD2	1:B:160:ILE:HG12	2.45	0.51
1:D:271:LEU:HD12	1:D:386:PRO:HB3	1.93	0.51
1:A:121:TYR:CD2	1:A:160:ILE:HG12	2.45	0.51
1:B:271:LEU:HD12	1:B:386:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:PHE:CD1	1:B:350:PHE:C	2.83	0.51
1:B:308:ASP:HA	1:D:367:ILE:O	2.11	0.51
1:A:350:PHE:CD1	1:A:350:PHE:C	2.82	0.51
1:C:211:GLN:HB3	1:C:212:PRO:HD2	1.92	0.51
1:B:45:ALA:HB2	1:B:132:TYR:CD1	2.45	0.51
1:C:45:ALA:HB2	1:C:132:TYR:CD1	2.45	0.51
1:D:121:TYR:CD2	1:D:160:ILE:HG12	2.45	0.51
1:A:27:ASN:HD21	1:A:407:CYS:HB2	1.76	0.51
1:D:244:MET:HE1	1:D:257:PHE:HD2	1.75	0.51
1:B:114:LEU:HD11	1:B:400:LEU:HD13	1.92	0.51
1:B:27:ASN:HD21	1:B:407:CYS:HB2	1.76	0.51
1:D:45:ALA:HB2	1:D:132:TYR:CD1	2.45	0.51
1:C:27:ASN:HD21	1:C:407:CYS:HB2	1.76	0.51
1:A:45:ALA:HB2	1:A:132:TYR:CD1	2.45	0.51
1:B:310:ILE:HG23	1:D:366:VAL:HG22	1.92	0.51
1:C:198:GLU:HA	1:C:356:LYS:O	2.11	0.51
1:C:271:LEU:HD12	1:C:386:PRO:HB3	1.92	0.50
1:B:198:GLU:HA	1:B:356:LYS:O	2.12	0.50
1:A:198:GLU:HA	1:A:356:LYS:O	2.12	0.50
1:A:114:LEU:CD1	1:A:400:LEU:HD13	2.42	0.50
1:A:114:LEU:HD11	1:A:400:LEU:HD13	1.92	0.50
1:B:114:LEU:CD1	1:B:400:LEU:HD13	2.42	0.50
1:B:211:GLN:HB3	1:B:212:PRO:HD2	1.92	0.50
1:D:114:LEU:HD11	1:D:400:LEU:HD13	1.92	0.50
1:C:368:ILE:HG21	1:D:27:ASN:O	2.12	0.50
1:C:114:LEU:HD11	1:C:400:LEU:HD13	1.92	0.50
1:A:211:GLN:HB3	1:A:212:PRO:HD2	1.92	0.50
1:A:271:LEU:HD12	1:A:386:PRO:HB3	1.92	0.50
1:C:258:ILE:HG23	1:C:387:PHE:HD2	1.76	0.50
1:D:27:ASN:HD21	1:D:407:CYS:HB2	1.76	0.50
1:C:244:MET:HE1	1:C:257:PHE:HD2	1.75	0.50
1:C:114:LEU:CD1	1:C:400:LEU:HD13	2.42	0.50
1:D:132:TYR:HE2	1:D:144:PRO:CG	2.24	0.50
1:B:310:ILE:HA	1:D:365:ALA:O	2.12	0.49
1:C:4:VAL:O	1:C:7:SER:HB3	2.12	0.49
1:A:244:MET:HE1	1:A:257:PHE:HD2	1.76	0.49
1:B:176:LEU:CD2	1:B:346:ILE:HG12	2.43	0.49
1:A:176:LEU:CD2	1:A:346:ILE:HG12	2.43	0.49
1:C:45:ALA:O	1:C:331:PHE:HA	2.12	0.49
1:B:4:VAL:O	1:B:7:SER:HB3	2.12	0.49
1:A:4:VAL:O	1:A:7:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:VAL:O	1:D:7:SER:HB3	2.12	0.49
1:A:132:TYR:HE2	1:A:144:PRO:CG	2.25	0.49
1:D:45:ALA:O	1:D:331:PHE:HA	2.12	0.49
1:B:132:TYR:HE2	1:B:144:PRO:CG	2.25	0.49
1:D:176:LEU:CD2	1:D:346:ILE:HG12	2.43	0.49
1:D:310:ILE:CG2	1:D:312:LEU:HD23	2.43	0.49
1:B:309:ARG:NH1	1:B:309:ARG:HG2	2.28	0.49
1:D:114:LEU:CD1	1:D:400:LEU:HD13	2.42	0.49
1:B:199:TRP:CE2	1:B:357:GLY:HA2	2.48	0.49
1:C:199:TRP:CE2	1:C:357:GLY:HA2	2.48	0.49
1:C:176:LEU:CD2	1:C:346:ILE:HG12	2.42	0.49
1:A:45:ALA:O	1:A:331:PHE:HA	2.13	0.49
1:A:354:ASP:OD2	1:A:357:GLY:N	2.46	0.49
1:D:155:GLN:O	1:D:156:SER:C	2.51	0.49
1:D:198:GLU:HA	1:D:356:LYS:O	2.12	0.49
1:A:309:ARG:HG2	1:A:309:ARG:NH1	2.28	0.49
1:B:354:ASP:OD2	1:B:357:GLY:N	2.46	0.49
1:C:354:ASP:OD2	1:C:357:GLY:N	2.46	0.49
1:B:155:GLN:O	1:B:156:SER:C	2.51	0.49
1:B:45:ALA:O	1:B:331:PHE:HA	2.12	0.48
1:D:95:HIS:CD2	1:D:140:TYR:OH	2.66	0.48
1:B:310:ILE:CG2	1:B:312:LEU:HD23	2.43	0.48
1:A:199:TRP:CE2	1:A:357:GLY:HA2	2.48	0.48
1:D:258:ILE:HG23	1:D:387:PHE:HD2	1.76	0.48
1:D:332:ARG:HA	1:D:335:THR:O	2.13	0.48
1:B:332:ARG:HA	1:B:335:THR:O	2.13	0.48
1:B:157:ARG:HB2	1:B:181:VAL:HG21	1.94	0.48
1:A:28:ILE:N	1:A:28:ILE:CD1	2.76	0.48
1:A:157:ARG:HB2	1:A:181:VAL:HG21	1.94	0.48
1:D:364:THR:O	1:D:364:THR:OG1	2.31	0.48
1:C:244:MET:CE	1:C:257:PHE:CD2	2.93	0.48
1:D:244:MET:CE	1:D:257:PHE:CD2	2.93	0.48
1:A:250:VAL:O	1:A:252:ARG:N	2.47	0.48
1:D:235:LEU:HD22	1:D:292:MET:HB2	1.96	0.48
1:A:155:GLN:O	1:A:156:SER:C	2.51	0.48
1:C:310:ILE:CG2	1:C:312:LEU:HD23	2.43	0.48
1:C:364:THR:OG1	1:C:364:THR:O	2.31	0.48
1:B:28:ILE:CD1	1:B:28:ILE:N	2.76	0.48
1:A:332:ARG:HA	1:A:335:THR:O	2.13	0.48
1:B:235:LEU:HD22	1:B:292:MET:HB2	1.96	0.48
1:D:309:ARG:NH1	1:D:309:ARG:HG2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ILE:HG23	1:A:387:PHE:HD2	1.76	0.48
1:C:372:THR:HG22	1:C:373:SER:N	2.28	0.48
1:D:157:ARG:HB2	1:D:181:VAL:HG21	1.94	0.48
1:A:310:ILE:CG2	1:A:312:LEU:HD23	2.43	0.48
1:D:354:ASP:OD2	1:D:357:GLY:N	2.46	0.48
1:D:199:TRP:CE2	1:D:357:GLY:HA2	2.48	0.48
1:B:161:ASN:N	1:B:161:ASN:HD22	2.12	0.48
1:C:132:TYR:HE2	1:C:144:PRO:CG	2.25	0.48
1:B:250:VAL:O	1:B:252:ARG:N	2.47	0.48
1:D:372:THR:CG2	1:D:373:SER:H	2.27	0.48
1:C:332:ARG:HA	1:C:335:THR:O	2.13	0.48
1:B:372:THR:HG22	1:B:373:SER:N	2.29	0.48
1:A:235:LEU:HD22	1:A:292:MET:HB2	1.96	0.48
1:C:309:ARG:NH1	1:C:309:ARG:HG2	2.28	0.48
1:C:250:VAL:O	1:C:252:ARG:N	2.47	0.48
1:D:47:LYS:O	1:D:330:ASP:HB3	2.14	0.48
1:C:373:SER:CB	2:D:442:HOH:O	2.62	0.48
1:A:372:THR:CG2	1:A:373:SER:H	2.27	0.48
1:D:236:ILE:HG22	1:D:237:MET:N	2.29	0.48
1:A:302:PRO:HD3	1:A:383:VAL:O	2.14	0.48
1:C:235:LEU:HD22	1:C:292:MET:HB2	1.96	0.48
1:B:302:PRO:HD3	1:B:383:VAL:O	2.14	0.48
1:D:302:PRO:HD3	1:D:383:VAL:O	2.14	0.48
1:D:250:VAL:O	1:D:252:ARG:N	2.47	0.48
1:D:161:ASN:N	1:D:161:ASN:HD22	2.12	0.48
1:C:372:THR:CG2	1:C:373:SER:H	2.27	0.48
1:A:372:THR:HG22	1:A:373:SER:N	2.28	0.48
1:C:236:ILE:HG22	1:C:237:MET:N	2.29	0.48
1:A:33:TRP:O	1:A:37:SER:OG	2.26	0.48
1:C:157:ARG:HB2	1:C:181:VAL:HG21	1.94	0.48
1:C:302:PRO:HD3	1:C:383:VAL:O	2.14	0.48
1:C:206:GLU:OE1	1:D:348:GLN:OE1	2.31	0.47
1:D:260:LEU:HD11	1:D:382:LYS:O	2.15	0.47
1:D:227:TYR:HA	1:D:299:LEU:O	2.14	0.47
1:D:372:THR:HG22	1:D:373:SER:N	2.28	0.47
1:C:155:GLN:O	1:C:156:SER:C	2.51	0.47
1:A:227:TYR:HA	1:A:299:LEU:O	2.14	0.47
1:D:288:ASP:OD1	1:D:397:LYS:HD3	2.14	0.47
1:A:364:THR:OG1	1:A:364:THR:O	2.31	0.47
1:A:161:ASN:N	1:A:161:ASN:HD22	2.12	0.47
1:A:260:LEU:HD11	1:A:382:LYS:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:TYR:HA	1:B:299:LEU:O	2.15	0.47
1:C:47:LYS:O	1:C:330:ASP:HB3	2.14	0.47
1:A:326:THR:O	1:A:341:ALA:HB2	2.15	0.47
1:B:23:ASN:C	1:B:25:ASP:H	2.17	0.47
1:C:161:ASN:N	1:C:161:ASN:HD22	2.12	0.47
1:A:215:LEU:HD21	1:A:406:CYS:O	2.15	0.47
1:B:215:LEU:HD21	1:B:406:CYS:O	2.15	0.47
1:D:326:THR:O	1:D:341:ALA:HB2	2.15	0.47
1:D:114:LEU:HD23	1:D:114:LEU:O	2.15	0.47
1:D:28:ILE:N	1:D:28:ILE:CD1	2.76	0.47
1:B:258:ILE:HG23	1:B:387:PHE:HD2	1.76	0.47
1:B:47:LYS:O	1:B:330:ASP:HB3	2.14	0.47
1:A:47:LYS:O	1:A:330:ASP:HB3	2.14	0.47
1:A:236:ILE:HG22	1:A:237:MET:N	2.29	0.47
1:C:227:TYR:HA	1:C:299:LEU:O	2.15	0.47
1:C:288:ASP:OD1	1:C:397:LYS:HD3	2.14	0.47
1:B:326:THR:O	1:B:341:ALA:HB2	2.15	0.47
1:A:114:LEU:O	1:A:114:LEU:HD23	2.15	0.47
1:B:114:LEU:O	1:B:114:LEU:HD23	2.15	0.47
1:D:215:LEU:HD21	1:D:406:CYS:O	2.15	0.47
1:A:288:ASP:OD1	1:A:397:LYS:HD3	2.14	0.47
1:D:235:LEU:HD12	1:D:236:ILE:N	2.30	0.47
1:C:326:THR:O	1:C:341:ALA:HB2	2.15	0.47
1:B:260:LEU:HD11	1:B:382:LYS:O	2.15	0.47
1:C:260:LEU:HD11	1:C:382:LYS:O	2.15	0.47
1:B:385:HIS:O	1:B:386:PRO:C	2.54	0.46
1:B:236:ILE:HG22	1:B:237:MET:N	2.29	0.46
1:C:194:TYR:O	1:C:195:PHE:HB2	2.15	0.46
1:D:194:TYR:O	1:D:195:PHE:HB2	2.15	0.46
1:C:95:HIS:CD2	1:C:140:TYR:OH	2.66	0.46
1:C:114:LEU:HD23	1:C:114:LEU:O	2.15	0.46
1:C:160:ILE:O	1:C:164:VAL:HG23	2.15	0.46
1:B:372:THR:CG2	1:B:373:SER:H	2.27	0.46
1:C:372:THR:CG2	1:C:373:SER:N	2.78	0.46
1:D:191:ASN:ND2	1:D:347:HIS:HA	2.31	0.46
1:B:160:ILE:O	1:B:164:VAL:HG23	2.15	0.46
1:D:385:HIS:O	1:D:386:PRO:C	2.54	0.46
1:A:23:ASN:C	1:A:25:ASP:H	2.18	0.46
1:D:23:ASN:C	1:D:25:ASP:H	2.18	0.46
1:C:44:LEU:O	1:C:44:LEU:CG	2.64	0.46
1:B:288:ASP:OD1	1:B:397:LYS:HD3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:TYR:HE1	1:B:145:GLN:HG3	1.81	0.46
1:A:160:ILE:O	1:A:164:VAL:HG23	2.16	0.46
1:C:310:ILE:HG22	1:C:312:LEU:HD23	1.97	0.46
1:C:235:LEU:HD12	1:C:236:ILE:N	2.30	0.46
1:A:194:TYR:O	1:A:195:PHE:HB2	2.15	0.46
1:B:194:TYR:O	1:B:195:PHE:HB2	2.15	0.46
1:A:95:HIS:CD2	1:A:140:TYR:OH	2.66	0.46
1:D:310:ILE:HG22	1:D:312:LEU:HD23	1.97	0.46
1:A:310:ILE:HG22	1:A:312:LEU:HD23	1.97	0.46
1:A:392:ARG:HG2	1:A:393:HIS:N	2.30	0.46
1:B:392:ARG:HG2	1:B:393:HIS:N	2.30	0.46
1:C:392:ARG:HG2	1:C:393:HIS:N	2.30	0.46
1:D:160:ILE:O	1:D:164:VAL:HG23	2.15	0.46
1:B:310:ILE:HG22	1:B:312:LEU:HD23	1.97	0.46
1:C:28:ILE:N	1:C:28:ILE:CD1	2.76	0.46
1:B:235:LEU:HD12	1:B:236:ILE:N	2.30	0.46
1:B:255:SER:OG	1:B:394:ASN:ND2	2.49	0.46
1:C:15:LEU:HD23	1:C:30:PHE:CE1	2.51	0.46
1:C:215:LEU:HD21	1:C:406:CYS:O	2.15	0.46
1:B:191:ASN:ND2	1:B:347:HIS:HA	2.31	0.46
1:C:121:TYR:HE1	1:C:145:GLN:HG3	1.81	0.46
1:A:385:HIS:O	1:A:386:PRO:C	2.54	0.46
1:D:379:LEU:HA	1:D:379:LEU:HD12	1.80	0.46
1:B:354:ASP:C	1:B:356:LYS:H	2.20	0.46
1:D:372:THR:CG2	1:D:373:SER:N	2.78	0.46
1:A:372:THR:CG2	1:A:373:SER:N	2.78	0.46
1:C:23:ASN:C	1:C:25:ASP:H	2.18	0.46
1:B:44:LEU:O	1:B:44:LEU:CG	2.64	0.46
1:D:16:PHE:O	1:D:17:ASN:C	2.55	0.46
1:A:15:LEU:HD23	1:A:30:PHE:CE1	2.51	0.46
1:C:279:THR:CG2	1:C:280:TYR:N	2.78	0.45
1:B:244:MET:CE	1:B:257:PHE:CD2	2.93	0.45
1:A:235:LEU:HD12	1:A:236:ILE:N	2.31	0.45
1:B:279:THR:CG2	1:B:280:TYR:N	2.78	0.45
1:C:191:ASN:ND2	1:C:347:HIS:HA	2.31	0.45
1:A:354:ASP:C	1:A:356:LYS:H	2.20	0.45
1:A:317:ARG:HE	1:D:282:ARG:NH2	2.14	0.45
1:A:44:LEU:CG	1:A:44:LEU:O	2.64	0.45
1:C:385:HIS:O	1:C:386:PRO:C	2.54	0.45
1:A:16:PHE:O	1:A:17:ASN:C	2.55	0.45
1:D:121:TYR:HE1	1:D:145:GLN:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASN:ND2	1:A:347:HIS:HA	2.31	0.45
1:D:392:ARG:HG2	1:D:393:HIS:N	2.30	0.45
1:C:331:PHE:C	1:C:333:GLY:H	2.20	0.45
1:A:121:TYR:HE1	1:A:145:GLN:HG3	1.81	0.45
1:C:255:SER:OG	1:C:394:ASN:ND2	2.49	0.45
1:C:371:THR:O	1:D:305:SER:HB3	2.16	0.45
1:B:331:PHE:C	1:B:333:GLY:H	2.20	0.45
1:D:32:PRO:HD2	1:D:400:LEU:O	2.17	0.45
1:B:372:THR:CG2	1:B:373:SER:N	2.78	0.45
1:B:15:LEU:HD23	1:B:30:PHE:CE1	2.51	0.45
1:D:44:LEU:CG	1:D:44:LEU:O	2.64	0.45
1:B:16:PHE:O	1:B:17:ASN:C	2.55	0.45
1:B:309:ARG:N	1:D:367:ILE:O	2.38	0.45
1:C:354:ASP:C	1:C:356:LYS:H	2.20	0.45
1:A:255:SER:OG	1:A:394:ASN:ND2	2.49	0.45
1:D:279:THR:CG2	1:D:280:TYR:N	2.78	0.45
1:A:95:HIS:CD2	1:A:95:HIS:O	2.70	0.45
1:C:95:HIS:CD2	1:C:95:HIS:O	2.70	0.45
1:C:152:ALA:N	1:C:153:PRO:CD	2.80	0.45
1:B:152:ALA:N	1:B:153:PRO:CD	2.80	0.45
1:C:362:ALA:O	1:C:363:ALA:HB2	2.17	0.45
1:A:279:THR:CG2	1:A:280:TYR:N	2.78	0.44
1:A:152:ALA:N	1:A:153:PRO:CD	2.80	0.44
1:A:362:ALA:O	1:A:363:ALA:HB2	2.17	0.44
1:D:15:LEU:HD23	1:D:30:PHE:CE1	2.51	0.44
1:D:331:PHE:C	1:D:333:GLY:H	2.20	0.44
1:A:139:TYR:CD1	1:A:139:TYR:N	2.85	0.44
1:B:95:HIS:CD2	1:B:140:TYR:OH	2.66	0.44
1:A:331:PHE:C	1:A:333:GLY:H	2.20	0.44
1:C:32:PRO:HD2	1:C:400:LEU:O	2.17	0.44
1:C:211:GLN:O	1:C:222:PRO:HA	2.18	0.44
1:B:95:HIS:O	1:B:95:HIS:CD2	2.70	0.44
1:D:271:LEU:HD22	1:D:388:HIS:HD2	1.83	0.44
1:D:12:THR:HG23	1:D:32:PRO:CB	2.46	0.44
1:A:130:PRO:O	1:A:131:THR:C	2.56	0.44
1:C:139:TYR:CD1	1:C:139:TYR:N	2.86	0.44
1:B:32:PRO:HD2	1:B:400:LEU:O	2.17	0.44
1:D:362:ALA:O	1:D:363:ALA:HB2	2.17	0.44
1:D:139:TYR:N	1:D:139:TYR:CD1	2.85	0.44
1:C:121:TYR:CE2	1:C:160:ILE:HG12	2.53	0.44
1:D:354:ASP:C	1:D:356:LYS:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASN:HD21	1:B:176:LEU:CB	2.31	0.44
1:A:211:GLN:O	1:A:222:PRO:HA	2.18	0.44
1:D:95:HIS:CD2	1:D:95:HIS:O	2.70	0.44
1:C:232:PHE:O	1:C:234:VAL:HG23	2.18	0.44
1:B:300:HIS:HB2	1:B:382:LYS:HA	2.00	0.44
1:B:23:ASN:C	1:B:25:ASP:N	2.72	0.44
1:B:362:ALA:O	1:B:363:ALA:HB2	2.17	0.44
1:B:139:TYR:CD1	1:B:139:TYR:N	2.85	0.44
1:B:121:TYR:CE2	1:B:160:ILE:HG12	2.53	0.44
1:C:12:THR:HG23	1:C:32:PRO:CB	2.46	0.44
1:A:32:PRO:HD2	1:A:400:LEU:O	2.17	0.44
1:D:152:ALA:N	1:D:153:PRO:CD	2.80	0.44
1:B:211:GLN:O	1:B:222:PRO:HA	2.18	0.44
1:A:161:ASN:HD21	1:A:176:LEU:CB	2.31	0.43
1:C:130:PRO:O	1:C:131:THR:C	2.56	0.43
1:A:372:THR:HG22	1:A:373:SER:H	1.84	0.43
1:A:157:ARG:HD3	1:A:181:VAL:CG2	2.48	0.43
1:D:232:PHE:O	1:D:234:VAL:HG23	2.18	0.43
1:A:300:HIS:HB2	1:A:382:LYS:HA	2.00	0.43
1:D:300:HIS:HB2	1:D:382:LYS:HA	2.00	0.43
1:C:23:ASN:C	1:C:25:ASP:N	2.71	0.43
1:B:200:GLU:HG3	2:B:435:HOH:O	2.18	0.43
1:C:16:PHE:O	1:C:17:ASN:C	2.55	0.43
1:B:260:LEU:HD23	1:B:261:PRO:O	2.18	0.43
1:C:157:ARG:HD3	1:C:181:VAL:CG2	2.48	0.43
1:A:389:PHE:C	1:A:389:PHE:CD1	2.92	0.43
1:B:389:PHE:CD1	1:B:389:PHE:C	2.92	0.43
1:C:44:LEU:HD22	1:C:95:HIS:CE1	2.53	0.43
1:C:175:LEU:HG	1:C:346:ILE:HG21	2.01	0.43
1:D:157:ARG:HD3	1:D:181:VAL:CG2	2.48	0.43
1:A:31:SER:HB3	1:A:34:SER:HB3	2.01	0.43
1:C:31:SER:HB3	1:C:34:SER:HB3	2.01	0.43
1:B:379:LEU:HA	1:B:379:LEU:HD12	1.80	0.43
1:D:175:LEU:HG	1:D:346:ILE:HG21	2.01	0.43
1:C:98:PHE:O	1:C:102:LEU:CB	2.67	0.43
1:B:260:LEU:HD11	1:B:383:VAL:HA	2.00	0.43
1:C:271:LEU:HD22	1:C:388:HIS:HD2	1.83	0.43
1:C:161:ASN:HD21	1:C:176:LEU:CB	2.31	0.43
1:C:57:VAL:HG12	1:C:58:LEU:N	2.33	0.43
1:D:211:GLN:O	1:D:222:PRO:HA	2.18	0.43
1:B:234:VAL:HG12	1:B:235:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HB2	1:A:292:MET:HG3	2.00	0.43
1:C:260:LEU:HD11	1:C:383:VAL:HA	2.00	0.43
1:D:389:PHE:CD1	1:D:389:PHE:C	2.92	0.43
1:C:193:ILE:O	1:C:193:ILE:HG23	2.19	0.43
1:A:200:GLU:HG3	2:A:435:HOH:O	2.19	0.43
1:A:193:ILE:O	1:A:193:ILE:HG23	2.19	0.43
1:D:255:SER:OG	1:D:394:ASN:ND2	2.49	0.43
1:D:257:PHE:O	1:D:389:PHE:HA	2.19	0.43
1:B:44:LEU:HD22	1:B:95:HIS:CE1	2.53	0.43
1:A:121:TYR:CE2	1:A:160:ILE:HG12	2.53	0.43
1:D:121:TYR:CE2	1:D:160:ILE:HG12	2.53	0.43
1:D:118:ASN:N	1:D:118:ASN:ND2	2.67	0.43
1:A:234:VAL:HG12	1:A:235:LEU:N	2.34	0.43
1:D:260:LEU:HD11	1:D:383:VAL:HA	2.00	0.43
1:C:260:LEU:HD23	1:C:261:PRO:O	2.18	0.43
1:A:23:ASN:C	1:A:25:ASP:N	2.72	0.43
1:C:200:GLU:HG3	2:C:434:HOH:O	2.18	0.43
1:A:257:PHE:O	1:A:389:PHE:HA	2.19	0.43
1:B:175:LEU:HG	1:B:346:ILE:HG21	2.01	0.43
1:B:57:VAL:HG12	1:B:58:LEU:N	2.33	0.43
1:B:232:PHE:O	1:B:234:VAL:HG23	2.18	0.43
1:C:113:SER:O	1:C:195:PHE:HA	2.19	0.43
1:C:257:PHE:O	1:C:389:PHE:HA	2.19	0.43
1:A:175:LEU:HG	1:A:346:ILE:HG21	2.01	0.43
1:B:289:SER:C	1:B:291:MET:H	2.22	0.43
1:A:103:THR:O	1:A:107:LYS:N	2.39	0.43
1:A:57:VAL:HG12	1:A:58:LEU:N	2.33	0.43
1:D:235:LEU:HB2	1:D:292:MET:HG3	2.01	0.43
1:A:260:LEU:HD11	1:A:383:VAL:HA	2.00	0.43
1:B:113:SER:O	1:B:195:PHE:HA	2.19	0.43
1:B:31:SER:HB3	1:B:34:SER:HB3	2.00	0.43
1:A:245:ILE:HG13	1:A:246:GLU:N	2.34	0.42
1:C:118:ASN:ND2	1:C:118:ASN:N	2.67	0.42
1:D:57:VAL:HG12	1:D:58:LEU:N	2.33	0.42
1:D:234:VAL:HG12	1:D:235:LEU:N	2.34	0.42
1:C:235:LEU:HB2	1:C:292:MET:HG3	2.00	0.42
1:D:260:LEU:HD23	1:D:261:PRO:O	2.18	0.42
1:D:23:ASN:C	1:D:25:ASP:N	2.71	0.42
1:A:113:SER:O	1:A:195:PHE:HA	2.19	0.42
1:C:14:ASP:O	1:C:15:LEU:C	2.58	0.42
1:C:389:PHE:CD1	1:C:389:PHE:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PHE:O	1:B:389:PHE:HA	2.19	0.42
1:B:311:ASP:N	1:D:365:ALA:O	2.47	0.42
1:B:372:THR:HG22	1:B:373:SER:H	1.84	0.42
1:A:260:LEU:HD23	1:A:261:PRO:O	2.18	0.42
1:C:234:VAL:HG12	1:C:235:LEU:N	2.34	0.42
1:B:14:ASP:O	1:B:15:LEU:C	2.58	0.42
1:D:14:ASP:O	1:D:15:LEU:C	2.58	0.42
1:D:98:PHE:O	1:D:102:LEU:CB	2.67	0.42
1:A:44:LEU:HD22	1:A:95:HIS:CE1	2.53	0.42
1:A:118:ASN:N	1:A:118:ASN:ND2	2.67	0.42
1:B:98:PHE:O	1:B:102:LEU:CB	2.67	0.42
1:A:340:LEU:HD22	1:A:341:ALA:H	1.85	0.42
1:A:98:PHE:O	1:A:102:LEU:CB	2.67	0.42
1:D:189:LEU:O	1:D:345:VAL:HA	2.20	0.42
1:D:31:SER:HB3	1:D:34:SER:HB3	2.01	0.42
1:B:245:ILE:HG13	1:B:246:GLU:N	2.34	0.42
1:B:312:LEU:HB3	1:B:316:LEU:CD1	2.50	0.42
1:D:289:SER:C	1:D:291:MET:H	2.22	0.42
1:B:157:ARG:HD3	1:B:181:VAL:CG2	2.48	0.42
1:A:232:PHE:O	1:A:234:VAL:HG23	2.18	0.42
1:A:116:SER:HA	1:A:193:ILE:HA	2.02	0.42
1:B:18:LYS:O	1:B:19:LEU:C	2.58	0.42
1:B:364:THR:OG1	1:B:364:THR:O	2.32	0.42
1:A:27:ASN:ND2	1:A:407:CYS:HB2	2.35	0.42
1:B:236:ILE:CG2	1:B:237:MET:N	2.83	0.42
1:A:312:LEU:HB3	1:A:316:LEU:CD1	2.50	0.42
1:A:200:GLU:O	1:A:201:VAL:HB	2.20	0.42
1:D:44:LEU:HD22	1:D:95:HIS:CE1	2.53	0.42
1:C:245:ILE:HG13	1:C:246:GLU:N	2.35	0.42
1:C:289:SER:C	1:C:291:MET:H	2.22	0.42
1:C:372:THR:HG22	1:C:373:SER:H	1.84	0.42
1:C:103:THR:O	1:C:107:LYS:N	2.39	0.42
1:B:227:TYR:CG	1:B:228:MET:N	2.88	0.42
1:D:113:SER:O	1:D:195:PHE:HA	2.19	0.42
1:B:116:SER:HA	1:B:193:ILE:HA	2.02	0.42
1:B:340:LEU:C	1:B:340:LEU:HD13	2.40	0.42
1:A:271:LEU:HD22	1:A:388:HIS:HD2	1.83	0.42
1:A:12:THR:HG23	1:A:32:PRO:CB	2.46	0.42
1:B:199:TRP:CD1	1:B:357:GLY:N	2.88	0.42
1:C:199:TRP:CD1	1:C:357:GLY:N	2.88	0.42
1:D:161:ASN:HD21	1:D:176:LEU:CB	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:TYR:C	1:C:112:TYR:CD1	2.93	0.42
1:B:235:LEU:HB2	1:B:292:MET:HG3	2.01	0.42
1:B:200:GLU:O	1:B:201:VAL:HB	2.20	0.42
1:C:116:SER:HA	1:C:193:ILE:HA	2.02	0.42
1:B:193:ILE:HG23	1:B:193:ILE:O	2.19	0.42
1:D:200:GLU:HG3	2:D:436:HOH:O	2.18	0.42
1:A:282:ARG:HH21	1:D:317:ARG:HH21	1.67	0.42
1:B:392:ARG:CD	1:B:397:LYS:HA	2.46	0.42
1:D:330:ASP:C	1:D:332:ARG:H	2.24	0.42
1:A:289:SER:C	1:A:291:MET:H	2.22	0.42
1:D:130:PRO:O	1:D:131:THR:C	2.56	0.42
1:D:312:LEU:HB3	1:D:316:LEU:CD1	2.50	0.42
1:D:227:TYR:CG	1:D:228:MET:N	2.88	0.42
1:C:200:GLU:O	1:C:201:VAL:HB	2.20	0.42
1:D:16:PHE:CD1	1:D:28:ILE:HG21	2.55	0.42
1:B:330:ASP:C	1:B:332:ARG:H	2.24	0.42
1:C:330:ASP:C	1:C:332:ARG:H	2.24	0.42
1:A:189:LEU:O	1:A:345:VAL:HA	2.20	0.42
1:C:27:ASN:ND2	1:C:407:CYS:HB2	2.35	0.42
1:C:300:HIS:HB2	1:C:382:LYS:HA	2.00	0.42
1:B:215:LEU:CD2	1:B:406:CYS:O	2.68	0.42
1:A:14:ASP:O	1:A:15:LEU:C	2.58	0.42
1:B:27:ASN:ND2	1:B:407:CYS:HB2	2.35	0.41
1:A:244:MET:CE	1:A:257:PHE:CD2	2.93	0.41
1:A:16:PHE:CD1	1:A:28:ILE:HG21	2.55	0.41
1:A:330:ASP:C	1:A:332:ARG:H	2.24	0.41
1:C:373:SER:CB	1:C:374:VAL:HG23	2.50	0.41
1:A:112:TYR:C	1:A:112:TYR:CD1	2.93	0.41
1:D:236:ILE:CG2	1:D:237:MET:N	2.83	0.41
1:D:347:HIS:ND1	1:D:348:GLN:N	2.69	0.41
1:A:347:HIS:ND1	1:A:348:GLN:N	2.69	0.41
1:C:42:THR:HB	1:C:331:PHE:CE2	2.55	0.41
1:D:42:THR:HB	1:D:331:PHE:CE2	2.55	0.41
1:B:271:LEU:HD22	1:B:388:HIS:HD2	1.83	0.41
1:B:340:LEU:HD22	1:B:341:ALA:H	1.85	0.41
1:A:199:TRP:CD1	1:A:357:GLY:N	2.88	0.41
1:A:215:LEU:CD2	1:A:406:CYS:O	2.68	0.41
1:B:255:SER:CB	1:B:394:ASN:HD21	2.33	0.41
1:D:255:SER:CB	1:D:394:ASN:HD21	2.33	0.41
1:D:193:ILE:O	1:D:193:ILE:HG23	2.19	0.41
1:D:340:LEU:HD22	1:D:341:ALA:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:PHE:CD1	1:C:28:ILE:HG21	2.55	0.41
1:A:379:LEU:HD12	1:A:379:LEU:HA	1.80	0.41
1:C:236:ILE:CG2	1:C:237:MET:N	2.83	0.41
1:B:347:HIS:ND1	1:B:348:GLN:N	2.69	0.41
1:D:372:THR:HG22	1:D:373:SER:H	1.84	0.41
1:C:189:LEU:O	1:C:345:VAL:HA	2.20	0.41
1:D:27:ASN:ND2	1:D:407:CYS:HB2	2.35	0.41
1:C:227:TYR:CG	1:C:228:MET:N	2.88	0.41
1:D:10:ASN:O	1:D:11:PHE:C	2.58	0.41
1:C:347:HIS:ND1	1:C:348:GLN:N	2.68	0.41
1:D:254:LEU:HA	1:D:392:ARG:O	2.20	0.41
1:A:340:LEU:HD13	1:A:340:LEU:C	2.40	0.41
1:A:227:TYR:CG	1:A:228:MET:N	2.88	0.41
1:C:331:PHE:C	1:C:333:GLY:N	2.74	0.41
1:D:199:TRP:CD1	1:D:357:GLY:N	2.88	0.41
1:D:200:GLU:O	1:D:201:VAL:HB	2.20	0.41
1:D:116:SER:HA	1:D:193:ILE:HA	2.02	0.41
1:B:10:ASN:O	1:B:11:PHE:C	2.58	0.41
1:D:331:PHE:C	1:D:333:GLY:N	2.74	0.41
1:B:16:PHE:CD1	1:B:28:ILE:HG21	2.55	0.41
1:A:373:SER:CB	1:A:374:VAL:HG23	2.50	0.41
1:B:189:LEU:O	1:B:345:VAL:HA	2.20	0.41
1:C:312:LEU:HB3	1:C:316:LEU:CD1	2.50	0.41
1:C:18:LYS:O	1:C:19:LEU:C	2.58	0.41
1:D:98:PHE:HB3	1:D:140:TYR:HE1	1.86	0.41
1:D:340:LEU:C	1:D:340:LEU:HD13	2.40	0.41
1:A:236:ILE:CG2	1:A:237:MET:N	2.83	0.41
1:C:215:LEU:CD2	1:C:406:CYS:O	2.68	0.41
1:D:200:GLU:C	1:D:201:VAL:HG23	2.41	0.41
1:D:364:THR:HG1	1:D:367:ILE:HD11	1.85	0.41
1:B:254:LEU:HA	1:B:392:ARG:O	2.20	0.41
1:C:254:LEU:HA	1:C:392:ARG:O	2.20	0.41
1:A:42:THR:HB	1:A:331:PHE:CE2	2.55	0.41
1:C:340:LEU:C	1:C:340:LEU:HD13	2.40	0.41
1:B:12:THR:HG23	1:B:32:PRO:CB	2.46	0.41
1:D:373:SER:CB	1:D:374:VAL:HG23	2.50	0.41
1:D:103:THR:O	1:D:107:LYS:N	2.39	0.41
1:B:112:TYR:C	1:B:112:TYR:CD1	2.94	0.41
1:D:260:LEU:HD23	1:D:260:LEU:C	2.42	0.41
1:C:260:LEU:HD23	1:C:260:LEU:C	2.42	0.41
1:C:255:SER:CB	1:C:394:ASN:HD21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:HA	1:A:392:ARG:O	2.20	0.41
1:B:392:ARG:HD2	1:B:397:LYS:CA	2.45	0.41
1:A:120:ILE:HD13	1:A:334:MET:HE1	2.03	0.41
1:D:245:ILE:HG13	1:D:246:GLU:N	2.34	0.41
1:B:130:PRO:O	1:B:131:THR:C	2.56	0.41
1:A:260:LEU:C	1:A:260:LEU:HD23	2.42	0.41
1:A:255:SER:CB	1:A:394:ASN:HD21	2.33	0.41
1:C:10:ASN:O	1:C:11:PHE:C	2.58	0.40
1:B:42:THR:HB	1:B:331:PHE:CE2	2.55	0.40
1:D:350:PHE:C	1:D:350:PHE:HD1	2.24	0.40
1:D:215:LEU:CD2	1:D:406:CYS:O	2.68	0.40
1:B:39:LEU:HA	1:B:39:LEU:HD23	1.96	0.40
1:A:18:LYS:O	1:A:19:LEU:C	2.58	0.40
1:D:392:ARG:HD2	1:D:397:LYS:CA	2.45	0.40
1:B:373:SER:CB	1:B:374:VAL:HG23	2.50	0.40
1:B:331:PHE:C	1:B:333:GLY:N	2.74	0.40
1:B:36:SER:O	1:B:40:ALA:N	2.54	0.40
1:D:112:TYR:C	1:D:112:TYR:CD1	2.94	0.40
1:C:200:GLU:C	1:C:201:VAL:HG23	2.41	0.40
1:D:18:LYS:O	1:D:19:LEU:C	2.58	0.40
1:D:246:GLU:HG2	1:D:248:PRO:HG3	2.04	0.40
1:A:346:ILE:CD1	1:A:346:ILE:N	2.84	0.40
1:C:346:ILE:N	1:C:346:ILE:CD1	2.84	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	354/423 (84%)	275 (78%)	61 (17%)	18 (5%)	2 15
1	B	354/423 (84%)	275 (78%)	61 (17%)	18 (5%)	2 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	354/423 (84%)	276 (78%)	60 (17%)	18 (5%)	2 15
1	D	354/423 (84%)	275 (78%)	61 (17%)	18 (5%)	2 15
All	All	1416/1692 (84%)	1101 (78%)	243 (17%)	72 (5%)	2 15

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	LYS
1	A	108	PRO
1	A	130	PRO
1	A	173	LYS
1	A	251	LYS
1	A	359	GLU
1	A	363	ALA
1	A	365	ALA
1	B	107	LYS
1	B	108	PRO
1	B	130	PRO
1	B	173	LYS
1	B	251	LYS
1	B	359	GLU
1	B	363	ALA
1	B	365	ALA
1	C	107	LYS
1	C	108	PRO
1	C	130	PRO
1	C	173	LYS
1	C	251	LYS
1	C	359	GLU
1	C	363	ALA
1	C	365	ALA
1	D	107	LYS
1	D	108	PRO
1	D	130	PRO
1	D	173	LYS
1	D	251	LYS
1	D	359	GLU
1	D	363	ALA
1	D	365	ALA
1	A	141	LYS
1	B	141	LYS

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Mol	Chain	Res	Type
1	C	141	LYS
1	D	141	LYS
1	A	195	PHE
1	B	195	PHE
1	C	195	PHE
1	D	195	PHE
1	A	201	VAL
1	A	394	ASN
1	A	406	CYS
1	B	201	VAL
1	B	394	ASN
1	B	406	CYS
1	C	201	VAL
1	C	394	ASN
1	C	406	CYS
1	D	201	VAL
1	D	394	ASN
1	D	406	CYS
1	A	237	MET
1	B	237	MET
1	C	237	MET
1	D	237	MET
1	A	193	ILE
1	A	345	VAL
1	B	193	ILE
1	B	345	VAL
1	C	193	ILE
1	C	345	VAL
1	D	193	ILE
1	D	345	VAL
1	A	250	VAL
1	B	250	VAL
1	C	250	VAL
1	D	250	VAL
1	A	386	PRO
1	B	386	PRO
1	C	386	PRO
1	D	386	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	270/379 (71%)	251 (93%)	19 (7%)	19 55
1	B	270/379 (71%)	251 (93%)	19 (7%)	19 55
1	C	270/379 (71%)	251 (93%)	19 (7%)	19 55
1	D	270/379 (71%)	251 (93%)	19 (7%)	19 55
All	All	1080/1516 (71%)	1004 (93%)	76 (7%)	19 55

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	LEU
1	A	125	THR
1	A	130	PRO
1	A	131	THR
1	A	139	TYR
1	A	143	GLU
1	A	145	GLN
1	A	179	ASP
1	A	190	VAL
1	A	191	ASN
1	A	204	GLN
1	A	244	MET
1	A	250	VAL
1	A	263	ASP
1	A	283	LEU
1	A	298	ASP
1	A	326	THR
1	A	364	THR
1	A	378	VAL
1	B	114	LEU
1	B	125	THR
1	B	130	PRO
1	B	131	THR
1	B	139	TYR

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Mol	Chain	Res	Type
1	B	143	GLU
1	B	145	GLN
1	B	179	ASP
1	B	190	VAL
1	B	191	ASN
1	B	204	GLN
1	B	244	MET
1	B	250	VAL
1	B	263	ASP
1	B	283	LEU
1	B	298	ASP
1	B	326	THR
1	B	364	THR
1	B	378	VAL
1	C	114	LEU
1	C	125	THR
1	C	130	PRO
1	C	131	THR
1	C	139	TYR
1	C	143	GLU
1	C	145	GLN
1	C	179	ASP
1	C	190	VAL
1	C	191	ASN
1	C	204	GLN
1	C	244	MET
1	C	250	VAL
1	C	263	ASP
1	C	283	LEU
1	C	298	ASP
1	C	326	THR
1	C	364	THR
1	C	378	VAL
1	D	114	LEU
1	D	125	THR
1	D	130	PRO
1	D	131	THR
1	D	139	TYR
1	D	143	GLU
1	D	145	GLN
1	D	179	ASP
1	D	190	VAL

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Mol	Chain	Res	Type
1	D	191	ASN
1	D	204	GLN
1	D	244	MET
1	D	250	VAL
1	D	263	ASP
1	D	283	LEU
1	D	298	ASP
1	D	326	THR
1	D	364	THR
1	D	378	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	20	ASN
1	A	27	ASN
1	A	106	ASN
1	A	118	ASN
1	A	161	ASN
1	A	191	ASN
1	A	204	GLN
1	A	211	GLN
1	A	347	HIS
1	B	10	ASN
1	B	20	ASN
1	B	27	ASN
1	B	106	ASN
1	B	118	ASN
1	B	161	ASN
1	B	174	ASN
1	B	191	ASN
1	B	204	GLN
1	B	211	GLN
1	B	347	HIS
1	C	10	ASN
1	C	20	ASN
1	C	27	ASN
1	C	106	ASN
1	C	118	ASN
1	C	161	ASN
1	C	191	ASN

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Mol	Chain	Res	Type
1	C	204	GLN
1	C	211	GLN
1	C	347	HIS
1	D	10	ASN
1	D	20	ASN
1	D	27	ASN
1	D	106	ASN
1	D	118	ASN
1	D	161	ASN
1	D	191	ASN
1	D	204	GLN
1	D	211	GLN
1	D	347	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	366/423 (86%)	-0.09	1 (0%)	94	84	15, 40, 75, 99	0
1	B	366/423 (86%)	-0.15	1 (0%)	94	84	15, 40, 75, 99	0
1	C	366/423 (86%)	-0.15	2 (0%)	91	76	15, 40, 75, 99	0
1	D	366/423 (86%)	-0.17	1 (0%)	94	84	15, 40, 75, 99	0
All	All	1464/1692 (86%)	-0.14	5 (0%)	94	84	15, 40, 76, 99	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	410	GLU	2.5
1	C	364	THR	2.3
1	D	4	VAL	2.2
1	C	368	ILE	2.0
1	A	263	ASP	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.