



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 08:07 pm GMT

PDB ID : 4APL  
Title : Crystal Structure of AMA1 from Neospora caninum  
Authors : Tonkin, M.L.; Crawford, J.; Lebrun, M.L.; Boulanger, M.J.  
Deposited on : 2012-04-04  
Resolution : 2.90 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

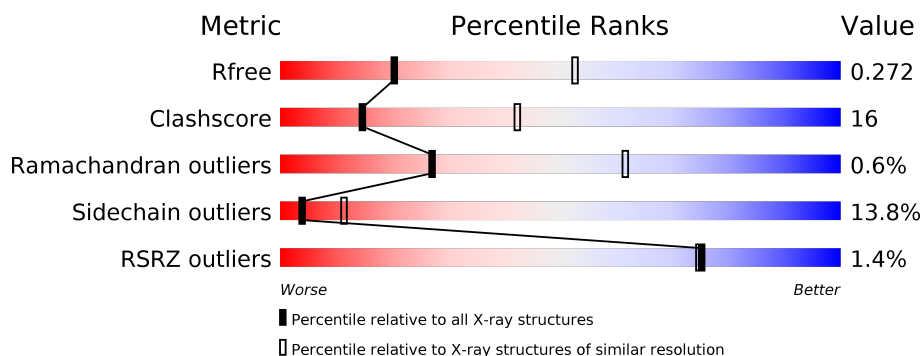
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	111664	1716 (2.90-2.90)
Clashscore	122126	1924 (2.90-2.90)
Ramachandran outliers	120053	1884 (2.90-2.90)
Sidechain outliers	120020	1886 (2.90-2.90)
RSRZ outliers	108989	1669 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	431	
1	B	431	
1	D	431	
1	E	431	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12647 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 APICAL MEMBRANE ANTIGEN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	0	1	0
			3155	1975	541	618	21			
1	B	394	Total	C	N	O	S	0	1	0
			3123	1958	533	611	21			
1	D	395	Total	C	N	O	S	0	1	0
			3133	1963	537	612	21			
1	E	390	Total	C	N	O	S	0	1	0
			3094	1940	529	604	21			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	GLY	-	expression tag	UNP A2A114
A	55	SER	-	expression tag	UNP A2A114
A	56	ALA	-	expression tag	UNP A2A114
A	57	MET	-	expression tag	UNP A2A114
A	58	GLY	-	expression tag	UNP A2A114
A	479	ALA	-	expression tag	UNP A2A114
A	480	ALA	-	expression tag	UNP A2A114
A	481	LEU	-	expression tag	UNP A2A114
A	482	VAL	-	expression tag	UNP A2A114
A	483	PRO	-	expression tag	UNP A2A114
A	484	ARG	-	expression tag	UNP A2A114
B	54	GLY	-	expression tag	UNP A2A114
B	55	SER	-	expression tag	UNP A2A114
B	56	ALA	-	expression tag	UNP A2A114
B	57	MET	-	expression tag	UNP A2A114
B	58	GLY	-	expression tag	UNP A2A114
B	479	ALA	-	expression tag	UNP A2A114
B	480	ALA	-	expression tag	UNP A2A114
B	481	LEU	-	expression tag	UNP A2A114
B	482	VAL	-	expression tag	UNP A2A114
B	483	PRO	-	expression tag	UNP A2A114

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Chain	Residue	Modelled	Actual	Comment	Reference
B	484	ARG	-	expression tag	UNP A2A114
D	54	GLY	-	expression tag	UNP A2A114
D	55	SER	-	expression tag	UNP A2A114
D	56	ALA	-	expression tag	UNP A2A114
D	57	MET	-	expression tag	UNP A2A114
D	58	GLY	-	expression tag	UNP A2A114
D	479	ALA	-	expression tag	UNP A2A114
D	480	ALA	-	expression tag	UNP A2A114
D	481	LEU	-	expression tag	UNP A2A114
D	482	VAL	-	expression tag	UNP A2A114
D	483	PRO	-	expression tag	UNP A2A114
D	484	ARG	-	expression tag	UNP A2A114
E	54	GLY	-	expression tag	UNP A2A114
E	55	SER	-	expression tag	UNP A2A114
E	56	ALA	-	expression tag	UNP A2A114
E	57	MET	-	expression tag	UNP A2A114
E	58	GLY	-	expression tag	UNP A2A114
E	479	ALA	-	expression tag	UNP A2A114
E	480	ALA	-	expression tag	UNP A2A114
E	481	LEU	-	expression tag	UNP A2A114
E	482	VAL	-	expression tag	UNP A2A114
E	483	PRO	-	expression tag	UNP A2A114
E	484	ARG	-	expression tag	UNP A2A114

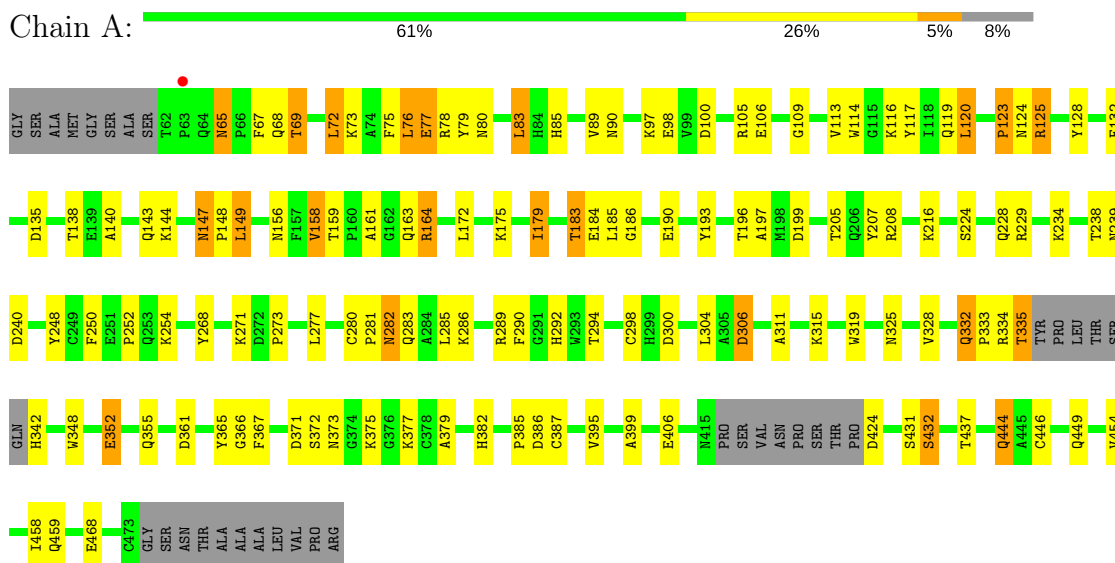
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	45	Total O 45 45	0	0
2	B	33	Total O 33 33	0	0
2	D	45	Total O 45 45	0	0
2	E	19	Total O 19 19	0	0

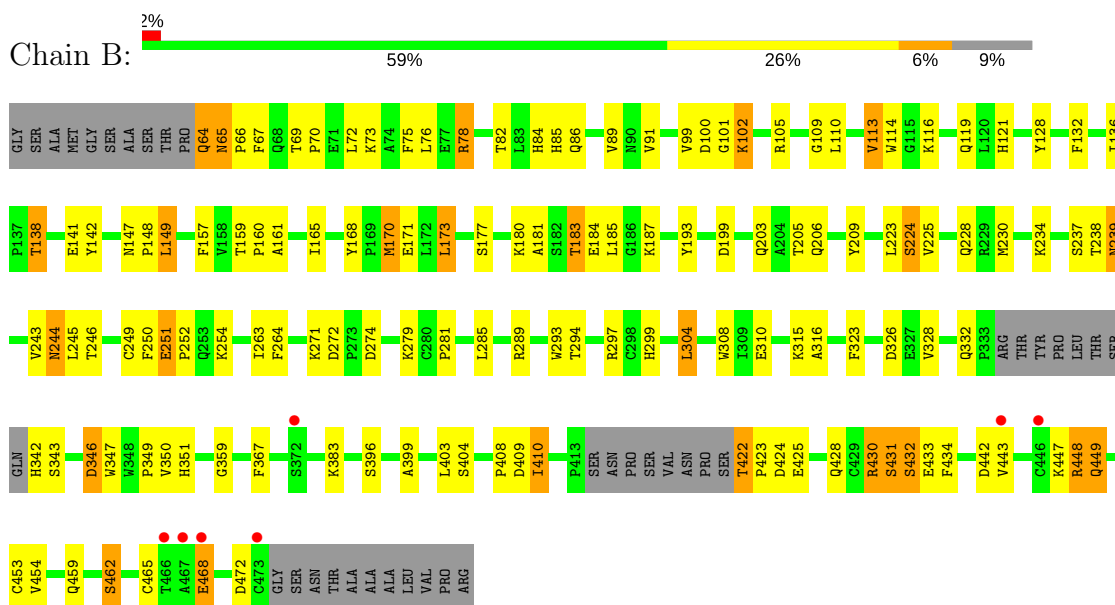
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: APICAL MEMBRANE ANTIGEN 1

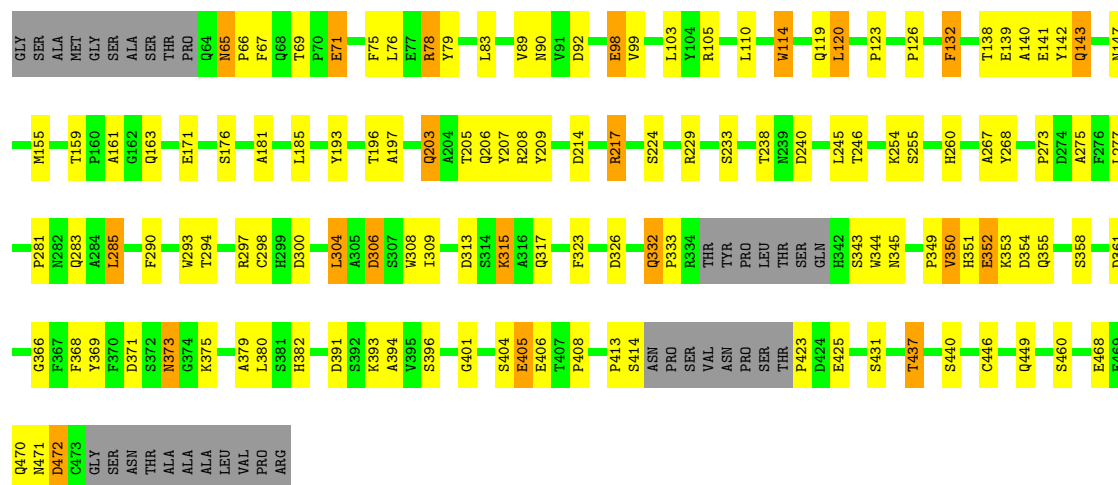


#### • Molecule 1: APICAL MEMBRANE ANTIGEN 1



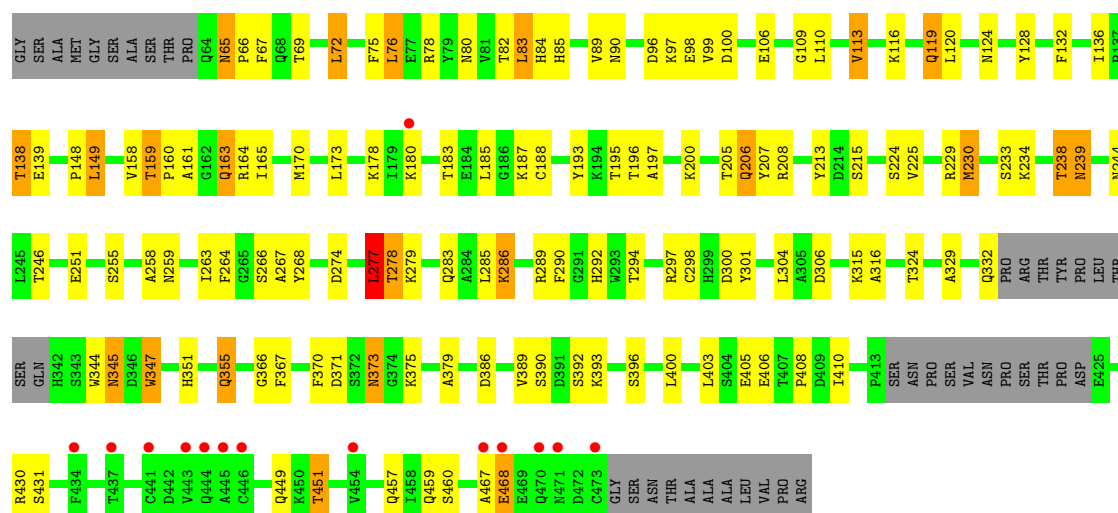
#### • Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain D:  62% 25% 5% 8%



• Molecule 1: APICAL MEMBRANE ANTIGEN 1

Chain E:  3% 59% 26% 5% 10%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	251.56Å 51.00Å 145.34Å 90.00° 90.93° 90.00°	Depositor
Resolution (Å)	48.44 – 2.90 47.31 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.44-2.90) 98.8 (47.31-2.90)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.193 , 0.271 0.193 , 0.272	Depositor DCC
$R_{free}$ test set	2078 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.0365e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.50	1/3244 (0.0%)	0.55	0/4401
1	B	0.50	2/3212 (0.1%)	0.53	0/4358
1	D	0.52	1/3222 (0.0%)	0.56	0/4369
1	E	0.49	1/3181 (0.0%)	0.53	0/4313
All	All	0.50	5/12859 (0.0%)	0.54	0/17441

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	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	TRP	CD2-CE2	5.21	1.47	1.41
1	B	293	TRP	CD2-CE2	5.11	1.47	1.41
1	E	347	TRP	CD2-CE2	5.10	1.47	1.41
1	B	308	TRP	CD2-CE2	5.04	1.47	1.41
1	D	114	TRP	CD2-CE2	5.00	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	353	LYS	Peptide
1	E	277	LEU	Peptide



## 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	3155	0	2950	96	0
1	B	3123	0	2919	109	0
1	D	3133	0	2931	94	0
1	E	3094	0	2894	100	0
2	A	45	0	0	1	0
2	B	33	0	0	0	0
2	D	45	0	0	5	0
2	E	19	0	0	1	0
All	All	12647	0	11694	396	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (396) 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:A:69:THR:HG22	1:A:72:LEU:HB2	1.26	1.18
1:B:422:THR:HB	1:B:423:PRO:CD	1.76	1.13
1:A:183:THR:HG22	1:A:186:GLY:H	1.10	1.12
1:D:205:THR:HG22	1:D:207:TYR:H	1.15	1.11
1:D:217:ARG:HH11	1:D:217:ARG:HG2	1.11	1.08
1:B:205:THR:HG22	1:B:206:GLN:H	1.14	1.07
1:A:332:GLN:HA	1:A:332:GLN:HE21	1.17	1.06
1:B:422:THR:HB	1:B:423:PRO:HD3	1.38	1.03
1:B:159:THR:HG22	1:B:161:ALA:H	1.25	1.00
1:D:65:ASN:C	1:D:65:ASN:HD22	1.68	0.97
1:D:159:THR:HG22	1:D:161:ALA:H	1.25	0.95
1:E:205:THR:HG22	1:E:207:TYR:H	1.31	0.95
1:B:136:ILE:HD11	1:B:224:SER:HB3	1.46	0.94
1:A:75:PHE:O	1:A:78:ARG:HG2	1.68	0.94
1:B:423:PRO:HB2	1:B:424:ASP:HA	1.51	0.92
1:D:65:ASN:ND2	1:D:67:PHE:H	1.67	0.92
1:A:159:THR:HG22	1:A:161:ALA:H	1.36	0.91
1:B:136:ILE:HD11	1:B:224:SER:CB	2.01	0.91
1:B:138:THR:HG22	1:B:141:GLU:H	1.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:ILE:CD1	1:E:224:SER:HB3	2.02	0.88
1:D:283:GLN:HG2	2:D:2025:HOH:O	1.74	0.87
1:B:205:THR:HG22	1:B:206:GLN:N	1.90	0.87
1:B:422:THR:CB	1:B:423:PRO:HD3	2.03	0.87
1:A:100:ASP:OD1	1:A:199:ASP:HB2	1.75	0.85
1:D:217:ARG:HH11	1:D:217:ARG:CG	1.90	0.85
1:D:217:ARG:HG2	1:D:217:ARG:NH1	1.89	0.84
1:D:205:THR:HG22	1:D:206:GLN:N	1.92	0.84
1:D:138:THR:HG22	1:D:140:ALA:H	1.45	0.82
1:B:136:ILE:CD1	1:B:224:SER:CB	2.57	0.82
1:D:332:GLN:HE21	1:D:332:GLN:HA	1.45	0.82
1:A:332:GLN:HA	1:A:332:GLN:NE2	1.92	0.81
1:B:136:ILE:CD1	1:B:224:SER:HB3	2.09	0.81
1:B:423:PRO:HA	1:B:425:GLU:H	1.44	0.81
1:B:422:THR:CB	1:B:423:PRO:CD	2.57	0.80
1:B:99:VAL:HG22	1:B:205:THR:HG21	1.63	0.79
1:A:282:ASN:ND2	1:A:282:ASN:H	1.76	0.79
1:A:183:THR:HG22	1:A:186:GLY:N	1.94	0.79
1:B:85:HIS:CE1	1:B:109:GLY:HA3	2.18	0.79
1:A:205:THR:HG23	1:A:207:TYR:H	1.48	0.79
1:D:105:ARG:HB2	1:D:349:PRO:HG2	1.65	0.78
1:D:205:THR:HG22	1:D:207:TYR:N	1.97	0.78
1:D:65:ASN:HD22	1:D:66:PRO:N	1.82	0.78
1:A:69:THR:CG2	1:A:72:LEU:HB2	2.13	0.78
1:E:373:ASN:HD22	1:E:373:ASN:N	1.80	0.77
1:A:332:GLN:HE21	1:A:332:GLN:CA	1.96	0.77
1:B:423:PRO:CB	1:B:424:ASP:HA	2.13	0.77
1:A:432:SER:HB2	2:A:2040:HOH:O	1.84	0.76
1:A:77:GLU:HG2	1:A:83:LEU:HD23	1.66	0.76
1:E:298:CYS:H	1:E:449:GLN:NE2	1.82	0.76
1:A:183:THR:CG2	1:A:186:GLY:H	1.93	0.76
1:E:316:ALA:HA	1:E:403:LEU:HD11	1.66	0.76
1:D:205:THR:CG2	1:D:206:GLN:N	2.50	0.75
1:B:159:THR:HG22	1:B:161:ALA:N	2.01	0.75
1:B:205:THR:CG2	1:B:206:GLN:H	1.95	0.74
1:A:454:VAL:HB	1:A:459:GLN:HG3	1.67	0.74
1:D:65:ASN:ND2	1:D:65:ASN:C	2.40	0.73
1:A:97:LYS:HE3	1:A:106:GLU:OE1	1.88	0.73
1:D:90:ASN:ND2	1:D:229:ARG:NH2	2.36	0.73
1:B:114:TRP:O	1:B:254:LYS:HE2	1.89	0.72
1:D:332:GLN:NE2	1:D:333:PRO:HD2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:ILE:HD12	1:E:410:ILE:H	1.53	0.72
1:B:65:ASN:ND2	1:B:67:PHE:H	1.86	0.72
1:A:298:CYS:H	1:A:449:GLN:NE2	1.88	0.72
1:B:430:ARG:HD2	1:B:431:SER:H	1.56	0.71
1:B:430:ARG:HD2	1:B:431:SER:N	2.06	0.71
1:A:135:ASP:OD1	1:A:164:ARG:NH2	2.24	0.71
1:B:75:PHE:O	1:B:78:ARG:HD2	1.91	0.70
1:A:229:ARG:HD2	1:A:332:GLN:HG2	1.73	0.70
1:D:155:MET:HE1	1:D:209:TYR:CE2	2.27	0.70
1:E:205:THR:HG22	1:E:206:GLN:N	2.07	0.69
1:D:437:THR:HG23	2:D:2042:HOH:O	1.92	0.69
1:E:136:ILE:HD12	1:E:224:SER:HB3	1.73	0.69
1:E:65:ASN:ND2	1:E:67:PHE:H	1.90	0.69
1:E:97:LYS:HD2	1:E:206:GLN:HB3	1.74	0.69
1:D:139:GLU:O	1:D:143:GLN:HG2	1.92	0.69
1:A:90:ASN:HD21	1:A:229:ARG:NH2	1.90	0.69
1:D:437:THR:CG2	2:D:2042:HOH:O	2.41	0.68
1:B:99:VAL:CG2	1:B:205:THR:HG21	2.23	0.68
1:B:181:ALA:HB3	1:B:187:LYS:HG2	1.76	0.67
1:D:313:ASP:H	1:D:317:GLN:HE21	1.41	0.67
1:E:468:GLU:HG2	1:E:468:GLU:O	1.94	0.67
1:B:422:THR:CG2	1:B:423:PRO:HD3	2.23	0.67
1:B:425:GLU:HA	1:B:428:GLN:NE2	2.10	0.67
1:B:422:THR:HB	1:B:423:PRO:HD2	1.73	0.67
1:A:373:ASN:HB2	1:A:375:LYS:HE3	1.77	0.67
1:A:75:PHE:HE1	1:A:424:ASP:HB2	1.60	0.67
1:A:90:ASN:ND2	1:A:229:ARG:HH21	1.93	0.66
1:A:371:ASP:HB2	1:A:375:LYS:H	1.60	0.66
1:D:138:THR:HB	1:D:141:GLU:HG3	1.77	0.66
1:B:136:ILE:CD1	1:B:224:SER:HB2	2.26	0.66
1:D:147:ASN:HB3	1:D:245:LEU:O	1.95	0.66
1:B:86:GLN:O	1:B:359:GLY:HA2	1.95	0.66
1:E:128:TYR:OH	1:E:148:PRO:HD2	1.97	0.65
1:D:313:ASP:H	1:D:317:GLN:NE2	1.95	0.64
1:A:179:ILE:HG22	1:A:179:ILE:O	1.96	0.64
1:D:138:THR:HG22	1:D:140:ALA:N	2.11	0.64
1:A:282:ASN:HD22	1:A:282:ASN:H	1.45	0.63
1:E:65:ASN:HD22	1:E:65:ASN:C	2.01	0.63
1:B:159:THR:CG2	1:B:161:ALA:H	2.07	0.63
1:B:193:TYR:CZ	1:B:271:LYS:HG3	2.33	0.63
1:D:205:THR:CG2	1:D:206:GLN:H	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ASN:HD22	1:D:67:PHE:H	1.47	0.63
1:B:170:MET:HE3	1:B:184:GLU:O	1.98	0.63
1:E:238:THR:O	1:E:239:ASN:HB2	1.97	0.63
1:D:69:THR:HG22	1:D:71:GLU:H	1.64	0.63
1:B:65:ASN:HD22	1:B:66:PRO:N	1.96	0.62
1:E:159:THR:HG22	1:E:161:ALA:H	1.64	0.62
1:D:99:VAL:HG22	1:D:205:THR:HG21	1.80	0.62
1:B:442:ASP:HB3	1:B:447:LYS:O	2.00	0.61
1:B:454:VAL:HB	1:B:459:GLN:HG3	1.83	0.61
1:D:205:THR:CG2	1:D:207:TYR:H	2.04	0.60
1:A:75:PHE:CE1	1:A:424:ASP:HB2	2.37	0.60
1:D:142:TYR:OH	1:D:147:ASN:ND2	2.34	0.60
1:E:205:THR:CG2	1:E:206:GLN:N	2.64	0.60
1:E:99:VAL:HG22	1:E:205:THR:HG21	1.83	0.60
1:D:351:HIS:C	1:D:352:GLU:HG2	2.21	0.60
1:D:351:HIS:O	1:D:352:GLU:HG2	2.01	0.59
1:D:358:SER:O	1:D:361:ASP:HB3	2.01	0.59
1:A:120:LEU:HD12	1:A:250:PHE:HB3	1.85	0.59
1:E:69:THR:HG22	1:E:72:LEU:H	1.67	0.59
1:A:158:VAL:HB	1:A:163:GLN:O	2.02	0.59
1:E:208:ARG:HB3	1:E:267:ALA:CB	2.32	0.58
1:A:90:ASN:ND2	1:A:229:ARG:NH2	2.49	0.58
1:A:286:LYS:HA	1:A:395:VAL:HG22	1.85	0.58
1:D:306:ASP:N	1:D:306:ASP:OD1	2.31	0.58
1:D:114:TRP:O	1:D:254:LYS:HE2	2.03	0.58
1:D:75:PHE:O	1:D:78:ARG:HD2	2.04	0.58
1:E:124:ASN:ND2	1:E:239:ASN:HD21	2.02	0.57
1:E:119:GLN:NE2	1:E:251:GLU:OE2	2.38	0.57
1:E:451:THR:HG23	1:E:460:SER:HB2	1.87	0.57
1:E:351:HIS:HA	1:E:355:GLN:NE2	2.20	0.57
1:A:138:THR:HG22	1:A:140:ALA:H	1.69	0.56
1:B:65:ASN:HD22	1:B:66:PRO:CD	2.18	0.56
1:A:282:ASN:N	1:A:282:ASN:ND2	2.51	0.56
1:A:125:ARG:NH2	1:A:240:ASP:OD2	2.39	0.56
1:A:120:LEU:HG	1:A:248:TYR:CE1	2.40	0.56
1:A:65:ASN:HB3	1:A:68:GLN:HB2	1.87	0.56
1:E:298:CYS:H	1:E:449:GLN:HE21	1.53	0.56
1:B:184:GLU:OE1	1:B:410:ILE:HG22	2.04	0.56
1:B:432:SER:C	1:B:434:PHE:H	2.09	0.56
1:A:65:ASN:ND2	1:A:67:PHE:H	2.03	0.56
1:D:90:ASN:HD21	1:D:229:ARG:NH2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:ALA:O	1:E:205:THR:HB	2.06	0.55
1:E:263:ILE:N	1:E:263:ILE:HD12	2.22	0.55
1:A:298:CYS:H	1:A:449:GLN:HE21	1.53	0.55
1:B:100:ASP:O	1:B:102:LYS:HE3	2.07	0.55
1:D:371:ASP:HB3	1:D:373:ASN:H	1.71	0.55
1:D:65:ASN:HD21	1:D:67:PHE:H	1.48	0.55
1:E:113:VAL:HG22	1:E:116:LYS:HB2	1.89	0.55
1:D:470:GLN:C	1:D:472:ASP:H	2.10	0.54
1:D:65:ASN:HB2	1:D:293:TRP:CE2	2.41	0.54
1:A:366:GLY:HA2	1:A:379:ALA:O	2.07	0.54
1:B:136:ILE:HD11	1:B:224:SER:HB2	1.81	0.54
1:D:197:ALA:O	1:D:205:THR:HB	2.08	0.54
1:D:65:ASN:HB2	1:D:293:TRP:CD2	2.43	0.54
1:A:144:LYS:HG2	1:A:144:LYS:O	2.07	0.54
1:E:80:ASN:OD1	1:E:82:THR:HB	2.08	0.54
1:A:183:THR:HG23	1:A:184:GLU:N	2.23	0.53
1:B:78:ARG:NH2	1:B:423:PRO:HG3	2.24	0.53
1:B:159:THR:HG23	1:B:160:PRO:HD2	1.90	0.53
1:E:274:ASP:O	1:E:277:LEU:HB2	2.09	0.53
1:E:72:LEU:O	1:E:75:PHE:HB3	2.07	0.53
1:D:468:GLU:OE2	1:E:244:ASN:HA	2.08	0.53
1:E:371:ASP:CB	1:E:375:LYS:HG2	2.39	0.53
1:D:159:THR:HG22	1:D:161:ALA:N	2.09	0.53
1:B:289:ARG:HB3	1:B:367:PHE:CE2	2.43	0.52
1:A:65:ASN:HD22	1:A:67:PHE:H	1.57	0.52
1:B:254:LYS:NZ	1:B:399:ALA:O	2.40	0.52
1:B:65:ASN:C	1:B:65:ASN:HD22	2.10	0.52
1:B:65:ASN:HD22	1:B:66:PRO:HD2	1.74	0.52
1:A:371:ASP:OD2	1:A:375:LYS:HB2	2.09	0.52
1:A:371:ASP:HB3	1:A:373:ASN:H	1.75	0.52
1:B:142:TYR:OH	1:B:147:ASN:ND2	2.40	0.52
1:D:206:GLN:NE2	1:D:208:ARG:HH12	2.08	0.52
1:B:64:GLN:HE21	1:B:64:GLN:CA	2.22	0.52
1:E:316:ALA:HA	1:E:403:LEU:CD1	2.38	0.52
1:A:147:ASN:N	1:A:147:ASN:HD22	2.07	0.51
1:B:149:LEU:HD22	1:B:246:THR:O	2.10	0.51
1:E:159:THR:CG2	1:E:161:ALA:H	2.23	0.51
1:D:208:ARG:HD2	1:D:268:TYR:CZ	2.45	0.51
1:A:366:GLY:CA	1:A:379:ALA:O	2.58	0.51
1:A:138:THR:HG22	1:A:140:ALA:N	2.25	0.51
1:E:370:PHE:CD2	1:E:393:LYS:HE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TYR:CE2	1:A:119:GLN:HG2	2.45	0.51
1:D:254:LYS:HE3	1:D:323:PHE:CD2	2.45	0.51
1:E:159:THR:HG22	1:E:161:ALA:N	2.26	0.51
1:A:69:THR:HG23	1:A:72:LEU:H	1.76	0.50
1:B:434:PHE:HD2	1:B:453:CYS:HB2	1.75	0.50
1:E:106:GLU:OE2	1:E:268:TYR:OH	2.25	0.50
1:A:135:ASP:HB3	1:A:156:ASN:HB3	1.94	0.50
1:A:334:ARG:O	1:A:335:THR:HG23	2.11	0.50
1:D:297:ARG:HB2	1:D:449:GLN:HE21	1.76	0.50
1:E:371:ASP:HB3	1:E:375:LYS:HG2	1.94	0.50
1:E:229:ARG:HG3	1:E:230:MET:N	2.27	0.50
1:E:278:THR:HG22	1:E:279:LYS:HG3	1.94	0.50
1:A:208:ARG:HD2	1:A:268:TYR:CZ	2.46	0.50
1:B:168:TYR:CE2	1:B:173:LEU:HD13	2.46	0.49
1:E:468:GLU:CG	1:E:468:GLU:O	2.60	0.49
1:B:408:PRO:HB2	1:B:410:ILE:HD13	1.95	0.49
1:E:65:ASN:HD21	1:E:67:PHE:HB2	1.76	0.49
1:E:85:HIS:CE1	1:E:109:GLY:HA3	2.46	0.49
1:A:69:THR:CG2	1:A:72:LEU:H	2.25	0.49
1:A:179:ILE:CG2	1:A:179:ILE:O	2.57	0.49
1:B:65:ASN:C	1:B:65:ASN:ND2	2.66	0.49
1:B:367:PHE:HB3	1:B:396:SER:OG	2.12	0.49
1:E:100:ASP:OD1	1:E:200:LYS:HB2	2.12	0.49
1:A:117:TYR:HE2	1:A:119:GLN:HG2	1.78	0.49
1:E:205:THR:HG22	1:E:207:TYR:N	2.12	0.49
1:E:188:CYS:SG	1:E:213:TYR:HD1	2.36	0.49
1:B:168:TYR:HE2	1:B:173:LEU:HD13	1.78	0.49
1:D:159:THR:HB	1:D:163:GLN:HB2	1.93	0.49
1:E:264:PHE:C	1:E:264:PHE:CD1	2.85	0.49
1:A:332:GLN:NE2	1:A:333:PRO:HD2	2.28	0.49
1:A:468:GLU:HA	1:A:468:GLU:OE1	2.12	0.49
1:A:114:TRP:O	1:A:254:LYS:HE2	2.13	0.48
1:E:159:THR:HG23	1:E:160:PRO:HD2	1.95	0.48
1:A:197:ALA:O	1:A:205:THR:HG22	2.13	0.48
1:A:73:LYS:O	1:A:77:GLU:HB2	2.13	0.48
1:B:78:ARG:NH2	1:B:423:PRO:CG	2.76	0.48
1:D:171:GLU:CG	2:D:2016:HOH:O	2.62	0.48
1:E:213:TYR:CE2	1:E:215:SER:HA	2.48	0.48
1:B:316:ALA:HA	1:B:403:LEU:HD11	1.96	0.48
1:D:368:PHE:O	1:D:394:ALA:HA	2.14	0.48
1:A:444:GLN:O	1:A:444:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HG22	1:A:72:LEU:CB	2.19	0.48
1:E:292:HIS:CD2	1:E:386:ASP:OD2	2.67	0.48
1:E:300:ASP:HB3	1:E:389:VAL:HG21	1.96	0.48
1:E:65:ASN:HD22	1:E:67:PHE:H	1.59	0.48
1:B:209:TYR:HB3	1:B:223:LEU:O	2.14	0.47
1:B:250:PHE:C	1:B:251:GLU:HG3	2.34	0.47
1:D:155:MET:HE1	1:D:209:TYR:CD2	2.47	0.47
1:B:183:THR:O	1:B:187:LYS:HG3	2.14	0.47
1:D:123:PRO:HG3	1:D:240:ASP:HB2	1.95	0.47
1:E:373:ASN:ND2	1:E:373:ASN:N	2.53	0.47
1:D:159:THR:CB	1:D:163:GLN:HB2	2.45	0.47
1:D:309:ILE:HD13	1:D:369:TYR:OH	2.14	0.47
1:D:298:CYS:H	1:D:449:GLN:NE2	2.13	0.47
1:B:105:ARG:HB2	1:B:349:PRO:HB2	1.96	0.47
1:D:332:GLN:HE21	1:D:333:PRO:HD2	1.80	0.47
1:E:136:ILE:HD11	1:E:225:VAL:HG23	1.96	0.47
1:E:410:ILE:CD1	1:E:410:ILE:H	2.26	0.47
1:A:89:VAL:HG21	1:A:399:ALA:HB1	1.96	0.47
1:E:373:ASN:HB2	1:E:375:LYS:HD3	1.96	0.47
1:D:283:GLN:OE1	1:D:408:PRO:HD3	2.14	0.47
1:D:142:TYR:OH	1:D:246:THR:HG23	2.15	0.47
1:D:308:TRP:HB2	1:D:380:LEU:HB2	1.95	0.47
1:D:78:ARG:NH2	1:D:423:PRO:HD2	2.31	0.46
1:E:170:MET:O	1:E:173:LEU:HB2	2.15	0.46
1:E:65:ASN:C	1:E:65:ASN:ND2	2.67	0.46
1:E:163:GLN:HG2	1:E:164:ARG:N	2.29	0.46
1:B:128:TYR:OH	1:B:148:PRO:HD2	2.15	0.46
1:D:78:ARG:NH2	1:D:423:PRO:CD	2.79	0.46
1:A:280:CYS:O	1:A:282:ASN:ND2	2.49	0.46
1:A:352:GLU:H	1:A:355:GLN:NE2	2.14	0.46
1:A:77:GLU:CG	1:A:83:LEU:HD23	2.41	0.46
1:B:448:ARG:HG2	1:B:465:CYS:SG	2.56	0.46
1:B:228:GLN:O	1:B:252:PRO:HD3	2.16	0.46
1:E:215:SER:HB2	1:E:410:ILE:HG12	1.98	0.46
1:A:124:ASN:HD22	1:E:324:THR:HB	1.80	0.46
1:D:98:GLU:HG2	1:D:103:LEU:HD13	1.97	0.46
1:E:205:THR:CG2	1:E:206:GLN:H	2.29	0.46
1:E:459:GLN:HB2	2:E:2019:HOH:O	2.16	0.46
1:A:128:TYR:OH	1:A:148:PRO:HD2	2.16	0.46
1:E:195:THR:O	1:E:208:ARG:HG2	2.16	0.46
1:A:113:VAL:CG2	1:A:116:LYS:HB3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASP:N	1:A:306:ASP:OD1	2.43	0.45
1:A:183:THR:CG2	1:A:184:GLU:N	2.79	0.45
1:B:430:ARG:CD	1:B:431:SER:N	2.78	0.45
1:B:297:ARG:HB2	1:B:449:GLN:HB2	1.99	0.45
1:D:344:TRP:CG	1:D:345:ASN:N	2.84	0.45
1:D:69:THR:HG22	1:D:71:GLU:N	2.28	0.45
1:D:92:ASP:OD1	1:D:92:ASP:C	2.55	0.45
1:E:119:GLN:HE21	1:E:119:GLN:HB3	1.51	0.45
1:E:80:ASN:HB3	1:E:83:LEU:HB2	1.98	0.45
1:B:310:GLU:OE2	1:D:126:PRO:HD3	2.15	0.45
1:B:121:HIS:NE2	1:B:251:GLU:OE2	2.44	0.45
1:A:123:PRO:HD2	1:A:128:TYR:CG	2.52	0.45
1:A:65:ASN:C	1:A:65:ASN:HD22	2.20	0.45
1:B:136:ILE:HD12	1:B:224:SER:HB2	1.96	0.45
1:E:113:VAL:CG2	1:E:116:LYS:HB2	2.46	0.45
1:A:105:ARG:HD2	1:A:355:GLN:NE2	2.32	0.44
1:B:304:LEU:HA	1:B:304:LEU:HD12	1.74	0.44
1:B:69:THR:O	1:B:70:PRO:C	2.55	0.44
1:D:65:ASN:ND2	1:D:67:PHE:N	2.51	0.44
1:E:345:ASN:O	1:E:347:TRP:N	2.50	0.44
1:D:275:ALA:O	1:D:277:LEU:N	2.51	0.44
1:B:351:HIS:CD2	1:B:351:HIS:C	2.90	0.44
1:D:366:GLY:HA2	1:D:379:ALA:O	2.18	0.44
1:B:113:VAL:HG22	1:B:116:LYS:HB3	2.00	0.44
1:B:100:ASP:OD1	1:B:199:ASP:HB2	2.18	0.44
1:B:422:THR:HG22	1:B:423:PRO:HD3	1.99	0.44
1:A:311:ALA:HA	1:A:377:LYS:HG3	1.99	0.44
1:B:157:PHE:O	1:B:165:ILE:HG12	2.17	0.44
1:B:199:ASP:OD2	1:B:203:GLN:HB2	2.17	0.44
1:B:343:SER:O	1:B:346:ASP:HB2	2.16	0.44
1:B:64:GLN:HE21	1:B:64:GLN:HA	1.81	0.44
1:A:289:ARG:HB3	1:A:367:PHE:CE2	2.53	0.44
1:B:454:VAL:HB	1:B:459:GLN:CG	2.48	0.44
1:D:171:GLU:HG2	2:D:2016:HOH:O	2.17	0.44
1:E:193:TYR:CD1	1:E:208:ARG:HD3	2.52	0.44
1:A:290:PHE:HB3	1:A:385:PRO:HB3	1.99	0.44
1:D:181:ALA:HB2	1:D:273:PRO:HB2	2.00	0.44
1:E:297:ARG:HB2	1:E:449:GLN:HE21	1.83	0.44
1:D:99:VAL:CG2	1:D:205:THR:HG21	2.45	0.44
1:D:214:ASP:OD1	1:D:214:ASP:C	2.57	0.43
1:B:297:ARG:NH1	1:B:462:SER:OG	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:VAL:HG22	1:E:116:LYS:CB	2.48	0.43
1:B:294:THR:HG23	1:B:299:HIS:ND1	2.33	0.43
1:B:323:PHE:O	1:B:328:VAL:HG11	2.19	0.43
1:D:79:TYR:OH	1:D:285:LEU:HG	2.18	0.43
1:E:258:ALA:O	1:E:259:ASN:HB2	2.18	0.43
1:E:289:ARG:HD3	1:E:367:PHE:CE1	2.53	0.43
1:E:345:ASN:ND2	1:E:345:ASN:H	2.16	0.43
1:A:85:HIS:CE1	1:A:109:GLY:HA3	2.54	0.43
1:B:237:SER:HB3	1:B:245:LEU:HB2	2.01	0.43
1:D:300:ASP:C	1:D:300:ASP:OD1	2.57	0.43
1:D:315:LYS:HB3	1:D:368:PHE:CD2	2.54	0.43
1:E:75:PHE:HD2	1:E:76:LEU:HD13	1.83	0.43
1:A:300:ASP:C	1:A:300:ASP:OD1	2.57	0.43
1:B:239:ASN:C	1:B:239:ASN:HD22	2.21	0.43
1:E:90:ASN:ND2	1:E:229:ARG:HH22	2.17	0.43
1:D:405:GLU:H	1:D:405:GLU:HG2	1.64	0.43
1:B:423:PRO:HB2	1:B:424:ASP:CA	2.35	0.42
1:A:128:TYR:CZ	1:A:148:PRO:HD2	2.54	0.42
1:E:344:TRP:CE2	1:E:345:ASN:OD1	2.72	0.42
1:E:366:GLY:HA2	1:E:379:ALA:O	2.19	0.42
1:A:76:LEU:HD21	1:A:387:CYS:HA	1.99	0.42
1:B:410:ILE:HD13	1:B:410:ILE:H	1.84	0.42
1:E:96:ASP:OD2	1:E:351:HIS:ND1	2.52	0.42
1:D:350:VAL:O	1:D:355:GLN:OE1	2.37	0.42
1:D:470:GLN:C	1:D:472:ASP:N	2.71	0.42
1:E:138:THR:O	1:E:139:GLU:C	2.58	0.42
1:B:65:ASN:HD21	1:B:67:PHE:HD1	1.66	0.42
1:D:193:TYR:HA	1:D:267:ALA:HB1	2.01	0.42
1:E:65:ASN:HD22	1:E:66:PRO:N	2.16	0.42
1:A:325:ASN:O	1:A:328:VAL:HG12	2.20	0.42
1:D:366:GLY:CA	1:D:379:ALA:O	2.68	0.42
1:D:143:GLN:HG2	1:D:143:GLN:H	1.51	0.42
1:D:290:PHE:CZ	1:D:396:SER:HB3	2.55	0.42
1:E:128:TYR:CZ	1:E:148:PRO:HD2	2.54	0.42
1:B:468:GLU:H	1:B:468:GLU:HG3	1.59	0.42
1:A:80:ASN:HB3	1:A:83:LEU:HB2	2.02	0.42
1:B:272:ASP:O	1:B:274:ASP:N	2.52	0.42
1:E:278:THR:CG2	1:E:278:THR:O	2.67	0.42
1:A:149:LEU:HA	1:A:149:LEU:HD12	1.92	0.42
1:A:135:ASP:CG	1:A:164:ARG:HH22	2.23	0.42
1:B:230:MET:O	1:B:249:CYS:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HG13	1:B:228:GLN:HB2	2.02	0.42
1:A:79:TYR:O	1:A:365:TYR:HE1	2.03	0.41
1:B:113:VAL:HG13	1:B:264:PHE:O	2.20	0.41
1:A:254:LYS:HD3	1:A:319:TRP:CZ2	2.55	0.41
1:B:245:LEU:HA	1:B:245:LEU:HD23	1.94	0.41
1:B:263:ILE:N	1:B:263:ILE:HD12	2.35	0.41
1:B:433:GLU:O	1:B:433:GLU:CG	2.67	0.41
1:D:255:SER:O	1:D:260:HIS:HE1	2.03	0.41
1:D:391:ASP:OD1	1:D:391:ASP:C	2.59	0.41
1:E:225:VAL:HA	1:E:347:TRP:HB3	2.02	0.41
1:E:290:PHE:CZ	1:E:396:SER:HB3	2.54	0.41
1:D:120:LEU:HD11	1:D:132:PHE:HB3	2.01	0.41
1:E:286:LYS:H	1:E:286:LYS:HG2	1.43	0.41
1:E:290:PHE:HB2	1:E:301:TYR:CE2	2.55	0.41
1:E:292:HIS:HD2	1:E:386:ASP:OD2	2.03	0.41
1:E:238:THR:O	1:E:239:ASN:CB	2.67	0.41
1:E:278:THR:HG23	1:E:278:THR:O	2.21	0.41
1:B:423:PRO:HA	1:B:425:GLU:N	2.23	0.41
1:D:114:TRP:HB2	1:D:401:GLY:O	2.21	0.41
1:B:78:ARG:O	1:B:281:PRO:HG3	2.20	0.41
1:E:430:ARG:HG3	1:E:431:SER:N	2.35	0.41
1:A:193:TYR:CZ	1:A:271:LYS:HG3	2.56	0.41
1:A:285:LEU:HA	1:A:285:LEU:HD23	1.94	0.41
1:B:423:PRO:CB	1:B:424:ASP:CA	2.94	0.41
1:D:203:GLN:HE21	1:D:203:GLN:CA	2.32	0.41
1:E:183:THR:O	1:E:187:LYS:HG3	2.21	0.41
1:A:78:ARG:O	1:A:281:PRO:HD3	2.21	0.41
1:B:430:ARG:CD	1:B:431:SER:H	2.27	0.41
1:B:454:VAL:CG2	1:B:459:GLN:HG3	2.51	0.41
1:E:124:ASN:H	1:E:124:ASN:ND2	2.18	0.41
1:E:183:THR:HG21	1:E:277:LEU:HD11	2.03	0.41
1:E:83:LEU:HB3	1:E:84[B]:HIS:CD2	2.56	0.41
1:E:406:GLU:O	1:E:408:PRO:HD3	2.20	0.41
1:A:159:THR:HG22	1:A:161:ALA:N	2.18	0.40
1:D:304:LEU:HD12	1:D:304:LEU:HA	1.88	0.40
1:E:124:ASN:HD22	1:E:124:ASN:H	1.67	0.40
1:E:163:GLN:HB3	1:E:163:GLN:HE21	1.61	0.40
1:A:228:GLN:O	1:A:252:PRO:HD3	2.22	0.40
1:E:149:LEU:HD22	1:E:246:THR:HG22	2.02	0.40
1:B:84[A]:HIS:CD2	1:B:279:LYS:O	2.75	0.40
1:E:351:HIS:HA	1:E:355:GLN:HE21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:HIS:HA	1:A:386:ASP:OD1	2.21	0.40
1:A:72:LEU:HD21	1:A:458:ILE:CD1	2.51	0.40
1:B:225:VAL:HA	1:B:347:TRP:HB3	2.04	0.40
1:B:432:SER:C	1:B:434:PHE:N	2.73	0.40
1:A:190:GLU:HG3	1:A:273:PRO:HG3	2.02	0.40
1:B:119:GLN:HB3	1:B:119:GLN:HE21	1.63	0.40
1:B:244:ASN:HA	1:B:244:ASN:HD22	1.74	0.40
1:B:272:ASP:C	1:B:274:ASP:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	393/431 (91%)	371 (94%)	22 (6%)	0	100	100
1	B	389/431 (90%)	353 (91%)	35 (9%)	1 (0%)	43	75
1	D	390/431 (90%)	358 (92%)	26 (7%)	6 (2%)	11	37
1	E	385/431 (89%)	345 (90%)	38 (10%)	2 (0%)	31	65
All	All	1557/1724 (90%)	1427 (92%)	121 (8%)	9 (1%)	27	61

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	326	ASP
1	D	471	ASN
1	D	472	ASP
1	E	467	ALA
1	D	233	SER
1	D	281	PRO
1	D	413	PRO

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Mol	Chain	Res	Type
1	E	329	ALA
1	B	101	GLY

### 5.3.2 Protein sidechains ⓘ

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	348/372 (94%)	301 (86%)	47 (14%)	4	12
1	B	344/372 (92%)	294 (86%)	50 (14%)	3	10
1	D	345/372 (93%)	302 (88%)	43 (12%)	5	15
1	E	340/372 (91%)	290 (85%)	50 (15%)	3	10
All	All	1377/1488 (92%)	1187 (86%)	190 (14%)	4	11

All (190) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	69	THR
1	A	72	LEU
1	A	76	LEU
1	A	77	GLU
1	A	83	LEU
1	A	98	GLU
1	A	120	LEU
1	A	123	PRO
1	A	125	ARG
1	A	132	PHE
1	A	143	GLN
1	A	147	ASN
1	A	149	LEU
1	A	158	VAL
1	A	164	ARG
1	A	172	LEU
1	A	175	LYS
1	A	179	ILE

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Mol	Chain	Res	Type
1	A	183	THR
1	A	185	LEU
1	A	196	THR
1	A	216	LYS
1	A	224	SER
1	A	234	LYS
1	A	238	THR
1	A	239	ASN
1	A	277	LEU
1	A	282	ASN
1	A	283	GLN
1	A	294	THR
1	A	304	LEU
1	A	306	ASP
1	A	315	LYS
1	A	332	GLN
1	A	335	THR
1	A	342	HIS
1	A	352	GLU
1	A	361	ASP
1	A	372	SER
1	A	382	HIS
1	A	406	GLU
1	A	431	SER
1	A	432	SER
1	A	437	THR
1	A	444	GLN
1	A	446	CYS
1	B	64	GLN
1	B	65	ASN
1	B	72	LEU
1	B	73	LYS
1	B	76	LEU
1	B	78	ARG
1	B	82	THR
1	B	89	VAL
1	B	102	LYS
1	B	110	LEU
1	B	113	VAL
1	B	132	PHE
1	B	138	THR
1	B	149	LEU

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Mol	Chain	Res	Type
1	B	170	MET
1	B	171	GLU
1	B	173	LEU
1	B	177	SER
1	B	180	LYS
1	B	183	THR
1	B	185	LEU
1	B	224	SER
1	B	234	LYS
1	B	238	THR
1	B	239	ASN
1	B	243	VAL
1	B	244	ASN
1	B	251	GLU
1	B	285	LEU
1	B	304	LEU
1	B	315	LYS
1	B	326	ASP
1	B	332	GLN
1	B	342	HIS
1	B	346	ASP
1	B	350	VAL
1	B	383	LYS
1	B	404	SER
1	B	409	ASP
1	B	410	ILE
1	B	422	THR
1	B	430	ARG
1	B	431	SER
1	B	432	SER
1	B	443	VAL
1	B	448	ARG
1	B	449	GLN
1	B	462	SER
1	B	468	GLU
1	B	472	ASP
1	D	65	ASN
1	D	71	GLU
1	D	76	LEU
1	D	78	ARG
1	D	83	LEU
1	D	89	VAL

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Mol	Chain	Res	Type
1	D	98	GLU
1	D	110	LEU
1	D	119	GLN
1	D	120	LEU
1	D	132	PHE
1	D	143	GLN
1	D	176	SER
1	D	185	LEU
1	D	196	THR
1	D	203	GLN
1	D	217	ARG
1	D	224	SER
1	D	238	THR
1	D	285	LEU
1	D	294	THR
1	D	304	LEU
1	D	306	ASP
1	D	315	LYS
1	D	332	GLN
1	D	343	SER
1	D	350	VAL
1	D	352	GLU
1	D	354	ASP
1	D	373	ASN
1	D	375	LYS
1	D	382	HIS
1	D	393	LYS
1	D	404	SER
1	D	405	GLU
1	D	406	GLU
1	D	414	SER
1	D	425	GLU
1	D	431	SER
1	D	437	THR
1	D	440	SER
1	D	446	CYS
1	D	460	SER
1	E	65	ASN
1	E	72	LEU
1	E	76	LEU
1	E	78	ARG
1	E	83	LEU

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Mol	Chain	Res	Type
1	E	89	VAL
1	E	98	GLU
1	E	110	LEU
1	E	113	VAL
1	E	119	GLN
1	E	120	LEU
1	E	132	PHE
1	E	138	THR
1	E	149	LEU
1	E	158	VAL
1	E	159	THR
1	E	163	GLN
1	E	165	ILE
1	E	178	LYS
1	E	180	LYS
1	E	185	LEU
1	E	196	THR
1	E	206	GLN
1	E	230	MET
1	E	233	SER
1	E	234	LYS
1	E	238	THR
1	E	239	ASN
1	E	255	SER
1	E	266	SER
1	E	277	LEU
1	E	278	THR
1	E	283	GLN
1	E	285	LEU
1	E	286	LYS
1	E	294	THR
1	E	304	LEU
1	E	306	ASP
1	E	315	LYS
1	E	332	GLN
1	E	345	ASN
1	E	355	GLN
1	E	373	ASN
1	E	390	SER
1	E	392	SER
1	E	400	LEU
1	E	405	GLU

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Mol	Chain	Res	Type
1	E	451	THR
1	E	457	GLN
1	E	468	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	90	ASN
1	A	143	GLN
1	A	147	ASN
1	A	154	ASN
1	A	282	ASN
1	A	292	HIS
1	A	295	ASN
1	A	299	HIS
1	A	332	GLN
1	A	351	HIS
1	A	355	GLN
1	A	357	HIS
1	A	373	ASN
1	A	449	GLN
1	A	470	GLN
1	A	471	ASN
1	B	64	GLN
1	B	65	ASN
1	B	90	ASN
1	B	119	GLN
1	B	147	ASN
1	B	154	ASN
1	B	244	ASN
1	B	317	GLN
1	B	355	GLN
1	B	373	ASN
1	B	428	GLN
1	B	449	GLN
1	D	65	ASN
1	D	90	ASN
1	D	95	GLN
1	D	119	GLN
1	D	124	ASN
1	D	147	ASN

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Mol	Chain	Res	Type
1	D	154	ASN
1	D	203	GLN
1	D	206	GLN
1	D	260	HIS
1	D	317	GLN
1	D	332	GLN
1	D	355	GLN
1	D	444	GLN
1	D	449	GLN
1	D	470	GLN
1	E	65	ASN
1	E	68	GLN
1	E	90	ASN
1	E	119	GLN
1	E	124	ASN
1	E	147	ASN
1	E	163	GLN
1	E	292	HIS
1	E	317	GLN
1	E	332	GLN
1	E	355	GLN
1	E	373	ASN
1	E	382	HIS
1	E	449	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	398/431 (92%)	-0.24	1 (0%) 93 94	19, 33, 59, 79	0
1	B	394/431 (91%)	-0.11	7 (1%) 68 67	17, 35, 71, 97	0
1	D	395/431 (91%)	-0.28	0 100 100	18, 32, 56, 80	0
1	E	390/431 (90%)	0.00	14 (3%) 42 37	21, 42, 79, 95	0
All	All	1577/1724 (91%)	-0.16	22 (1%) 75 75	17, 35, 69, 97	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	467	ALA	3.6
1	E	443	VAL	3.4
1	B	468	GLU	3.2
1	E	467	ALA	3.2
1	E	444	GLN	3.1
1	E	473	CYS	3.0
1	B	473	CYS	3.0
1	B	443	VAL	2.9
1	E	446	CYS	2.8
1	E	180	LYS	2.8
1	E	471	ASN	2.8
1	B	446	CYS	2.8
1	A	63	PRO	2.8
1	E	468	GLU	2.7
1	E	470	GLN	2.5
1	E	441	CYS	2.5
1	E	445	ALA	2.4
1	E	434	PHE	2.3
1	E	437	THR	2.2
1	B	466	THR	2.2
1	B	372	SER	2.1
1	E	454	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.