Full wwPDB X-ray Structure Validation Report ⓘ

Apr 30, 2025 – 12:13 PM JST

PDB ID	:	9IJF / pdb_00009ijf
Title	:	Structure of ATP-dependent diazotase CmaA6
Authors	:	Katsuyama, Y.; Kawai, S.; Ohnishi, Y.
Deposited on	:	2024-06-22
Resolution	:	2.73 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 ⓘ 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 ⓘ) were used in the production of this report:

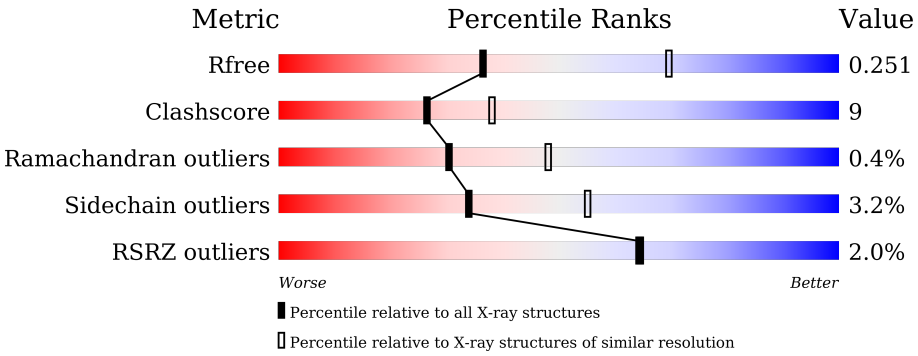
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.73 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}	164625	1649 (2.76-2.72)
Clashscore	180529	1744 (2.76-2.72)
Ramachandran outliers	177936	1710 (2.76-2.72)
Sidechain outliers	177891	1711 (2.76-2.72)
RSRZ outliers	164620	1649 (2.76-2.72)

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	569	7% 73% 21% • 5%
1	B	569	% 71% 19% • 8%
1	D	569	% 75% 16% 8%
1	E	569	72% 19% • 8%
1	F	569	% 68% 23% • 8%
1	G	569	3% 71% 20% • 8%

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Mol	Chain	Length	Quality of chain
1	H	569	2% 70% 22% 8%
1	I	569	71% 21% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 32117 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative AMP-binding enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4104	2581	726	784	13			
1	B	523	Total	C	N	O	S	0	0	0
			3996	2514	706	763	13			
1	D	523	Total	C	N	O	S	0	0	0
			3996	2514	706	763	13			
1	E	521	Total	C	N	O	S	0	0	0
			3982	2507	704	758	13			
1	F	523	Total	C	N	O	S	0	0	0
			3996	2514	706	763	13			
1	G	523	Total	C	N	O	S	0	0	0
			3996	2514	706	763	13			
1	H	523	Total	C	N	O	S	0	0	0
			3996	2514	706	763	13			
1	I	524	Total	C	N	O	S	0	0	0
			4006	2520	709	764	13			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP W5W4E6
A	-14	ASN	-	expression tag	UNP W5W4E6
A	-13	HIS	-	expression tag	UNP W5W4E6
A	-12	LYS	-	expression tag	UNP W5W4E6
A	-11	VAL	-	expression tag	UNP W5W4E6
A	-10	HIS	-	expression tag	UNP W5W4E6
A	-9	HIS	-	expression tag	UNP W5W4E6
A	-8	HIS	-	expression tag	UNP W5W4E6
A	-7	HIS	-	expression tag	UNP W5W4E6
A	-6	HIS	-	expression tag	UNP W5W4E6
A	-5	HIS	-	expression tag	UNP W5W4E6
A	-4	ILE	-	expression tag	UNP W5W4E6
A	-3	GLU	-	expression tag	UNP W5W4E6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP W5W4E6
A	-1	ARG	-	expression tag	UNP W5W4E6
A	0	HIS	-	expression tag	UNP W5W4E6
B	-15	MET	-	initiating methionine	UNP W5W4E6
B	-14	ASN	-	expression tag	UNP W5W4E6
B	-13	HIS	-	expression tag	UNP W5W4E6
B	-12	LYS	-	expression tag	UNP W5W4E6
B	-11	VAL	-	expression tag	UNP W5W4E6
B	-10	HIS	-	expression tag	UNP W5W4E6
B	-9	HIS	-	expression tag	UNP W5W4E6
B	-8	HIS	-	expression tag	UNP W5W4E6
B	-7	HIS	-	expression tag	UNP W5W4E6
B	-6	HIS	-	expression tag	UNP W5W4E6
B	-5	HIS	-	expression tag	UNP W5W4E6
B	-4	ILE	-	expression tag	UNP W5W4E6
B	-3	GLU	-	expression tag	UNP W5W4E6
B	-2	GLY	-	expression tag	UNP W5W4E6
B	-1	ARG	-	expression tag	UNP W5W4E6
B	0	HIS	-	expression tag	UNP W5W4E6
D	-15	MET	-	initiating methionine	UNP W5W4E6
D	-14	ASN	-	expression tag	UNP W5W4E6
D	-13	HIS	-	expression tag	UNP W5W4E6
D	-12	LYS	-	expression tag	UNP W5W4E6
D	-11	VAL	-	expression tag	UNP W5W4E6
D	-10	HIS	-	expression tag	UNP W5W4E6
D	-9	HIS	-	expression tag	UNP W5W4E6
D	-8	HIS	-	expression tag	UNP W5W4E6
D	-7	HIS	-	expression tag	UNP W5W4E6
D	-6	HIS	-	expression tag	UNP W5W4E6
D	-5	HIS	-	expression tag	UNP W5W4E6
D	-4	ILE	-	expression tag	UNP W5W4E6
D	-3	GLU	-	expression tag	UNP W5W4E6
D	-2	GLY	-	expression tag	UNP W5W4E6
D	-1	ARG	-	expression tag	UNP W5W4E6
D	0	HIS	-	expression tag	UNP W5W4E6
E	-15	MET	-	initiating methionine	UNP W5W4E6
E	-14	ASN	-	expression tag	UNP W5W4E6
E	-13	HIS	-	expression tag	UNP W5W4E6
E	-12	LYS	-	expression tag	UNP W5W4E6
E	-11	VAL	-	expression tag	UNP W5W4E6
E	-10	HIS	-	expression tag	UNP W5W4E6
E	-9	HIS	-	expression tag	UNP W5W4E6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-8	HIS	-	expression tag	UNP W5W4E6
E	-7	HIS	-	expression tag	UNP W5W4E6
E	-6	HIS	-	expression tag	UNP W5W4E6
E	-5	HIS	-	expression tag	UNP W5W4E6
E	-4	ILE	-	expression tag	UNP W5W4E6
E	-3	GLU	-	expression tag	UNP W5W4E6
E	-2	GLY	-	expression tag	UNP W5W4E6
E	-1	ARG	-	expression tag	UNP W5W4E6
E	0	HIS	-	expression tag	UNP W5W4E6
F	-15	MET	-	initiating methionine	UNP W5W4E6
F	-14	ASN	-	expression tag	UNP W5W4E6
F	-13	HIS	-	expression tag	UNP W5W4E6
F	-12	LYS	-	expression tag	UNP W5W4E6
F	-11	VAL	-	expression tag	UNP W5W4E6
F	-10	HIS	-	expression tag	UNP W5W4E6
F	-9	HIS	-	expression tag	UNP W5W4E6
F	-8	HIS	-	expression tag	UNP W5W4E6
F	-7	HIS	-	expression tag	UNP W5W4E6
F	-6	HIS	-	expression tag	UNP W5W4E6
F	-5	HIS	-	expression tag	UNP W5W4E6
F	-4	ILE	-	expression tag	UNP W5W4E6
F	-3	GLU	-	expression tag	UNP W5W4E6
F	-2	GLY	-	expression tag	UNP W5W4E6
F	-1	ARG	-	expression tag	UNP W5W4E6
F	0	HIS	-	expression tag	UNP W5W4E6
G	-15	MET	-	initiating methionine	UNP W5W4E6
G	-14	ASN	-	expression tag	UNP W5W4E6
G	-13	HIS	-	expression tag	UNP W5W4E6
G	-12	LYS	-	expression tag	UNP W5W4E6
G	-11	VAL	-	expression tag	UNP W5W4E6
G	-10	HIS	-	expression tag	UNP W5W4E6
G	-9	HIS	-	expression tag	UNP W5W4E6
G	-8	HIS	-	expression tag	UNP W5W4E6
G	-7	HIS	-	expression tag	UNP W5W4E6
G	-6	HIS	-	expression tag	UNP W5W4E6
G	-5	HIS	-	expression tag	UNP W5W4E6
G	-4	ILE	-	expression tag	UNP W5W4E6
G	-3	GLU	-	expression tag	UNP W5W4E6
G	-2	GLY	-	expression tag	UNP W5W4E6
G	-1	ARG	-	expression tag	UNP W5W4E6
G	0	HIS	-	expression tag	UNP W5W4E6
H	-15	MET	-	initiating methionine	UNP W5W4E6

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-14	ASN	-	expression tag	UNP W5W4E6
H	-13	HIS	-	expression tag	UNP W5W4E6
H	-12	LYS	-	expression tag	UNP W5W4E6
H	-11	VAL	-	expression tag	UNP W5W4E6
H	-10	HIS	-	expression tag	UNP W5W4E6
H	-9	HIS	-	expression tag	UNP W5W4E6
H	-8	HIS	-	expression tag	UNP W5W4E6
H	-7	HIS	-	expression tag	UNP W5W4E6
H	-6	HIS	-	expression tag	UNP W5W4E6
H	-5	HIS	-	expression tag	UNP W5W4E6
H	-4	ILE	-	expression tag	UNP W5W4E6
H	-3	GLU	-	expression tag	UNP W5W4E6
H	-2	GLY	-	expression tag	UNP W5W4E6
H	-1	ARG	-	expression tag	UNP W5W4E6
H	0	HIS	-	expression tag	UNP W5W4E6
I	-15	MET	-	initiating methionine	UNP W5W4E6
I	-14	ASN	-	expression tag	UNP W5W4E6
I	-13	HIS	-	expression tag	UNP W5W4E6
I	-12	LYS	-	expression tag	UNP W5W4E6
I	-11	VAL	-	expression tag	UNP W5W4E6
I	-10	HIS	-	expression tag	UNP W5W4E6
I	-9	HIS	-	expression tag	UNP W5W4E6
I	-8	HIS	-	expression tag	UNP W5W4E6
I	-7	HIS	-	expression tag	UNP W5W4E6
I	-6	HIS	-	expression tag	UNP W5W4E6
I	-5	HIS	-	expression tag	UNP W5W4E6
I	-4	ILE	-	expression tag	UNP W5W4E6
I	-3	GLU	-	expression tag	UNP W5W4E6
I	-2	GLY	-	expression tag	UNP W5W4E6
I	-1	ARG	-	expression tag	UNP W5W4E6
I	0	HIS	-	expression tag	UNP W5W4E6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	3	Total O 3 3	0	0
2	D	11	Total O 11 11	0	0
2	E	4	Total O 4 4	0	0

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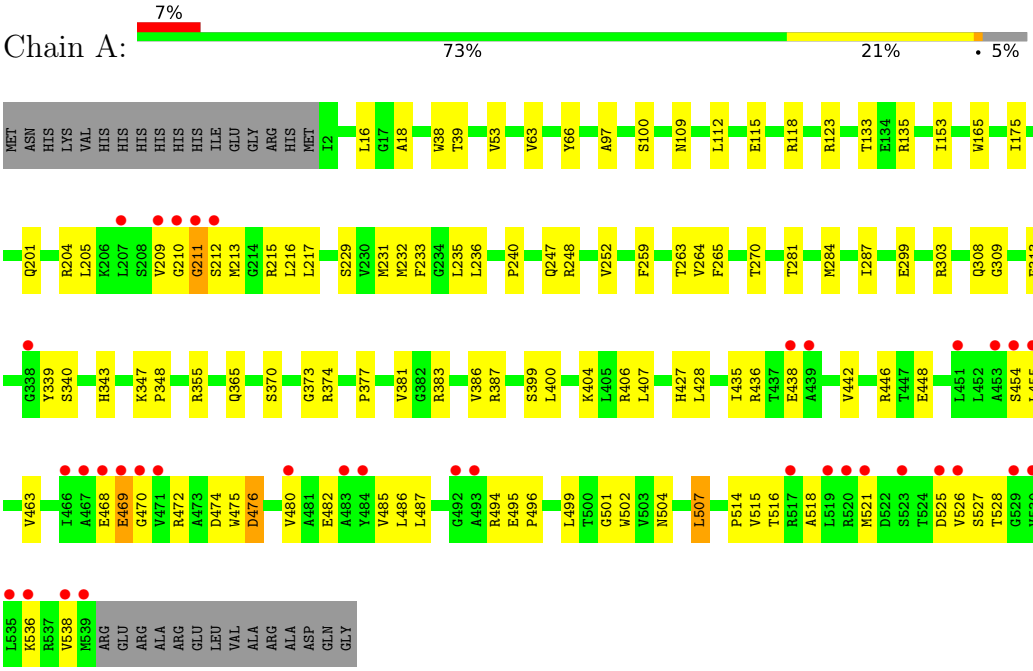
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	3	Total O 3 3	0	0
2	G	4	Total O 4 4	0	0
2	H	4	Total O 4 4	0	0
2	I	6	Total O 6 6	0	0

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.

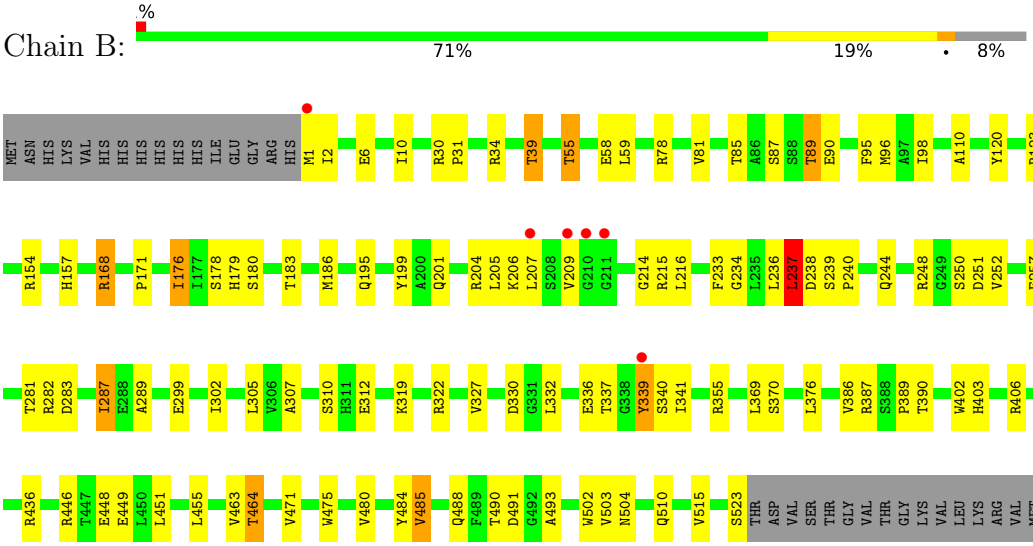
• Molecule 1: Putative AMP-binding enzyme

Chain A:



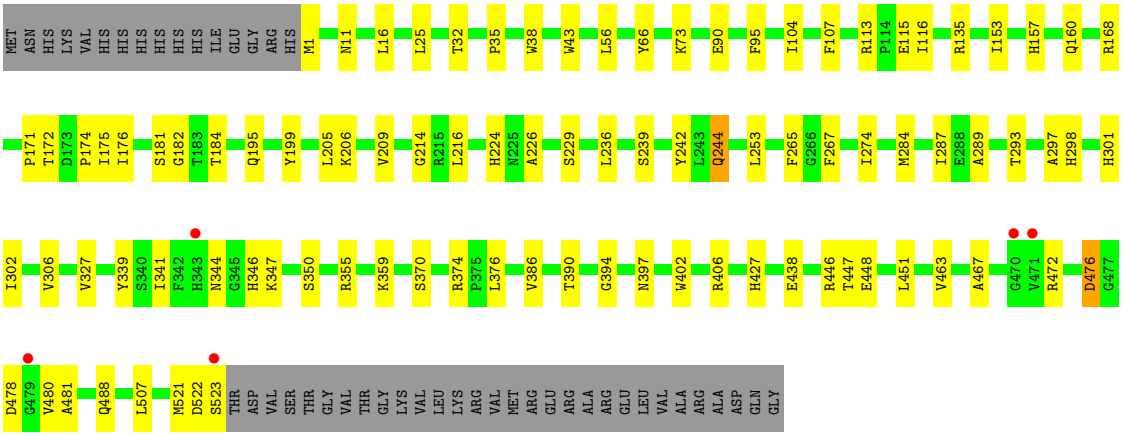
• Molecule 1: Putative AMP-binding enzyme

Chain B:



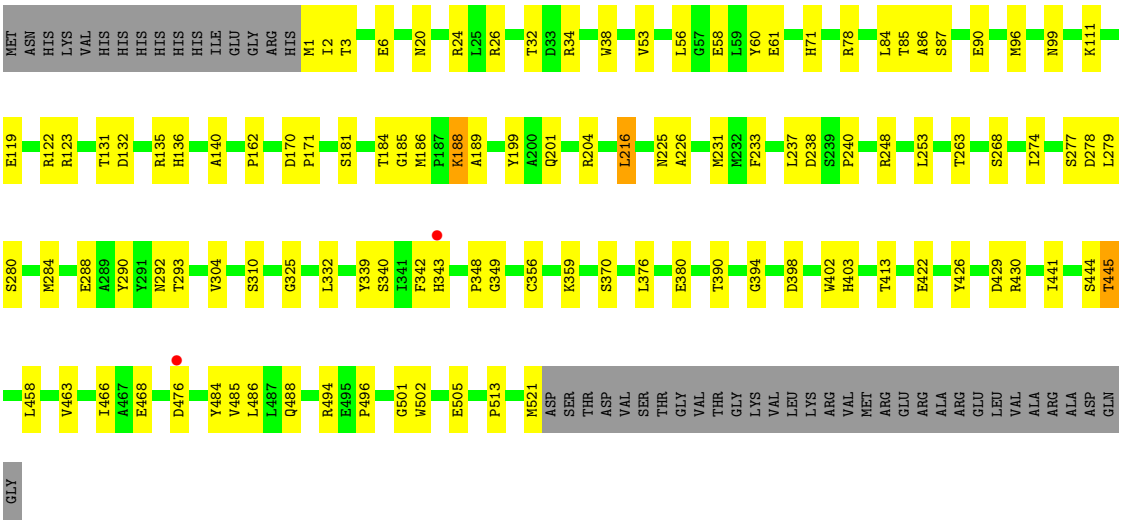
• Molecule 1: Putative AMP-binding enzyme

Chain D:



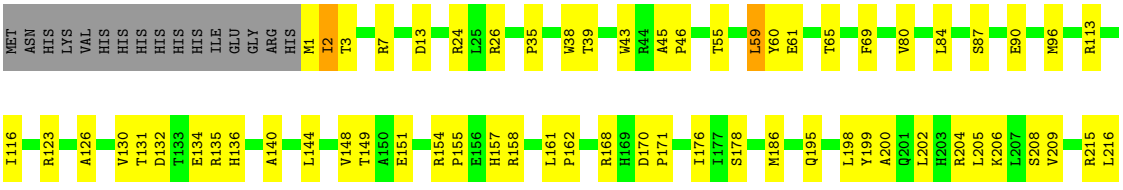
• Molecule 1: Putative AMP-binding enzyme

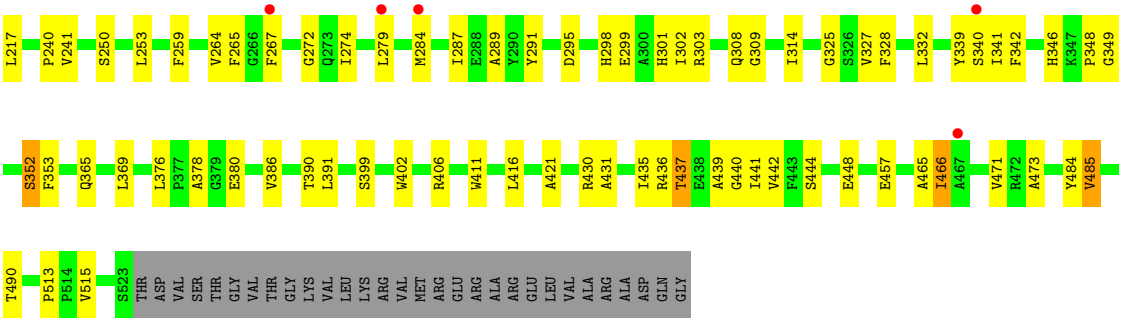
Chain E:



• Molecule 1: Putative AMP-binding enzyme

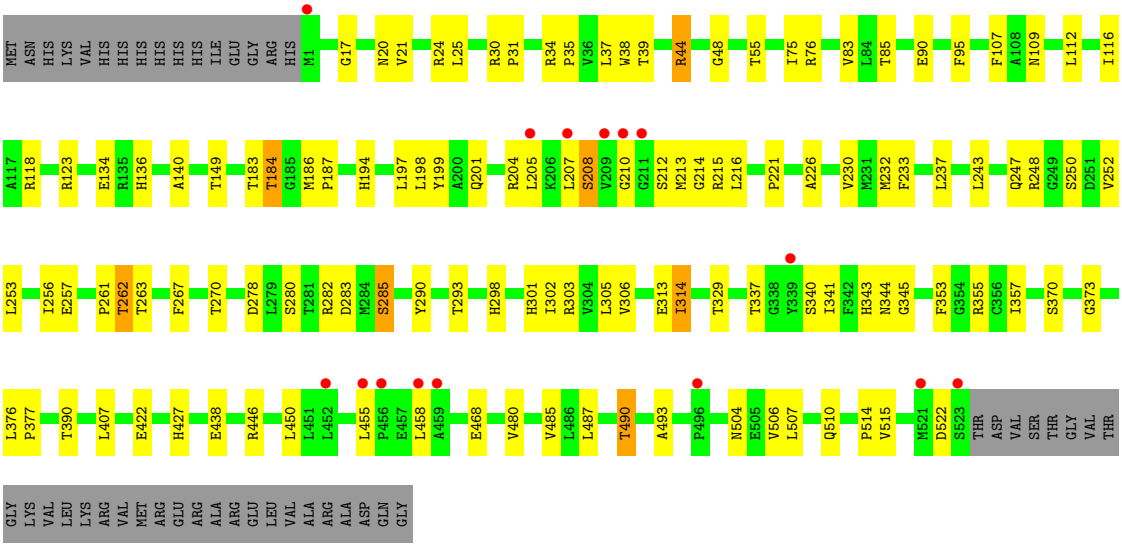
Chain F:





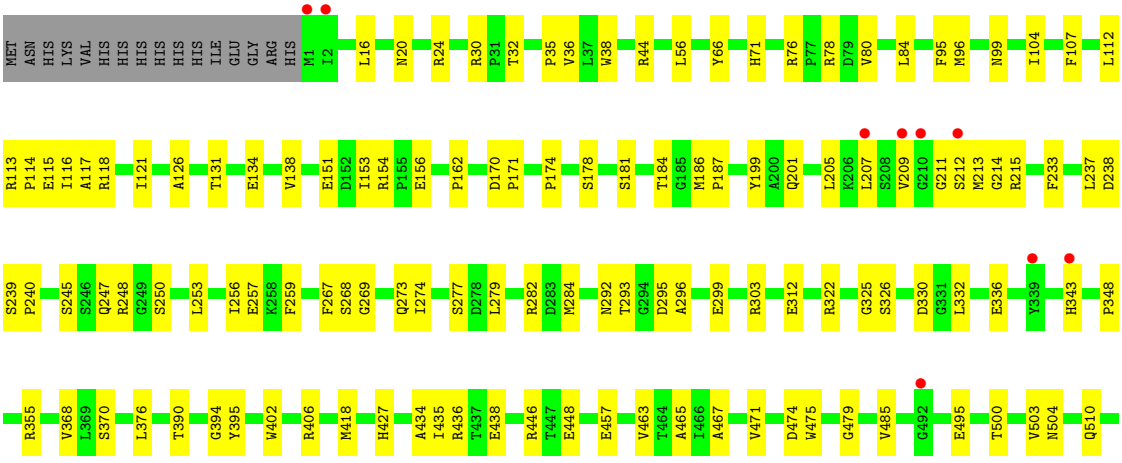
• Molecule 1: Putative AMP-binding enzyme

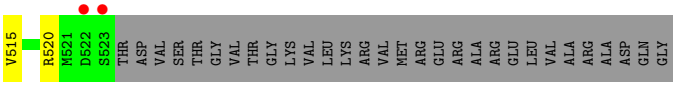
Chain G:



• Molecule 1: Putative AMP-binding enzyme

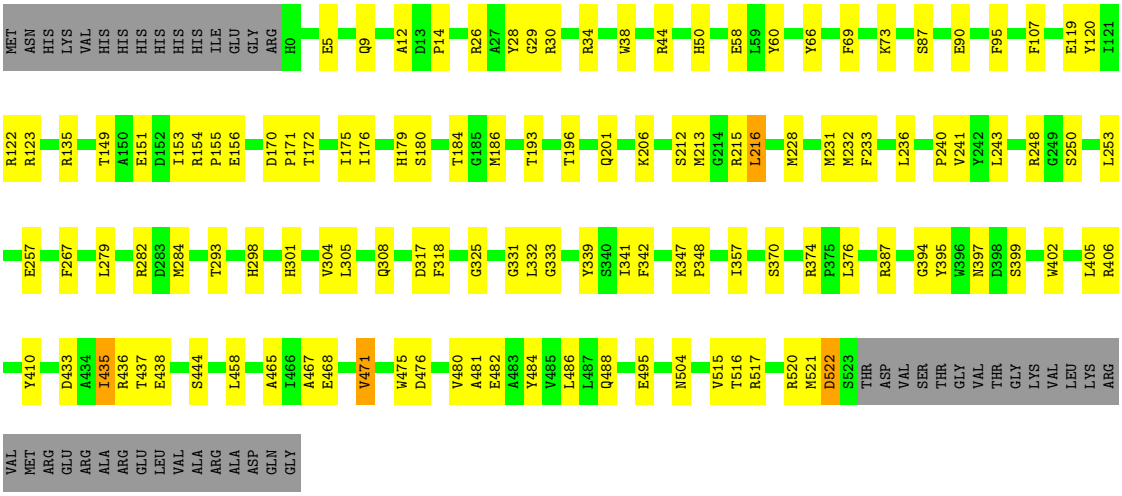
Chain H:





• Molecule 1: Putative AMP-binding enzyme

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	94.16Å 101.07Å 157.41Å 76.31° 88.05° 62.28°	Depositor
Resolution (Å)	65.95 – 2.73 65.95 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.6 (65.95-2.73) 98.6 (65.95-2.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.194 , 0.251 0.197 , 0.251	Depositor DCC
R_{free} test set	3676 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.048 for h,h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	32117	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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

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	0.40	0/4204	0.55	0/5720
1	B	0.38	0/4096	0.60	2/5574 (0.0%)
1	D	0.41	0/4096	0.60	2/5574 (0.0%)
1	E	0.41	0/4082	0.62	0/5555
1	F	0.35	0/4096	0.56	0/5574
1	G	0.37	0/4096	0.56	0/5574
1	H	0.39	0/4096	0.56	0/5574
1	I	0.40	0/4107	0.60	0/5589
All	All	0.39	0/32873	0.58	4/44734 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	181	SER	CA-C-N	-8.03	105.68	121.41
1	D	181	SER	C-N-CA	-8.03	105.68	121.41
1	B	237	LEU	CA-C-N	-6.57	109.00	121.54
1	B	237	LEU	C-N-CA	-6.57	109.00	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	182	GLY	Peptide
1	H	78	ARG	Sidechain

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	4104	0	3997	82	0
1	B	3996	0	3878	70	0
1	D	3996	0	3878	63	0
1	E	3982	0	3869	69	1
1	F	3996	0	3878	82	0
1	G	3996	0	3878	79	0
1	H	3996	0	3878	79	0
1	I	4006	0	3885	81	1
2	A	10	0	0	1	0
2	B	3	0	0	0	0
2	D	11	0	0	0	0
2	E	4	0	0	0	0
2	F	3	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	6	0	0	0	0
All	All	32117	0	31141	584	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 9.

All (584) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:458:LEU:O	1:I:34:ARG:NH1	1.90	1.05
1:G:31:PRO:HG2	1:G:34:ARG:HD2	1.50	0.94
1:B:39:THR:HB	1:B:89:THR:HG21	1.50	0.93
1:H:186:MET:HE3	1:H:187:PRO:HD2	1.51	0.91
1:H:279:LEU:HD21	1:H:284:MET:HE3	1.55	0.88
1:A:487:LEU:HD11	1:A:518:ALA:HB1	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:332:LEU:HD13	1:I:357:ILE:HG23	1.60	0.83
1:D:11:ASN:O	1:D:206:LYS:NZ	2.11	0.83
1:A:215:ARG:NH1	1:A:259:PHE:O	2.13	0.82
1:F:437:THR:HG22	1:F:439:ALA:H	1.46	0.79
1:D:438:GLU:N	1:D:438:GLU:OE1	2.17	0.77
1:F:279:LEU:HD21	1:F:284:MET:HG2	1.65	0.76
1:I:436:ARG:NH2	1:I:475:TRP:O	2.17	0.76
1:B:30:ARG:NH1	1:B:236:LEU:O	2.18	0.76
1:I:248:ARG:HE	1:I:250:SER:H	1.34	0.75
1:I:293:THR:HG23	1:I:339:TYR:HB3	1.69	0.75
1:A:507:LEU:HD23	1:A:514:PRO:HA	1.67	0.74
1:I:488:GLN:HB2	1:I:521:MET:HE3	1.69	0.74
1:I:231:MET:CE	1:I:232:MET:HE3	2.20	0.72
1:D:472:ARG:HH21	1:D:476:ASP:HB2	1.53	0.71
1:A:284:MET:HE3	1:A:308:GLN:HG3	1.71	0.71
1:G:340:SER:HB2	1:G:343:HIS:CE1	2.25	0.71
1:H:112:LEU:HD22	1:H:116:ILE:HD11	1.71	0.70
1:H:267:PHE:HE1	1:H:293:THR:HB	1.55	0.70
1:H:215:ARG:NH1	1:H:259:PHE:O	2.26	0.69
1:G:355:ARG:HD2	1:G:446:ARG:HD2	1.75	0.68
1:D:472:ARG:NH2	1:D:476:ASP:HB2	2.08	0.68
1:I:5:GLU:CD	1:I:5:GLU:H	2.01	0.68
1:A:109:ASN:HB3	1:A:112:LEU:HD13	1.76	0.68
1:I:279:LEU:HD13	1:I:284:MET:HE2	1.76	0.68
1:F:151:GLU:H	1:F:151:GLU:CD	2.01	0.68
1:G:134:GLU:OE2	1:G:134:GLU:N	2.20	0.67
1:H:214:GLY:O	1:H:239:SER:HB2	1.95	0.66
1:E:2:ILE:HG23	1:E:6:GLU:HG3	1.77	0.66
1:G:248:ARG:NH1	1:G:250:SER:OG	2.28	0.66
1:F:43:TRP:HD1	1:F:90:GLU:HG3	1.61	0.66
1:D:1:MET:HE1	1:D:214:GLY:HA2	1.77	0.66
1:A:428:LEU:O	1:A:446:ARG:NH1	2.27	0.65
1:B:123:ARG:NH1	1:B:186:MET:HG2	2.11	0.65
1:D:16:LEU:HD21	1:D:236:LEU:HD11	1.78	0.65
1:A:118:ARG:HD3	2:A:610:HOH:O	1.95	0.65
1:A:494:ARG:H	1:A:494:ARG:HD2	1.60	0.65
1:H:253:LEU:HD23	1:H:256:ILE:HD12	1.79	0.64
1:I:370:SER:HB3	1:I:376:LEU:HD21	1.78	0.64
1:D:355:ARG:HD3	1:D:427:HIS:O	1.98	0.64
1:D:293:THR:HB	1:D:339:TYR:HB2	1.79	0.64
1:D:157:HIS:HD2	1:D:160:GLN:HE22	1.45	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:LYS:N	1:D:350:SER:OG	2.32	0.63
1:E:3:THR:OG1	1:E:6:GLU:HG2	1.98	0.63
1:F:84:LEU:HB3	1:F:131:THR:HG22	1.80	0.63
1:F:199:TYR:HB3	1:F:390:THR:HG22	1.81	0.63
1:A:204:ARG:NH2	1:A:339:TYR:OH	2.31	0.63
1:I:495:GLU:OE1	1:I:520:ARG:NH1	2.32	0.62
1:D:224:HIS:CD2	1:D:226:ALA:H	2.17	0.62
1:E:279:LEU:HD13	1:E:284:MET:HE2	1.81	0.62
1:D:171:PRO:O	1:D:195:GLN:HG2	1.99	0.62
1:D:224:HIS:HD2	1:D:226:ALA:H	1.48	0.62
1:E:486:LEU:HD12	1:E:521:MET:HB3	1.81	0.62
1:F:7:ARG:HH12	1:F:208:SER:HA	1.63	0.62
1:G:507:LEU:HD23	1:G:514:PRO:HA	1.81	0.61
1:H:16:LEU:HD13	1:H:24:ARG:HG3	1.82	0.61
1:I:231:MET:HE1	1:I:232:MET:HE3	1.82	0.61
1:A:406:ARG:NH2	1:D:172:THR:OG1	2.33	0.61
1:E:466:ILE:HD11	1:E:484:TYR:CE2	2.36	0.61
1:I:201:GLN:HB3	1:I:233:PHE:CE1	2.35	0.61
1:F:217:LEU:HB3	1:F:264:VAL:HG22	1.81	0.61
1:A:210:GLY:O	1:A:212:SER:N	2.34	0.61
1:G:233:PHE:CZ	1:G:237:LEU:HD11	2.36	0.61
1:B:387:ARG:HH21	1:B:409:GLY:HA3	1.66	0.61
1:D:32:THR:HA	1:D:56:LEU:HB3	1.83	0.61
1:A:16:LEU:HD21	1:A:236:LEU:HD11	1.83	0.60
1:F:43:TRP:CD1	1:F:90:GLU:HG3	2.35	0.60
1:D:157:HIS:CD2	1:D:160:GLN:HE22	2.19	0.60
1:A:355:ARG:HD3	1:A:427:HIS:O	2.02	0.60
1:E:201:GLN:HB3	1:E:233:PHE:CE2	2.35	0.60
1:E:468:GLU:N	1:E:468:GLU:OE1	2.33	0.60
1:F:272:GLY:HA2	1:F:301:HIS:CD2	2.37	0.60
1:F:325:GLY:HA3	1:F:348:PRO:HG3	1.82	0.60
1:A:213:MET:HB3	1:A:216:LEU:HD21	1.83	0.59
1:G:355:ARG:HD3	1:G:427:HIS:O	2.01	0.59
1:B:199:TYR:HB3	1:B:390:THR:HG22	1.84	0.59
1:G:44:ARG:HE	1:G:48:GLY:HA2	1.67	0.59
1:G:490:THR:HG22	1:G:493:ALA:HB2	1.83	0.59
1:H:303:ARG:HG3	1:H:303:ARG:HH11	1.68	0.59
1:I:437:THR:HA	1:I:480:VAL:HG13	1.84	0.59
1:B:485:VAL:HG22	1:B:515:VAL:HG11	1.83	0.59
1:A:38:TRP:CZ3	1:A:240:PRO:HB3	2.38	0.59
1:A:210:GLY:C	1:A:212:SER:H	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:118:ARG:NH2	1:G:140:ALA:O	2.35	0.59
1:G:329:THR:HG21	1:G:343:HIS:HD2	1.67	0.59
1:H:154:ARG:HB3	1:H:156:GLU:OE2	2.02	0.59
1:B:387:ARG:HG3	1:B:410:TYR:CD2	2.38	0.59
1:H:325:GLY:HA3	1:H:348:PRO:HG3	1.85	0.59
1:A:472:ARG:NE	1:A:474:ASP:OD1	2.33	0.59
1:A:66:TYR:CE2	1:A:153:ILE:HD13	2.38	0.58
1:F:303:ARG:HH12	1:F:349:GLY:H	1.50	0.58
1:F:123:ARG:HH12	1:F:186:MET:HG2	1.68	0.58
1:G:215:ARG:H	1:G:262:THR:HG23	1.67	0.58
1:E:278:ASP:OD1	1:E:280:SER:OG	2.17	0.58
1:F:35:PRO:HA	1:F:55:THR:HA	1.86	0.58
1:I:26:ARG:O	1:I:29:GLY:N	2.27	0.58
1:E:253:LEU:HD11	1:E:274:ILE:HG23	1.83	0.58
1:F:13:ASP:OD2	1:F:24:ARG:HD3	2.03	0.58
1:F:135:ARG:HH11	1:F:135:ARG:HG2	1.67	0.58
1:D:448:GLU:HG3	1:D:463:VAL:HG23	1.85	0.58
1:A:383:ARG:HH22	1:A:476:ASP:HB3	1.69	0.58
1:D:113:ARG:HB3	1:D:116:ILE:HD12	1.86	0.58
1:B:87:SER:HB3	1:B:90:GLU:HB3	1.86	0.57
1:B:205:LEU:HD11	1:B:237:LEU:HD21	1.85	0.57
1:F:208:SER:HB3	1:G:377:PRO:HA	1.87	0.57
1:I:482:GLU:HG2	1:I:516:THR:HG21	1.85	0.57
1:E:370:SER:HB3	1:E:376:LEU:HD21	1.84	0.57
1:G:303:ARG:HA	1:G:306:VAL:HG22	1.86	0.57
1:B:299:GLU:HA	1:B:302:ILE:HD12	1.85	0.57
1:F:284:MET:SD	1:F:308:GLN:HB3	2.45	0.57
1:G:337:THR:HB	1:G:341:ILE:HD11	1.85	0.57
1:H:402:TRP:CE2	1:H:406:ARG:HD2	2.40	0.57
1:B:168:ARG:O	1:B:168:ARG:HG3	2.04	0.57
1:I:435:ILE:HD13	1:I:465:ALA:HB2	1.86	0.57
1:D:157:HIS:HA	1:D:160:GLN:NE2	2.20	0.56
1:I:215:ARG:HG2	1:I:240:PRO:HG2	1.87	0.56
1:B:30:ARG:HG2	1:B:31:PRO:HD2	1.87	0.56
1:G:438:GLU:HG2	1:G:480:VAL:HG11	1.88	0.56
1:B:123:ARG:HH11	1:B:186:MET:HG2	1.71	0.56
1:A:458:LEU:HD11	1:A:487:LEU:HD23	1.86	0.56
1:D:267:PHE:HE1	1:D:293:THR:OG1	1.89	0.56
1:H:248:ARG:HH12	1:H:250:SER:HB3	1.70	0.56
1:A:216:LEU:HD22	1:A:265:PHE:HE1	1.70	0.56
1:A:365:GLN:HG2	1:A:387:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLN:O	1:B:204:ARG:HB2	2.05	0.56
1:G:123:ARG:NH1	1:G:186:MET:HG2	2.21	0.56
1:B:488:GLN:HG3	1:B:523:SER:HA	1.87	0.56
1:H:343:HIS:O	1:H:343:HIS:ND1	2.36	0.56
1:H:448:GLU:HG3	1:H:463:VAL:HG23	1.87	0.56
1:A:299:GLU:HG2	1:A:303:ARG:NH2	2.21	0.56
1:F:113:ARG:HB3	1:F:116:ILE:HD12	1.88	0.56
1:D:267:PHE:HE1	1:D:293:THR:HG1	1.52	0.55
1:H:355:ARG:HD3	1:H:427:HIS:O	2.06	0.55
1:D:95:PHE:HB2	1:D:107:PHE:HZ	1.71	0.55
1:F:267:PHE:HE1	1:F:295:ASP:H	1.55	0.55
1:A:436:ARG:NH1	1:A:475:TRP:O	2.39	0.55
1:F:457:GLU:O	1:F:490:THR:HG22	2.07	0.55
1:G:253:LEU:HD22	1:G:282:ARG:HD2	1.88	0.55
1:H:245:SER:O	1:H:247:GLN:NE2	2.39	0.55
1:H:355:ARG:HD2	1:H:446:ARG:CD	2.36	0.55
1:E:394:GLY:HA2	1:E:402:TRP:CD2	2.43	0.54
1:I:394:GLY:HA2	1:I:402:TRP:CD2	2.43	0.54
1:E:84:LEU:HB3	1:E:131:THR:HG22	1.88	0.54
1:G:213:MET:HB2	1:G:216:LEU:HD21	1.89	0.54
1:F:161:LEU:HD12	1:F:162:PRO:HD2	1.89	0.54
1:F:378:ALA:H	1:G:208:SER:HB2	1.72	0.54
1:D:43:TRP:CD1	1:D:90:GLU:HG3	2.43	0.54
1:F:253:LEU:HD21	1:F:274:ILE:HG23	1.89	0.54
1:F:332:LEU:HB3	1:F:342:PHE:HB2	1.90	0.54
1:H:118:ARG:HD3	1:H:138:VAL:O	2.07	0.54
1:A:435:ILE:HB	1:A:442:VAL:CG1	2.38	0.54
1:A:531:THR:OG1	1:A:532:GLY:N	2.38	0.54
1:E:216:LEU:HD12	1:E:263:THR:HB	1.90	0.54
1:A:355:ARG:HD2	1:A:446:ARG:CD	2.38	0.53
1:F:87:SER:HB3	1:F:90:GLU:HB2	1.90	0.53
1:G:221:PRO:HG2	1:G:267:PHE:CE1	2.43	0.53
1:G:450:LEU:HD21	1:G:510:GLN:HG3	1.89	0.53
1:A:448:GLU:HG3	1:A:463:VAL:HG23	1.90	0.53
1:G:25:LEU:HB3	1:G:30:ARG:HG3	1.91	0.53
1:G:199:TYR:HB3	1:G:390:THR:HG22	1.90	0.53
1:I:123:ARG:NH1	1:I:186:MET:HG2	2.23	0.53
1:I:213:MET:HE3	1:I:216:LEU:CD1	2.39	0.53
1:H:471:VAL:HG22	1:H:479:GLY:HA3	1.90	0.53
1:B:1:MET:SD	1:B:1:MET:N	2.66	0.53
1:H:292:ASN:ND2	1:H:295:ASP:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ARG:HG2	1:D:168:ARG:HH22	1.72	0.53
1:B:30:ARG:CG	1:B:31:PRO:HD2	2.38	0.53
1:E:188:LYS:NZ	1:E:189:ALA:H	2.07	0.53
1:E:413:THR:O	1:E:430:ARG:NH2	2.40	0.53
1:A:100:SER:HB2	1:A:165:TRP:NE1	2.24	0.52
1:D:253:LEU:HD21	1:D:274:ILE:HG23	1.92	0.52
1:E:199:TYR:HB3	1:E:390:THR:HG22	1.91	0.52
1:E:38:TRP:CD1	1:E:53:VAL:HG22	2.45	0.52
1:E:136:HIS:CE1	1:E:140:ALA:HB2	2.44	0.52
1:B:244:GLN:HG2	1:B:252:VAL:HG22	1.92	0.52
1:F:299:GLU:HA	1:F:302:ILE:HD12	1.90	0.52
1:G:215:ARG:HB2	1:G:261:PRO:HA	1.89	0.52
1:D:199:TYR:HB3	1:D:390:THR:HG22	1.92	0.52
1:G:345:GLY:O	1:G:353:PHE:HZ	1.93	0.52
1:H:32:THR:HA	1:H:56:LEU:HB3	1.91	0.52
1:H:80:VAL:HB	1:H:126:ALA:HA	1.91	0.52
1:F:287:ILE:O	1:F:309:GLY:HA3	2.09	0.52
1:G:35:PRO:HB2	1:G:38:TRP:CH2	2.45	0.52
1:G:201:GLN:HG2	1:G:233:PHE:HB2	1.91	0.52
1:I:438:GLU:HG2	1:I:480:VAL:HG11	1.92	0.52
1:B:55:THR:HG22	1:B:58:GLU:H	1.75	0.52
1:D:104:ILE:HG12	1:D:174:PRO:HB2	1.92	0.52
1:E:429:ASP:OD1	1:E:445:THR:HG23	2.10	0.52
1:H:104:ILE:HG12	1:H:174:PRO:HB2	1.92	0.52
1:I:484:TYR:CE1	1:I:517:ARG:HB3	2.45	0.52
1:D:467:ALA:HB2	1:D:481:ALA:HA	1.92	0.52
1:G:136:HIS:CE1	1:G:140:ALA:HB2	2.45	0.51
1:A:215:ARG:HG2	1:A:240:PRO:HG2	1.92	0.51
1:B:78:ARG:HD2	1:E:403:HIS:HB3	1.92	0.51
1:D:25:LEU:HD21	1:D:236:LEU:HD23	1.93	0.51
1:E:188:LYS:HZ1	1:E:189:ALA:H	1.58	0.51
1:D:216:LEU:HD22	1:D:265:PHE:HE1	1.74	0.51
1:B:81:VAL:HB	1:B:98:ILE:HD13	1.92	0.51
1:B:257:GLU:OE2	1:B:282:ARG:HA	2.10	0.51
1:A:340:SER:HB2	1:A:343:HIS:HE1	1.74	0.51
1:D:355:ARG:HD2	1:D:446:ARG:CD	2.41	0.51
1:F:26:ARG:HG3	1:F:60:TYR:CE2	2.46	0.51
1:I:333:GLY:HA3	1:I:339:TYR:HA	1.93	0.51
1:E:184:THR:OG1	1:E:185:GLY:N	2.44	0.51
1:G:253:LEU:HB3	1:G:282:ARG:HD2	1.93	0.51
1:I:107:PHE:HE2	1:I:228:MET:HE3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:N	1:A:135:ARG:HD2	2.26	0.51
1:A:527:SER:O	1:A:531:THR:HG23	2.11	0.51
1:G:213:MET:HB3	1:G:263:THR:OG1	2.11	0.51
1:G:298:HIS:HB2	1:G:301:HIS:ND1	2.25	0.51
1:A:355:ARG:HD2	1:A:446:ARG:HD2	1.93	0.50
1:D:35:PRO:HB2	1:D:38:TRP:CH2	2.45	0.50
1:G:278:ASP:OD2	1:G:280:SER:OG	2.30	0.50
1:I:135:ARG:HD2	1:I:135:ARG:N	2.26	0.50
1:A:231:MET:HE3	1:A:235:LEU:HD11	1.92	0.50
1:H:343:HIS:HD1	1:H:343:HIS:C	2.19	0.50
1:H:418:MET:HE1	1:I:318:PHE:HB3	1.93	0.50
1:B:2:ILE:HB	1:B:6:GLU:HB3	1.94	0.50
1:E:135:ARG:HD2	1:E:135:ARG:N	2.26	0.50
1:B:10:ILE:HG12	1:B:236:LEU:HD22	1.92	0.50
1:G:17:GLY:HA3	1:G:194:HIS:CE1	2.47	0.50
1:A:216:LEU:HD22	1:A:265:PHE:CE1	2.46	0.50
1:E:332:LEU:HD23	1:E:342:PHE:HB2	1.94	0.50
1:G:252:VAL:O	1:G:256:ILE:HG13	2.12	0.50
1:B:403:HIS:HB3	1:E:78:ARG:HD2	1.92	0.50
1:E:136:HIS:ND1	1:E:140:ALA:HB2	2.26	0.50
1:H:186:MET:HE3	1:H:187:PRO:CD	2.35	0.50
1:H:186:MET:CE	1:H:187:PRO:HD2	2.33	0.50
1:H:296:ALA:HA	1:H:330:ASP:OD1	2.12	0.50
1:H:370:SER:HB3	1:H:376:LEU:HD21	1.93	0.50
1:I:467:ALA:HB2	1:I:481:ALA:HA	1.93	0.50
1:A:355:ARG:HA	1:A:355:ARG:NE	2.25	0.50
1:E:293:THR:HB	1:E:339:TYR:HB2	1.93	0.50
1:B:448:GLU:HG3	1:B:463:VAL:HG23	1.94	0.49
1:E:359:LYS:NZ	1:E:422:GLU:O	2.45	0.49
1:G:344:ASN:HD21	1:G:357:ILE:HA	1.77	0.49
1:E:26:ARG:HG2	1:E:60:TYR:CZ	2.48	0.49
1:G:204:ARG:O	1:G:205:LEU:HD22	2.12	0.49
1:I:66:TYR:CE2	1:I:153:ILE:HD13	2.48	0.49
1:F:303:ARG:NH1	1:F:349:GLY:H	2.11	0.49
1:G:197:LEU:HD23	1:G:232:MET:HE1	1.93	0.49
1:A:204:ARG:HG3	1:A:205:LEU:N	2.27	0.49
1:A:499:LEU:HD22	1:A:502:TRP:CE3	2.47	0.49
1:E:2:ILE:HD11	1:E:238:ASP:HB2	1.94	0.49
1:H:36:VAL:HG11	1:H:56:LEU:HD13	1.93	0.49
1:F:435:ILE:HG12	1:F:465:ALA:HB2	1.95	0.49
1:G:247:GLN:O	1:G:270:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:279:LEU:HD23	1:H:282:ARG:HB2	1.94	0.49
1:I:95:PHE:HB2	1:I:107:PHE:HZ	1.77	0.49
1:A:458:LEU:HD21	1:A:487:LEU:HB3	1.94	0.48
1:F:123:ARG:NH1	1:F:186:MET:HG2	2.28	0.48
1:F:202:LEU:O	1:F:206:LYS:HG2	2.12	0.48
1:D:402:TRP:CE2	1:D:406:ARG:HD2	2.48	0.48
1:E:444:SER:HB2	1:E:463:VAL:HB	1.93	0.48
1:G:257:GLU:CD	1:G:282:ARG:HD3	2.38	0.48
1:G:370:SER:HB3	1:G:376:LEU:HD21	1.95	0.48
1:B:355:ARG:HD3	1:B:427:HIS:O	2.13	0.48
1:F:132:ASP:OD1	1:F:135:ARG:HG2	2.12	0.48
1:H:205:LEU:HD11	1:H:237:LEU:CD2	2.43	0.48
1:E:325:GLY:HA3	1:E:348:PRO:HG3	1.95	0.48
1:G:75:ILE:O	1:G:76:ARG:HD3	2.14	0.48
1:A:252:VAL:HG21	1:A:270:THR:HG21	1.94	0.48
1:D:370:SER:HB3	1:D:376:LEU:HD21	1.95	0.48
1:E:188:LYS:HE2	1:E:398:ASP:OD2	2.14	0.48
1:H:170:ASP:CG	1:H:171:PRO:HD2	2.39	0.48
1:H:436:ARG:NH2	1:H:475:TRP:O	2.41	0.48
1:E:356:CYS:HB2	1:E:426:TYR:CE2	2.49	0.48
1:H:253:LEU:HD21	1:H:274:ILE:HG23	1.96	0.48
1:B:370:SER:HB3	1:B:376:LEU:HD21	1.96	0.48
1:G:37:LEU:HD11	1:G:243:LEU:HD12	1.95	0.48
1:H:114:PRO:HB2	1:H:118:ARG:NH1	2.29	0.48
1:B:234:GLY:O	1:B:237:LEU:O	2.32	0.48
1:D:242:TYR:HE1	1:D:244:GLN:HG2	1.78	0.48
1:G:298:HIS:HB2	1:G:301:HIS:CE1	2.49	0.48
1:I:44:ARG:HD3	1:I:151:GLU:OE2	2.14	0.48
1:I:170:ASP:CG	1:I:171:PRO:HD2	2.39	0.48
1:B:10:ILE:HG21	1:B:205:LEU:HD23	1.94	0.48
1:D:66:TYR:CE2	1:D:153:ILE:HD13	2.49	0.48
1:A:347:LYS:HG2	1:A:348:PRO:HD2	1.95	0.47
1:B:59:LEU:HD21	1:B:96:MET:HE1	1.96	0.47
1:I:44:ARG:HB3	1:I:50:HIS:CE1	2.49	0.47
1:I:175:ILE:HD12	1:I:176:ILE:HG22	1.96	0.47
1:A:216:LEU:HD23	1:A:263:THR:HB	1.95	0.47
1:B:248:ARG:HB2	1:B:251:ASP:OD2	2.15	0.47
1:D:447:THR:HG23	1:D:507:LEU:HD11	1.97	0.47
1:G:136:HIS:HD2	1:G:149:THR:HG23	1.79	0.47
1:A:436:ARG:HB2	1:A:480:VAL:HA	1.96	0.47
1:F:151:GLU:OE2	1:F:151:GLU:N	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ILE:HD12	1:D:176:ILE:HG22	1.96	0.47
1:G:253:LEU:HD13	1:G:282:ARG:NH1	2.29	0.47
1:H:38:TRP:CZ3	1:H:240:PRO:HB3	2.50	0.47
1:A:485:VAL:C	1:A:486:LEU:HD23	2.38	0.47
1:F:302:ILE:HG12	1:F:328:PHE:CD2	2.50	0.47
1:H:394:GLY:HA2	1:H:402:TRP:CD2	2.50	0.47
1:F:406:ARG:HH22	1:I:172:THR:CB	2.27	0.47
1:H:35:PRO:HB2	1:H:38:TRP:CH2	2.50	0.47
1:A:115:GLU:CD	1:A:115:GLU:H	2.23	0.47
1:F:61:GLU:HG3	1:F:158:ARG:HH12	1.80	0.47
1:A:201:GLN:HB3	1:A:233:PHE:CD1	2.50	0.46
1:A:299:GLU:O	1:A:303:ARG:HG3	2.14	0.46
1:A:533:LYS:O	1:A:536:LYS:HB3	2.15	0.46
1:D:476:ASP:OD1	1:D:476:ASP:N	2.48	0.46
1:E:71:HIS:CE1	1:E:162:PRO:HB3	2.49	0.46
1:F:38:TRP:CZ3	1:F:240:PRO:HB3	2.50	0.46
1:G:458:LEU:HD21	1:G:487:LEU:HB3	1.98	0.46
1:A:381:VAL:HG13	1:A:428:LEU:HD12	1.97	0.46
1:E:96:MET:O	1:E:99:ASN:HB2	2.14	0.46
1:F:168:ARG:HD2	1:I:374:ARG:NH1	2.30	0.46
1:I:267:PHE:HE1	1:I:293:THR:HB	1.80	0.46
1:I:332:LEU:HB2	1:I:342:PHE:HB2	1.97	0.46
1:B:2:ILE:HG23	1:B:238:ASP:H	1.80	0.46
1:D:341:ILE:HD12	1:D:386:VAL:HG11	1.97	0.46
1:F:200:ALA:O	1:F:204:ARG:HG3	2.16	0.46
1:F:416:LEU:HG	1:F:431:ALA:HA	1.97	0.46
1:H:44:ARG:NE	1:H:151:GLU:HG3	2.31	0.46
1:A:209:VAL:HG13	1:A:211:GLY:N	2.30	0.46
1:A:482:GLU:CD	1:A:516:THR:HG21	2.40	0.46
1:H:253:LEU:O	1:H:257:GLU:HG3	2.15	0.46
1:I:5:GLU:CD	1:I:5:GLU:N	2.69	0.46
1:B:132:ASP:OD1	1:B:135:ARG:HB2	2.15	0.46
1:F:130:VAL:HG23	1:F:148:VAL:HG23	1.98	0.46
1:F:402:TRP:CE2	1:F:406:ARG:HD3	2.51	0.46
1:F:485:VAL:HG22	1:F:515:VAL:HG11	1.97	0.46
1:H:510:GLN:O	1:I:317:ASP:HB3	2.14	0.46
1:G:373:GLY:HA2	1:G:407:LEU:HG	1.98	0.46
1:I:201:GLN:HB3	1:I:233:PHE:CZ	2.51	0.46
1:A:313:GLU:O	1:A:320:PRO:HA	2.16	0.46
1:H:84:LEU:O	1:H:131:THR:HA	2.16	0.46
1:F:303:ARG:NH1	1:F:348:PRO:HA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:485:VAL:CG2	1:G:515:VAL:HG11	2.44	0.46
1:H:279:LEU:HD21	1:H:284:MET:CE	2.36	0.46
1:I:257:GLU:OE1	1:I:282:ARG:NH1	2.37	0.46
1:A:123:ARG:NH1	1:A:186:MET:HG2	2.32	0.46
1:A:496:PRO:HG2	1:A:502:TRP:CD2	2.50	0.46
1:E:248:ARG:HH11	1:E:248:ARG:HG3	1.81	0.46
1:F:61:GLU:CG	1:F:158:ARG:HH12	2.28	0.46
1:F:205:LEU:HD23	1:F:205:LEU:HA	1.77	0.46
1:H:30:ARG:NH1	1:H:238:ASP:HB2	2.30	0.46
1:H:299:GLU:O	1:H:303:ARG:HG2	2.16	0.46
1:A:468:GLU:HB3	1:A:469:GLU:H	1.60	0.45
1:B:339:TYR:CG	1:B:340:SER:N	2.83	0.45
1:D:289:ALA:HA	1:D:327:VAL:O	2.15	0.45
1:D:347:LYS:O	1:D:350:SER:OG	2.32	0.45
1:E:268:SER:HB3	1:E:292:ASN:HD21	1.81	0.45
1:F:80:VAL:HB	1:F:126:ALA:HA	1.97	0.45
1:E:476:ASP:OD2	1:E:476:ASP:N	2.49	0.45
1:H:199:TYR:HB3	1:H:390:THR:HG22	1.99	0.45
1:I:284:MET:HB2	1:I:308:GLN:HB3	1.97	0.45
1:B:337:THR:HB	1:B:341:ILE:HD11	1.98	0.45
1:A:370:SER:OG	1:A:374:ARG:HB2	2.16	0.45
1:E:288:GLU:HG2	1:E:310:SER:O	2.16	0.45
1:I:154:ARG:HB3	1:I:156:GLU:OE1	2.17	0.45
1:E:1:MET:HG3	1:E:2:ILE:H	1.81	0.45
1:E:123:ARG:NH1	1:E:186:MET:HG2	2.32	0.45
1:F:45:ALA:HB1	1:F:46:PRO:HD2	1.98	0.45
1:G:21:VAL:O	1:G:25:LEU:HG	2.17	0.45
1:I:395:TYR:HE2	1:I:405:LEU:HD12	1.80	0.45
1:B:463:VAL:HG22	1:B:485:VAL:HG13	1.99	0.45
1:A:340:SER:HB2	1:A:343:HIS:CE1	2.52	0.45
1:D:302:ILE:HD13	1:D:346:HIS:ND1	2.32	0.45
1:H:467:ALA:HB1	1:H:471:VAL:HG13	1.99	0.45
1:I:30:ARG:NH2	1:I:236:LEU:O	2.50	0.45
1:I:44:ARG:HD3	1:I:151:GLU:CD	2.42	0.45
1:B:34:ARG:HD3	1:B:238:ASP:OD1	2.17	0.45
1:B:171:PRO:O	1:B:195:GLN:HG2	2.16	0.45
1:F:7:ARG:NH1	1:F:208:SER:HA	2.31	0.45
1:G:109:ASN:O	1:G:112:LEU:HB2	2.17	0.45
1:H:435:ILE:HG12	1:H:465:ALA:HB2	1.97	0.45
1:A:63:VAL:HG13	1:A:97:ALA:HA	1.99	0.44
1:G:455:LEU:HD12	1:G:458:LEU:HD12	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:312:GLU:HG3	1:H:322:ARG:NH2	2.32	0.44
1:A:204:ARG:HD3	1:A:209:VAL:HA	2.00	0.44
1:B:248:ARG:NH1	1:B:273:GLN:HE22	2.15	0.44
1:B:490:THR:HG22	1:B:493:ALA:HB2	1.99	0.44
1:E:111:LYS:HA	1:E:111:LYS:HD3	1.83	0.44
1:F:1:MET:HE3	1:F:1:MET:HB2	1.79	0.44
1:F:69:PHE:HZ	1:F:148:VAL:HG11	1.81	0.44
1:E:496:PRO:HG2	1:E:502:TRP:CD2	2.53	0.44
1:F:289:ALA:HA	1:F:327:VAL:O	2.17	0.44
1:G:283:ASP:OD1	1:G:285:SER:HB3	2.18	0.44
1:E:20:ASN:O	1:E:24:ARG:HG2	2.17	0.44
1:F:299:GLU:OE1	1:F:352:SER:HB2	2.17	0.44
1:H:418:MET:CE	1:I:318:PHE:HB3	2.47	0.44
1:I:119:GLU:CD	1:I:122:ARG:HE	2.25	0.44
1:A:377:PRO:HB3	1:B:209:VAL:HG23	2.00	0.44
1:D:522:ASP:OD1	1:D:523:SER:N	2.50	0.44
1:E:441:ILE:O	1:E:513:PRO:HG2	2.18	0.44
1:G:207:LEU:O	1:G:208:SER:HB3	2.17	0.44
1:I:435:ILE:CD1	1:I:465:ALA:HB2	2.47	0.44
1:A:217:LEU:HB3	1:A:264:VAL:HG22	2.00	0.44
1:B:95:PHE:HE1	1:B:176:ILE:HB	1.83	0.44
1:F:339:TYR:CG	1:F:340:SER:N	2.85	0.44
1:H:95:PHE:HB2	1:H:107:PHE:HZ	1.83	0.44
1:E:1:MET:HG3	1:E:2:ILE:N	2.33	0.44
1:E:38:TRP:CZ3	1:E:240:PRO:HB3	2.53	0.44
1:E:349:GLY:HA2	1:I:155:PRO:HB2	2.00	0.44
1:F:442:VAL:HG22	1:F:513:PRO:HB2	2.00	0.44
1:I:87:SER:HB3	1:I:90:GLU:HB3	1.98	0.44
1:I:120:TYR:OH	1:I:179:HIS:HB3	2.17	0.44
1:I:325:GLY:HA3	1:I:348:PRO:HG3	1.99	0.44
1:I:476:ASP:OD1	1:I:476:ASP:N	2.50	0.44
1:A:501:GLY:HA2	1:A:504:ASN:HB2	2.00	0.44
1:D:298:HIS:HB3	1:D:301:HIS:ND1	2.33	0.44
1:E:58:GLU:O	1:E:61:GLU:HB3	2.18	0.44
1:G:184:THR:O	1:G:184:THR:OG1	2.36	0.44
1:H:343:HIS:ND1	1:H:343:HIS:C	2.76	0.44
1:H:485:VAL:CG2	1:H:515:VAL:HG11	2.48	0.44
1:E:85:THR:OG1	1:E:86:ALA:N	2.50	0.44
1:F:84:LEU:O	1:F:131:THR:HA	2.18	0.44
1:H:336:GLU:OE2	1:H:395:TYR:OH	2.29	0.44
1:E:274:ILE:O	1:E:277:SER:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:474:ASP:OD1	1:H:474:ASP:N	2.44	0.43
1:I:26:ARG:HG2	1:I:60:TYR:CZ	2.53	0.43
1:F:65:THR:HG21	1:F:155:PRO:HA	2.00	0.43
1:F:391:LEU:HD21	1:F:411:TRP:HB2	1.99	0.43
1:F:399:SER:N	1:I:397:ASN:OD1	2.52	0.43
1:I:231:MET:HG3	1:I:243:LEU:HD21	2.00	0.43
1:B:85:THR:O	1:B:110:ALA:HB2	2.18	0.43
1:B:355:ARG:HD2	1:B:446:ARG:CD	2.47	0.43
1:B:464:THR:HG22	1:B:484:TYR:HB2	1.99	0.43
1:D:327:VAL:HG13	1:D:347:LYS:HE3	2.00	0.43
1:I:436:ARG:HH21	1:I:475:TRP:C	2.22	0.43
1:B:120:TYR:OH	1:B:179:HIS:HB3	2.18	0.43
1:D:43:TRP:HD1	1:D:90:GLU:HG3	1.82	0.43
1:D:242:TYR:CE1	1:D:244:GLN:HG2	2.54	0.43
1:E:394:GLY:HA2	1:E:402:TRP:CE2	2.53	0.43
1:F:441:ILE:O	1:F:513:PRO:HG2	2.18	0.43
1:G:450:LEU:HD12	1:G:450:LEU:HA	1.80	0.43
1:I:347:LYS:HB2	1:I:348:PRO:HD2	1.99	0.43
1:I:433:ASP:HB3	1:I:444:SER:HB2	2.00	0.43
1:D:394:GLY:HA2	1:D:402:TRP:CD2	2.53	0.43
1:E:188:LYS:HD2	1:E:188:LYS:HA	1.43	0.43
1:F:444:SER:O	1:F:448:GLU:HG3	2.18	0.43
1:G:20:ASN:O	1:G:24:ARG:HG2	2.18	0.43
1:G:522:ASP:OD1	1:G:522:ASP:N	2.50	0.43
1:G:198:LEU:HD23	1:G:198:LEU:HA	1.80	0.43
1:H:434:ALA:O	1:H:474:ASP:HA	2.19	0.43
1:E:501:GLY:O	1:E:505:GLU:HG3	2.18	0.43
1:F:154:ARG:H	1:F:157:HIS:CD2	2.36	0.43
1:G:201:GLN:HA	1:G:204:ARG:HG2	2.00	0.43
1:I:331:GLY:C	1:I:332:LEU:HG	2.43	0.43
1:F:298:HIS:HB3	1:F:301:HIS:ND1	2.34	0.43
1:H:71:HIS:CG	1:H:162:PRO:HG3	2.54	0.43
1:I:387:ARG:HG3	1:I:410:TYR:CD2	2.53	0.43
1:B:214:GLY:O	1:B:240:PRO:HD2	2.18	0.43
1:F:198:LEU:HD23	1:F:198:LEU:HA	1.89	0.43
1:H:96:MET:O	1:H:99:ASN:HB2	2.19	0.43
1:H:303:ARG:HG3	1:H:303:ARG:NH1	2.32	0.43
1:H:495:GLU:OE1	1:H:520:ARG:HD3	2.19	0.43
1:I:69:PHE:O	1:I:73:LYS:HG2	2.18	0.43
1:I:95:PHE:HB2	1:I:107:PHE:CZ	2.54	0.43
1:I:298:HIS:HB2	1:I:301:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:468:GLU:O	1:I:471:VAL:HG13	2.19	0.43
1:F:437:THR:HB	1:F:440:GLY:O	2.18	0.42
1:H:269:GLY:O	1:H:273:GLN:HG3	2.18	0.42
1:A:454:SER:O	1:A:455:LEU:HG	2.19	0.42
1:D:297:ALA:HB3	1:D:302:ILE:HD11	2.01	0.42
1:B:199:TYR:CE2	1:B:389:PRO:HG2	2.54	0.42
1:F:170:ASP:CG	1:F:171:PRO:HD2	2.44	0.42
1:G:75:ILE:HD13	1:G:75:ILE:HA	1.86	0.42
1:G:95:PHE:HB2	1:G:107:PHE:HZ	1.84	0.42
1:G:329:THR:HG21	1:G:343:HIS:CD2	2.52	0.42
1:A:38:TRP:CD1	1:A:53:VAL:HG22	2.55	0.42
1:A:374:ARG:HG2	1:D:168:ARG:NH2	2.34	0.42
1:B:310:SER:O	1:B:322:ARG:NH2	2.52	0.42
1:B:446:ARG:NH2	1:B:449:GLU:OE1	2.52	0.42
1:D:438:GLU:OE2	1:D:480:VAL:HG21	2.19	0.42
1:F:216:LEU:HD12	1:F:265:PHE:HE1	1.84	0.42
1:F:436:ARG:HB2	1:F:473:ALA:O	2.20	0.42
1:G:267:PHE:HD2	1:G:267:PHE:HA	1.74	0.42
1:G:313:GLU:HG3	1:G:314:ILE:N	2.35	0.42
1:H:504:ASN:OD1	1:H:515:VAL:HG22	2.19	0.42
1:D:284:MET:HE2	1:D:287:ILE:HD12	2.02	0.42
1:H:134:GLU:OE2	1:H:134:GLU:N	2.51	0.42
1:I:341:ILE:HG22	1:I:342:PHE:CD2	2.54	0.42
1:A:231:MET:O	1:A:235:LEU:HG	2.19	0.42
1:B:287:ILE:O	1:B:287:ILE:HG12	2.18	0.42
1:I:357:ILE:HA	1:I:357:ILE:HD13	1.78	0.42
1:A:248:ARG:O	1:A:252:VAL:HG23	2.20	0.42
1:A:400:LEU:HG	1:A:404:LYS:HE2	2.00	0.42
1:F:421:ALA:HA	1:G:210:GLY:HA2	2.00	0.42
1:G:248:ARG:O	1:G:252:VAL:HG23	2.20	0.42
1:G:302:ILE:O	1:G:306:VAL:HG22	2.19	0.42
1:H:114:PRO:HB2	1:H:118:ARG:HH12	1.84	0.42
1:I:9:GLN:OE1	1:I:28:TYR:HA	2.20	0.42
1:B:451:LEU:HD21	1:B:503:VAL:HG13	2.02	0.42
1:F:1:MET:HG2	1:F:2:ILE:H	1.84	0.42
1:F:303:ARG:HH12	1:F:348:PRO:HA	1.84	0.42
1:E:204:ARG:NH2	1:E:340:SER:OG	2.50	0.42
1:E:225:ASN:OD1	1:E:226:ALA:N	2.52	0.42
1:D:135:ARG:HD2	1:D:135:ARG:N	2.34	0.42
1:F:346:HIS:CD2	1:F:353:PHE:HE1	2.38	0.42
1:A:458:LEU:HD21	1:A:487:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:GLU:CD	1:E:122:ARG:HE	2.28	0.41
1:F:215:ARG:HB3	1:F:259:PHE:CE2	2.55	0.41
1:G:226:ALA:O	1:G:230:VAL:HG22	2.19	0.41
1:G:353:PHE:N	1:G:353:PHE:CD1	2.88	0.41
1:I:149:THR:OG1	1:I:151:GLU:OE1	2.32	0.41
1:I:305:LEU:HD23	1:I:305:LEU:HA	1.86	0.41
1:A:495:GLU:HG2	1:A:496:PRO:O	2.20	0.41
1:D:302:ILE:O	1:D:306:VAL:HG22	2.20	0.41
1:E:32:THR:HA	1:E:56:LEU:HB3	2.01	0.41
1:B:206:LYS:HA	1:B:206:LYS:HD2	1.83	0.41
1:B:319:LYS:HE3	1:B:319:LYS:HB3	1.63	0.41
1:E:87:SER:HB3	1:E:90:GLU:HB3	2.03	0.41
1:F:265:PHE:CD2	1:F:291:TYR:HB2	2.54	0.41
1:F:466:ILE:HD13	1:F:484:TYR:CG	2.55	0.41
1:H:113:ARG:HD3	1:H:115:GLU:OE2	2.21	0.41
1:I:504:ASN:OD1	1:I:515:VAL:HG22	2.21	0.41
1:A:210:GLY:C	1:A:212:SER:N	2.77	0.41
1:A:316:PRO:HB2	1:B:510:GLN:HG3	2.03	0.41
1:A:468:GLU:O	1:A:470:GLY:N	2.45	0.41
1:D:478:ASP:OD1	1:D:478:ASP:N	2.53	0.41
1:E:466:ILE:HD11	1:E:484:TYR:CD2	2.54	0.41
1:H:211:GLY:O	1:H:213:MET:N	2.54	0.41
1:H:368:VAL:HG12	1:H:376:LEU:HD12	2.03	0.41
1:A:287:ILE:O	1:A:309:GLY:HA3	2.21	0.41
1:B:154:ARG:H	1:B:157:HIS:CE1	2.39	0.41
1:B:289:ALA:HA	1:B:327:VAL:O	2.20	0.41
1:D:205:LEU:HA	1:D:205:LEU:HD12	1.58	0.41
1:D:359:LYS:NZ	1:E:343:HIS:CE1	2.88	0.41
1:H:279:LEU:CD2	1:H:284:MET:HE3	2.38	0.41
1:I:486:LEU:HD23	1:I:521:MET:HB3	2.03	0.41
1:A:18:ALA:HB1	1:A:232:MET:HE1	2.02	0.41
1:B:402:TRP:O	1:B:406:ARG:HG3	2.21	0.41
1:E:231:MET:HE2	1:E:231:MET:HB3	2.00	0.41
1:G:458:LEU:HD11	1:G:487:LEU:HD22	2.03	0.41
1:A:399:SER:N	1:D:397:ASN:OD1	2.53	0.41
1:B:201:GLN:HG2	1:B:233:PHE:CG	2.56	0.41
1:B:215:ARG:HD3	1:B:260:LYS:O	2.20	0.41
1:B:504:ASN:OD1	1:B:515:VAL:HG22	2.21	0.41
1:D:451:LEU:HD21	1:D:507:LEU:HD13	2.02	0.41
1:E:132:ASP:OD1	1:E:135:ARG:HD3	2.21	0.41
1:E:488:GLN:OE1	1:E:521:MET:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:494:ARG:NH1	1:I:212:SER:OG	2.54	0.41
1:F:376:LEU:HD22	1:F:380:GLU:OE1	2.21	0.41
1:I:12:ALA:O	1:I:14:PRO:HD3	2.20	0.41
1:I:38:TRP:CZ3	1:I:240:PRO:HB3	2.56	0.41
1:I:253:LEU:HD23	1:I:253:LEU:HA	1.92	0.41
1:A:373:GLY:HA2	1:A:407:LEU:HG	2.02	0.41
1:B:336:GLU:OE1	1:B:336:GLU:N	2.47	0.41
1:G:35:PRO:HA	1:G:55:THR:HA	2.02	0.41
1:H:113:ARG:HB2	1:H:114:PRO:HD2	2.02	0.41
1:A:463:VAL:HG22	1:A:485:VAL:HG22	2.02	0.41
1:B:305:LEU:C	1:B:307:ALA:H	2.29	0.41
1:G:305:LEU:HD23	1:G:305:LEU:HA	1.87	0.41
1:H:296:ALA:HB2	1:H:332:LEU:HD21	2.03	0.41
1:D:195:GLN:O	1:D:199:TYR:HB2	2.21	0.40
1:D:488:GLN:NE2	1:D:521:MET:SD	2.94	0.40
1:E:170:ASP:CG	1:E:171:PRO:HD2	2.47	0.40
1:F:171:PRO:O	1:F:195:GLN:HB3	2.21	0.40
1:G:83:VAL:HG12	1:G:85:THR:HG22	2.02	0.40
1:G:455:LEU:HD21	1:G:506:VAL:HG21	2.02	0.40
1:I:193:THR:OG1	1:I:196:THR:HG23	2.21	0.40
1:B:87:SER:HB3	1:B:90:GLU:CB	2.51	0.40
1:B:237:LEU:C	1:B:239:SER:H	2.29	0.40
1:F:59:LEU:HD21	1:F:96:MET:HE1	2.02	0.40
1:F:134:GLU:HB3	1:F:135:ARG:NH1	2.36	0.40
1:G:183:THR:CG2	1:G:187:PRO:HG3	2.52	0.40
1:H:66:TYR:CE2	1:H:153:ILE:HD13	2.57	0.40
1:H:446:ARG:H	1:H:446:ARG:HG2	1.71	0.40
1:A:536:LYS:C	1:A:538:VAL:N	2.78	0.40
1:B:455:LEU:HD13	1:B:502:TRP:CZ2	2.56	0.40
1:D:113:ARG:HG3	1:D:115:GLU:CD	2.46	0.40
1:H:76:ARG:HA	1:H:76:ARG:HD3	1.85	0.40
1:H:84:LEU:HB3	1:H:131:THR:HG22	2.03	0.40
1:H:117:ALA:O	1:H:121:ILE:HG12	2.21	0.40
1:H:201:GLN:HB3	1:H:233:PHE:CD1	2.56	0.40
1:I:267:PHE:HD1	1:I:267:PHE:HA	1.69	0.40
1:I:522:ASP:OD1	1:I:522:ASP:N	2.54	0.40
1:B:330:ASP:O	1:B:332:LEU:HD22	2.21	0.40
1:B:436:ARG:NH2	1:B:475:TRP:O	2.36	0.40
1:B:455:LEU:HD13	1:B:502:TRP:CH2	2.57	0.40
1:E:233:PHE:CZ	1:E:237:LEU:HD11	2.57	0.40
1:F:136:HIS:CE1	1:F:140:ALA:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:TYR:CD1	1:G:199:TYR:C	3.00	0.40
1:G:504:ASN:HD21	1:G:514:PRO:HB2	1.85	0.40
1:A:247:GLN:O	1:A:270:THR:HG23	2.21	0.40
1:H:205:LEU:HD11	1:H:237:LEU:HD21	2.02	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:E:34:ARG:NH2	1:I:458:LEU:O[1_655]	2.09	0.11

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	536/569 (94%)	499 (93%)	31 (6%)	6 (1%)	12	21
1	B	521/569 (92%)	490 (94%)	29 (6%)	2 (0%)	30	48
1	D	521/569 (92%)	498 (96%)	21 (4%)	2 (0%)	30	48
1	E	519/569 (91%)	498 (96%)	21 (4%)	0	100	100
1	F	521/569 (92%)	489 (94%)	32 (6%)	0	100	100
1	G	521/569 (92%)	494 (95%)	22 (4%)	5 (1%)	13	23
1	H	521/569 (92%)	501 (96%)	18 (4%)	2 (0%)	30	48
1	I	522/569 (92%)	502 (96%)	20 (4%)	0	100	100
All	All	4182/4552 (92%)	3971 (95%)	194 (5%)	17 (0%)	30	48

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	TYR

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Mol	Chain	Res	Type
1	G	422	GLU
1	A	211	GLY
1	A	438	GLU
1	A	469	GLU
1	A	507	LEU
1	A	525	ASP
1	D	344	ASN
1	G	208	SER
1	G	214	GLY
1	H	212	SER
1	A	521	MET
1	B	283	ASP
1	G	212	SER
1	G	468	GLU
1	H	20	ASN
1	D	209	VAL

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	429/455 (94%)	416 (97%)	13 (3%)	36	57
1	B	416/455 (91%)	394 (95%)	22 (5%)	19	34
1	D	416/455 (91%)	409 (98%)	7 (2%)	56	73
1	E	414/455 (91%)	406 (98%)	8 (2%)	52	71
1	F	416/455 (91%)	394 (95%)	22 (5%)	19	34
1	G	416/455 (91%)	405 (97%)	11 (3%)	41	62
1	H	416/455 (91%)	404 (97%)	12 (3%)	37	58
1	I	417/455 (92%)	405 (97%)	12 (3%)	37	58
All	All	3340/3640 (92%)	3233 (97%)	107 (3%)	34	55

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	133	THR
1	A	175	ILE
1	A	183	THR
1	A	184	THR
1	A	229	SER
1	A	281	THR
1	A	386	VAL
1	A	457	GLU
1	A	476	ASP
1	A	515	VAL
1	A	526	VAL
1	A	528	THR
1	B	39	THR
1	B	55	THR
1	B	89	THR
1	B	168	ARG
1	B	176	ILE
1	B	178	SER
1	B	180	SER
1	B	183	THR
1	B	207	LEU
1	B	216	LEU
1	B	237	LEU
1	B	250	SER
1	B	281	THR
1	B	287	ILE
1	B	312	GLU
1	B	369	LEU
1	B	386	VAL
1	B	464	THR
1	B	471	VAL
1	B	480	VAL
1	B	485	VAL
1	B	491	ASP
1	D	73	LYS
1	D	184	THR
1	D	229	SER
1	D	239	SER
1	D	244	GLN
1	D	374	ARG
1	D	476	ASP
1	E	181	SER

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Mol	Chain	Res	Type
1	E	188	LYS
1	E	216	LEU
1	E	290	TYR
1	E	304	VAL
1	E	380	GLU
1	E	445	THR
1	E	485	VAL
1	F	2	ILE
1	F	3	THR
1	F	39	THR
1	F	59	LEU
1	F	144	LEU
1	F	149	THR
1	F	176	ILE
1	F	178	SER
1	F	209	VAL
1	F	241	VAL
1	F	250	SER
1	F	314	ILE
1	F	341	ILE
1	F	352	SER
1	F	365	GLN
1	F	369	LEU
1	F	386	VAL
1	F	430	ARG
1	F	437	THR
1	F	466	ILE
1	F	471	VAL
1	F	485	VAL
1	G	39	THR
1	G	44	ARG
1	G	90	GLU
1	G	116	ILE
1	G	184	THR
1	G	262	THR
1	G	285	SER
1	G	290	TYR
1	G	293	THR
1	G	314	ILE
1	G	490	THR
1	H	178	SER
1	H	181	SER

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Mol	Chain	Res	Type
1	H	184	THR
1	H	207	LEU
1	H	209	VAL
1	H	268	SER
1	H	277	SER
1	H	326	SER
1	H	438	GLU
1	H	457	GLU
1	H	500	THR
1	H	503	VAL
1	I	58	GLU
1	I	180	SER
1	I	184	THR
1	I	206	LYS
1	I	216	LEU
1	I	241	VAL
1	I	304	VAL
1	I	399	SER
1	I	406	ARG
1	I	435	ILE
1	I	471	VAL
1	I	522	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	HIS
1	B	109	ASN
1	B	136	HIS
1	B	160	GLN
1	B	224	HIS
1	B	247	GLN
1	B	292	ASN
1	B	365	GLN
1	B	403	HIS
1	D	11	ASN
1	D	71	HIS
1	D	160	GLN
1	D	224	HIS
1	D	244	GLN
1	D	365	GLN
1	D	488	GLN

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Mol	Chain	Res	Type
1	E	23	HIS
1	E	160	GLN
1	F	20	ASN
1	F	136	HIS
1	F	160	GLN
1	F	403	HIS
1	F	424	ASN
1	F	510	GLN
1	G	23	HIS
1	G	71	HIS
1	G	169	HIS
1	G	308	GLN
1	G	343	HIS
1	G	344	ASN
1	H	9	GLN
1	H	346	HIS
1	H	365	GLN
1	H	424	ASN
1	H	488	GLN
1	H	510	GLN
1	I	20	ASN
1	I	163	GLN
1	I	403	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	538/569 (94%)	-0.03	39 (7%)	23	26	17, 44, 92, 118	0
1	B	523/569 (91%)	-0.16	6 (1%)	77	79	21, 44, 74, 94	0
1	D	523/569 (91%)	-0.40	5 (0%)	79	81	16, 36, 68, 97	0
1	E	521/569 (91%)	-0.41	2 (0%)	89	90	19, 35, 59, 93	0
1	F	523/569 (91%)	0.04	5 (0%)	79	81	24, 51, 84, 104	0
1	G	523/569 (91%)	-0.01	15 (2%)	54	54	21, 50, 80, 114	0
1	H	523/569 (91%)	-0.25	11 (2%)	63	63	20, 43, 75, 106	0
1	I	524/569 (92%)	-0.41	0	100	100	21, 36, 62, 94	0
All	All	4198/4552 (92%)	-0.20	83 (1%)	64	64	16, 42, 79, 118	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	210	GLY	5.3
1	A	209	VAL	3.9
1	A	526	VAL	3.9
1	A	470	GLY	3.7
1	A	212	SER	3.6
1	G	339	TYR	3.6
1	H	212	SER	3.5
1	A	519	LEU	3.4
1	A	466	ILE	3.3
1	D	523	SER	3.2
1	A	538	VAL	3.2
1	A	210	GLY	3.2
1	A	467	ALA	3.2
1	G	456	PRO	3.1
1	A	539	MET	3.1
1	H	209	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	279	LEU	3.0
1	G	211	GLY	3.0
1	A	517	ARG	2.9
1	A	536	LYS	2.9
1	A	525	ASP	2.9
1	G	209	VAL	2.9
1	H	2	ILE	2.8
1	A	480	VAL	2.8
1	F	267	PHE	2.8
1	A	211	GLY	2.8
1	A	456	PRO	2.8
1	A	207	LEU	2.8
1	H	343	HIS	2.8
1	A	483	ALA	2.7
1	A	471	VAL	2.7
1	B	211	GLY	2.7
1	A	521	MET	2.7
1	B	339	TYR	2.6
1	H	339	TYR	2.6
1	F	284	MET	2.6
1	A	338	GLY	2.6
1	G	1	MET	2.5
1	G	458	LEU	2.5
1	D	470	GLY	2.5
1	A	454	SER	2.5
1	D	343	HIS	2.5
1	A	455	LEU	2.5
1	A	535	LEU	2.5
1	A	530	VAL	2.4
1	B	1	MET	2.4
1	A	439	ALA	2.4
1	H	207	LEU	2.4
1	A	520	ARG	2.4
1	A	523	SER	2.4
1	G	523	SER	2.4
1	A	492	GLY	2.4
1	G	207	LEU	2.4
1	B	210	GLY	2.4
1	A	459	ALA	2.3
1	H	492	GLY	2.3
1	A	529	GLY	2.3
1	G	455	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	534	VAL	2.3
1	D	479	GLY	2.3
1	G	459	ALA	2.3
1	A	493	ALA	2.2
1	H	523	SER	2.2
1	A	484	TYR	2.2
1	G	205	LEU	2.2
1	H	210	GLY	2.2
1	A	438	GLU	2.2
1	A	469	GLU	2.2
1	D	471	VAL	2.2
1	H	1	MET	2.2
1	F	467	ALA	2.1
1	E	343	HIS	2.1
1	G	452	LEU	2.1
1	H	522	ASP	2.1
1	A	453	ALA	2.1
1	A	468	GLU	2.1
1	G	496	PRO	2.1
1	F	340	SER	2.1
1	B	209	VAL	2.1
1	A	451	LEU	2.1
1	E	476	ASP	2.1
1	B	207	LEU	2.0
1	G	521	MET	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.