Full wwPDB X-ray Structure Validation Report (i)

Oct 7, 2023 – 02:44 PM EDT

PDB ID	:	6DHJ
Title	:	Crystal structures of cyanuric acid hydrolase from Moorella thermoacetica
Authors	:	Shi, K.; Aihara, H.
Deposited on	:	2018-05-20
Resolution	:	3.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

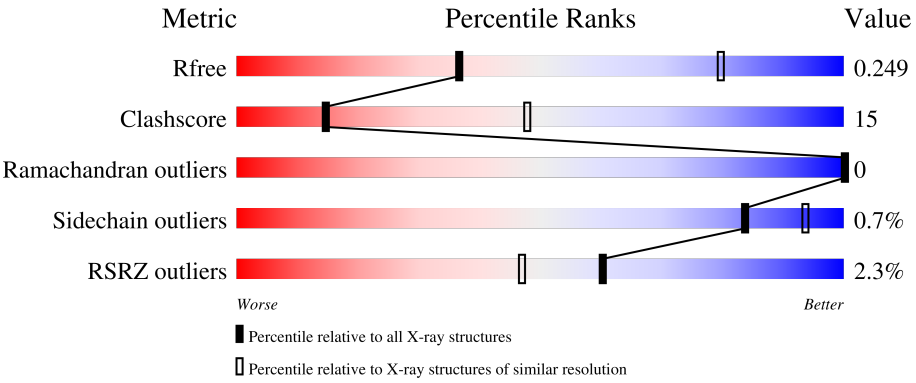
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	370	2% 74% 24%
1	B	370	% 76% 22%
1	C	370	2% 73% 25%
1	D	370	76% 22%
1	E	370	2% 73% 25%

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Mol	Chain	Length	Quality of chain
1	F	370	
1	G	370	
1	H	370	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 21566 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 Cyanuric acid amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2707	1677	484	533	13			
1	B	363	Total	C	N	O	S	0	0	0
			2688	1666	480	529	13			
1	C	362	Total	C	N	O	S	0	0	0
			2680	1660	479	528	13			
1	D	364	Total	C	N	O	S	0	0	0
			2697	1671	481	532	13			
1	E	364	Total	C	N	O	S	0	0	0
			2697	1671	481	532	13			
1	F	357	Total	C	N	O	S	0	0	0
			2647	1640	473	522	12			
1	G	359	Total	C	N	O	S	0	0	0
			2658	1645	476	525	12			
1	H	363	Total	C	N	O	S	0	0	0
			2688	1666	480	529	13			

There are 224 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	SER	CYS	engineered mutation	UNP Q2RGM7
A	53	CYS	GLY	engineered mutation	UNP Q2RGM7
A	103	ALA	GLN	engineered mutation	UNP Q2RGM7
A	104	ALA	GLU	engineered mutation	UNP Q2RGM7
A	107	ALA	LYS	engineered mutation	UNP Q2RGM7
A	162	ALA	CYS	engineered mutation	UNP Q2RGM7
A	218	VAL	CYS	engineered mutation	UNP Q2RGM7
A	235	CYS	GLU	engineered mutation	UNP Q2RGM7
A	279	ILE	LEU	engineered mutation	UNP Q2RGM7
A	280	ARG	LYS	engineered mutation	UNP Q2RGM7
A	281	SER	PHE	engineered mutation	UNP Q2RGM7
A	?	-	CYS	deletion	UNP Q2RGM7
A	?	-	CYS	deletion	UNP Q2RGM7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP Q2RGM7
A	?	-	PRO	deletion	UNP Q2RGM7
A	?	-	ALA	deletion	UNP Q2RGM7
A	283	ASP	GLU	engineered mutation	UNP Q2RGM7
A	290	MET	LEU	engineered mutation	UNP Q2RGM7
A	291	ASP	ALA	engineered mutation	UNP Q2RGM7
A	292	ARG	LYS	engineered mutation	UNP Q2RGM7
A	368	LEU	-	expression tag	UNP Q2RGM7
A	369	GLU	-	expression tag	UNP Q2RGM7
A	370	HIS	-	expression tag	UNP Q2RGM7
A	371	HIS	-	expression tag	UNP Q2RGM7
A	372	HIS	-	expression tag	UNP Q2RGM7
A	373	HIS	-	expression tag	UNP Q2RGM7
A	374	HIS	-	expression tag	UNP Q2RGM7
A	375	HIS	-	expression tag	UNP Q2RGM7
B	46	SER	CYS	engineered mutation	UNP Q2RGM7
B	53	CYS	GLY	engineered mutation	UNP Q2RGM7
B	103	ALA	GLN	engineered mutation	UNP Q2RGM7
B	104	ALA	GLU	engineered mutation	UNP Q2RGM7
B	107	ALA	LYS	engineered mutation	UNP Q2RGM7
B	162	ALA	CYS	engineered mutation	UNP Q2RGM7
B	218	VAL	CYS	engineered mutation	UNP Q2RGM7
B	235	CYS	GLU	engineered mutation	UNP Q2RGM7
B	279	ILE	LEU	engineered mutation	UNP Q2RGM7
B	280	ARG	LYS	engineered mutation	UNP Q2RGM7
B	281	SER	PHE	engineered mutation	UNP Q2RGM7
B	?	-	CYS	deletion	UNP Q2RGM7
B	?	-	CYS	deletion	UNP Q2RGM7
B	?	-	PRO	deletion	UNP Q2RGM7
B	?	-	PRO	deletion	UNP Q2RGM7
B	?	-	ALA	deletion	UNP Q2RGM7
B	283	ASP	GLU	engineered mutation	UNP Q2RGM7
B	290	MET	LEU	engineered mutation	UNP Q2RGM7
B	291	ASP	ALA	engineered mutation	UNP Q2RGM7
B	292	ARG	LYS	engineered mutation	UNP Q2RGM7
B	368	LEU	-	expression tag	UNP Q2RGM7
B	369	GLU	-	expression tag	UNP Q2RGM7
B	370	HIS	-	expression tag	UNP Q2RGM7
B	371	HIS	-	expression tag	UNP Q2RGM7
B	372	HIS	-	expression tag	UNP Q2RGM7
B	373	HIS	-	expression tag	UNP Q2RGM7
B	374	HIS	-	expression tag	UNP Q2RGM7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	375	HIS	-	expression tag	UNP Q2RGM7
C	46	SER	CYS	engineered mutation	UNP Q2RGM7
C	53	CYS	GLY	engineered mutation	UNP Q2RGM7
C	103	ALA	GLN	engineered mutation	UNP Q2RGM7
C	104	ALA	GLU	engineered mutation	UNP Q2RGM7
C	107	ALA	LYS	engineered mutation	UNP Q2RGM7
C	162	ALA	CYS	engineered mutation	UNP Q2RGM7
C	218	VAL	CYS	engineered mutation	UNP Q2RGM7
C	235	CYS	GLU	engineered mutation	UNP Q2RGM7
C	279	ILE	LEU	engineered mutation	UNP Q2RGM7
C	280	ARG	LYS	engineered mutation	UNP Q2RGM7
C	281	SER	PHE	engineered mutation	UNP Q2RGM7
C	?	-	CYS	deletion	UNP Q2RGM7
C	?	-	CYS	deletion	UNP Q2RGM7
C	?	-	PRO	deletion	UNP Q2RGM7
C	?	-	PRO	deletion	UNP Q2RGM7
C	?	-	ALA	deletion	UNP Q2RGM7
C	283	ASP	GLU	engineered mutation	UNP Q2RGM7
C	290	MET	LEU	engineered mutation	UNP Q2RGM7
C	291	ASP	ALA	engineered mutation	UNP Q2RGM7
C	292	ARG	LYS	engineered mutation	UNP Q2RGM7
C	368	LEU	-	expression tag	UNP Q2RGM7
C	369	GLU	-	expression tag	UNP Q2RGM7
C	370	HIS	-	expression tag	UNP Q2RGM7
C	371	HIS	-	expression tag	UNP Q2RGM7
C	372	HIS	-	expression tag	UNP Q2RGM7
C	373	HIS	-	expression tag	UNP Q2RGM7
C	374	HIS	-	expression tag	UNP Q2RGM7
C	375	HIS	-	expression tag	UNP Q2RGM7
D	46	SER	CYS	engineered mutation	UNP Q2RGM7
D	53	CYS	GLY	engineered mutation	UNP Q2RGM7
D	103	ALA	GLN	engineered mutation	UNP Q2RGM7
D	104	ALA	GLU	engineered mutation	UNP Q2RGM7
D	107	ALA	LYS	engineered mutation	UNP Q2RGM7
D	162	ALA	CYS	engineered mutation	UNP Q2RGM7
D	218	VAL	CYS	engineered mutation	UNP Q2RGM7
D	235	CYS	GLU	engineered mutation	UNP Q2RGM7
D	279	ILE	LEU	engineered mutation	UNP Q2RGM7
D	280	ARG	LYS	engineered mutation	UNP Q2RGM7
D	281	SER	PHE	engineered mutation	UNP Q2RGM7
D	?	-	CYS	deletion	UNP Q2RGM7
D	?	-	CYS	deletion	UNP Q2RGM7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP Q2RGM7
D	?	-	PRO	deletion	UNP Q2RGM7
D	?	-	ALA	deletion	UNP Q2RGM7
D	283	ASP	GLU	engineered mutation	UNP Q2RGM7
D	290	MET	LEU	engineered mutation	UNP Q2RGM7
D	291	ASP	ALA	engineered mutation	UNP Q2RGM7
D	292	ARG	LYS	engineered mutation	UNP Q2RGM7
D	368	LEU	-	expression tag	UNP Q2RGM7
D	369	GLU	-	expression tag	UNP Q2RGM7
D	370	HIS	-	expression tag	UNP Q2RGM7
D	371	HIS	-	expression tag	UNP Q2RGM7
D	372	HIS	-	expression tag	UNP Q2RGM7
D	373	HIS	-	expression tag	UNP Q2RGM7
D	374	HIS	-	expression tag	UNP Q2RGM7
D	375	HIS	-	expression tag	UNP Q2RGM7
E	46	SER	CYS	engineered mutation	UNP Q2RGM7
E	53	CYS	GLY	engineered mutation	UNP Q2RGM7
E	103	ALA	GLN	engineered mutation	UNP Q2RGM7
E	104	ALA	GLU	engineered mutation	UNP Q2RGM7
E	107	ALA	LYS	engineered mutation	UNP Q2RGM7
E	162	ALA	CYS	engineered mutation	UNP Q2RGM7
E	218	VAL	CYS	engineered mutation	UNP Q2RGM7
E	235	CYS	GLU	engineered mutation	UNP Q2RGM7
E	279	ILE	LEU	engineered mutation	UNP Q2RGM7
E	280	ARG	LYS	engineered mutation	UNP Q2RGM7
E	281	SER	PHE	engineered mutation	UNP Q2RGM7
E	?	-	CYS	deletion	UNP Q2RGM7
E	?	-	CYS	deletion	UNP Q2RGM7
E	?	-	PRO	deletion	UNP Q2RGM7
E	?	-	PRO	deletion	UNP Q2RGM7
E	?	-	ALA	deletion	UNP Q2RGM7
E	283	ASP	GLU	engineered mutation	UNP Q2RGM7
E	290	MET	LEU	engineered mutation	UNP Q2RGM7
E	291	ASP	ALA	engineered mutation	UNP Q2RGM7
E	292	ARG	LYS	engineered mutation	UNP Q2RGM7
E	368	LEU	-	expression tag	UNP Q2RGM7
E	369	GLU	-	expression tag	UNP Q2RGM7
E	370	HIS	-	expression tag	UNP Q2RGM7
E	371	HIS	-	expression tag	UNP Q2RGM7
E	372	HIS	-	expression tag	UNP Q2RGM7
E	373	HIS	-	expression tag	UNP Q2RGM7
E	374	HIS	-	expression tag	UNP Q2RGM7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	375	HIS	-	expression tag	UNP Q2RGM7
F	46	SER	CYS	engineered mutation	UNP Q2RGM7
F	53	CYS	GLY	engineered mutation	UNP Q2RGM7
F	103	ALA	GLN	engineered mutation	UNP Q2RGM7
F	104	ALA	GLU	engineered mutation	UNP Q2RGM7
F	107	ALA	LYS	engineered mutation	UNP Q2RGM7
F	162	ALA	CYS	engineered mutation	UNP Q2RGM7
F	218	VAL	CYS	engineered mutation	UNP Q2RGM7
F	235	CYS	GLU	engineered mutation	UNP Q2RGM7
F	279	ILE	LEU	engineered mutation	UNP Q2RGM7
F	280	ARG	LYS	engineered mutation	UNP Q2RGM7
F	281	SER	PHE	engineered mutation	UNP Q2RGM7
F	?	-	CYS	deletion	UNP Q2RGM7
F	?	-	CYS	deletion	UNP Q2RGM7
F	?	-	PRO	deletion	UNP Q2RGM7
F	?	-	PRO	deletion	UNP Q2RGM7
F	?	-	ALA	deletion	UNP Q2RGM7
F	283	ASP	GLU	engineered mutation	UNP Q2RGM7
F	290	MET	LEU	engineered mutation	UNP Q2RGM7
F	291	ASP	ALA	engineered mutation	UNP Q2RGM7
F	292	ARG	LYS	engineered mutation	UNP Q2RGM7
F	368	LEU	-	expression tag	UNP Q2RGM7
F	369	GLU	-	expression tag	UNP Q2RGM7
F	370	HIS	-	expression tag	UNP Q2RGM7
F	371	HIS	-	expression tag	UNP Q2RGM7
F	372	HIS	-	expression tag	UNP Q2RGM7
F	373	HIS	-	expression tag	UNP Q2RGM7
F	374	HIS	-	expression tag	UNP Q2RGM7
F	375	HIS	-	expression tag	UNP Q2RGM7
G	46	SER	CYS	engineered mutation	UNP Q2RGM7
G	53	CYS	GLY	engineered mutation	UNP Q2RGM7
G	103	ALA	GLN	engineered mutation	UNP Q2RGM7
G	104	ALA	GLU	engineered mutation	UNP Q2RGM7
G	107	ALA	LYS	engineered mutation	UNP Q2RGM7
G	162	ALA	CYS	engineered mutation	UNP Q2RGM7
G	218	VAL	CYS	engineered mutation	UNP Q2RGM7
G	235	CYS	GLU	engineered mutation	UNP Q2RGM7
G	279	ILE	LEU	engineered mutation	UNP Q2RGM7
G	280	ARG	LYS	engineered mutation	UNP Q2RGM7
G	281	SER	PHE	engineered mutation	UNP Q2RGM7
G	?	-	CYS	deletion	UNP Q2RGM7
G	?	-	CYS	deletion	UNP Q2RGM7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	PRO	deletion	UNP Q2RGM7
G	?	-	PRO	deletion	UNP Q2RGM7
G	?	-	ALA	deletion	UNP Q2RGM7
G	283	ASP	GLU	engineered mutation	UNP Q2RGM7
G	290	MET	LEU	engineered mutation	UNP Q2RGM7
G	291	ASP	ALA	engineered mutation	UNP Q2RGM7
G	292	ARG	LYS	engineered mutation	UNP Q2RGM7
G	368	LEU	-	expression tag	UNP Q2RGM7
G	369	GLU	-	expression tag	UNP Q2RGM7
G	370	HIS	-	expression tag	UNP Q2RGM7
G	371	HIS	-	expression tag	UNP Q2RGM7
G	372	HIS	-	expression tag	UNP Q2RGM7
G	373	HIS	-	expression tag	UNP Q2RGM7
G	374	HIS	-	expression tag	UNP Q2RGM7
G	375	HIS	-	expression tag	UNP Q2RGM7
H	46	SER	CYS	engineered mutation	UNP Q2RGM7
H	53	CYS	GLY	engineered mutation	UNP Q2RGM7
H	103	ALA	GLN	engineered mutation	UNP Q2RGM7
H	104	ALA	GLU	engineered mutation	UNP Q2RGM7
H	107	ALA	LYS	engineered mutation	UNP Q2RGM7
H	162	ALA	CYS	engineered mutation	UNP Q2RGM7
H	218	VAL	CYS	engineered mutation	UNP Q2RGM7
H	235	CYS	GLU	engineered mutation	UNP Q2RGM7
H	279	ILE	LEU	engineered mutation	UNP Q2RGM7
H	280	ARG	LYS	engineered mutation	UNP Q2RGM7
H	281	SER	PHE	engineered mutation	UNP Q2RGM7
H	?	-	CYS	deletion	UNP Q2RGM7
H	?	-	CYS	deletion	UNP Q2RGM7
H	?	-	PRO	deletion	UNP Q2RGM7
H	?	-	PRO	deletion	UNP Q2RGM7
H	?	-	ALA	deletion	UNP Q2RGM7
H	283	ASP	GLU	engineered mutation	UNP Q2RGM7
H	290	MET	LEU	engineered mutation	UNP Q2RGM7
H	291	ASP	ALA	engineered mutation	UNP Q2RGM7
H	292	ARG	LYS	engineered mutation	UNP Q2RGM7
H	368	LEU	-	expression tag	UNP Q2RGM7
H	369	GLU	-	expression tag	UNP Q2RGM7
H	370	HIS	-	expression tag	UNP Q2RGM7
H	371	HIS	-	expression tag	UNP Q2RGM7
H	372	HIS	-	expression tag	UNP Q2RGM7
H	373	HIS	-	expression tag	UNP Q2RGM7
H	374	HIS	-	expression tag	UNP Q2RGM7

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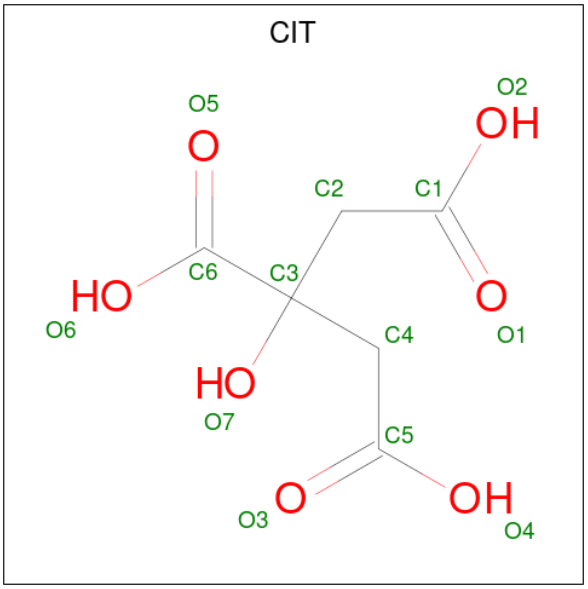
Chain	Residue	Modelled	Actual	Comment	Reference
H	375	HIS	-	expression tag	UNP Q2RGM7

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



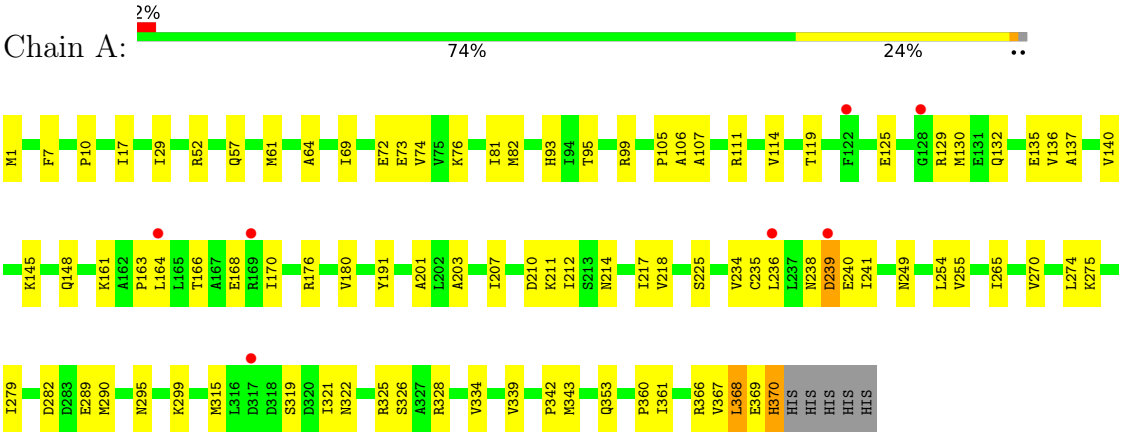
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0
2	G	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0

3 Residue-property plots (i)

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

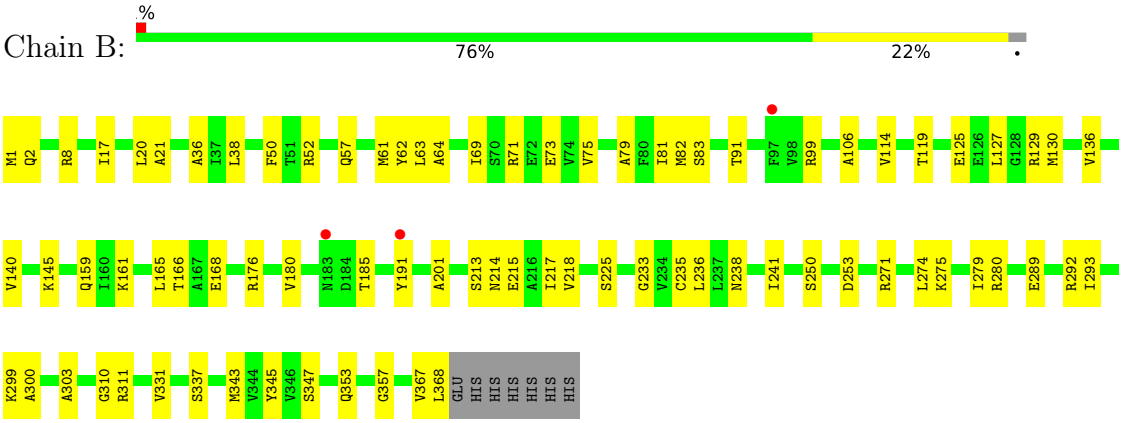
• Molecule 1: Cyanuric acid amidohydrolase

Chain A:



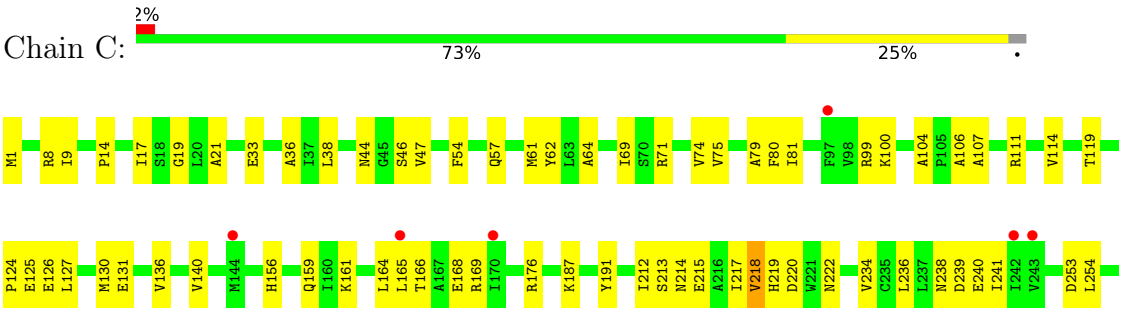
• Molecule 1: Cyanuric acid amidohydrolase

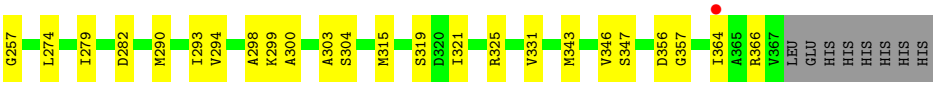
Chain B:



• Molecule 1: Cyanuric acid amidohydrolase

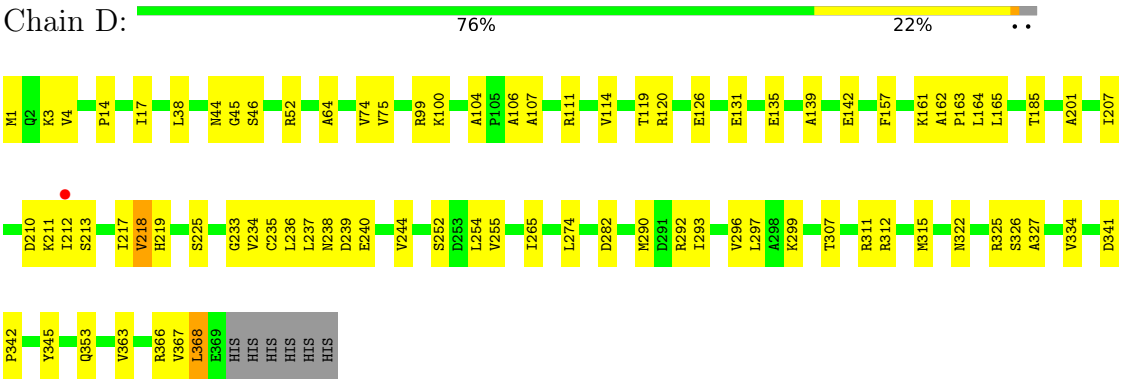
Chain C:





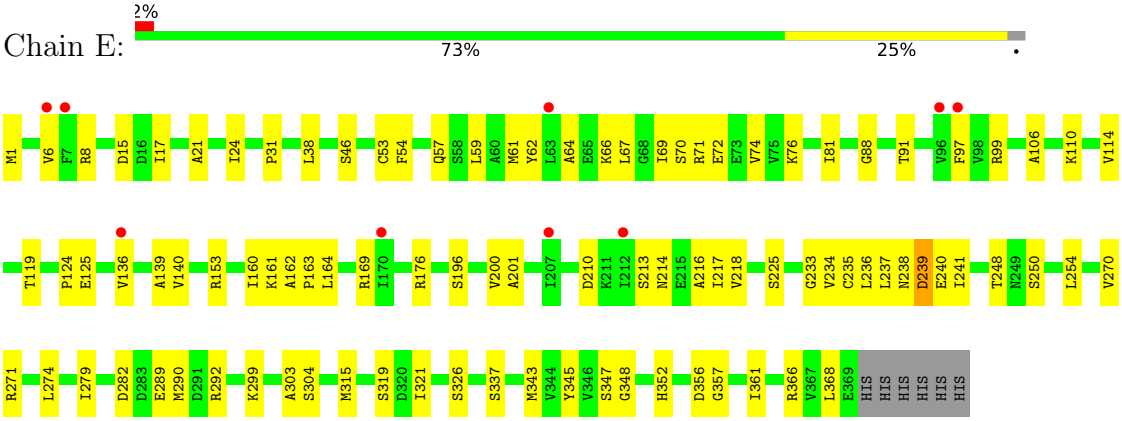
• Molecule 1: Cyanuric acid amidohydrolase

Chain D:



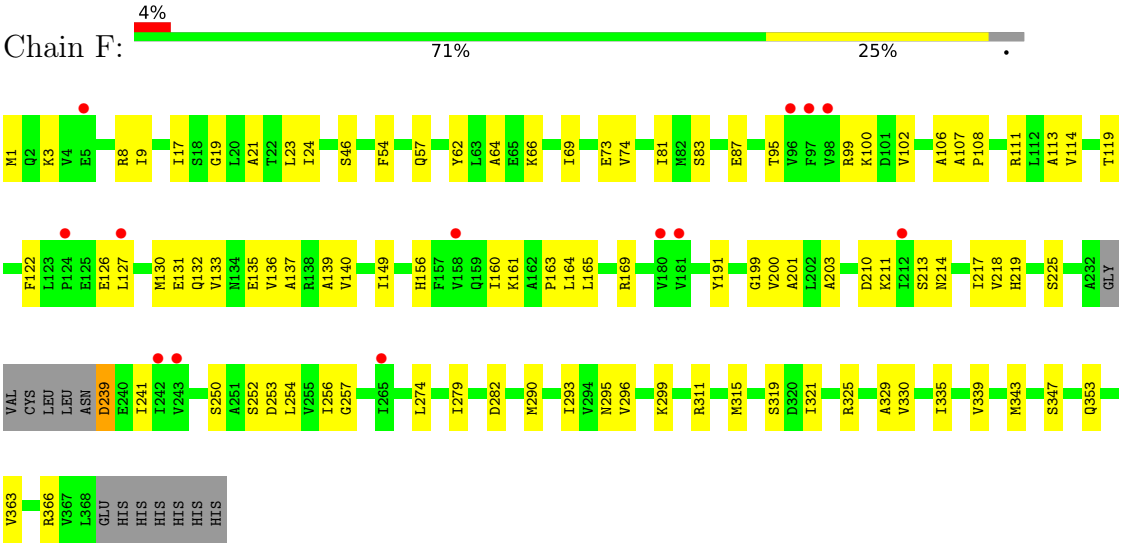
• Molecule 1: Cyanuric acid amidohydrolase

Chain E:



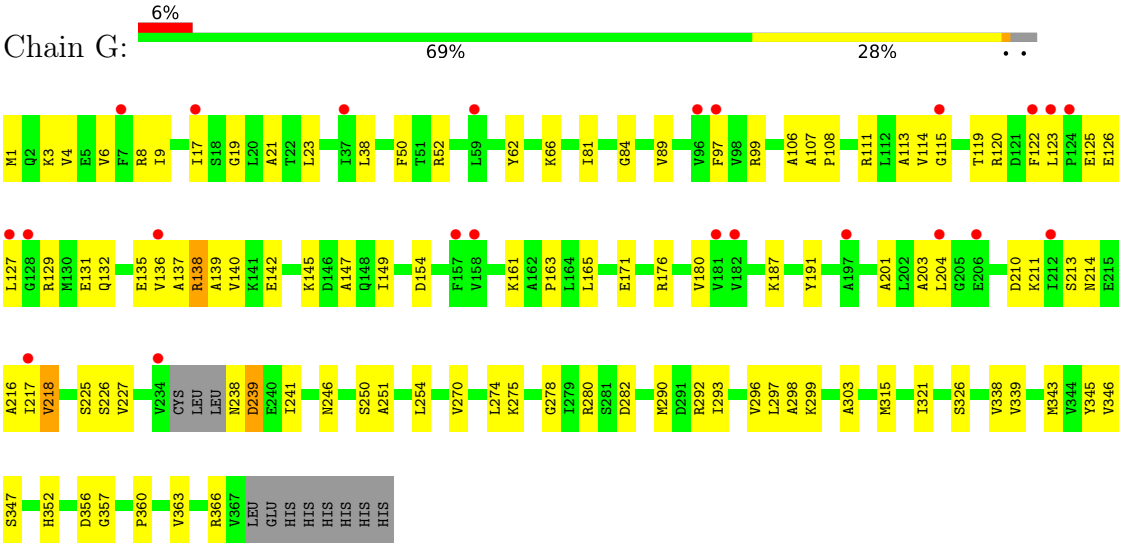
• Molecule 1: Cyanuric acid amidohydrolase

Chain F:



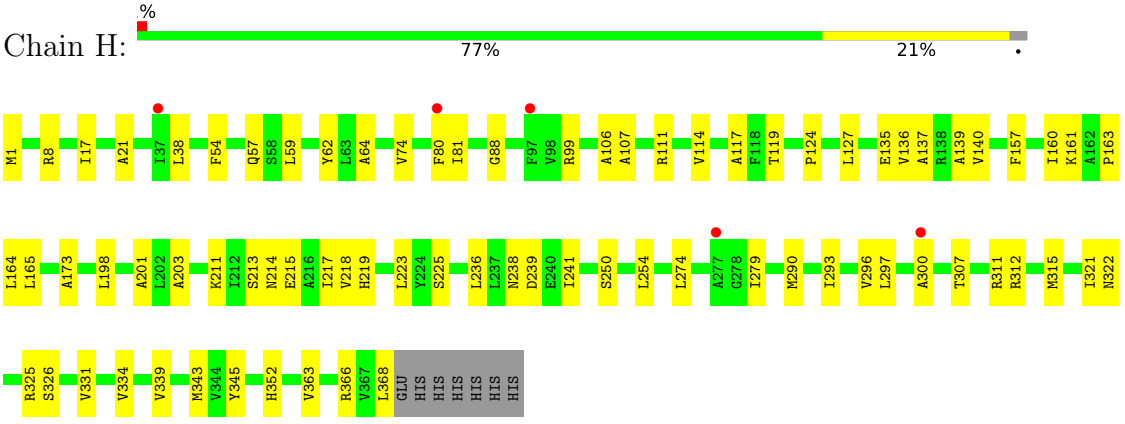
• Molecule 1: Cyanuric acid amidohydrolase

Chain G:



• Molecule 1: Cyanuric acid amidohydrolase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.91Å 164.56Å 202.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.80 – 3.20 127.80 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.6 (127.80-3.20) 95.7 (127.80-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.208 , 0.250 0.210 , 0.249	Depositor DCC
R_{free} test set	2807 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	118.7	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 86.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21566	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CIT

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	0.32	0/2740	0.57	0/3710
1	B	0.34	0/2720	0.60	0/3683
1	C	0.33	0/2712	0.58	0/3672
1	D	0.35	0/2729	0.63	0/3695
1	E	0.31	0/2729	0.56	0/3695
1	F	0.29	0/2678	0.54	0/3624
1	G	0.28	0/2689	0.52	0/3639
1	H	0.33	0/2720	0.60	0/3683
All	All	0.32	0/21717	0.58	0/29401

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2707	0	2733	92	0
1	B	2688	0	2718	88	1
1	C	2680	0	2707	86	0
1	D	2697	0	2722	81	0
1	E	2697	0	2725	89	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2647	0	2675	92	0
1	G	2658	0	2681	93	0
1	H	2688	0	2712	79	0
2	A	13	0	5	2	0
2	B	13	0	5	3	0
2	C	13	0	5	0	0
2	D	13	0	5	2	0
2	E	13	0	5	3	0
2	F	13	0	5	2	0
2	G	13	0	5	2	0
2	H	13	0	5	0	0
All	All	21566	0	21713	664	1

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 15.

All (664) 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:C:161:LYS:HG2	1:C:238:ASN:HB2	1.29	1.08
1:H:1:MET:HE2	1:H:106:ALA:HA	1.29	1.08
1:H:160:ILE:HG12	1:H:241:ILE:HD13	1.37	1.06
1:H:80:PHE:O	1:H:161:LYS:NZ	1.88	1.05
1:E:161:LYS:HE3	1:E:233:GLY:HA2	1.38	1.05
1:E:1:MET:HE2	1:E:106:ALA:HA	1.31	1.04
1:A:57:GLN:HE21	1:E:57:GLN:HE21	1.10	0.97
1:A:111:ARG:HH22	1:A:370:HIS:HB2	1.30	0.96
1:F:119:THR:HB	1:F:135:GLU:HG3	1.47	0.96
1:C:161:LYS:CG	1:C:238:ASN:HB2	1.95	0.95
1:F:107:ALA:HB1	1:F:108:PRO:HD2	1.51	0.92
1:G:217:ILE:O	1:G:352:HIS:NE2	2.02	0.92
1:B:1:MET:HE2	1:B:106:ALA:HA	1.49	0.91
1:E:110:LYS:HE3	1:E:248:THR:HG22	1.55	0.89
1:G:201:ALA:HB2	1:G:225:SER:HB2	1.55	0.87
1:G:296:VAL:HG22	1:G:363:VAL:HG22	1.57	0.86
1:D:239:ASP:O	1:D:240:GLU:HG3	1.76	0.84
1:G:315:MET:HE2	1:G:326:SER:HB3	1.60	0.83
1:B:161:LYS:HG3	1:B:238:ASN:HB3	1.61	0.83
1:A:111:ARG:NH2	1:A:370:HIS:HB2	1.93	0.82
1:F:164:LEU:O	1:F:169:ARG:NH1	2.12	0.82
1:H:163:PRO:CB	1:H:238:ASN:OD1	2.24	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:ASP:OD1	1:F:211:LYS:HE3	1.79	0.82
1:H:1:MET:CE	1:H:106:ALA:HA	2.10	0.82
1:C:1:MET:CE	1:C:106:ALA:HB2	2.09	0.81
1:E:162:ALA:O	1:E:233:GLY:N	2.12	0.81
1:G:119:THR:HB	1:G:135:GLU:HG3	1.62	0.81
1:F:139:ALA:HB3	1:F:241:ILE:HD12	1.63	0.80
1:G:210:ASP:OD1	1:G:211:LYS:HE3	1.81	0.80
1:A:210:ASP:OD1	1:A:211:LYS:HE3	1.80	0.79
1:G:163:PRO:HD3	1:G:239:ASP:OD1	1.82	0.79
1:C:75:VAL:HG11	1:C:236:LEU:HD12	1.64	0.78
1:G:211:LYS:HA	1:G:211:LYS:HE2	1.63	0.78
1:D:210:ASP:OD1	1:D:211:LYS:HE3	1.83	0.78
1:B:129:ARG:NH2	1:B:180:VAL:HA	1.98	0.78
1:A:10:PRO:HA	1:A:343:MET:HE3	1.66	0.78
1:E:119:THR:HG22	1:E:139:ALA:HB2	1.66	0.78
1:F:8:ARG:HG2	1:F:343:MET:HE3	1.65	0.78
1:A:211:LYS:HE2	1:A:211:LYS:HA	1.65	0.77
1:C:161:LYS:HG2	1:C:238:ASN:CB	2.12	0.77
1:F:1:MET:CE	1:F:106:ALA:HB2	2.14	0.77
1:E:1:MET:CE	1:E:106:ALA:HA	2.14	0.77
1:G:99:ARG:HD3	1:G:114:VAL:HG13	1.66	0.77
1:D:233:GLY:H	1:D:238:ASN:HD22	1.31	0.76
1:B:300:ALA:HB1	1:B:331:VAL:HG21	1.67	0.76
1:C:161:LYS:CD	1:C:238:ASN:HB2	2.15	0.76
1:E:161:LYS:O	1:E:239:ASP:HA	1.86	0.75
1:D:162:ALA:O	1:D:238:ASN:ND2	2.20	0.74
1:G:99:ARG:HD3	1:G:114:VAL:CG1	2.17	0.74
1:A:368:LEU:HD22	1:A:369:GLU:H	1.50	0.74
1:F:119:THR:HB	1:F:135:GLU:CG	2.17	0.74
1:D:211:LYS:HA	1:D:211:LYS:HE2	1.69	0.74
1:C:1:MET:HE1	1:C:106:ALA:HB2	1.69	0.73
1:D:322:ASN:HB2	1:D:325:ARG:HG3	1.68	0.73
1:A:368:LEU:HD22	1:A:369:GLU:N	2.03	0.73
1:D:163:PRO:HA	1:D:238:ASN:HD21	1.54	0.73
1:F:1:MET:HE2	1:F:106:ALA:HB2	1.71	0.73
1:F:139:ALA:CB	1:F:241:ILE:HD12	2.19	0.72
1:E:201:ALA:HB2	1:E:225:SER:HB2	1.71	0.72
1:H:99:ARG:HD3	1:H:114:VAL:HG13	1.71	0.72
1:E:213:SER:O	1:E:217:ILE:HG13	1.90	0.71
1:B:214:ASN:HA	1:B:217:ILE:HD12	1.72	0.71
1:E:110:LYS:HD2	1:E:110:LYS:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:214:ASN:HA	1:H:217:ILE:HD12	1.72	0.71
1:F:211:LYS:HE2	1:F:211:LYS:HA	1.73	0.71
1:H:307:THR:HG22	1:H:312:ARG:HA	1.73	0.71
1:C:61:MET:HG2	1:C:71:ARG:HD3	1.72	0.69
1:A:119:THR:HB	1:A:135:GLU:HG3	1.73	0.69
1:G:282:ASP:O	1:G:290:MET:HG2	1.91	0.69
1:F:81:ILE:HD11	1:F:161:LYS:HB2	1.74	0.69
1:B:214:ASN:HA	1:B:217:ILE:CD1	2.23	0.69
1:A:1:MET:CE	1:A:106:ALA:HB2	2.23	0.69
1:A:107:ALA:HB3	1:A:111:ARG:HG3	1.75	0.69
1:E:254:LEU:CD2	1:E:366:ARG:HG2	2.23	0.69
1:B:83:SER:OG	2:B:401:CIT:O7	2.11	0.68
1:E:53:CYS:SG	1:E:234:VAL:HG21	2.33	0.68
1:H:315:MET:HE2	1:H:326:SER:HB3	1.76	0.68
1:A:282:ASP:O	1:A:290:MET:HG2	1.93	0.68
1:C:79:ALA:HA	1:C:240:GLU:OE1	1.94	0.68
1:G:213:SER:H	1:G:216:ALA:HB3	1.59	0.68
1:D:161:LYS:HG2	1:D:238:ASN:HB2	1.76	0.68
1:G:119:THR:HB	1:G:135:GLU:CG	2.23	0.68
1:H:163:PRO:HB3	1:H:238:ASN:OD1	1.92	0.67
1:E:234:VAL:HG13	1:E:235:CYS:SG	2.34	0.67
1:D:119:THR:OG1	1:D:239:ASP:OD2	2.11	0.67
1:B:75:VAL:HG11	1:B:236:LEU:HD12	1.76	0.67
1:E:279:ILE:HD11	1:E:292:ARG:HB2	1.77	0.67
1:B:299:LYS:HE2	1:B:353:GLN:OE1	1.96	0.66
1:C:119:THR:OG1	1:C:239:ASP:OD1	2.11	0.66
1:A:129:ARG:HG2	1:A:214:ASN:ND2	2.11	0.66
1:D:38:LEU:HD11	1:D:345:TYR:CZ	2.30	0.66
1:A:166:THR:OG1	1:A:168:GLU:OE2	2.12	0.66
1:C:75:VAL:CG1	1:C:236:LEU:HD12	2.25	0.66
1:C:124:PRO:HB3	1:C:169:ARG:HB3	1.78	0.66
1:H:296:VAL:HG22	1:H:363:VAL:HG22	1.77	0.66
1:A:328:ARG:NH1	2:A:401:CIT:O6	2.30	0.65
1:C:213:SER:O	1:C:217:ILE:HG13	1.96	0.65
1:D:163:PRO:HA	1:D:238:ASN:ND2	2.10	0.65
1:E:161:LYS:CE	1:E:233:GLY:HA2	2.22	0.65
1:F:139:ALA:HB3	1:F:241:ILE:CD1	2.27	0.65
1:H:211:LYS:HE2	1:H:223:LEU:HD21	1.78	0.65
1:A:105:PRO:HG3	1:D:341:ASP:HB2	1.78	0.65
1:E:282:ASP:O	1:E:290:MET:HG2	1.96	0.65
1:B:64:ALA:HB1	1:B:69:ILE:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:99:ARG:HD3	1:H:114:VAL:CG1	2.26	0.65
1:B:166:THR:OG1	1:B:168:GLU:OE2	2.15	0.65
1:B:271:ARG:O	1:B:275:LYS:HG3	1.97	0.65
1:H:81:ILE:CD1	1:H:161:LYS:HD2	2.27	0.65
1:A:64:ALA:CA	1:A:74:VAL:HG21	2.27	0.65
1:B:75:VAL:CG1	1:B:236:LEU:HD12	2.27	0.65
1:E:214:ASN:HA	1:E:217:ILE:HD12	1.79	0.65
1:A:279:ILE:HG23	1:A:289:GLU:HB2	1.79	0.64
1:B:300:ALA:CB	1:B:331:VAL:HG21	2.26	0.64
1:B:129:ARG:HG2	1:B:214:ASN:ND2	2.13	0.64
1:A:145:LYS:NZ	1:G:171:GLU:HG2	2.13	0.64
1:B:279:ILE:HD11	1:B:292:ARG:HB2	1.78	0.64
1:D:233:GLY:H	1:D:238:ASN:ND2	1.95	0.64
1:E:164:LEU:O	1:E:169:ARG:NH1	2.31	0.64
1:C:131:GLU:OE1	1:C:131:GLU:N	2.31	0.64
1:D:1:MET:CE	1:D:106:ALA:HB2	2.28	0.64
1:H:201:ALA:HB2	1:H:225:SER:HB2	1.78	0.63
1:B:21:ALA:HA	1:B:62:TYR:OH	1.98	0.63
1:E:17:ILE:HG22	1:E:59:LEU:HD23	1.79	0.63
1:D:161:LYS:NZ	1:D:236:LEU:HD21	2.12	0.63
2:E:401:CIT:O4	2:E:401:CIT:O7	2.16	0.63
1:H:81:ILE:HD13	1:H:161:LYS:HD2	1.79	0.63
1:B:215:GLU:OE2	1:B:215:GLU:N	2.32	0.63
1:G:139:ALA:HB3	1:G:241:ILE:HD12	1.80	0.63
1:H:163:PRO:CG	1:H:238:ASN:OD1	2.47	0.62
1:F:156:HIS:CE1	1:F:257:GLY:HA2	2.34	0.62
1:H:161:LYS:CE	1:H:236:LEU:HD21	2.29	0.62
1:B:1:MET:CE	1:B:106:ALA:HA	2.26	0.62
1:A:119:THR:HB	1:A:135:GLU:CG	2.29	0.62
1:C:161:LYS:HD3	1:C:238:ASN:HB2	1.82	0.62
1:G:303:ALA:HB2	1:G:357:GLY:HA3	1.82	0.62
1:H:213:SER:O	1:H:217:ILE:HG13	1.99	0.62
1:B:161:LYS:CG	1:B:238:ASN:HB3	2.29	0.62
1:D:1:MET:HE3	1:D:106:ALA:HB2	1.82	0.62
1:D:201:ALA:HB2	1:D:225:SER:HB2	1.80	0.62
1:H:160:ILE:HG12	1:H:241:ILE:CD1	2.24	0.62
1:H:236:LEU:H	1:H:236:LEU:HD23	1.64	0.62
1:D:99:ARG:HD3	1:D:114:VAL:HG13	1.82	0.61
2:F:401:CIT:O3	2:F:401:CIT:O7	2.17	0.61
1:H:161:LYS:HE2	1:H:236:LEU:HD21	1.82	0.61
1:D:218:VAL:HG13	1:D:218:VAL:O	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:107:ALA:HB3	1:F:111:ARG:CZ	2.31	0.61
1:G:122:PHE:CE1	1:G:132:GLN:HA	2.35	0.61
1:C:61:MET:CG	1:C:71:ARG:HD3	2.31	0.61
1:A:1:MET:HE3	1:B:310:GLY:HA3	1.82	0.61
1:C:127:LEU:HD12	1:C:165:LEU:HG	1.81	0.61
1:D:292:ARG:HD3	1:D:368:LEU:HD22	1.82	0.61
1:C:166:THR:OG1	1:C:168:GLU:OE2	2.15	0.60
1:C:214:ASN:HA	1:C:217:ILE:HD12	1.82	0.60
1:A:163:PRO:HA	1:A:236:LEU:CD2	2.31	0.60
1:C:127:LEU:HD12	1:C:165:LEU:CD2	2.31	0.60
1:G:138:ARG:NH2	1:G:142:GLU:HG3	2.16	0.60
1:E:254:LEU:HD23	1:E:366:ARG:HA	1.84	0.60
1:F:299:LYS:HE2	1:F:353:GLN:OE1	2.01	0.60
1:H:163:PRO:HG3	1:H:238:ASN:OD1	2.01	0.60
1:C:1:MET:HG3	1:C:104:ALA:O	2.00	0.60
1:A:265:ILE:HA	1:A:334:VAL:HG21	1.83	0.60
1:B:161:LYS:HG3	1:B:238:ASN:CB	2.31	0.60
1:E:254:LEU:HD21	1:E:366:ARG:HG2	1.83	0.60
1:F:156:HIS:ND1	1:F:257:GLY:HA2	2.18	0.59
1:G:274:LEU:HD11	1:G:339:VAL:HG12	1.84	0.59
1:E:218:VAL:HG12	1:E:218:VAL:O	2.02	0.59
1:F:130:MET:HG2	1:F:214:ASN:OD1	2.02	0.59
1:H:161:LYS:HZ3	1:H:236:LEU:HD11	1.68	0.59
1:G:161:LYS:O	1:G:239:ASP:HA	2.03	0.59
1:D:296:VAL:HG22	1:D:363:VAL:HG22	1.84	0.58
1:G:125:GLU:O	1:G:129:ARG:HD2	2.04	0.58
1:D:161:LYS:HZ3	1:D:236:LEU:HD21	1.69	0.58
1:B:52:ARG:HD3	2:B:401:CIT:O4	2.04	0.57
1:F:296:VAL:HG22	1:F:363:VAL:HG22	1.85	0.57
1:A:319:SER:HB3	1:H:322:ASN:HD21	1.68	0.57
1:D:282:ASP:O	1:D:290:MET:HG2	2.04	0.57
1:E:319:SER:HG	1:F:46:SER:CB	2.16	0.57
1:F:127:LEU:HD12	1:F:165:LEU:CD2	2.34	0.57
1:H:127:LEU:HD12	1:H:165:LEU:CD2	2.34	0.57
1:H:214:ASN:HA	1:H:217:ILE:CD1	2.34	0.57
1:B:57:GLN:OE1	1:C:54:PHE:HE1	1.87	0.57
1:G:137:ALA:HA	1:G:203:ALA:HB2	1.86	0.57
1:A:57:GLN:NE2	1:E:57:GLN:HE21	1.92	0.57
1:B:201:ALA:HB2	1:B:225:SER:HB2	1.85	0.57
1:F:119:THR:OG1	1:F:239:ASP:HB2	2.04	0.57
1:H:218:VAL:HG13	1:H:219:HIS:ND1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:CYS:HB2	1:D:236:LEU:HD22	1.86	0.57
1:E:21:ALA:HA	1:E:62:TYR:OH	2.04	0.57
1:F:69:ILE:HD11	1:F:74:VAL:HG22	1.87	0.57
1:A:164:LEU:N	1:A:236:LEU:HD22	2.20	0.57
1:H:161:LYS:NZ	1:H:236:LEU:HD21	2.20	0.57
1:C:8:ARG:HG2	1:C:343:MET:HE3	1.86	0.57
1:F:218:VAL:HG23	1:F:219:HIS:CE1	2.39	0.57
1:A:64:ALA:HA	1:A:74:VAL:HG21	1.87	0.56
1:D:315:MET:HE2	1:D:327:ALA:N	2.20	0.56
1:F:133:VAL:HG13	1:F:199:GLY:HA2	1.85	0.56
1:G:84:GLY:N	2:G:401:CIT:O4	2.36	0.56
1:E:214:ASN:HA	1:E:217:ILE:CD1	2.35	0.56
1:E:234:VAL:HG13	1:E:235:CYS:N	2.20	0.56
1:B:50:PHE:CE2	1:C:14:PRO:HD2	2.40	0.56
1:G:299:LYS:HD2	1:G:347:SER:OG	2.05	0.56
1:H:136:VAL:O	1:H:140:VAL:HG23	2.06	0.56
1:A:1:MET:CE	1:B:310:GLY:HA3	2.36	0.56
1:A:145:LYS:HZ1	1:G:171:GLU:HG2	1.69	0.56
1:E:110:LYS:HG3	1:E:248:THR:HG22	1.88	0.56
1:E:8:ARG:HG2	1:E:343:MET:HE3	1.87	0.56
1:C:64:ALA:CA	1:C:74:VAL:HG21	2.35	0.56
1:B:127:LEU:HD12	1:B:165:LEU:CD2	2.36	0.55
1:C:299:LYS:HD2	1:C:347:SER:OG	2.06	0.55
1:F:119:THR:HG22	1:F:139:ALA:HB2	1.89	0.55
1:E:124:PRO:HG3	1:E:169:ARG:HB3	1.89	0.55
1:H:274:LEU:HD13	1:H:290:MET:CE	2.37	0.55
1:F:254:LEU:HD23	1:F:366:ARG:HA	1.89	0.55
1:A:1:MET:HE1	1:A:106:ALA:HB2	1.89	0.55
1:A:99:ARG:HD3	1:A:114:VAL:HG13	1.88	0.55
1:C:130:MET:SD	1:C:212:ILE:HG22	2.47	0.55
1:C:300:ALA:CB	1:C:331:VAL:HG21	2.36	0.55
1:E:213:SER:H	1:E:216:ALA:HB3	1.72	0.55
1:E:279:ILE:HD12	1:E:289:GLU:O	2.07	0.55
1:G:297:LEU:HD23	1:G:345:TYR:HB3	1.89	0.55
1:B:99:ARG:HD3	1:B:114:VAL:CG1	2.36	0.55
1:G:254:LEU:CD2	1:G:366:ARG:HG2	2.36	0.55
1:H:38:LEU:HD11	1:H:345:TYR:CZ	2.41	0.55
1:G:125:GLU:OE1	1:G:176:ARG:NH2	2.40	0.55
1:H:218:VAL:HG13	1:H:219:HIS:CE1	2.42	0.55
1:B:69:ILE:HB	1:B:73:GLU:OE1	2.07	0.55
1:F:1:MET:HE1	1:F:106:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:CYS:HB2	1:B:236:LEU:HD22	1.88	0.54
1:C:38:LEU:HD21	1:C:159:GLN:HG3	1.88	0.54
1:D:14:PRO:HD2	1:G:50:PHE:CE2	2.42	0.54
1:D:119:THR:HB	1:D:135:GLU:HG3	1.88	0.54
1:F:163:PRO:HD3	1:F:239:ASP:OD1	2.07	0.54
1:G:125:GLU:CD	1:G:176:ARG:HH22	2.10	0.54
1:H:127:LEU:HD12	1:H:165:LEU:HD23	1.89	0.54
1:H:21:ALA:HA	1:H:62:TYR:OH	2.07	0.54
1:D:4:VAL:H	1:D:252:SER:HB3	1.71	0.54
1:A:125:GLU:CD	1:A:176:ARG:HH22	2.11	0.54
1:C:75:VAL:HG11	1:C:236:LEU:CD1	2.37	0.54
1:D:64:ALA:CA	1:D:74:VAL:HG21	2.36	0.54
1:B:1:MET:HE1	1:B:106:ALA:CB	2.38	0.54
1:B:99:ARG:HD3	1:B:114:VAL:HG13	1.90	0.54
1:D:52:ARG:NH2	1:D:234:VAL:HG11	2.23	0.54
1:D:161:LYS:HD3	1:D:240:GLU:OE2	2.08	0.54
1:H:17:ILE:HG22	1:H:59:LEU:HD23	1.90	0.54
1:B:119:THR:HG23	1:B:241:ILE:CD1	2.38	0.53
1:E:17:ILE:HD12	1:E:17:ILE:C	2.28	0.53
1:E:61:MET:CG	1:E:71:ARG:HD3	2.37	0.53
1:G:211:LYS:HE2	1:G:211:LYS:CA	2.37	0.53
1:A:137:ALA:HA	1:A:203:ALA:HB2	1.89	0.53
1:F:57:GLN:CD	1:H:57:GLN:HE21	2.12	0.53
1:A:299:LYS:HE2	1:A:353:GLN:OE1	2.08	0.53
1:B:213:SER:O	1:B:217:ILE:HG13	2.07	0.53
1:F:24:ILE:HD12	1:F:62:TYR:HE2	1.72	0.53
1:G:138:ARG:HD3	1:G:139:ALA:N	2.23	0.53
1:D:265:ILE:HA	1:D:334:VAL:HG21	1.89	0.53
1:A:99:ARG:HD3	1:A:114:VAL:CG1	2.38	0.53
1:G:138:ARG:CZ	1:G:142:GLU:HG3	2.39	0.53
1:A:81:ILE:CD1	1:A:161:LYS:HD3	2.39	0.53
1:F:214:ASN:HA	1:F:217:ILE:HD12	1.90	0.53
1:G:213:SER:O	1:G:217:ILE:HG13	2.09	0.53
1:C:107:ALA:HB3	1:C:111:ARG:HG3	1.91	0.53
1:D:99:ARG:HD3	1:D:114:VAL:CG1	2.38	0.53
1:E:46:SER:HB2	1:F:319:SER:OG	2.08	0.53
1:G:21:ALA:HA	1:G:62:TYR:OH	2.08	0.53
1:C:319:SER:HB3	1:D:322:ASN:HD21	1.73	0.53
1:G:127:LEU:HD12	1:G:165:LEU:CD2	2.39	0.53
1:F:99:ARG:HD3	1:F:114:VAL:HG13	1.90	0.52
1:A:164:LEU:HG	1:A:236:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:HG22	1:A:361:ILE:CD1	2.39	0.52
1:A:275:LYS:HA	1:A:279:ILE:O	2.08	0.52
1:C:99:ARG:HD3	1:C:114:VAL:HG13	1.90	0.52
1:E:321:ILE:HG12	1:H:321:ILE:HG12	1.90	0.52
1:F:279:ILE:HD13	1:F:293:ILE:HG13	1.91	0.52
1:A:319:SER:HB3	1:H:322:ASN:ND2	2.24	0.52
1:D:368:LEU:HD12	1:D:368:LEU:O	2.09	0.52
1:G:4:VAL:CG2	1:G:114:VAL:HG12	2.39	0.52
1:G:191:TYR:CE1	1:G:218:VAL:HB	2.44	0.52
1:B:191:TYR:CE1	1:B:218:VAL:HG21	2.44	0.52
1:D:1:MET:HG3	1:D:104:ALA:O	2.08	0.52
1:D:254:LEU:HD23	1:D:366:ARG:HA	1.91	0.52
1:F:64:ALA:HB1	1:F:69:ILE:O	2.10	0.52
1:A:315:MET:HE2	1:A:326:SER:C	2.30	0.52
1:H:107:ALA:CB	1:H:111:ARG:HG3	2.39	0.52
1:B:129:ARG:HG2	1:B:214:ASN:HD22	1.75	0.52
1:B:279:ILE:HD12	1:B:289:GLU:O	2.08	0.52
1:F:83:SER:OG	2:F:401:CIT:O5	2.06	0.52
1:F:137:ALA:HA	1:F:203:ALA:HB2	1.91	0.52
1:A:163:PRO:HA	1:A:236:LEU:HD22	1.92	0.52
1:D:75:VAL:HG11	1:D:236:LEU:HD12	1.91	0.52
1:F:107:ALA:HB1	1:F:108:PRO:CD	2.33	0.52
1:G:38:LEU:HD11	1:G:345:TYR:CE2	2.45	0.52
1:H:119:THR:HB	1:H:135:GLU:HG3	1.90	0.52
1:E:348:GLY:H	2:E:401:CIT:C6	2.23	0.52
1:B:300:ALA:HB1	1:B:331:VAL:CG2	2.37	0.51
1:C:46:SER:OG	1:C:47:VAL:N	2.42	0.51
1:A:93:HIS:HB3	1:A:343:MET:HE3	1.91	0.51
1:G:214:ASN:HA	1:G:217:ILE:CD1	2.41	0.51
1:C:215:GLU:O	1:C:219:HIS:HB2	2.11	0.51
1:F:253:ASP:O	1:F:254:LEU:HD23	2.11	0.51
1:A:125:GLU:OE1	1:A:176:ARG:NH2	2.40	0.51
1:A:217:ILE:O	1:A:217:ILE:HG22	2.11	0.51
1:E:125:GLU:OE2	1:E:176:ARG:NH2	2.28	0.51
1:H:124:PRO:HG2	1:H:173:ALA:HB2	1.93	0.51
1:H:236:LEU:HD23	1:H:236:LEU:N	2.26	0.51
1:A:64:ALA:N	1:A:74:VAL:HG21	2.26	0.51
1:H:215:GLU:O	1:H:219:HIS:HB2	2.10	0.51
1:A:255:VAL:HG13	1:A:367:VAL:CG1	2.41	0.51
1:C:282:ASP:O	1:C:290:MET:HG2	2.11	0.51
1:F:99:ARG:HD3	1:F:114:VAL:CG1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PRO:HA	1:A:236:LEU:HD23	1.93	0.50
1:D:3:LYS:HB3	1:D:100:LYS:HG3	1.92	0.50
1:D:75:VAL:CG1	1:D:236:LEU:HD12	2.41	0.50
1:G:113:ALA:HB3	1:G:149:ILE:HD11	1.93	0.50
1:H:160:ILE:CG1	1:H:241:ILE:HD13	2.26	0.50
1:B:274:LEU:HD21	1:B:293:ILE:HD11	1.93	0.50
1:B:300:ALA:HB2	1:B:331:VAL:HG11	1.93	0.50
1:H:322:ASN:HB2	1:H:325:ARG:HG3	1.93	0.50
1:B:299:LYS:HD2	1:B:347:SER:O	2.12	0.50
1:E:61:MET:HG2	1:E:71:ARG:HD3	1.94	0.50
1:A:164:LEU:HG	1:A:236:LEU:CD1	2.42	0.50
1:G:1:MET:HE1	1:G:106:ALA:HB2	1.94	0.50
1:B:61:MET:HG3	1:B:71:ARG:HD3	1.94	0.50
1:B:83:SER:HG	2:B:401:CIT:HO7	1.50	0.50
1:E:217:ILE:O	1:E:352:HIS:NE2	2.40	0.50
1:A:321:ILE:HG12	1:F:321:ILE:HG12	1.92	0.50
1:C:187:LYS:HG2	1:C:191:TYR:HE2	1.75	0.50
1:D:52:ARG:CZ	1:D:234:VAL:HG11	2.41	0.50
1:G:142:GLU:OE1	1:G:142:GLU:HA	2.12	0.50
1:B:1:MET:HE1	1:B:106:ALA:HB2	1.93	0.50
1:C:126:GLU:OE2	1:C:131:GLU:HB3	2.11	0.50
1:C:254:LEU:CD2	1:C:366:ARG:HG2	2.41	0.50
1:F:95:THR:OG1	1:F:295:ASN:ND2	2.43	0.50
1:D:52:ARG:NH1	2:D:401:CIT:O4	2.45	0.50
1:D:142:GLU:HA	1:D:142:GLU:OE1	2.12	0.50
1:H:119:THR:HG22	1:H:139:ALA:HB2	1.93	0.49
1:D:236:LEU:O	1:D:237:LEU:C	2.49	0.49
1:D:44:ASN:OD1	1:D:46:SER:OG	2.24	0.49
1:E:303:ALA:HB2	1:E:357:GLY:HA3	1.93	0.49
1:F:81:ILE:CD1	1:F:161:LYS:HB2	2.41	0.49
1:G:138:ARG:HD3	1:G:138:ARG:C	2.33	0.49
1:A:130:MET:HG2	1:A:214:ASN:OD1	2.12	0.49
1:E:91:THR:OG1	1:H:311:ARG:HB3	2.12	0.49
1:H:1:MET:HE3	1:H:250:SER:CA	2.43	0.49
1:E:237:LEU:HD12	1:E:237:LEU:N	2.28	0.49
1:F:17:ILE:C	1:F:17:ILE:HD12	2.32	0.49
1:F:136:VAL:O	1:F:140:VAL:HG23	2.11	0.49
1:E:160:ILE:HD11	1:E:200:VAL:CG2	2.42	0.49
1:B:81:ILE:HD12	1:B:159:GLN:HG2	1.95	0.49
1:C:21:ALA:HA	1:C:62:TYR:OH	2.13	0.49
1:C:127:LEU:HD12	1:C:165:LEU:CG	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:MET:HE3	1:F:330:VAL:HG21	1.95	0.49
1:A:191:TYR:CE1	1:A:218:VAL:HG21	2.48	0.49
1:A:299:LYS:HB2	1:A:360:PRO:HD2	1.94	0.49
1:F:274:LEU:HD22	1:F:293:ILE:HD11	1.95	0.49
1:C:64:ALA:N	1:C:74:VAL:HG21	2.28	0.48
1:F:57:GLN:NE2	1:H:54:PHE:HE1	2.11	0.48
1:G:107:ALA:HB1	1:G:111:ARG:CZ	2.42	0.48
1:A:17:ILE:HD12	1:A:17:ILE:C	2.33	0.48
1:G:204:LEU:CD1	1:G:227:VAL:HG21	2.43	0.48
1:H:107:ALA:HB3	1:H:111:ARG:HG3	1.95	0.48
1:C:99:ARG:HD3	1:C:114:VAL:CG1	2.42	0.48
1:C:136:VAL:O	1:C:140:VAL:HG23	2.12	0.48
1:E:53:CYS:SG	1:E:234:VAL:CG2	3.00	0.48
1:F:87:GLU:HG2	1:F:325:ARG:HB3	1.95	0.48
1:H:218:VAL:HG22	1:H:218:VAL:O	2.14	0.48
1:B:38:LEU:HD11	1:B:345:TYR:CZ	2.47	0.48
1:B:61:MET:CG	1:B:71:ARG:HD3	2.43	0.48
1:B:119:THR:HG23	1:B:241:ILE:HD11	1.96	0.48
1:C:80:PHE:O	1:C:161:LYS:NZ	2.43	0.48
1:A:136:VAL:O	1:A:140:VAL:HG23	2.14	0.48
1:B:61:MET:HE3	1:C:71:ARG:NH2	2.28	0.48
1:E:15:ASP:HB3	1:E:54:PHE:CZ	2.48	0.48
1:F:156:HIS:CD2	1:F:256:ILE:HG23	2.49	0.48
1:F:156:HIS:CG	1:F:256:ILE:HG23	2.49	0.48
1:C:218:VAL:HG13	1:C:218:VAL:O	2.14	0.48
1:D:239:ASP:C	1:D:240:GLU:HG3	2.35	0.48
1:D:255:VAL:HG13	1:D:367:VAL:CG1	2.43	0.48
1:D:299:LYS:HE2	1:D:353:GLN:OE1	2.14	0.48
1:F:282:ASP:O	1:F:290:MET:HG2	2.13	0.48
1:E:124:PRO:CG	1:E:169:ARG:HB3	2.44	0.48
1:B:81:ILE:HD12	1:B:159:GLN:CG	2.43	0.47
1:B:125:GLU:CD	1:B:176:ARG:HH22	2.17	0.47
1:D:119:THR:HG22	1:D:139:ALA:HB2	1.96	0.47
1:E:299:LYS:HD2	1:E:347:SER:OG	2.14	0.47
1:A:10:PRO:CA	1:A:343:MET:HE3	2.42	0.47
1:A:64:ALA:HA	1:A:74:VAL:CG2	2.43	0.47
1:C:36:ALA:CB	1:C:79:ALA:HB3	2.44	0.47
1:F:213:SER:O	1:F:217:ILE:HG13	2.14	0.47
1:A:119:THR:CG2	1:A:239:ASP:HB2	2.45	0.47
1:B:119:THR:CG2	1:B:241:ILE:HD11	2.44	0.47
1:E:161:LYS:HG3	1:E:236:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ILE:CD1	1:B:159:GLN:HG3	2.44	0.47
1:F:191:TYR:CE1	1:F:218:VAL:HG21	2.49	0.47
1:D:126:GLU:OE2	1:D:131:GLU:HB3	2.14	0.47
1:E:62:TYR:CZ	1:E:66:LYS:HG3	2.49	0.47
1:F:214:ASN:HA	1:F:217:ILE:CD1	2.45	0.47
1:H:163:PRO:HG3	1:H:238:ASN:O	2.13	0.47
1:C:33:GLU:OE1	1:C:100:LYS:HG2	2.14	0.47
1:C:303:ALA:HB2	1:C:357:GLY:HA3	1.97	0.47
1:C:38:LEU:HG	1:C:81:ILE:HB	1.96	0.47
1:C:321:ILE:CD1	1:G:321:ILE:HG12	2.45	0.47
1:D:17:ILE:C	1:D:17:ILE:HD12	2.35	0.47
1:E:69:ILE:HG12	1:E:70:SER:H	1.80	0.47
1:G:81:ILE:HD11	1:G:161:LYS:HB2	1.95	0.47
1:G:123:LEU:HB2	1:G:126:GLU:HG3	1.96	0.47
1:G:274:LEU:CD2	1:G:293:ILE:HD11	2.45	0.47
1:G:278:GLY:O	1:G:292:ARG:NH2	2.47	0.47
1:E:236:LEU:HD12	1:E:238:ASN:OD1	2.15	0.47
1:F:122:PHE:CE1	1:F:132:GLN:HA	2.49	0.47
1:A:69:ILE:HB	1:A:73:GLU:OE1	2.15	0.47
1:B:1:MET:HG3	1:B:2:GLN:N	2.30	0.47
1:C:119:THR:O	1:C:239:ASP:OD2	2.32	0.47
1:E:24:ILE:HD12	1:E:62:TYR:HE2	1.80	0.47
1:B:129:ARG:HH22	1:B:180:VAL:HA	1.75	0.47
1:F:9:ILE:CG2	1:F:19:GLY:HA3	2.45	0.47
1:G:125:GLU:HA	1:G:180:VAL:HG12	1.97	0.47
1:G:163:PRO:HG3	1:G:238:ASN:OD1	2.15	0.47
1:A:129:ARG:HG2	1:A:214:ASN:HD22	1.80	0.46
1:A:163:PRO:HD3	1:A:239:ASP:OD1	2.14	0.46
1:B:130:MET:HG2	1:B:214:ASN:OD1	2.14	0.46
1:D:164:LEU:HD12	1:D:164:LEU:C	2.36	0.46
1:E:234:VAL:CG1	1:E:235:CYS:N	2.78	0.46
1:G:38:LEU:HD11	1:G:345:TYR:CZ	2.50	0.46
1:A:93:HIS:CB	1:A:343:MET:CE	2.94	0.46
1:B:236:LEU:HD23	1:B:236:LEU:N	2.31	0.46
1:F:9:ILE:HD11	1:F:23:LEU:HD12	1.98	0.46
1:G:297:LEU:CD2	1:G:345:TYR:HB3	2.45	0.46
1:A:211:LYS:HE2	1:A:211:LYS:CA	2.39	0.46
1:C:161:LYS:HG2	1:C:238:ASN:HD22	1.80	0.46
1:E:64:ALA:HB1	1:E:69:ILE:O	2.16	0.46
1:F:107:ALA:HB3	1:F:111:ARG:NH1	2.31	0.46
1:A:207:ILE:HG13	1:A:212:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:TYR:HE1	1:G:66:LYS:HZ3	1.63	0.46
1:D:1:MET:HE1	1:D:106:ALA:HB2	1.98	0.46
1:G:6:VAL:HG22	1:G:97:PHE:CD2	2.51	0.46
1:G:136:VAL:O	1:G:140:VAL:HG23	2.16	0.46
1:G:139:ALA:CB	1:G:241:ILE:HD12	2.44	0.46
1:G:275:LYS:O	1:G:280:ARG:NH1	2.49	0.46
1:A:234:VAL:O	1:A:236:LEU:HG	2.16	0.46
1:B:81:ILE:CD1	1:B:159:GLN:CG	2.94	0.46
1:E:24:ILE:HG21	1:E:66:LYS:HE2	1.96	0.46
1:E:218:VAL:O	1:E:218:VAL:CG1	2.63	0.46
1:F:279:ILE:CD1	1:F:293:ILE:HG13	2.45	0.46
1:H:198:LEU:HD11	1:H:352:HIS:CE1	2.50	0.46
1:C:38:LEU:HA	1:C:81:ILE:O	2.16	0.46
1:D:274:LEU:CD2	1:D:293:ILE:HD11	2.45	0.46
1:F:21:ALA:HA	1:F:62:TYR:OH	2.16	0.46
1:G:187:LYS:HG2	1:G:191:TYR:HE2	1.81	0.46
1:B:125:GLU:O	1:B:129:ARG:CZ	2.64	0.46
1:C:1:MET:HE3	1:C:106:ALA:HB2	1.96	0.46
1:C:161:LYS:HG2	1:C:238:ASN:ND2	2.30	0.46
1:E:271:ARG:HA	1:E:274:LEU:HD12	1.98	0.46
1:F:87:GLU:HB3	1:F:329:ALA:HB2	1.97	0.46
1:F:254:LEU:CD2	1:F:366:ARG:HG2	2.45	0.46
1:A:52:ARG:NH1	2:A:401:CIT:O3	2.49	0.46
1:B:81:ILE:HD13	1:B:159:GLN:NE2	2.31	0.46
1:D:236:LEU:HD23	1:D:236:LEU:N	2.31	0.46
1:E:88:GLY:HA2	1:H:315:MET:HE2	1.98	0.46
1:G:120:ARG:HG2	1:G:135:GLU:HG2	1.98	0.46
1:B:274:LEU:CD2	1:B:293:ILE:HD11	2.46	0.45
1:C:214:ASN:HA	1:C:217:ILE:CD1	2.46	0.45
1:C:279:ILE:CD1	1:C:293:ILE:HG13	2.46	0.45
1:F:69:ILE:HB	1:F:73:GLU:OE1	2.16	0.45
1:A:234:VAL:HG23	1:A:235:CYS:N	2.31	0.45
1:B:337:SER:HB3	1:D:334:VAL:HG22	1.98	0.45
1:G:315:MET:CE	1:G:326:SER:HB3	2.40	0.45
1:A:322:ASN:HB3	1:A:325:ARG:HG3	1.98	0.45
1:C:64:ALA:HB1	1:C:69:ILE:O	2.16	0.45
1:F:126:GLU:OE2	1:F:131:GLU:HG2	2.15	0.45
1:G:126:GLU:OE2	1:G:131:GLU:HG2	2.16	0.45
1:C:156:HIS:CE1	1:C:257:GLY:HA2	2.51	0.45
1:E:1:MET:HE3	1:E:250:SER:N	2.32	0.45
1:G:1:MET:HE3	1:G:250:SER:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:ALA:HB1	1:G:108:PRO:HD2	1.98	0.45
1:H:119:THR:HB	1:H:135:GLU:CG	2.46	0.45
1:B:303:ALA:HB2	1:B:357:GLY:HA3	1.98	0.45
1:G:81:ILE:HD13	1:G:161:LYS:HD3	1.98	0.45
1:B:36:ALA:CB	1:B:79:ALA:HB3	2.47	0.45
1:B:165:LEU:O	1:B:185:THR:HG22	2.17	0.45
1:F:299:LYS:HD3	1:F:347:SER:OG	2.17	0.45
1:H:279:ILE:CD1	1:H:293:ILE:HG13	2.47	0.45
1:A:270:VAL:HG22	1:A:361:ILE:HD13	1.97	0.45
1:C:298:ALA:O	1:C:346:VAL:HA	2.17	0.45
1:D:161:LYS:O	1:D:238:ASN:O	2.35	0.45
1:E:270:VAL:HG22	1:E:361:ILE:CD1	2.46	0.45
1:G:303:ALA:HA	1:G:356:ASP:OD1	2.17	0.45
1:C:125:GLU:CD	1:C:176:ARG:HH22	2.21	0.45
1:F:8:ARG:HG2	1:F:343:MET:CE	2.40	0.45
1:A:7:PHE:CD1	1:A:29:ILE:HD11	2.51	0.45
1:A:93:HIS:HB3	1:A:343:MET:CE	2.47	0.45
1:A:201:ALA:HB2	1:A:225:SER:HB2	1.99	0.45
1:D:45:GLY:HA2	2:D:401:CIT:O3	2.17	0.45
1:F:1:MET:HB3	1:F:102:VAL:O	2.17	0.45
1:H:1:MET:HE3	1:H:250:SER:C	2.37	0.45
1:H:17:ILE:HD12	1:H:17:ILE:C	2.38	0.45
1:B:136:VAL:O	1:B:140:VAL:HG23	2.16	0.44
1:C:321:ILE:HD11	1:G:321:ILE:HG12	1.98	0.44
1:E:17:ILE:HG22	1:E:59:LEU:CD2	2.46	0.44
1:F:217:ILE:O	1:F:217:ILE:HG22	2.17	0.44
1:G:140:VAL:HG23	1:G:241:ILE:HD13	1.98	0.44
1:A:72:GLU:O	1:A:76:LYS:HG3	2.17	0.44
1:B:253:ASP:O	1:B:367:VAL:HG22	2.17	0.44
1:F:160:ILE:HD11	1:F:200:VAL:CG2	2.47	0.44
1:H:137:ALA:HA	1:H:203:ALA:HB2	1.99	0.44
1:C:17:ILE:HD12	1:C:17:ILE:C	2.38	0.44
1:C:236:LEU:N	1:C:236:LEU:HD23	2.32	0.44
1:D:38:LEU:HD11	1:D:345:TYR:OH	2.17	0.44
1:G:191:TYR:OH	1:G:218:VAL:HG11	2.18	0.44
1:H:64:ALA:CA	1:H:74:VAL:HG21	2.46	0.44
1:H:163:PRO:CG	1:H:238:ASN:CG	2.85	0.44
1:C:294:VAL:HB	1:C:364:ILE:HG22	1.99	0.44
1:C:300:ALA:HB1	1:C:331:VAL:HG21	2.00	0.44
1:D:292:ARG:NH1	1:D:368:LEU:HD23	2.32	0.44
1:E:99:ARG:NH2	1:E:114:VAL:O	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:PRO:HD3	1:E:239:ASP:OD1	2.16	0.44
1:B:75:VAL:CG1	1:B:236:LEU:CD1	2.95	0.44
1:C:315:MET:HE3	1:G:89:VAL:HG13	1.99	0.44
1:D:254:LEU:CD2	1:D:366:ARG:HG2	2.47	0.44
1:D:315:MET:HE2	1:D:326:SER:C	2.38	0.44
1:B:161:LYS:HE3	1:B:233:GLY:HA3	1.99	0.44
1:E:38:LEU:HA	1:E:81:ILE:O	2.18	0.44
1:F:211:LYS:HE2	1:F:211:LYS:CA	2.46	0.44
1:G:17:ILE:C	1:G:17:ILE:HD12	2.38	0.44
1:G:254:LEU:HD23	1:G:366:ARG:HG2	1.99	0.44
1:C:75:VAL:CG1	1:C:236:LEU:CD1	2.94	0.44
1:D:120:ARG:HG2	1:D:135:GLU:CD	2.37	0.44
1:E:31:PRO:HB2	1:E:67:LEU:HD21	2.00	0.44
1:E:38:LEU:HD11	1:E:345:TYR:CZ	2.53	0.44
1:E:69:ILE:HG23	1:E:74:VAL:HG23	1.99	0.44
1:A:61:MET:SD	1:E:61:MET:SD	3.16	0.44
1:A:105:PRO:HD3	1:D:341:ASP:OD2	2.17	0.44
1:B:20:LEU:HD21	1:B:63:LEU:HD21	2.00	0.44
1:E:110:LYS:HE3	1:E:248:THR:CG2	2.35	0.44
1:D:64:ALA:HA	1:D:74:VAL:HG21	1.99	0.43
1:B:81:ILE:HD13	1:B:159:GLN:HE21	1.81	0.43
1:G:145:LYS:HE2	1:G:145:LYS:HB3	1.87	0.43
1:H:161:LYS:HZ3	1:H:236:LEU:CD1	2.28	0.43
1:G:1:MET:HE2	1:G:106:ALA:HA	2.00	0.43
1:H:8:ARG:HG2	1:H:343:MET:HE3	2.00	0.43
1:A:10:PRO:HA	1:A:343:MET:CE	2.43	0.43
1:A:119:THR:O	1:A:238:ASN:HB2	2.19	0.43
1:D:213:SER:O	1:D:217:ILE:HG13	2.18	0.43
1:D:292:ARG:HD3	1:D:368:LEU:CD2	2.45	0.43
1:E:110:LYS:CE	1:E:248:THR:HG22	2.39	0.43
1:F:87:GLU:CB	1:F:329:ALA:HB2	2.48	0.43
1:F:119:THR:CB	1:F:135:GLU:HG3	2.34	0.43
1:A:148:GLN:OE1	1:A:249:ASN:ND2	2.52	0.43
1:B:57:GLN:NE2	1:C:57:GLN:HG2	2.34	0.43
1:D:157:PHE:HB3	1:D:244:VAL:HB	2.00	0.43
1:E:1:MET:HE3	1:E:250:SER:C	2.39	0.43
1:F:1:MET:HE3	1:F:250:SER:C	2.39	0.43
1:H:217:ILE:HG22	1:H:217:ILE:O	2.18	0.43
1:B:17:ILE:C	1:B:17:ILE:HD12	2.39	0.43
1:B:311:ARG:HG3	1:D:342:PRO:HD2	2.00	0.43
1:D:274:LEU:HD22	1:D:293:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:54:PHE:HE1	1:H:57:GLN:OE1	2.00	0.43
1:G:1:MET:HE3	1:G:250:SER:N	2.34	0.43
1:H:38:LEU:HD11	1:H:345:TYR:CE2	2.53	0.43
1:D:307:THR:HG22	1:D:312:ARG:HA	2.00	0.43
1:E:6:VAL:HG22	1:E:97:PHE:CD2	2.54	0.43
1:H:164:LEU:C	1:H:164:LEU:HD12	2.39	0.43
1:A:164:LEU:HG	1:A:236:LEU:HD22	2.00	0.43
1:B:368:LEU:N	1:B:368:LEU:HD12	2.33	0.43
1:E:38:LEU:HD11	1:E:345:TYR:CE2	2.54	0.43
1:E:140:VAL:HG21	1:E:200:VAL:HA	2.01	0.43
1:F:111:ARG:HB3	1:F:252:SER:O	2.19	0.43
1:F:3:LYS:HB3	1:F:100:LYS:HG3	2.01	0.42
1:C:234:VAL:O	1:C:234:VAL:HG22	2.19	0.42
1:E:136:VAL:HG11	1:E:196:SER:O	2.19	0.42
1:B:145:LYS:HE2	1:B:145:LYS:HB3	1.95	0.42
1:C:164:LEU:HD21	1:C:234:VAL:HB	2.01	0.42
1:G:3:LYS:HG3	1:G:251:ALA:O	2.20	0.42
1:G:9:ILE:HD11	1:G:23:LEU:HD12	2.01	0.42
1:C:9:ILE:CG2	1:C:19:GLY:HA3	2.49	0.42
1:D:165:LEU:O	1:D:185:THR:HG22	2.18	0.42
1:G:9:ILE:HG21	1:G:19:GLY:HA3	2.02	0.42
1:H:17:ILE:HG22	1:H:59:LEU:CD2	2.48	0.42
1:A:240:GLU:C	1:A:241:ILE:HD12	2.39	0.42
1:B:61:MET:HE1	1:C:71:ARG:NE	2.35	0.42
1:B:161:LYS:CE	1:B:233:GLY:HA3	2.48	0.42
1:C:119:THR:N	1:C:239:ASP:OD2	2.53	0.42
1:F:201:ALA:HB2	1:F:225:SER:HB2	2.00	0.42
1:H:300:ALA:CB	1:H:331:VAL:HG21	2.49	0.42
1:B:8:ARG:HG2	1:B:343:MET:HE3	2.01	0.42
1:B:125:GLU:HA	1:B:129:ARG:NH2	2.34	0.42
1:D:368:LEU:HA	1:D:368:LEU:HD13	1.78	0.42
1:E:304:SER:OG	1:E:356:ASP:OD2	2.14	0.42
1:E:315:MET:HE2	1:H:88:GLY:HA2	2.00	0.42
1:H:117:ALA:O	1:H:241:ILE:HB	2.19	0.42
1:D:233:GLY:HA3	1:D:238:ASN:HB3	2.01	0.42
1:E:136:VAL:O	1:E:140:VAL:HG23	2.19	0.42
1:E:315:MET:HE2	1:E:326:SER:HB3	2.01	0.42
1:G:4:VAL:HG22	1:G:114:VAL:HG12	2.01	0.42
1:G:52:ARG:HH11	2:G:401:CIT:C5	2.33	0.42
1:B:127:LEU:HD12	1:B:165:LEU:HD23	2.01	0.42
1:C:44:ASN:OD1	1:C:325:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:GLU:O	1:E:76:LYS:HG3	2.19	0.42
1:E:348:GLY:N	2:E:401:CIT:O6	2.51	0.42
1:F:133:VAL:HG13	1:F:199:GLY:CA	2.48	0.42
1:A:52:ARG:HD2	1:A:82:MET:O	2.20	0.42
1:B:1:MET:HE3	1:B:250:SER:CA	2.49	0.42
1:F:113:ALA:HB3	1:F:149:ILE:HD11	2.02	0.42
1:G:270:VAL:HG12	1:G:338:VAL:HG11	2.02	0.42
1:G:298:ALA:O	1:G:346:VAL:HA	2.20	0.42
1:A:342:PRO:HD2	1:F:311:ARG:HG3	2.02	0.41
1:B:91:THR:OG1	1:D:311:ARG:HB3	2.19	0.41
1:F:274:LEU:CD2	1:F:293:ILE:HD11	2.50	0.41
1:G:8:ARG:HG2	1:G:343:MET:HE3	2.02	0.41
1:A:254:LEU:HD23	1:A:366:ARG:HA	2.02	0.41
1:F:57:GLN:HE22	1:H:54:PHE:HE1	1.68	0.41
1:G:81:ILE:CD1	1:G:161:LYS:HB2	2.49	0.41
1:A:93:HIS:CB	1:A:343:MET:HE2	2.50	0.41
1:B:217:ILE:O	1:B:217:ILE:HG22	2.20	0.41
1:D:207:ILE:CD1	1:D:212:ILE:HD11	2.50	0.41
1:F:9:ILE:CD1	1:F:23:LEU:HD12	2.49	0.41
1:F:274:LEU:HD23	1:F:363:VAL:HG21	2.03	0.41
1:H:64:ALA:HB2	1:H:74:VAL:HG21	2.03	0.41
1:C:64:ALA:HA	1:C:74:VAL:HG21	2.02	0.41
1:D:297:LEU:HD23	1:D:345:TYR:HB3	2.01	0.41
1:F:127:LEU:HD12	1:F:165:LEU:HD21	2.02	0.41
1:G:115:GLY:N	1:G:147:ALA:HB2	2.36	0.41
1:C:80:PHE:O	1:C:161:LYS:HE3	2.21	0.41
1:F:119:THR:HG22	1:F:139:ALA:CB	2.51	0.41
1:A:234:VAL:HG23	1:A:235:CYS:H	1.85	0.41
1:C:217:ILE:HG22	1:C:217:ILE:O	2.20	0.41
1:C:274:LEU:CD2	1:C:293:ILE:HD11	2.50	0.41
1:D:107:ALA:HB3	1:D:111:ARG:HG3	2.02	0.41
1:E:61:MET:HG3	1:E:71:ARG:HD3	2.02	0.41
1:G:1:MET:CE	1:G:106:ALA:HB2	2.50	0.41
1:G:4:VAL:HG21	1:G:114:VAL:HG12	2.02	0.41
1:H:157:PHE:CZ	1:H:297:LEU:HD13	2.54	0.41
1:A:10:PRO:CA	1:A:343:MET:CE	2.98	0.41
1:B:52:ARG:HD2	1:B:82:MET:O	2.21	0.41
1:F:8:ARG:CG	1:F:343:MET:HE3	2.44	0.41
1:F:62:TYR:HE1	1:F:66:LYS:HZ3	1.61	0.41
1:A:132:GLN:O	1:A:136:VAL:HG23	2.21	0.41
1:A:119:THR:HG21	1:A:239:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ASP:O	1:C:254:LEU:HD23	2.21	0.41
1:D:3:LYS:HG3	1:D:252:SER:HA	2.03	0.41
1:E:240:GLU:C	1:E:241:ILE:HD12	2.41	0.41
1:F:57:GLN:NE2	1:H:54:PHE:CE1	2.88	0.41
1:A:93:HIS:CB	1:A:343:MET:HE3	2.51	0.41
1:A:95:THR:OG1	1:A:295:ASN:ND2	2.54	0.41
1:B:1:MET:CE	1:B:106:ALA:CA	2.98	0.41
1:B:368:LEU:HD12	1:B:368:LEU:H	1.85	0.41
1:E:110:LYS:HG3	1:E:248:THR:CG2	2.50	0.41
1:G:154:ASP:HB3	1:G:246:ASN:O	2.21	0.41
1:D:211:LYS:HE2	1:D:211:LYS:CA	2.44	0.40
1:G:9:ILE:CG2	1:G:19:GLY:HA3	2.51	0.40
1:H:254:LEU:HD23	1:H:366:ARG:HA	2.03	0.40
1:A:274:LEU:HD11	1:A:339:VAL:HG12	2.03	0.40
1:C:220:ASP:OD1	1:C:222:ASN:HB2	2.21	0.40
1:C:274:LEU:HD13	1:C:290:MET:CE	2.51	0.40
1:E:31:PRO:HG2	1:E:67:LEU:HD21	2.02	0.40
1:A:170:ILE:HG12	1:A:180:VAL:HG21	2.02	0.40
1:C:240:GLU:C	1:C:241:ILE:HD12	2.41	0.40
1:C:304:SER:OG	1:C:356:ASP:OD2	2.34	0.40
1:E:361:ILE:O	1:E:361:ILE:HG23	2.21	0.40
1:F:335:ILE:O	1:F:339:VAL:HG22	2.21	0.40
1:G:226:SER:O	1:G:360:PRO:HB3	2.21	0.40
1:H:274:LEU:HD11	1:H:339:VAL:HG12	2.03	0.40
1:D:217:ILE:O	1:D:217:ILE:HG22	2.21	0.40
1:E:337:SER:HB3	1:H:334:VAL:HG22	2.04	0.40
1:G:290:MET:HE1	1:G:338:VAL:O	2.22	0.40

All (1) 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)
1:B:280:ARG:NH1	1:E:210:ASP:OD2[4_455]	1.97	0.23

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	363/370 (98%)	351 (97%)	12 (3%)	0	100	100
1	B	361/370 (98%)	349 (97%)	12 (3%)	0	100	100
1	C	360/370 (97%)	345 (96%)	15 (4%)	0	100	100
1	D	362/370 (98%)	347 (96%)	15 (4%)	0	100	100
1	E	362/370 (98%)	351 (97%)	11 (3%)	0	100	100
1	F	353/370 (95%)	344 (98%)	9 (2%)	0	100	100
1	G	355/370 (96%)	347 (98%)	8 (2%)	0	100	100
1	H	361/370 (98%)	349 (97%)	12 (3%)	0	100	100
All	All	2877/2960 (97%)	2783 (97%)	94 (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	288/293 (98%)	285 (99%)	3 (1%)	76	90
1	B	286/293 (98%)	286 (100%)	0	100	100
1	C	285/293 (97%)	284 (100%)	1 (0%)	91	95
1	D	287/293 (98%)	284 (99%)	3 (1%)	76	90
1	E	287/293 (98%)	284 (99%)	3 (1%)	76	90
1	F	281/293 (96%)	280 (100%)	1 (0%)	91	95
1	G	282/293 (96%)	279 (99%)	3 (1%)	73	88
1	H	286/293 (98%)	284 (99%)	2 (1%)	84	94
All	All	2282/2344 (97%)	2266 (99%)	16 (1%)	84	94

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	ASP
1	A	368	LEU
1	A	370	HIS
1	C	218	VAL
1	D	218	VAL
1	D	219	HIS
1	D	368	LEU
1	E	153	ARG
1	E	239	ASP
1	E	368	LEU
1	F	239	ASP
1	G	138	ARG
1	G	218	VAL
1	G	239	ASP
1	H	239	ASP
1	H	368	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	183	ASN
1	A	214	ASN
1	B	57	GLN
1	B	148	GLN
1	B	159	GLN
1	B	214	ASN
1	B	238	ASN
1	C	57	GLN
1	C	249	ASN
1	C	322	ASN
1	D	57	GLN
1	D	238	ASN
1	D	322	ASN
1	F	57	GLN
1	F	134	ASN
1	G	57	GLN
1	H	57	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CIT	A	401	-	12,12,12	1.14	0	17,17,17	1.63	4 (23%)
2	CIT	C	401	-	12,12,12	1.02	0	17,17,17	2.09	4 (23%)
2	CIT	D	401	-	12,12,12	1.21	1 (8%)	17,17,17	2.10	6 (35%)
2	CIT	E	401	-	12,12,12	1.08	0	17,17,17	1.47	1 (5%)
2	CIT	F	401	-	12,12,12	0.96	0	17,17,17	1.71	3 (17%)
2	CIT	G	401	-	12,12,12	1.04	0	17,17,17	1.69	1 (5%)
2	CIT	B	401	-	12,12,12	1.04	0	17,17,17	1.94	5 (29%)
2	CIT	H	401	-	12,12,12	1.26	1 (8%)	17,17,17	1.81	6 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	A	401	-	-	9/16/16/16	-
2	CIT	C	401	-	-	2/16/16/16	-
2	CIT	D	401	-	-	7/16/16/16	-
2	CIT	E	401	-	-	9/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	F	401	-	-	10/16/16/16	-
2	CIT	G	401	-	-	12/16/16/16	-
2	CIT	B	401	-	-	7/16/16/16	-
2	CIT	H	401	-	-	10/16/16/16	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	CIT	C3-C6	2.20	1.55	1.53
2	H	401	CIT	C3-C6	2.14	1.55	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	CIT	O6-C6-C3	5.81	123.15	113.05
2	D	401	CIT	O6-C6-C3	5.56	122.71	113.05
2	G	401	CIT	O6-C6-C3	4.60	121.05	113.05
2	F	401	CIT	O6-C6-C3	4.56	120.96	113.05
2	B	401	CIT	O6-C6-C3	4.41	120.71	113.05
2	E	401	CIT	O6-C6-C3	4.12	120.21	113.05
2	H	401	CIT	O6-C6-C3	4.10	120.17	113.05
2	A	401	CIT	O5-C6-C3	2.97	126.45	122.25
2	B	401	CIT	O7-C3-C2	-2.77	102.92	109.40
2	B	401	CIT	O4-C5-C4	2.67	122.92	114.35
2	H	401	CIT	O2-C1-O1	-2.66	116.68	123.30
2	D	401	CIT	C3-C4-C5	-2.62	107.46	113.81
2	D	401	CIT	O2-C1-O1	-2.59	116.84	123.30
2	C	401	CIT	O5-C6-C3	-2.59	118.59	122.25
2	A	401	CIT	O2-C1-C2	2.44	122.18	114.35
2	A	401	CIT	O2-C1-O1	-2.37	117.39	123.30
2	C	401	CIT	C2-C3-C6	2.33	115.11	110.11
2	D	401	CIT	O4-C5-C4	2.31	121.78	114.35
2	D	401	CIT	O2-C1-C2	2.24	121.55	114.35
2	H	401	CIT	O4-C5-O3	-2.20	117.80	123.30
2	F	401	CIT	O2-C1-C2	2.19	121.38	114.35
2	H	401	CIT	O4-C5-C4	2.19	121.37	114.35
2	H	401	CIT	O2-C1-C2	2.13	121.18	114.35
2	B	401	CIT	O2-C1-C2	2.12	121.16	114.35
2	B	401	CIT	C2-C3-C6	2.10	114.61	110.11
2	F	401	CIT	C3-C4-C5	-2.08	108.78	113.81
2	C	401	CIT	O2-C1-O1	-2.06	118.16	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	CIT	O6-C6-O5	-2.04	117.34	123.82
2	D	401	CIT	O6-C6-O5	-2.02	117.39	123.82
2	H	401	CIT	O7-C3-C6	-2.00	106.06	108.86

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CIT	C2-C3-C4-C5
2	A	401	CIT	O7-C3-C4-C5
2	A	401	CIT	C6-C3-C4-C5
2	A	401	CIT	C2-C3-C6-O5
2	A	401	CIT	C2-C3-C6-O6
2	A	401	CIT	O7-C3-C6-O5
2	A	401	CIT	O7-C3-C6-O6
2	B	401	CIT	O7-C3-C6-O5
2	B	401	CIT	O7-C3-C6-O6
2	B	401	CIT	C4-C3-C6-O5
2	B	401	CIT	C4-C3-C6-O6
2	D	401	CIT	C2-C3-C4-C5
2	D	401	CIT	O7-C3-C4-C5
2	D	401	CIT	C6-C3-C4-C5
2	D	401	CIT	O7-C3-C6-O5
2	D	401	CIT	O7-C3-C6-O6
2	D	401	CIT	C4-C3-C6-O5
2	D	401	CIT	C4-C3-C6-O6
2	E	401	CIT	C2-C3-C4-C5
2	E	401	CIT	O7-C3-C4-C5
2	E	401	CIT	C6-C3-C4-C5
2	E	401	CIT	O7-C3-C6-O5
2	E	401	CIT	O7-C3-C6-O6
2	E	401	CIT	C4-C3-C6-O5
2	E	401	CIT	C4-C3-C6-O6
2	F	401	CIT	O7-C3-C6-O5
2	F	401	CIT	O7-C3-C6-O6
2	F	401	CIT	C4-C3-C6-O5
2	F	401	CIT	C4-C3-C6-O6
2	G	401	CIT	C2-C3-C6-O5
2	G	401	CIT	C2-C3-C6-O6
2	G	401	CIT	O7-C3-C6-O5
2	G	401	CIT	O7-C3-C6-O6
2	H	401	CIT	C1-C2-C3-O7

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Mol	Chain	Res	Type	Atoms
2	H	401	CIT	C1-C2-C3-C4
2	H	401	CIT	C1-C2-C3-C6
2	H	401	CIT	C2-C3-C6-O5
2	H	401	CIT	C2-C3-C6-O6
2	H	401	CIT	O7-C3-C6-O5
2	H	401	CIT	O7-C3-C6-O6
2	F	401	CIT	C1-C2-C3-C4
2	F	401	CIT	C1-C2-C3-C6
2	H	401	CIT	C4-C3-C6-O6
2	C	401	CIT	C1-C2-C3-O7
2	F	401	CIT	C1-C2-C3-O7
2	F	401	CIT	C2-C3-C6-O5
2	F	401	CIT	C2-C3-C6-O6
2	G	401	CIT	C1-C2-C3-C4
2	E	401	CIT	C3-C4-C5-O3
2	E	401	CIT	C3-C4-C5-O4
2	G	401	CIT	C1-C2-C3-C6
2	H	401	CIT	C4-C3-C6-O5
2	B	401	CIT	C1-C2-C3-O7
2	C	401	CIT	C1-C2-C3-C4
2	G	401	CIT	O7-C3-C4-C5
2	G	401	CIT	C6-C3-C4-C5
2	H	401	CIT	C6-C3-C4-C5
2	G	401	CIT	C4-C3-C6-O6
2	A	401	CIT	O2-C1-C2-C3
2	A	401	CIT	O1-C1-C2-C3
2	G	401	CIT	O1-C1-C2-C3
2	G	401	CIT	O2-C1-C2-C3
2	B	401	CIT	O1-C1-C2-C3
2	B	401	CIT	O2-C1-C2-C3
2	F	401	CIT	O7-C3-C4-C5
2	G	401	CIT	C2-C3-C4-C5

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	CIT	2	0
2	D	401	CIT	2	0
2	E	401	CIT	3	0
2	F	401	CIT	2	0
2	G	401	CIT	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	CIT	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	365/370 (98%)	-0.08	7 (1%)	66	53	62, 112, 196, 251	0
1	B	363/370 (98%)	-0.05	3 (0%)	86	78	68, 114, 179, 254	0
1	C	362/370 (97%)	-0.00	7 (1%)	66	53	86, 133, 196, 242	0
1	D	364/370 (98%)	-0.10	1 (0%)	94	92	75, 114, 166, 230	0
1	E	364/370 (98%)	-0.10	9 (2%)	57	43	84, 137, 210, 259	0
1	F	357/370 (96%)	0.05	13 (3%)	42	27	91, 165, 230, 306	0
1	G	359/370 (97%)	0.13	23 (6%)	19	11	90, 166, 236, 297	0
1	H	363/370 (98%)	0.04	5 (1%)	75	63	77, 126, 179, 254	0
All	All	2897/2960 (97%)	-0.02	68 (2%)	60	47	62, 131, 212, 306	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	157	PHE	5.6
1	G	136	VAL	5.0
1	G	122	PHE	4.5
1	G	181	VAL	4.4
1	F	5	GLU	4.3
1	G	158	VAL	4.1
1	E	6	VAL	4.0
1	F	243	VAL	4.0
1	A	239	ASP	3.9
1	G	7	PHE	3.8
1	G	124	PRO	3.7
1	F	127	LEU	3.4
1	H	37	ILE	3.3
1	F	180	VAL	3.3
1	C	144	MET	3.1
1	G	212	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	115	GLY	3.1
1	F	97	PHE	3.0
1	G	128	GLY	3.0
1	B	183	ASN	3.0
1	G	182	VAL	3.0
1	C	242	ILE	3.0
1	H	97	PHE	2.9
1	F	242	ILE	2.8
1	E	170	ILE	2.8
1	F	158	VAL	2.8
1	H	300	ALA	2.7
1	F	98	VAL	2.6
1	G	97	PHE	2.6
1	G	59	LEU	2.6
1	A	164	LEU	2.5
1	G	37	ILE	2.5
1	E	96	VAL	2.5
1	C	364	ILE	2.5
1	G	96	VAL	2.4
1	C	243	VAL	2.4
1	E	97	PHE	2.4
1	F	265	ILE	2.3
1	G	234	VAL	2.3
1	A	236	LEU	2.3
1	H	80	PHE	2.3
1	B	97	PHE	2.2
1	E	136	VAL	2.2
1	G	197	ALA	2.2
1	F	181	VAL	2.2
1	G	206	GLU	2.2
1	F	124	PRO	2.2
1	C	165	LEU	2.2
1	E	207	ILE	2.2
1	A	122	PHE	2.2
1	A	317	ASP	2.2
1	G	127	LEU	2.2
1	C	170	ILE	2.1
1	A	128	GLY	2.1
1	E	63	LEU	2.1
1	G	217	ILE	2.1
1	D	212	ILE	2.1
1	G	17	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	204	LEU	2.1
1	C	97	PHE	2.1
1	A	169	ARG	2.1
1	G	123	LEU	2.1
1	B	191	TYR	2.1
1	E	7	PHE	2.1
1	H	277	ALA	2.1
1	F	212	ILE	2.1
1	F	96	VAL	2.0
1	E	212	ILE	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
2	CIT	D	401	13/13	0.80	0.13	93,100,109,110	0
2	CIT	H	401	13/13	0.87	0.18	87,111,122,123	0
2	CIT	G	401	13/13	0.89	0.12	126,140,153,154	0
2	CIT	E	401	13/13	0.91	0.10	96,109,113,115	0
2	CIT	B	401	13/13	0.93	0.12	73,85,90,91	0
2	CIT	C	401	13/13	0.93	0.13	87,105,119,119	0
2	CIT	A	401	13/13	0.93	0.13	84,104,116,116	0
2	CIT	F	401	13/13	0.94	0.12	101,139,147,148	0

6.5 Other polymers (i)

There are no such residues in this entry.