Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:43 AM GMT

PDB ID	:	2E2K
Title	:	Helicobacter pylori formamidase AmiF contains a fine-tuned cysteine-glutamate-lysine catalytic triad
Authors	:	Wang, W.C.; Hung, C.L.
Deposited on	:	2006-11-14
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

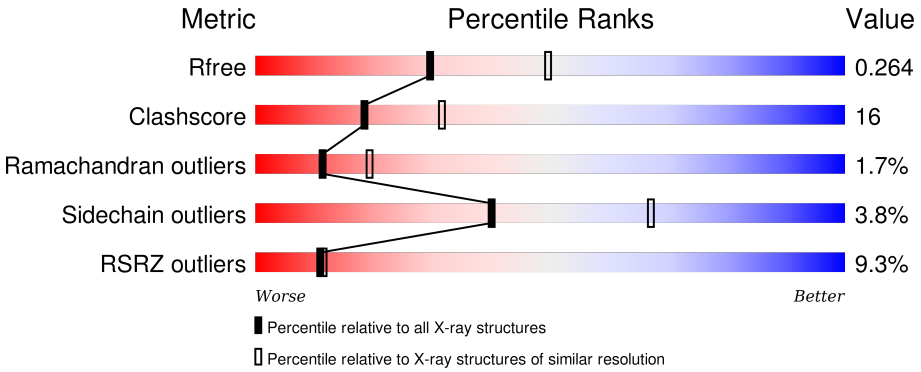
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	8% 75% 16% • 6%
1	B	334	8% 74% 18% • 6%
1	C	334	7% 74% 17% • 6%
1	D	334	8% 73% 18% • 7%
1	E	334	10% 74% 17% • 6%

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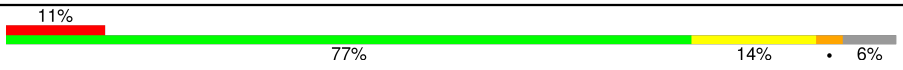
Mol	Chain	Length	Quality of chain
1	F	334	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15744 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 Formamidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2482	1597	416	458	11			
1	B	314	Total	C	N	O	S	0	0	0
			2485	1598	417	459	11			
1	C	314	Total	C	N	O	S	0	0	0
			2489	1600	417	461	11			
1	D	311	Total	C	N	O	S	0	0	0
			2458	1581	412	454	11			
1	E	315	Total	C	N	O	S	0	0	0
			2493	1602	419	461	11			
1	F	314	Total	C	N	O	S	0	0	0
			2487	1601	415	460	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	166	SER	CYS	ENGINEERED	UNP O25836
B	166	SER	CYS	ENGINEERED	UNP O25836
C	166	SER	CYS	ENGINEERED	UNP O25836
D	166	SER	CYS	ENGINEERED	UNP O25836
E	166	SER	CYS	ENGINEERED	UNP O25836
F	166	SER	CYS	ENGINEERED	UNP O25836

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	148	Total	O	0	0
			148	148		
2	B	151	Total	O	0	0
			151	151		
2	C	133	Total	O	0	0
			133	133		

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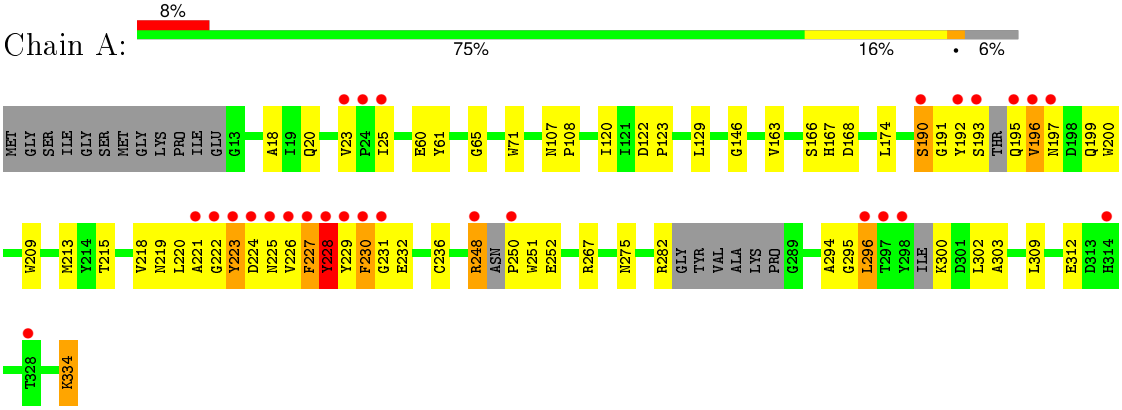
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	159	Total O 159 159	0	0
2	E	138	Total O 138 138	0	0
2	F	121	Total O 121 121	0	0

3 Residue-property plots (i)

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

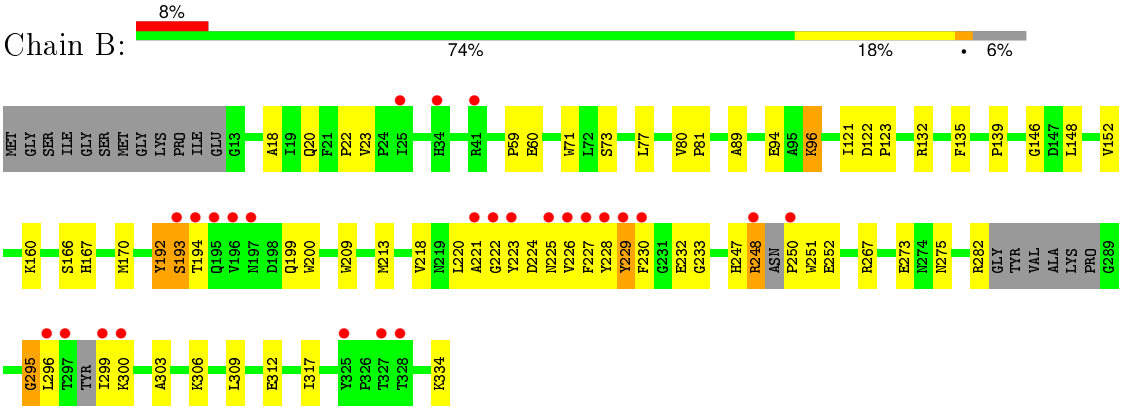
- Molecule 1: Formamidase

Chain A:



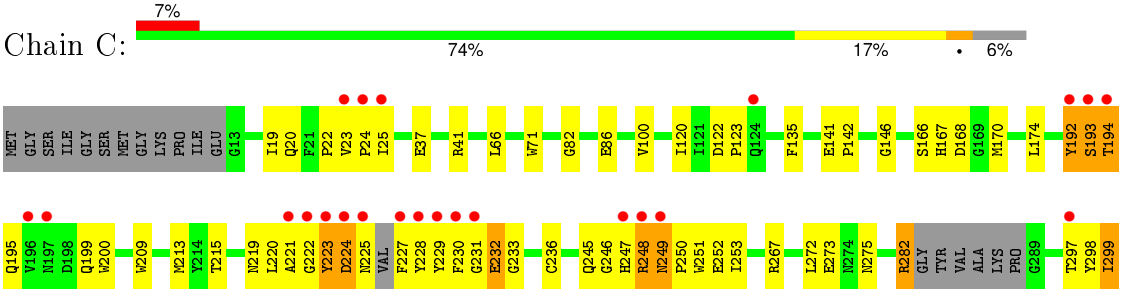
- Molecule 1: Formamidase

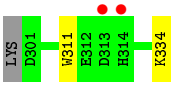
Chain B:



- Molecule 1: Formamidase

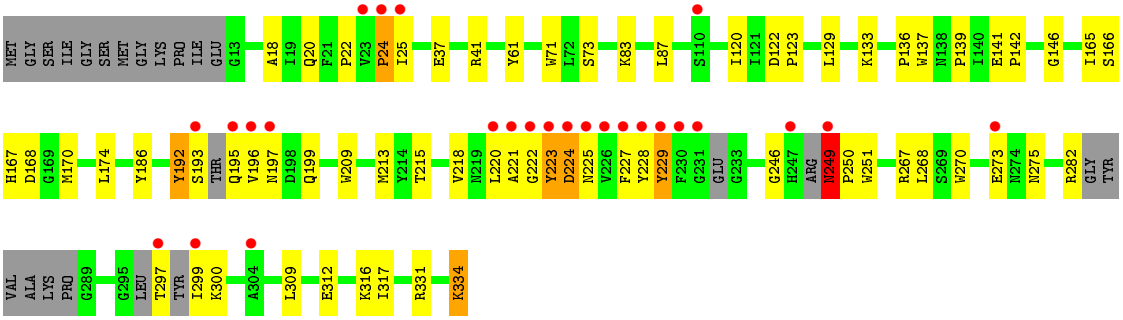
Chain C:





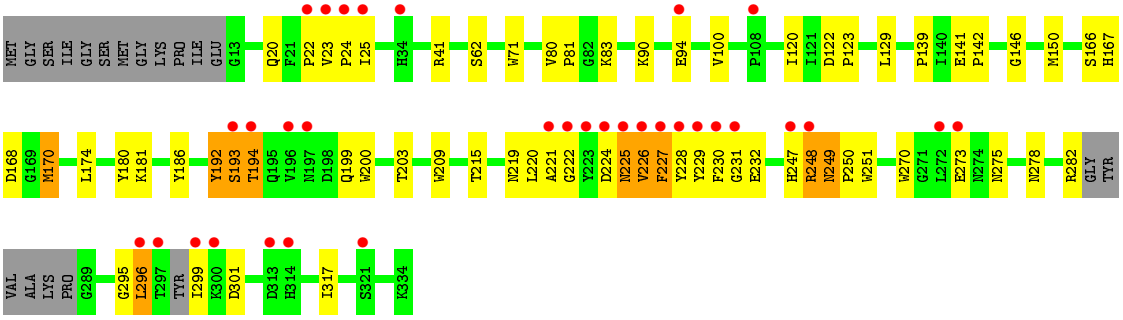
• Molecule 1: Formamidase

Chain D:



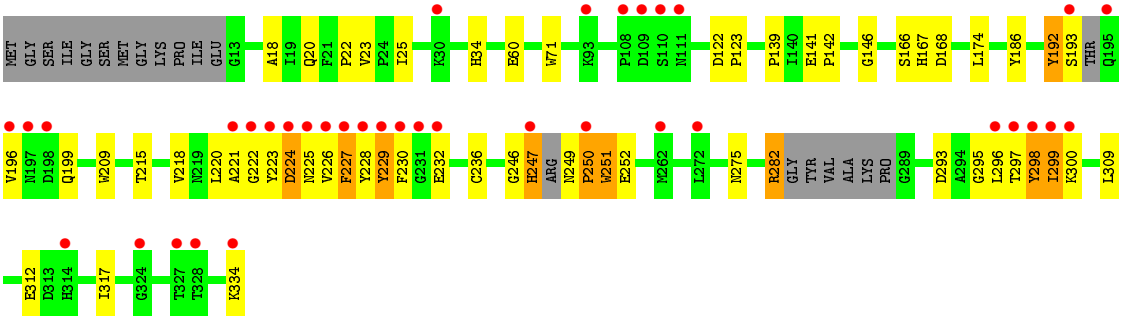
• Molecule 1: Formamidase

Chain E:



• Molecule 1: Formamidase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.72Å 130.53Å 144.59Å 90.00° 99.44° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 26.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.50) 99.8 (26.90-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	13.24 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.256 , 0.294 0.256 , 0.264	Depositor DCC
R_{free} test set	3744 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	13.2	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 74588 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	15744	wwPDB-VP
Average B, all atoms (Å^2)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.26	0/2550	0.46	0/3459
1	B	0.27	0/2553	0.47	0/3465
1	C	0.26	0/2558	0.47	0/3474
1	D	0.27	0/2523	0.46	0/3421
1	E	0.27	0/2562	0.46	0/3480
1	F	0.26	0/2556	0.47	0/3471
All	All	0.27	0/15302	0.46	0/20770

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	249	ASN	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	2482	0	2407	111	0
1	B	2485	0	2417	84	0
1	C	2489	0	2409	101	0
1	D	2458	0	2382	83	0
1	E	2493	0	2423	92	0
1	F	2487	0	2411	75	0
2	A	148	0	0	6	0
2	B	151	0	0	1	0
2	C	133	0	0	6	0
2	D	159	0	0	4	0
2	E	138	0	0	3	0
2	F	121	0	0	0	0
All	All	15744	0	14449	455	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 (455) 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:F:192:TYR:HB3	1:F:193:SER:CA	1.69	1.23
1:E:248:ARG:HD3	1:E:248:ARG:H	1.06	1.20
1:A:192:TYR:CB	1:A:193:SER:HA	1.73	1.18
1:D:192:TYR:HB3	1:D:193:SER:CA	1.76	1.14
1:C:192:TYR:HB3	1:C:193:SER:CA	1.78	1.13
1:E:192:TYR:HB3	1:E:193:SER:CA	1.79	1.13
1:C:227:PHE:CE1	1:C:229:TYR:HB2	1.85	1.11
1:A:224:ASP:N	1:A:225:ASN:HA	1.64	1.10
1:A:192:TYR:HB3	1:A:193:SER:HA	1.11	1.09
1:A:223:TYR:HB3	1:A:227:PHE:CD2	1.87	1.08
1:C:209:TRP:HE1	1:D:170:MET:HE3	1.12	1.08
1:C:192:TYR:HB3	1:C:193:SER:HA	1.34	1.08
1:A:223:TYR:C	1:A:225:ASN:HA	1.74	1.08
1:B:192:TYR:HB3	1:B:193:SER:CA	1.83	1.07
1:A:219:ASN:HB3	1:A:231:GLY:HA2	1.34	1.04
1:F:192:TYR:HB3	1:F:193:SER:HA	1.06	1.02
1:A:223:TYR:HB3	1:A:227:PHE:HD2	1.18	1.02
1:B:192:TYR:HB3	1:B:193:SER:HA	1.35	1.02
1:D:192:TYR:HB3	1:D:193:SER:HA	1.01	1.00
1:E:192:TYR:HB3	1:E:193:SER:HA	1.39	1.00
1:C:248:ARG:HH11	1:C:248:ARG:HG3	0.85	1.00
1:B:222:GLY:HA2	1:B:227:PHE:O	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:TYR:HB3	1:E:193:SER:CB	1.91	0.99
1:C:248:ARG:NH1	1:C:248:ARG:HG3	1.65	0.98
1:F:23:VAL:HG22	1:F:220:LEU:HD23	1.42	0.97
1:E:192:TYR:CB	1:E:193:SER:HB3	1.95	0.97
1:F:192:TYR:CB	1:F:193:SER:HA	1.95	0.97
1:C:248:ARG:CG	1:C:248:ARG:HH11	1.78	0.96
1:C:192:TYR:HB3	1:C:193:SER:CB	1.95	0.96
1:D:249:ASN:ND2	1:F:229:TYR:O	1.98	0.96
1:E:248:ARG:HD3	1:E:248:ARG:N	1.73	0.95
1:A:224:ASP:H	1:A:226:VAL:H	1.11	0.93
1:F:23:VAL:HB	1:F:222:GLY:O	1.69	0.93
1:A:223:TYR:CD2	1:A:227:PHE:HB3	2.04	0.93
1:D:192:TYR:CB	1:D:193:SER:HA	1.96	0.91
1:D:270:TRP:CE3	1:D:273:GLU:HB2	2.06	0.91
1:B:228:TYR:O	1:B:250:PRO:HG3	1.70	0.90
1:A:192:TYR:HB3	1:A:193:SER:CA	2.00	0.90
1:D:221:ALA:HB1	1:D:228:TYR:O	1.73	0.89
1:C:209:TRP:HE1	1:D:170:MET:CE	1.86	0.89
1:C:248:ARG:H	1:E:248:ARG:HH12	0.95	0.89
1:A:225:ASN:HB2	2:A:386:HOH:O	1.73	0.88
1:F:282:ARG:NH1	1:F:293:ASP:O	2.06	0.88
1:B:248:ARG:HB2	1:B:250:PRO:HD3	1.54	0.88
1:B:251:TRP:HB2	1:E:227:PHE:HD1	1.35	0.88
1:F:299:ILE:HG22	1:F:299:ILE:O	1.71	0.87
1:B:222:GLY:CA	1:B:228:TYR:HA	2.04	0.87
1:B:22:PRO:HA	1:B:221:ALA:HB3	1.57	0.87
1:F:22:PRO:HA	1:F:221:ALA:HB3	1.56	0.87
1:E:170:MET:HE2	1:F:209:TRP:HE1	1.40	0.87
1:E:224:ASP:OD1	1:E:227:PHE:HB3	1.74	0.86
1:B:192:TYR:HB3	1:B:193:SER:CB	2.04	0.86
1:A:192:TYR:CB	1:A:193:SER:CA	2.52	0.86
1:A:227:PHE:CZ	1:A:229:TYR:HB2	2.11	0.85
1:B:23:VAL:H	1:B:222:GLY:H	1.24	0.85
1:E:192:TYR:HB3	1:E:193:SER:HB3	1.54	0.85
1:B:23:VAL:HB	1:B:222:GLY:O	1.77	0.84
1:F:221:ALA:O	1:F:229:TYR:N	2.10	0.84
1:B:222:GLY:HA3	1:B:228:TYR:HA	1.60	0.83
1:E:170:MET:HE3	1:E:203:THR:HG21	1.59	0.83
1:A:223:TYR:HD2	1:A:227:PHE:HB3	1.42	0.83
1:A:303:ALA:HB1	1:B:300:LYS:HB3	1.61	0.82
1:B:251:TRP:HB2	1:E:227:PHE:CD1	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:TYR:HB2	1:E:193:SER:HB3	1.61	0.82
1:A:209:TRP:HE1	1:B:170:MET:CE	1.92	0.82
1:B:23:VAL:HB	1:B:222:GLY:C	2.01	0.81
1:C:248:ARG:N	1:E:248:ARG:HH12	1.76	0.81
1:A:224:ASP:N	1:A:225:ASN:CA	2.43	0.80
1:A:167:HIS:HA	1:A:192:TYR:OH	1.80	0.80
1:D:222:GLY:HA3	1:D:228:TYR:HA	1.62	0.80
1:E:20:GLN:NE2	1:E:232:GLU:O	2.15	0.79
1:D:192:TYR:CB	1:D:193:SER:CA	2.56	0.79
1:A:282:ARG:NH2	1:B:146:GLY:O	2.14	0.79
1:C:248:ARG:H	1:E:248:ARG:NH1	1.77	0.78
1:C:209:TRP:NE1	1:D:170:MET:HE3	1.94	0.78
1:A:20:GLN:NE2	1:A:232:GLU:O	2.16	0.78
1:F:227:PHE:N	1:F:227:PHE:CD1	2.50	0.78
1:F:23:VAL:HG22	1:F:220:LEU:CD2	2.13	0.77
1:F:23:VAL:HG23	1:F:222:GLY:H	1.49	0.77
1:F:192:TYR:HB3	1:F:193:SER:CB	2.14	0.77
1:A:223:TYR:H	1:A:226:VAL:N	1.83	0.77
1:B:192:TYR:HB3	1:B:193:SER:HB3	1.65	0.77
1:F:192:TYR:CB	1:F:193:SER:CA	2.58	0.77
1:A:223:TYR:CB	1:A:227:PHE:HD2	1.96	0.77
1:B:192:TYR:CB	1:B:193:SER:HB3	2.14	0.76
1:C:192:TYR:CB	1:C:193:SER:HB3	2.15	0.76
1:A:146:GLY:O	1:B:282:ARG:NH2	2.19	0.76
1:E:200:TRP:CZ3	1:E:232:GLU:HB2	2.21	0.76
1:A:223:TYR:CB	1:A:227:PHE:CD2	2.67	0.76
1:E:194:THR:HG22	1:E:230:PHE:HE1	1.49	0.76
1:F:227:PHE:N	1:F:227:PHE:HD1	1.83	0.75
1:C:282:ARG:NH2	1:D:146:GLY:O	2.18	0.75
1:C:192:TYR:HB3	1:C:193:SER:HB3	1.69	0.74
1:B:23:VAL:HG22	1:B:220:LEU:HD23	1.69	0.74
1:D:133:LYS:HD3	1:D:165:ILE:HB	1.70	0.73
1:C:167:HIS:HE1	1:D:275:ASN:HD22	1.38	0.72
1:E:170:MET:CE	1:F:209:TRP:HE1	2.02	0.71
1:C:194:THR:HG22	1:C:230:PHE:HE1	1.55	0.71
1:C:146:GLY:O	1:D:282:ARG:NH2	2.23	0.71
1:C:22:PRO:O	2:C:455:HOH:O	2.08	0.71
1:D:193:SER:O	1:D:195:GLN:N	2.24	0.71
1:D:249:ASN:CG	1:F:229:TYR:HB2	2.12	0.70
1:F:300:LYS:HG2	1:F:300:LYS:O	1.90	0.70
1:F:298:TYR:O	1:F:299:ILE:HG12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:LYS:H	1:D:334:LYS:HD3	1.56	0.69
1:A:221:ALA:O	2:A:471:HOH:O	2.10	0.69
1:A:209:TRP:HE1	1:B:170:MET:HE3	1.55	0.69
1:C:249:ASN:HA	2:C:452:HOH:O	1.93	0.69
1:A:191:GLY:HA3	1:A:219:ASN:OD1	1.93	0.68
1:A:334:LYS:H	1:A:334:LYS:HD3	1.57	0.68
1:C:248:ARG:HH12	1:E:249:ASN:ND2	1.91	0.68
1:E:219:ASN:HB3	1:E:231:GLY:HA2	1.74	0.68
1:A:190:SER:HB3	1:A:191:GLY:HA3	1.76	0.68
1:A:302:LEU:HG	1:B:296:LEU:HD11	1.76	0.68
1:C:170:MET:CE	1:D:209:TRP:HE1	2.07	0.67
1:D:220:LEU:HG	1:D:221:ALA:H	1.59	0.67
1:D:222:GLY:CA	1:D:228:TYR:HA	2.23	0.67
1:A:295:GLY:HA2	1:A:296:LEU:C	2.14	0.67
1:A:224:ASP:H	1:A:226:VAL:N	1.89	0.67
1:A:224:ASP:N	1:A:226:VAL:H	1.90	0.66
1:C:227:PHE:CD2	1:C:230:PHE:CE2	2.83	0.66
1:A:190:SER:CB	1:A:191:GLY:CA	2.73	0.66
1:E:170:MET:CE	1:E:203:THR:HG21	2.24	0.66
1:B:300:LYS:HB2	1:B:303:ALA:HB3	1.77	0.66
1:C:247:HIS:HB2	2:C:456:HOH:O	1.94	0.66
1:A:228:TYR:O	1:A:250:PRO:HD3	1.96	0.66
1:E:282:ARG:NH2	1:F:146:GLY:O	2.26	0.66
1:C:227:PHE:HD2	1:C:230:PHE:CE2	2.14	0.65
1:F:23:VAL:CG2	1:F:222:GLY:H	2.09	0.65
1:C:231:GLY:O	1:C:248:ARG:HD2	1.96	0.65
1:A:192:TYR:HB2	1:A:193:SER:HA	1.74	0.65
1:A:209:TRP:HE1	1:B:170:MET:HE1	1.61	0.65
1:C:275:ASN:ND2	1:D:167:HIS:HE1	1.95	0.65
1:C:209:TRP:NE1	1:D:170:MET:CE	2.57	0.65
1:B:200:TRP:HZ3	1:B:232:GLU:O	1.80	0.65
1:B:248:ARG:HB2	1:B:250:PRO:CD	2.25	0.64
1:E:224:ASP:OD1	1:E:227:PHE:CB	2.45	0.64
1:F:250:PRO:O	1:F:252:GLU:N	2.28	0.64
1:E:194:THR:HG22	1:E:230:PHE:CE1	2.30	0.64
1:C:170:MET:HE2	1:D:209:TRP:HE1	1.63	0.64
1:A:168:ASP:HB3	1:A:174:LEU:HD23	1.78	0.64
1:C:248:ARG:O	1:E:248:ARG:NH1	2.31	0.63
1:C:135:PHE:O	1:C:167:HIS:HD2	1.82	0.63
1:C:192:TYR:CB	1:C:193:SER:CA	2.66	0.63
1:E:192:TYR:CB	1:E:193:SER:CB	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TRP:CZ3	1:A:232:GLU:HB2	2.34	0.62
1:F:295:GLY:HA2	1:F:297:THR:N	2.13	0.62
1:D:270:TRP:HE3	1:D:273:GLU:HB2	1.63	0.62
1:A:190:SER:CB	1:A:191:GLY:HA3	2.28	0.62
1:E:90:LYS:O	1:E:94:GLU:HG2	1.98	0.62
1:C:167:HIS:HE1	1:D:275:ASN:ND2	1.97	0.62
1:D:25:ILE:N	1:D:25:ILE:HD12	2.16	0.61
1:B:23:VAL:HG22	1:B:220:LEU:CD2	2.30	0.61
1:B:251:TRP:CB	1:E:227:PHE:CD1	2.84	0.61
1:D:167:HIS:HA	1:D:192:TYR:OH	2.01	0.61
1:C:248:ARG:HA	1:C:252:GLU:OE1	1.99	0.60
1:D:250:PRO:O	1:D:251:TRP:HB2	1.99	0.60
1:C:192:TYR:CB	1:C:193:SER:HA	2.21	0.60
1:C:66:LEU:HD13	1:C:223:TYR:HB2	1.84	0.60
1:B:250:PRO:HG2	1:E:229:TYR:CZ	2.36	0.60
1:E:25:ILE:HD11	1:E:225:ASN:H	1.66	0.60
1:C:221:ALA:HA	1:C:230:PHE:H	1.65	0.60
1:A:275:ASN:HD22	1:B:167:HIS:HE1	1.50	0.59
1:C:227:PHE:HD2	1:C:230:PHE:CZ	2.19	0.59
1:D:192:TYR:HB2	1:D:193:SER:HB3	1.83	0.59
1:C:200:TRP:HZ3	1:C:232:GLU:O	1.85	0.59
1:C:249:ASN:HB2	1:C:250:PRO:HD2	1.85	0.59
1:E:248:ARG:N	1:E:248:ARG:CD	2.59	0.59
1:C:219:ASN:HB3	1:C:231:GLY:HA2	1.84	0.59
1:E:227:PHE:CG	1:E:228:TYR:N	2.71	0.58
1:D:270:TRP:CE3	1:D:273:GLU:CB	2.82	0.58
1:E:22:PRO:HA	1:E:221:ALA:HB3	1.85	0.58
1:B:167:HIS:HA	1:B:192:TYR:OH	2.04	0.58
1:F:295:GLY:N	1:F:296:LEU:HB2	2.18	0.58
1:A:229:TYR:HH	1:D:229:TYR:HE1	1.51	0.58
1:E:225:ASN:O	1:E:226:VAL:HB	2.04	0.58
1:A:228:TYR:HB2	1:A:250:PRO:HG3	1.85	0.57
1:C:248:ARG:HH12	1:E:249:ASN:HD21	1.51	0.57
1:C:248:ARG:CG	1:C:248:ARG:NH1	2.48	0.57
1:B:248:ARG:HH22	1:C:247:HIS:CG	2.23	0.57
1:F:299:ILE:CG2	1:F:299:ILE:O	2.45	0.57
1:E:275:ASN:ND2	1:F:167:HIS:HE1	2.03	0.57
1:C:192:TYR:HB2	1:C:193:SER:HB3	1.85	0.57
1:B:192:TYR:HB2	1:B:193:SER:HB3	1.85	0.57
1:F:221:ALA:O	1:F:228:TYR:C	2.42	0.57
1:B:23:VAL:HG22	1:B:220:LEU:CG	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:TYR:HB3	1:D:193:SER:CB	2.36	0.56
1:A:219:ASN:HB3	1:A:231:GLY:CA	2.22	0.56
1:D:224:ASP:O	1:D:225:ASN:HB2	2.05	0.56
1:F:223:TYR:CD1	1:F:224:ASP:HB2	2.40	0.56
1:A:295:GLY:N	1:A:296:LEU:HG	2.21	0.56
1:B:248:ARG:HH22	1:C:247:HIS:CE1	2.23	0.56
1:B:60:GLU:O	1:B:220:LEU:HD22	2.06	0.56
1:C:23:VAL:HG12	1:C:222:GLY:O	2.06	0.56
1:B:192:TYR:CB	1:B:193:SER:CA	2.70	0.56
1:D:20:GLN:HE22	1:D:246:GLY:HA3	1.70	0.55
1:C:193:SER:OG	1:C:194:THR:N	2.38	0.55
1:A:227:PHE:CG	1:F:251:TRP:HB2	2.40	0.55
1:D:168:ASP:HB3	1:D:174:LEU:HD23	1.89	0.55
1:A:209:TRP:NE1	1:B:170:MET:CE	2.67	0.55
1:E:167:HIS:CE1	1:F:275:ASN:HD22	2.25	0.55
1:E:228:TYR:O	1:E:250:PRO:HD3	2.07	0.55
1:A:227:PHE:CE1	1:A:229:TYR:HB2	2.42	0.55
1:A:167:HIS:HE1	1:B:275:ASN:ND2	2.05	0.55
1:A:220:LEU:O	1:A:231:GLY:N	2.37	0.55
1:E:170:MET:HE3	1:E:170:MET:HA	1.89	0.55
1:A:200:TRP:HZ3	1:A:232:GLU:HB2	1.71	0.55
1:E:275:ASN:HD22	1:F:167:HIS:HE1	1.55	0.55
1:C:229:TYR:CD1	1:C:250:PRO:HD3	2.42	0.55
1:E:222:GLY:HA2	1:E:227:PHE:CE2	2.41	0.55
1:E:167:HIS:HE1	1:F:275:ASN:ND2	2.05	0.55
1:E:227:PHE:CD1	1:E:229:TYR:HD2	2.24	0.55
1:F:249:ASN:HB2	1:F:250:PRO:HD2	1.88	0.55
1:E:167:HIS:CE1	1:F:275:ASN:ND2	2.75	0.55
1:B:152:VAL:HG12	1:B:160:LYS:HD2	1.88	0.54
1:A:251:TRP:HB2	1:D:227:PHE:CD1	2.42	0.54
1:A:60:GLU:N	1:A:190:SER:O	2.39	0.54
1:D:18:ALA:HB1	1:D:218:VAL:HB	1.89	0.54
1:B:132:ARG:HD2	1:B:148:LEU:HG	1.90	0.54
1:A:248:ARG:HD2	1:F:247:HIS:CE1	2.42	0.54
1:F:247:HIS:N	1:F:247:HIS:CD2	2.76	0.54
1:E:170:MET:SD	2:E:340:HOH:O	2.58	0.54
1:A:221:ALA:HA	1:A:230:PHE:HB2	1.90	0.54
1:C:20:GLN:HE22	1:C:246:GLY:HA3	1.73	0.54
1:E:295:GLY:N	1:E:296:LEU:HB2	2.23	0.54
1:B:222:GLY:HA2	1:B:228:TYR:HA	1.87	0.53
1:A:209:TRP:CD2	1:B:199:GLN:HG2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:HIS:CE1	1:D:275:ASN:ND2	2.76	0.53
1:C:248:ARG:O	1:C:249:ASN:HB3	2.09	0.53
1:D:192:TYR:CB	1:D:193:SER:CB	2.87	0.53
1:A:199:GLN:HG2	1:B:209:TRP:CD2	2.44	0.53
1:C:227:PHE:HB2	1:E:251:TRP:HB3	1.90	0.52
1:A:224:ASP:HA	2:A:477:HOH:O	2.09	0.52
1:D:299:ILE:HG13	1:D:300:LYS:N	2.24	0.52
1:D:249:ASN:HB3	1:F:229:TYR:CG	2.44	0.52
1:C:223:TYR:HE2	1:C:230:PHE:CE2	2.26	0.52
1:C:24:PRO:HD3	2:C:455:HOH:O	2.08	0.52
1:D:122:ASP:HB2	1:D:123:PRO:CD	2.39	0.52
1:A:227:PHE:O	1:A:229:TYR:N	2.41	0.52
1:A:229:TYR:OH	1:D:229:TYR:CE1	2.62	0.52
1:F:186:TYR:HB3	1:F:215:THR:HG22	1.91	0.52
1:F:168:ASP:HB3	1:F:174:LEU:HD23	1.91	0.52
1:A:196:VAL:HG13	1:A:196:VAL:O	2.09	0.52
1:B:23:VAL:HG23	1:B:222:GLY:N	2.25	0.52
1:A:275:ASN:ND2	1:B:167:HIS:HE1	2.07	0.51
1:C:170:MET:CE	1:D:209:TRP:NE1	2.73	0.51
1:F:228:TYR:O	1:F:250:PRO:HG3	2.10	0.51
1:D:24:PRO:HA	1:D:228:TYR:HE1	1.76	0.51
1:E:167:HIS:HE1	1:F:275:ASN:HD22	1.57	0.51
1:A:122:ASP:HB2	1:A:123:PRO:CD	2.41	0.51
1:E:250:PRO:O	1:E:251:TRP:HB2	2.11	0.50
1:B:200:TRP:CZ3	1:B:232:GLU:O	2.63	0.50
1:E:25:ILE:N	1:E:25:ILE:HD12	2.26	0.50
1:C:249:ASN:OD1	1:C:252:GLU:HB2	2.11	0.50
1:A:23:VAL:HG21	1:A:65:GLY:HA2	1.94	0.50
1:C:168:ASP:HB3	1:C:174:LEU:HD23	1.94	0.50
1:B:227:PHE:CZ	1:C:252:GLU:HA	2.46	0.50
1:E:209:TRP:CD2	1:F:199:GLN:HG2	2.46	0.50
1:A:229:TYR:OH	1:D:229:TYR:HE1	1.94	0.50
1:F:229:TYR:HB3	1:F:249:ASN:HA	1.93	0.50
1:B:221:ALA:O	1:B:229:TYR:N	2.45	0.49
1:C:20:GLN:NE2	1:C:233:GLY:H	2.10	0.49
1:F:221:ALA:O	1:F:229:TYR:CA	2.60	0.49
1:D:249:ASN:HB3	1:F:229:TYR:CD2	2.47	0.49
1:D:192:TYR:CB	1:D:193:SER:HB3	2.43	0.49
1:C:199:GLN:HG2	1:D:209:TRP:CD2	2.48	0.49
1:F:192:TYR:HB3	1:F:193:SER:HB3	1.93	0.49
1:C:227:PHE:CZ	1:C:229:TYR:HB2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HB2	1:A:312:GLU:HG3	1.94	0.49
1:C:82:GLY:O	1:C:86:GLU:HG2	2.13	0.49
1:C:229:TYR:CD1	1:E:249:ASN:OD1	2.65	0.49
1:E:249:ASN:N	1:E:249:ASN:ND2	2.61	0.49
1:F:18:ALA:HB1	1:F:218:VAL:HB	1.95	0.49
1:C:272:LEU:O	1:D:137:TRP:NE1	2.45	0.49
1:B:135:PHE:O	1:B:167:HIS:HD2	1.95	0.49
1:D:25:ILE:N	1:D:25:ILE:CD1	2.76	0.49
1:A:209:TRP:NE1	1:B:170:MET:HE1	2.26	0.48
1:B:192:TYR:CB	1:B:193:SER:HA	2.23	0.48
1:B:224:ASP:OD1	1:B:225:ASN:N	2.37	0.48
1:A:18:ALA:HB1	1:A:218:VAL:HB	1.94	0.48
1:B:222:GLY:HA3	1:B:228:TYR:CD1	2.49	0.48
1:E:222:GLY:CA	1:E:228:TYR:HA	2.44	0.48
1:B:282:ARG:HG3	2:B:358:HOH:O	2.14	0.48
1:C:273:GLU:N	1:C:273:GLU:OE1	2.47	0.48
1:C:248:ARG:HH22	1:E:249:ASN:ND2	2.12	0.48
1:A:223:TYR:N	1:A:227:PHE:H	2.12	0.48
1:E:146:GLY:O	1:F:282:ARG:NH2	2.47	0.48
1:C:282:ARG:HG2	2:C:338:HOH:O	2.14	0.48
1:E:295:GLY:N	1:E:296:LEU:CB	2.77	0.48
1:A:120:ILE:HD12	1:A:129:LEU:HD13	1.96	0.48
1:A:192:TYR:HB2	1:A:193:SER:CA	2.38	0.47
1:A:250:PRO:O	1:A:251:TRP:HB2	2.14	0.47
1:D:273:GLU:HA	2:D:411:HOH:O	2.13	0.47
1:A:167:HIS:HE1	1:B:275:ASN:HD22	1.63	0.47
1:C:170:MET:HE2	1:D:209:TRP:NE1	2.29	0.47
1:C:66:LEU:HD13	1:C:223:TYR:CB	2.44	0.47
1:A:224:ASP:HB3	1:A:226:VAL:HG12	1.95	0.47
1:E:194:THR:O	1:E:194:THR:HG23	2.14	0.47
1:B:20:GLN:NE2	1:B:233:GLY:H	2.12	0.47
1:E:23:VAL:CG2	1:E:62:SER:HA	2.44	0.47
1:B:295:GLY:N	1:B:296:LEU:HB2	2.30	0.47
1:F:221:ALA:O	1:F:230:PHE:N	2.48	0.47
1:D:331:ARG:HG3	1:D:334:LYS:HD2	1.96	0.47
1:A:296:LEU:N	2:A:465:HOH:O	2.47	0.47
1:C:200:TRP:CZ3	1:C:232:GLU:O	2.68	0.47
1:D:197:ASN:OD1	2:D:357:HOH:O	2.20	0.47
1:C:100:VAL:HG22	1:C:120:ILE:HG12	1.97	0.47
1:C:20:GLN:NE2	1:C:246:GLY:HA3	2.30	0.47
1:F:25:ILE:CD1	1:F:225:ASN:HB2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:TYR:HB3	1:D:215:THR:HG22	1.95	0.47
1:B:221:ALA:O	1:B:230:PHE:HD2	1.97	0.47
1:C:222:GLY:CA	1:C:228:TYR:HA	2.45	0.47
1:A:282:ARG:HG3	2:A:369:HOH:O	2.15	0.47
1:D:61:TYR:HB2	1:D:220:LEU:HD22	1.95	0.47
1:E:180:TYR:HE2	1:F:299:ILE:HD12	1.80	0.47
1:C:37:GLU:O	1:C:41:ARG:HG3	2.15	0.47
1:D:120:ILE:HD12	1:D:129:LEU:HD13	1.97	0.47
1:E:180:TYR:CE2	1:F:299:ILE:HD12	2.50	0.46
1:F:298:TYR:O	1:F:299:ILE:CG1	2.62	0.46
1:C:299:ILE:HG23	2:D:474:HOH:O	2.15	0.46
1:D:73:SER:HA	1:D:334:LYS:HA	1.98	0.46
1:B:250:PRO:O	1:E:229:TYR:CD2	2.69	0.46
1:B:309:LEU:HB2	1:B:312:GLU:HG3	1.97	0.46
1:F:192:TYR:CB	1:F:193:SER:HB3	2.45	0.46
1:A:224:ASP:CB	1:A:226:VAL:HG12	2.46	0.46
1:F:25:ILE:HD12	1:F:225:ASN:HB2	1.98	0.46
1:E:139:PRO:HG3	1:E:317:ILE:HG21	1.97	0.46
1:B:248:ARG:NH2	1:C:247:HIS:CE1	2.84	0.46
1:C:20:GLN:HE21	1:C:233:GLY:H	1.64	0.46
1:F:122:ASP:HB2	1:F:123:PRO:CD	2.46	0.46
1:B:23:VAL:HG22	1:B:220:LEU:HG	1.97	0.46
1:C:194:THR:HG22	1:C:230:PHE:CE1	2.42	0.46
1:A:252:GLU:HA	1:D:227:PHE:CZ	2.50	0.46
1:A:228:TYR:O	1:A:250:PRO:HG3	2.15	0.46
1:E:25:ILE:CD1	1:E:25:ILE:N	2.78	0.46
1:C:298:TYR:CE2	1:C:299:ILE:HD12	2.50	0.46
1:F:139:PRO:HG3	1:F:317:ILE:HG21	1.98	0.46
1:B:59:PRO:HB2	1:B:220:LEU:HD13	1.98	0.45
1:F:229:TYR:N	1:F:229:TYR:CD2	2.83	0.45
1:C:19:ILE:HG13	1:C:253:ILE:HG12	1.98	0.45
1:D:133:LYS:HE3	1:D:136:PRO:HA	1.99	0.45
1:A:223:TYR:HB3	1:A:227:PHE:CG	2.46	0.45
1:B:89:ALA:HA	1:B:121:ILE:HG21	1.98	0.45
1:B:227:PHE:CE2	1:B:230:PHE:CZ	3.05	0.45
1:C:23:VAL:HG12	1:C:220:LEU:HD21	1.98	0.45
1:A:227:PHE:HZ	1:F:252:GLU:HG3	1.82	0.45
1:B:221:ALA:O	1:B:230:PHE:CD2	2.70	0.45
1:C:122:ASP:HB2	1:C:123:PRO:CD	2.46	0.45
1:D:213:MET:HB3	1:D:267:ARG:NH2	2.32	0.45
1:E:299:ILE:HB	1:E:301:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TYR:CG	1:A:224:ASP:N	2.85	0.45
1:C:170:MET:HE3	1:D:209:TRP:HE1	1.78	0.45
1:D:37:GLU:O	1:D:41:ARG:HG3	2.17	0.45
1:E:150:MET:O	1:E:181:LYS:NZ	2.48	0.45
1:C:223:TYR:HE2	1:C:230:PHE:CZ	2.34	0.45
1:E:222:GLY:HA3	1:E:228:TYR:HA	1.99	0.45
1:A:224:ASP:N	1:A:226:VAL:N	2.57	0.45
1:A:190:SER:HB3	1:A:219:ASN:HA	1.99	0.45
1:F:215:THR:OG1	1:F:236:CYS:HB2	2.17	0.45
1:A:23:VAL:O	1:A:23:VAL:HG13	2.16	0.45
1:A:195:GLN:HG2	2:A:365:HOH:O	2.16	0.45
1:C:250:PRO:O	1:C:251:TRP:HB2	2.17	0.44
1:A:251:TRP:HB3	1:D:227:PHE:CG	2.52	0.44
1:D:229:TYR:CD2	1:D:229:TYR:N	2.85	0.44
1:F:23:VAL:HB	1:F:222:GLY:C	2.35	0.44
1:E:199:GLN:HG2	1:F:209:TRP:CD2	2.53	0.44
1:F:227:PHE:H	1:F:227:PHE:HD1	1.43	0.44
1:E:168:ASP:HB3	1:E:174:LEU:HD23	1.98	0.44
1:A:209:TRP:NE1	1:B:170:MET:HE3	2.30	0.44
1:B:96:LYS:HD3	1:B:123:PRO:HB3	1.99	0.44
1:E:186:TYR:HB3	1:E:215:THR:HG22	1.99	0.44
1:D:297:THR:HA	2:D:490:HOH:O	2.17	0.44
1:A:227:PHE:CE1	1:A:229:TYR:CD2	3.06	0.44
1:A:250:PRO:HG2	1:D:229:TYR:CE2	2.53	0.44
1:B:122:ASP:HB2	1:B:123:PRO:CD	2.47	0.44
1:B:273:GLU:N	1:B:273:GLU:OE1	2.51	0.44
1:D:309:LEU:HB2	1:D:312:GLU:HG3	2.00	0.44
1:C:228:TYR:O	1:C:250:PRO:HD3	2.18	0.43
1:B:251:TRP:CD1	1:E:227:PHE:HB2	2.53	0.43
1:A:275:ASN:ND2	1:B:167:HIS:CE1	2.86	0.43
1:E:23:VAL:HG21	1:E:62:SER:HA	2.00	0.43
1:A:192:TYR:CG	1:A:196:VAL:HG11	2.53	0.43
1:E:226:VAL:O	1:E:226:VAL:HG22	2.18	0.43
1:C:311:TRP:HB2	1:D:268:LEU:HD21	1.99	0.43
1:E:120:ILE:HD12	1:E:129:LEU:HD13	2.00	0.43
1:A:228:TYR:O	1:A:250:PRO:CD	2.63	0.43
1:D:25:ILE:HG12	1:D:225:ASN:HA	2.01	0.43
1:E:296:LEU:HD21	2:E:393:HOH:O	2.18	0.43
1:D:83:LYS:O	1:D:87:LEU:HG	2.19	0.43
1:B:295:GLY:HA2	1:B:296:LEU:C	2.39	0.43
1:A:213:MET:HB3	1:A:267:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:VAL:HG22	1:E:120:ILE:HG12	2.00	0.43
1:F:295:GLY:HA2	1:F:296:LEU:C	2.39	0.43
1:E:23:VAL:HG12	1:E:24:PRO:O	2.19	0.43
1:A:60:GLU:O	1:A:61:TYR:HB2	2.18	0.43
1:B:80:VAL:HA	1:B:81:PRO:HA	1.89	0.43
1:B:247:HIS:HB2	1:E:248:ARG:HG3	2.00	0.43
1:C:215:THR:OG1	1:C:236:CYS:HB2	2.19	0.43
1:B:228:TYR:O	1:B:250:PRO:CG	2.57	0.42
1:B:18:ALA:HB1	1:B:218:VAL:HB	2.01	0.42
1:C:245:GLN:O	1:C:247:HIS:CD2	2.72	0.42
1:A:225:ASN:HB3	1:A:230:PHE:HE2	1.84	0.42
1:C:222:GLY:HA2	1:C:228:TYR:HA	2.01	0.42
1:A:251:TRP:CB	1:D:227:PHE:CD1	3.02	0.42
1:E:232:GLU:HA	1:E:247:HIS:O	2.20	0.42
1:E:80:VAL:HA	1:E:81:PRO:HA	1.90	0.42
1:D:22:PRO:HB3	1:D:250:PRO:HB2	2.02	0.42
1:C:248:ARG:O	1:C:249:ASN:CB	2.68	0.42
1:A:167:HIS:CE1	1:B:275:ASN:ND2	2.87	0.42
1:E:275:ASN:ND2	1:F:167:HIS:CE1	2.86	0.42
1:F:309:LEU:HB2	1:F:312:GLU:HG3	2.02	0.42
1:A:107:ASN:HA	1:A:108:PRO:HD2	1.86	0.42
1:B:73:SER:O	1:B:77:LEU:HG	2.20	0.42
1:A:228:TYR:O	1:A:250:PRO:CG	2.68	0.42
1:E:122:ASP:HB2	1:E:123:PRO:CD	2.49	0.42
1:D:122:ASP:HB2	1:D:123:PRO:HD2	2.02	0.42
1:F:141:GLU:HA	1:F:142:PRO:HD3	1.89	0.42
1:A:190:SER:OG	1:A:191:GLY:HA2	2.20	0.41
1:A:222:GLY:CA	1:A:227:PHE:O	2.68	0.41
1:F:249:ASN:O	1:F:250:PRO:O	2.38	0.41
1:F:20:GLN:HE22	1:F:246:GLY:HA3	1.84	0.41
1:B:213:MET:HB3	1:B:267:ARG:NH2	2.35	0.41
1:A:227:PHE:CE1	1:A:229:TYR:HD2	2.38	0.41
1:D:249:ASN:N	1:D:249:ASN:OD1	2.54	0.41
1:C:209:TRP:CD2	1:D:199:GLN:HG2	2.55	0.41
1:C:195:GLN:HG2	2:C:405:HOH:O	2.20	0.41
1:D:141:GLU:HA	1:D:142:PRO:HD3	1.75	0.41
1:E:227:PHE:CD2	1:E:228:TYR:N	2.86	0.41
1:A:223:TYR:H	1:A:226:VAL:H	1.64	0.41
1:E:141:GLU:HA	1:E:142:PRO:HD3	1.80	0.41
1:E:270:TRP:CE3	1:E:273:GLU:HB2	2.56	0.41
1:B:251:TRP:CG	1:E:227:PHE:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ARG:NH1	1:E:249:ASN:ND2	2.63	0.41
1:A:248:ARG:CZ	1:F:247:HIS:HB2	2.50	0.41
1:E:249:ASN:HD22	1:E:249:ASN:N	2.18	0.41
1:E:247:HIS:CD2	2:E:446:HOH:O	2.74	0.41
1:F:60:GLU:O	1:F:220:LEU:HD22	2.21	0.41
1:C:224:ASP:O	1:C:225:ASN:HB2	2.20	0.41
1:F:22:PRO:HG3	1:F:250:PRO:HB3	2.03	0.41
1:A:282:ARG:HD2	1:A:294:ALA:HA	2.02	0.41
1:E:275:ASN:HA	1:E:278:ASN:HD22	1.86	0.41
1:C:141:GLU:HA	1:C:142:PRO:HD3	1.89	0.41
1:C:213:MET:HB3	1:C:267:ARG:NH2	2.36	0.41
1:A:228:TYR:O	1:A:229:TYR:CG	2.74	0.41
1:A:122:ASP:HB2	1:A:123:PRO:HD2	2.02	0.41
1:D:196:VAL:O	1:D:196:VAL:HG13	2.21	0.41
1:A:215:THR:OG1	1:A:236:CYS:HB2	2.21	0.41
1:A:168:ASP:HB3	1:A:174:LEU:CD2	2.47	0.40
1:C:275:ASN:HD22	1:D:167:HIS:HE1	1.64	0.40
1:D:133:LYS:HB2	1:D:165:ILE:HD12	2.03	0.40
1:A:295:GLY:HA2	1:A:296:LEU:O	2.20	0.40
1:F:122:ASP:HB2	1:F:123:PRO:HD2	2.04	0.40
1:C:248:ARG:CA	1:C:252:GLU:OE1	2.69	0.40
1:B:139:PRO:HG3	1:B:317:ILE:HG21	2.04	0.40
1:D:139:PRO:HG3	1:D:317:ILE:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	303/334 (91%)	282 (93%)	19 (6%)	2 (1%)	26 46
1	B	306/334 (92%)	282 (92%)	18 (6%)	6 (2%)	9 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	306/334 (92%)	287 (94%)	12 (4%)	7 (2%)	8 12
1	D	298/334 (89%)	278 (93%)	16 (5%)	4 (1%)	15 26
1	E	309/334 (92%)	281 (91%)	22 (7%)	6 (2%)	10 16
1	F	306/334 (92%)	278 (91%)	22 (7%)	6 (2%)	9 15
All	All	1828/2004 (91%)	1688 (92%)	109 (6%)	31 (2%)	11 19

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	194	THR
1	C	194	THR
1	E	194	THR
1	E	226	VAL
1	F	250	PRO
1	F	251	TRP
1	F	299	ILE
1	C	166	SER
1	C	192	TYR
1	D	166	SER
1	D	192	TYR
1	D	223	TYR
1	F	192	TYR
1	A	166	SER
1	A	228	TYR
1	B	166	SER
1	B	226	VAL
1	C	223	TYR
1	E	166	SER
1	E	193	SER
1	F	166	SER
1	F	224	ASP
1	B	192	TYR
1	C	232	GLU
1	E	192	TYR
1	E	220	LEU
1	B	193	SER
1	C	193	SER
1	B	295	GLY
1	C	249	ASN
1	D	24	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/277 (94%)	247 (95%)	14 (5%)	27	49
1	B	262/277 (95%)	252 (96%)	10 (4%)	40	67
1	C	262/277 (95%)	254 (97%)	8 (3%)	47	75
1	D	259/277 (94%)	252 (97%)	7 (3%)	52	79
1	E	263/277 (95%)	254 (97%)	9 (3%)	44	72
1	F	262/277 (95%)	251 (96%)	11 (4%)	36	62
All	All	1569/1662 (94%)	1510 (96%)	59 (4%)	40	67

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	71	TRP
1	A	163	VAL
1	A	190	SER
1	A	196	VAL
1	A	197	ASN
1	A	223	TYR
1	A	227	PHE
1	A	228	TYR
1	A	230	PHE
1	A	248	ARG
1	A	296	LEU
1	A	300	LYS
1	A	334	LYS
1	B	71	TRP
1	B	94	GLU
1	B	96	LYS
1	B	223	TYR
1	B	229	TYR
1	B	248	ARG
1	B	252	GLU
1	B	299	ILE

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Mol	Chain	Res	Type
1	B	306	LYS
1	B	334	LYS
1	C	25	ILE
1	C	71	TRP
1	C	224	ASP
1	C	248	ARG
1	C	282	ARG
1	C	297	THR
1	C	299	ILE
1	C	334	LYS
1	D	71	TRP
1	D	223	TYR
1	D	224	ASP
1	D	229	TYR
1	D	249	ASN
1	D	316	LYS
1	D	334	LYS
1	E	41	ARG
1	E	71	TRP
1	E	83	LYS
1	E	170	MET
1	E	225	ASN
1	E	227	PHE
1	E	248	ARG
1	E	249	ASN
1	E	296	LEU
1	F	34	HIS
1	F	71	TRP
1	F	196	VAL
1	F	226	VAL
1	F	227	PHE
1	F	229	TYR
1	F	232	GLU
1	F	247	HIS
1	F	282	ARG
1	F	298	TYR
1	F	334	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS

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Mol	Chain	Res	Type
1	A	197	ASN
1	A	210	HIS
1	A	275	ASN
1	A	278	ASN
1	A	292	HIS
1	B	20	GLN
1	B	167	HIS
1	B	210	HIS
1	B	225	ASN
1	B	275	ASN
1	B	278	ASN
1	C	20	GLN
1	C	167	HIS
1	C	210	HIS
1	C	247	HIS
1	C	275	ASN
1	C	278	ASN
1	C	281	HIS
1	C	292	HIS
1	D	20	GLN
1	D	35	ASN
1	D	167	HIS
1	D	197	ASN
1	D	210	HIS
1	D	247	HIS
1	D	275	ASN
1	D	278	ASN
1	D	281	HIS
1	E	20	GLN
1	E	167	HIS
1	E	195	GLN
1	E	210	HIS
1	E	225	ASN
1	E	249	ASN
1	E	275	ASN
1	E	278	ASN
1	F	20	GLN
1	F	167	HIS
1	F	210	HIS
1	F	247	HIS
1	F	275	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	313/334 (93%)	0.53	27 (8%)	13	14	2, 8, 20, 28	0
1	B	314/334 (94%)	0.48	26 (8%)	14	15	3, 8, 18, 25	0
1	C	314/334 (94%)	0.41	25 (7%)	15	16	2, 7, 15, 24	0
1	D	311/334 (93%)	0.47	26 (8%)	14	14	2, 7, 17, 28	0
1	E	315/334 (94%)	0.66	33 (10%)	8	8	3, 10, 21, 29	0
1	F	314/334 (94%)	0.66	37 (11%)	6	6	4, 10, 21, 26	0
All	All	1881/2004 (93%)	0.53	174 (9%)	11	11	2, 8, 20, 29	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	222	GLY	13.9
1	A	222	GLY	12.8
1	B	222	GLY	12.1
1	E	228	TYR	11.1
1	F	222	GLY	10.8
1	A	221	ALA	10.8
1	F	228	TYR	10.8
1	F	225	ASN	10.7
1	F	229	TYR	10.4
1	D	221	ALA	10.3
1	B	228	TYR	10.2
1	E	221	ALA	10.2
1	E	229	TYR	10.1
1	A	229	TYR	9.7
1	A	225	ASN	9.6
1	A	228	TYR	9.6
1	E	227	PHE	9.5
1	E	296	LEU	9.4
1	D	222	GLY	9.3

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Mol	Chain	Res	Type	RSRZ
1	D	226	VAL	9.2
1	C	229	TYR	9.2
1	C	225	ASN	9.0
1	B	229	TYR	8.9
1	C	228	TYR	8.7
1	B	297	THR	8.7
1	B	226	VAL	8.7
1	D	227	PHE	8.4
1	D	229	TYR	8.4
1	E	226	VAL	8.3
1	A	297	THR	8.3
1	E	297	THR	8.2
1	F	221	ALA	8.2
1	B	296	LEU	8.1
1	E	299	ILE	8.1
1	D	225	ASN	8.1
1	B	225	ASN	7.8
1	A	24	PRO	7.7
1	B	223	TYR	7.7
1	F	296	LEU	7.7
1	B	299	ILE	7.5
1	F	226	VAL	7.5
1	D	228	TYR	7.4
1	F	297	THR	7.4
1	B	227	PHE	7.4
1	A	227	PHE	7.3
1	A	296	LEU	6.9
1	B	221	ALA	6.9
1	A	230	PHE	6.8
1	E	24	PRO	6.5
1	F	298	TYR	6.4
1	C	24	PRO	6.4
1	A	223	TYR	6.4
1	C	223	TYR	6.4
1	E	225	ASN	6.4
1	D	193	SER	6.4
1	A	298	TYR	6.3
1	C	248	ARG	6.3
1	D	24	PRO	6.1
1	A	193	SER	6.1
1	C	222	GLY	6.0
1	C	297	THR	5.9

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Mol	Chain	Res	Type	RSRZ
1	D	249	ASN	5.7
1	C	227	PHE	5.6
1	D	223	TYR	5.6
1	B	193	SER	5.5
1	E	231	GLY	5.4
1	B	196	VAL	5.3
1	C	193	SER	5.2
1	D	230	PHE	5.2
1	E	23	VAL	5.1
1	B	230	PHE	5.0
1	F	227	PHE	5.0
1	E	223	TYR	5.0
1	F	223	TYR	4.9
1	E	193	SER	4.9
1	A	226	VAL	4.8
1	B	194	THR	4.8
1	D	297	THR	4.8
1	C	25	ILE	4.7
1	F	197	ASN	4.7
1	A	197	ASN	4.7
1	F	247	HIS	4.7
1	D	197	ASN	4.6
1	C	197	ASN	4.5
1	F	231	GLY	4.5
1	C	249	ASN	4.5
1	C	194	THR	4.4
1	C	23	VAL	4.3
1	D	247	HIS	4.2
1	F	300	LYS	4.2
1	E	230	PHE	4.2
1	F	230	PHE	4.1
1	D	196	VAL	4.1
1	E	194	THR	4.1
1	C	224	ASP	4.1
1	A	224	ASP	4.0
1	F	193	SER	4.0
1	C	230	PHE	4.0
1	B	300	LYS	3.9
1	D	231	GLY	3.9
1	A	196	VAL	3.9
1	F	232	GLU	3.8
1	B	197	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	23	VAL	3.7
1	F	196	VAL	3.5
1	A	328	THR	3.5
1	C	221	ALA	3.5
1	B	248	ARG	3.4
1	E	321	SER	3.3
1	A	314	HIS	3.3
1	D	224	ASP	3.3
1	E	197	ASN	3.3
1	F	110	SER	3.1
1	F	299	ILE	3.1
1	C	231	GLY	3.0
1	E	196	VAL	3.0
1	F	111	ASN	3.0
1	E	224	ASP	2.9
1	A	25	ILE	2.9
1	C	314	HIS	2.9
1	C	196	VAL	2.8
1	D	195	GLN	2.8
1	E	247	HIS	2.8
1	D	299	ILE	2.8
1	B	327	THR	2.8
1	A	190	SER	2.8
1	F	224	ASP	2.8
1	F	327	THR	2.8
1	F	195	GLN	2.7
1	E	25	ILE	2.7
1	E	108	PRO	2.7
1	C	313	ASP	2.6
1	E	313	ASP	2.6
1	F	30	LYS	2.6
1	A	195	GLN	2.6
1	C	247	HIS	2.6
1	B	25	ILE	2.6
1	A	248	ARG	2.6
1	D	25	ILE	2.5
1	B	34	HIS	2.4
1	B	328	THR	2.4
1	F	198	ASP	2.4
1	F	262	MET	2.3
1	F	334	LYS	2.3
1	D	273	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	41	ARG	2.3
1	D	110	SER	2.3
1	D	220	LEU	2.3
1	C	124	GLN	2.2
1	F	314	HIS	2.2
1	F	324	GLY	2.2
1	B	325	TYR	2.2
1	F	109	ASP	2.2
1	E	272	LEU	2.2
1	A	231	GLY	2.1
1	E	94	GLU	2.1
1	B	250	PRO	2.1
1	E	22	PRO	2.1
1	F	108	PRO	2.1
1	F	250	PRO	2.1
1	D	23	VAL	2.1
1	A	250	PRO	2.1
1	A	192	TYR	2.1
1	F	272	LEU	2.1
1	F	93	LYS	2.1
1	B	195	GLN	2.1
1	E	314	HIS	2.1
1	E	248	ARG	2.0
1	E	273	GLU	2.0
1	E	300	LYS	2.0
1	D	304	ALA	2.0
1	E	34	HIS	2.0
1	C	192	TYR	2.0
1	F	328	THR	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.