Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:27 AM GMT

PDB ID	:	3M2L
Title	:	Crystal structure of the M113F mutant of alpha-hemolysin
Authors	:	Montoya, M.; Gouaux, E.
Deposited on	:	2010-03-07
Resolution	:	2.10 Å(reported)

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

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

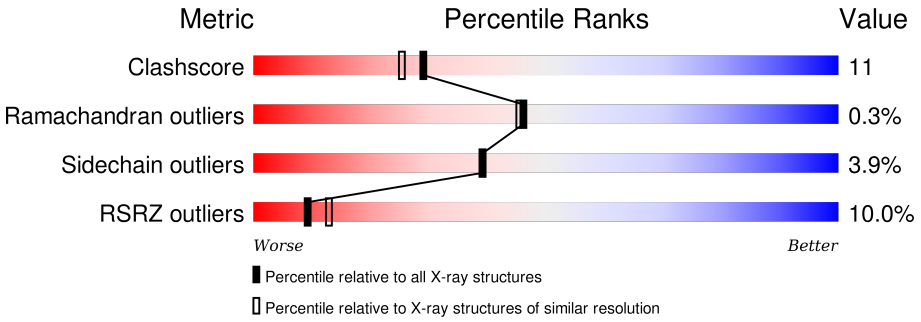
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	294	15% 79% 18% ·
1	B	294	13% 74% 23% ·
1	C	294	10% 79% 18% ·
1	D	294	6% 73% 24% ·
1	E	294	9% 78% 21% ·
1	F	294	11% 75% 22% ·
1	G	294	6% 78% 20% ·

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16733 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 Alpha-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	41	0	0
			2343	1472	400	465	6			
1	B	293	Total	C	N	O	S	45	0	0
			2348	1476	401	465	6			
1	C	293	Total	C	N	O	S	59	0	0
			2348	1476	401	465	6			
1	D	293	Total	C	N	O	S	66	0	0
			2348	1476	401	465	6			
1	E	293	Total	C	N	O	S	49	0	0
			2348	1476	401	465	6			
1	F	293	Total	C	N	O	S	62	0	0
			2348	1476	401	465	6			
1	G	293	Total	C	N	O	S	52	0	0
			2348	1476	401	465	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	UNP P09616
A	113	PHE	MET	ENGINEERED	UNP P09616
B	0	MET	-	INITIATING METHIONINE	UNP P09616
B	113	PHE	MET	ENGINEERED	UNP P09616
C	0	MET	-	INITIATING METHIONINE	UNP P09616
C	113	PHE	MET	ENGINEERED	UNP P09616
D	0	MET	-	INITIATING METHIONINE	UNP P09616
D	113	PHE	MET	ENGINEERED	UNP P09616
E	0	MET	-	INITIATING METHIONINE	UNP P09616
E	113	PHE	MET	ENGINEERED	UNP P09616
F	0	MET	-	INITIATING METHIONINE	UNP P09616
F	113	PHE	MET	ENGINEERED	UNP P09616
G	0	MET	-	INITIATING METHIONINE	UNP P09616
G	113	PHE	MET	ENGINEERED	UNP P09616

- Molecule 2 is water.

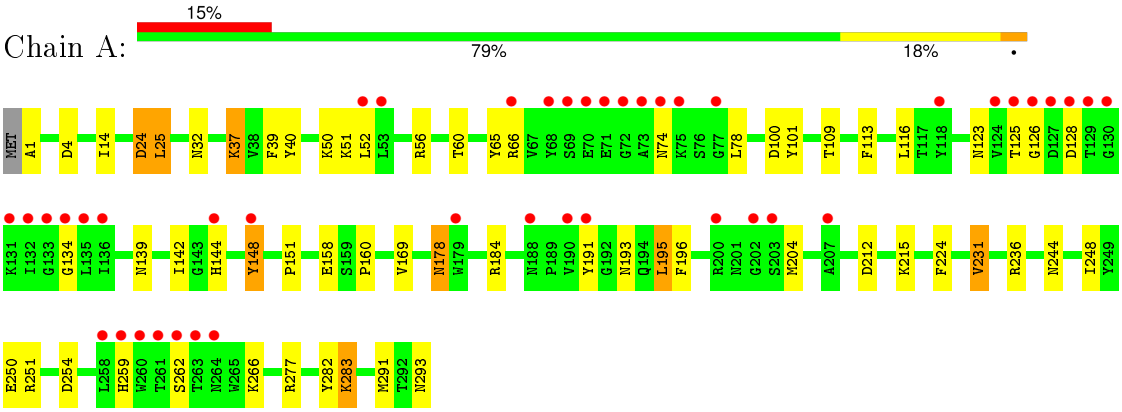
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	45	Total O 45 45	0	0
2	B	45	Total O 45 45	0	0
2	C	45	Total O 45 45	0	0
2	D	40	Total O 40 40	0	0
2	E	36	Total O 36 36	0	0
2	F	52	Total O 52 52	0	0
2	G	39	Total O 39 39	0	0

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.

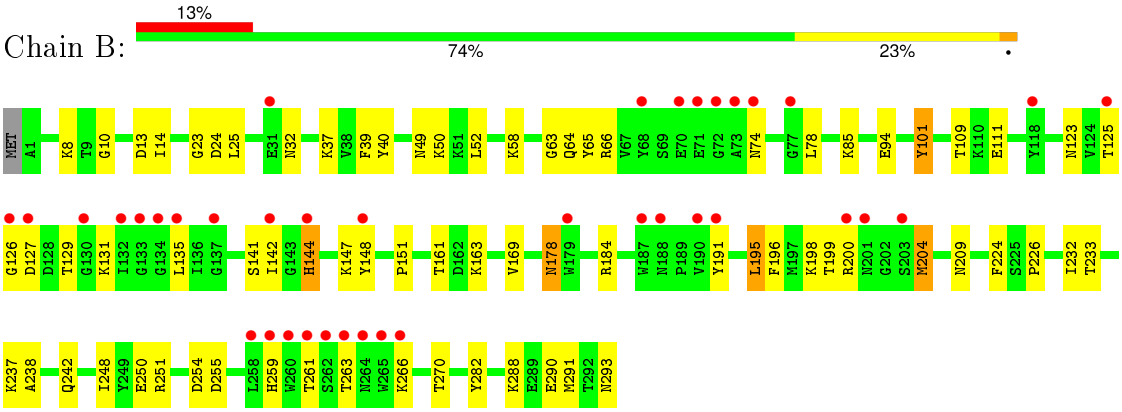
- Molecule 1: Alpha-hemolysin

Chain A:



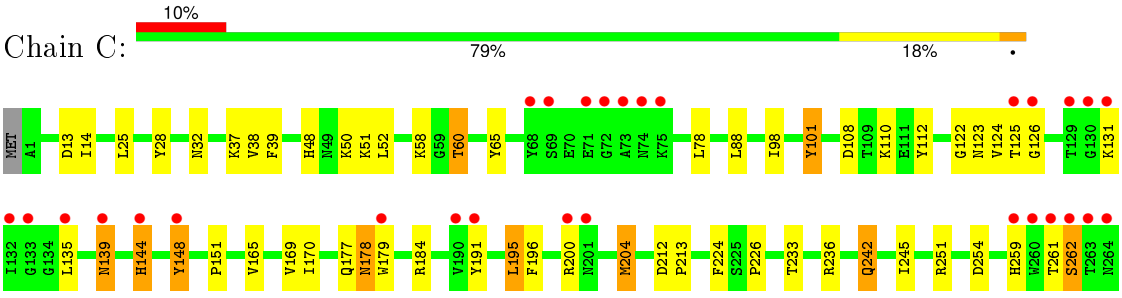
- Molecule 1: Alpha-hemolysin

Chain B:



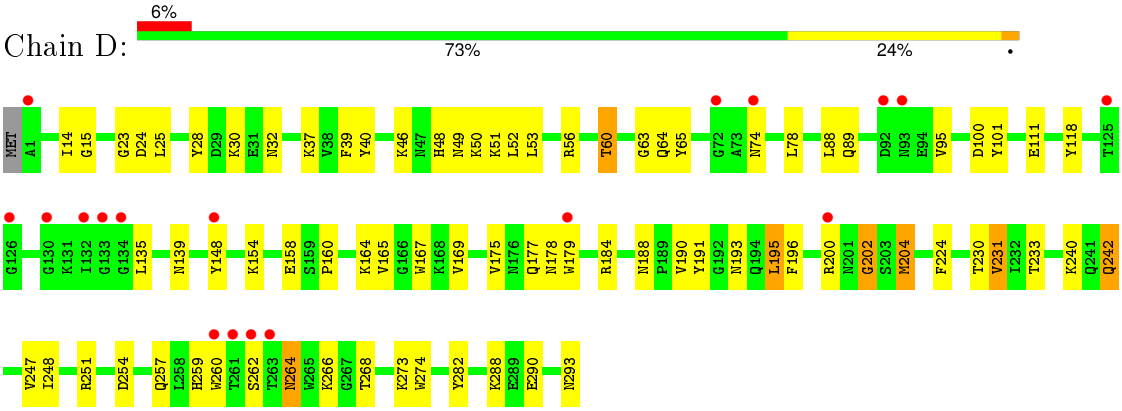
- Molecule 1: Alpha-hemolysin

Chain C:



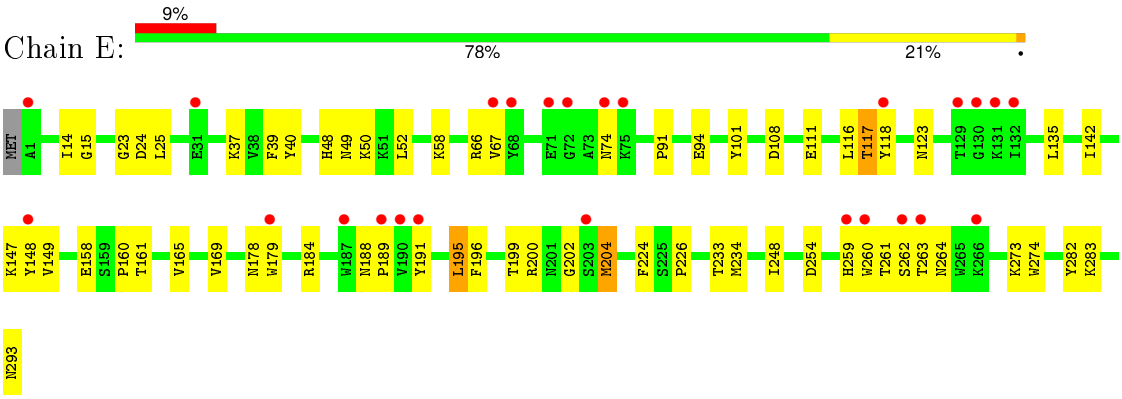
• Molecule 1: Alpha-hemolysin

Chain D:



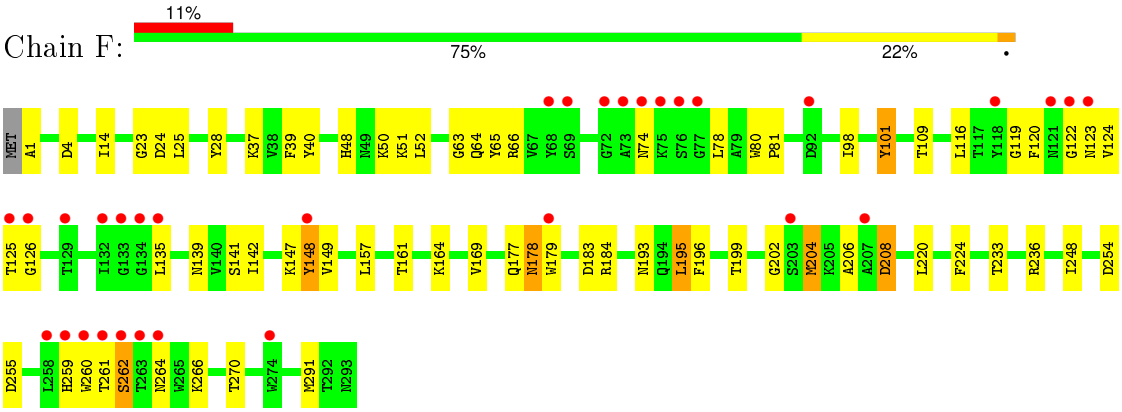
• Molecule 1: Alpha-hemolysin

Chain E:



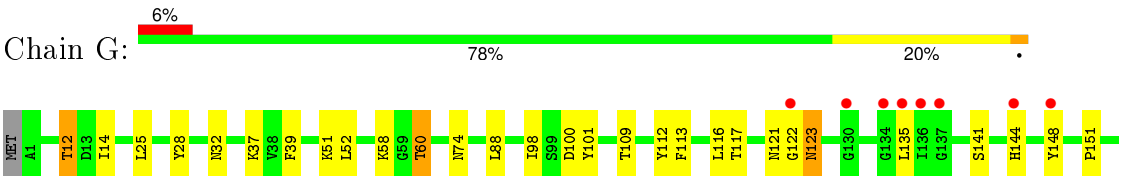
• Molecule 1: Alpha-hemolysin

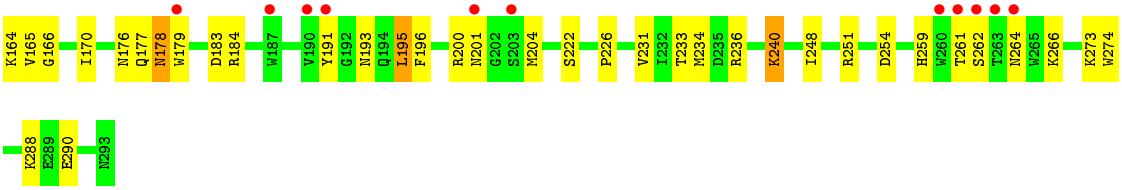
Chain F:



• Molecule 1: Alpha-hemolysin

Chain G:




K164
V165
G166
I170
N176
Q177
N178
W179
D183
R184
W187
V190
Y191
G192
N193
Q194
L195
F196
R200
N201
G202
S203
M204
S222
P226
V231
I232
T233
M234
D235
R236
K240
I248
R251
D254
H259
W260
T261
S262
T263
N264
W265
K266
K273
W274
K288
E289
E290
N293

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	151.19Å 134.80Å 132.89Å 90.00° 90.62° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 39.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.10) 87.1 (39.97-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.275 0.256 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	32.2	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.9	EDS
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 134871 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16733	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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	0.35	0/2396	0.62	0/3243
1	B	0.36	0/2401	0.64	0/3249
1	C	0.34	0/2401	0.62	0/3249
1	D	0.36	0/2401	0.63	0/3249
1	E	0.35	0/2401	0.62	0/3249
1	F	0.34	0/2401	0.62	0/3249
1	G	0.36	0/2401	0.64	0/3249
All	All	0.35	0/16802	0.63	0/22737

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2343	0	2258	52	0
1	B	2348	0	2270	65	0
1	C	2348	0	2270	58	0
1	D	2348	0	2270	71	0
1	E	2348	0	2270	46	0
1	F	2348	0	2270	64	0
1	G	2348	0	2270	63	0
2	A	45	0	0	1	0
2	B	45	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	45	0	0	1	0
2	D	40	0	0	3	0
2	E	36	0	0	0	0
2	F	52	0	0	2	0
2	G	39	0	0	0	0
All	All	16733	0	15878	358	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 11.

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASN:HB3	1:C:135:LEU:HB3	1.51	0.91
1:A:14:ILE:HD11	1:B:39:PHE:HE1	1.36	0.90
1:B:199:THR:H	1:B:209:ASN:HD21	1.20	0.89
1:G:123:ASN:HB3	1:G:135:LEU:HB3	1.54	0.89
1:B:123:ASN:HB3	1:B:135:LEU:HB3	1.54	0.88
1:A:212:ASP:HB3	1:A:215:LYS:HD2	1.59	0.84
1:G:51:LYS:HE3	1:G:236:ARG:HG2	1.62	0.81
1:B:178:ASN:HD22	1:B:178:ASN:N	1.79	0.81
1:D:52:LEU:HD22	1:D:233:THR:HG22	1.64	0.79
1:B:8:LYS:HD2	1:C:13:ASP:HB2	1.62	0.79
1:E:202:GLY:HA3	1:E:204:MET:HE3	1.66	0.79
1:A:178:ASN:HD22	1:A:178:ASN:N	1.78	0.78
1:D:167:TRP:HH2	1:D:230:THR:HG22	1.50	0.77
1:D:230:THR:HG23	2:D:294:HOH:O	1.84	0.76
1:C:242:GLN:HB2	1:C:283:LYS:HE3	1.68	0.75
1:A:39:PHE:HE1	1:G:14:ILE:HD11	1.50	0.75
1:F:123:ASN:HD21	1:G:135:LEU:HD11	1.52	0.74
1:E:91:PRO:HD2	1:E:94:GLU:HG3	1.69	0.74
1:A:14:ILE:HD11	1:B:39:PHE:CE1	2.22	0.74
1:G:100:ASP:HB3	1:G:231:VAL:CG1	2.18	0.73
1:F:148:TYR:OH	1:G:178:ASN:ND2	2.22	0.73
1:B:14:ILE:HD11	1:C:39:PHE:HE1	1.53	0.72
1:E:123:ASN:HB3	1:E:135:LEU:HB3	1.71	0.72
1:F:14:ILE:HD11	1:F:48:HIS:CE1	2.25	0.71
1:F:202:GLY:HA3	1:F:204:MET:HE3	1.71	0.71
1:A:56:ARG:NH2	1:G:12:THR:HG21	2.05	0.71
1:B:52:LEU:CD2	1:B:233:THR:HG22	2.21	0.70
1:C:178:ASN:HD22	1:C:178:ASN:N	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:ASN:ND2	1:G:135:LEU:HD11	2.08	0.69
1:F:123:ASN:HB3	1:F:135:LEU:HB3	1.75	0.68
1:F:124:VAL:O	1:G:135:LEU:HD12	1.94	0.68
1:G:191:TYR:CE2	1:G:200:ARG:HB3	2.29	0.68
1:F:178:ASN:HD22	1:F:178:ASN:N	1.91	0.68
1:E:52:LEU:CD2	1:E:233:THR:HG22	2.23	0.67
1:C:14:ILE:HD11	1:C:48:HIS:CE1	2.29	0.67
1:G:100:ASP:HB3	1:G:231:VAL:HG11	1.75	0.67
1:G:52:LEU:HD23	1:G:233:THR:HG22	1.77	0.66
1:A:123:ASN:OD1	1:B:135:LEU:HD11	1.95	0.66
1:D:52:LEU:CD2	1:D:233:THR:HG22	2.26	0.66
1:D:148:TYR:OH	1:E:178:ASN:ND2	2.28	0.66
1:B:199:THR:H	1:B:209:ASN:ND2	1.92	0.66
1:B:191:TYR:CE2	1:B:200:ARG:HB3	2.33	0.64
1:B:52:LEU:HD23	1:B:233:THR:HG22	1.79	0.64
1:D:167:TRP:CH2	1:D:230:THR:HG22	2.32	0.64
1:D:257:GLN:HB2	1:D:268:THR:CG2	2.29	0.63
1:C:148:TYR:OH	1:D:178:ASN:ND2	2.32	0.63
1:D:282:TYR:CD1	1:D:293:ASN:HB3	2.34	0.63
1:E:148:TYR:OH	1:F:178:ASN:ND2	2.32	0.63
1:A:148:TYR:OH	1:B:178:ASN:ND2	2.32	0.62
1:D:264:ASN:C	1:D:264:ASN:HD22	2.00	0.62
1:F:248:ILE:N	1:F:248:ILE:HD12	2.14	0.62
1:G:178:ASN:HD22	1:G:178:ASN:N	1.97	0.62
1:E:116:LEU:HD13	1:E:117:THR:N	2.15	0.62
1:B:111:GLU:OE1	1:B:147:LYS:HD3	2.00	0.62
1:A:100:ASP:HB3	1:A:231:VAL:HG13	1.83	0.61
1:B:259:HIS:CE1	1:B:266:LYS:HB3	2.36	0.61
1:B:144:HIS:C	1:B:144:HIS:CD2	2.73	0.61
1:D:240:LYS:HD2	1:D:242:GLN:NE2	2.16	0.61
1:F:177:GLN:O	1:F:179:TRP:HD1	1.84	0.60
1:C:14:ILE:HD11	1:D:39:PHE:HE1	1.65	0.60
1:A:56:ARG:HH22	1:G:12:THR:HG21	1.66	0.60
1:E:14:ILE:HD11	1:E:48:HIS:CE1	2.36	0.60
1:E:111:GLU:OE1	1:F:147:LYS:HE3	2.02	0.59
1:D:14:ILE:HD11	1:E:39:PHE:HE1	1.68	0.59
1:A:178:ASN:ND2	1:A:178:ASN:N	2.48	0.59
1:A:116:LEU:HD13	1:A:142:ILE:HD11	1.84	0.59
1:D:100:ASP:HB3	1:D:231:VAL:HG13	1.84	0.59
1:D:14:ILE:HD11	1:D:48:HIS:CE1	2.38	0.58
1:G:170:ILE:HD12	1:G:170:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:VAL:O	1:D:135:LEU:HD12	2.03	0.58
1:E:273:LYS:HD2	1:E:274:TRP:CE2	2.39	0.58
1:C:48:HIS:O	1:C:236:ARG:NH2	2.32	0.58
1:D:184:ARG:HD2	1:D:254:ASP:OD2	2.03	0.58
1:D:202:GLY:HA3	1:D:204:MET:CE	2.34	0.58
1:B:8:LYS:HD2	1:C:13:ASP:CB	2.32	0.57
1:D:195:LEU:HD13	1:D:196:PHE:CE2	2.39	0.57
1:D:49:ASN:O	1:D:50:LYS:HG3	2.05	0.57
1:F:74:ASN:O	1:F:259:HIS:HA	2.05	0.57
1:A:244:ASN:OD1	1:A:283:LYS:HE2	2.05	0.57
1:C:51:LYS:HG3	1:C:236:ARG:HG3	1.87	0.57
1:D:74:ASN:O	1:D:259:HIS:HA	2.04	0.56
1:A:178:ASN:ND2	1:G:148:TYR:OH	2.38	0.56
1:A:116:LEU:HD13	1:A:142:ILE:CD1	2.35	0.56
1:F:52:LEU:CD2	1:F:233:THR:HG22	2.34	0.56
1:G:117:THR:HG23	1:G:141:SER:HB3	1.86	0.56
1:C:37:LYS:C	1:C:37:LYS:HD2	2.26	0.56
1:F:261:THR:O	1:F:262:SER:CB	2.54	0.56
1:B:255:ASP:HB3	1:B:270:THR:OG1	2.06	0.56
1:D:240:LYS:CE	1:D:242:GLN:HE21	2.19	0.56
1:C:259:HIS:CE1	1:C:266:LYS:HB3	2.41	0.56
1:B:25:LEU:HD21	1:B:40:TYR:HE1	1.71	0.56
1:C:101:TYR:OH	1:D:60:THR:HG22	2.06	0.56
1:D:100:ASP:HB3	1:D:231:VAL:CG1	2.36	0.55
1:F:119:GLY:HA3	1:F:139:ASN:OD1	2.06	0.55
1:B:178:ASN:N	1:B:178:ASN:ND2	2.51	0.55
1:F:66:ARG:C	1:F:78:LEU:HD12	2.25	0.55
1:F:259:HIS:CE1	1:F:266:LYS:HB3	2.40	0.55
1:F:37:LYS:C	1:F:37:LYS:HD2	2.27	0.55
1:C:169:VAL:HG21	1:C:224:PHE:CZ	2.41	0.55
1:A:125:THR:HG22	1:A:126:GLY:H	1.71	0.55
1:C:261:THR:O	1:C:262:SER:HB3	2.07	0.55
1:B:148:TYR:OH	1:C:178:ASN:ND2	2.40	0.55
1:D:259:HIS:CE1	1:D:266:LYS:HB3	2.42	0.55
1:C:112:TYR:CE2	1:C:144:HIS:NE2	2.74	0.55
1:A:65:TYR:CE1	1:A:78:LEU:HD21	2.43	0.54
1:F:177:GLN:O	1:F:179:TRP:CD1	2.60	0.54
1:A:100:ASP:HB3	1:A:231:VAL:CG1	2.36	0.54
1:D:193:ASN:OD1	1:D:195:LEU:HB2	2.08	0.54
1:B:58:LYS:HA	1:B:226:PRO:O	2.07	0.54
1:C:52:LEU:CD2	1:C:233:THR:HG22	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LYS:HE3	1:C:236:ARG:HG2	1.89	0.54
1:E:116:LEU:HD23	1:E:142:ILE:HG12	1.90	0.54
1:E:248:ILE:N	1:E:248:ILE:HD12	2.23	0.54
1:B:199:THR:N	1:B:209:ASN:HD21	1.98	0.54
1:G:122:GLY:O	1:G:123:ASN:HB2	2.08	0.53
1:F:51:LYS:HG3	1:F:236:ARG:HG2	1.89	0.53
1:C:184:ARG:HD2	1:C:254:ASP:OD2	2.08	0.53
1:G:248:ILE:HD12	1:G:248:ILE:N	2.24	0.53
1:E:49:ASN:O	1:E:50:LYS:HG3	2.08	0.53
1:C:52:LEU:HD21	1:C:233:THR:HG22	1.89	0.53
1:B:125:THR:HG22	1:C:135:LEU:HD13	1.91	0.53
1:A:191:TYR:O	1:A:266:LYS:HA	2.09	0.53
1:E:169:VAL:HG21	1:E:224:PHE:CZ	2.44	0.53
1:D:32:ASN:O	1:D:251:ARG:NH2	2.35	0.53
1:C:126:GLY:HA2	1:C:131:LYS:O	2.08	0.53
1:F:261:THR:O	1:F:262:SER:HB2	2.08	0.53
1:B:109:THR:HG22	1:C:151:PRO:HA	1.91	0.53
1:C:139:ASN:HD22	1:C:139:ASN:N	2.06	0.53
1:G:74:ASN:O	1:G:259:HIS:HA	2.08	0.53
1:F:195:LEU:HD13	1:F:196:PHE:CE2	2.43	0.53
1:E:263:THR:HG23	1:E:264:ASN:OD1	2.09	0.52
1:G:184:ARG:HD2	1:G:254:ASP:OD2	2.09	0.52
1:C:242:GLN:CB	1:C:283:LYS:HE3	2.39	0.52
1:F:184:ARG:HD2	1:F:254:ASP:OD2	2.09	0.52
1:F:25:LEU:HD21	1:F:40:TYR:HE1	1.74	0.52
1:A:215:LYS:NZ	1:G:183:ASP:OD1	2.42	0.52
1:G:240:LYS:HB2	1:G:240:LYS:NZ	2.24	0.52
1:F:122:GLY:O	1:F:123:ASN:HB2	2.09	0.51
1:D:28:TYR:CE1	1:D:30:LYS:HG2	2.46	0.51
1:B:125:THR:HG22	1:C:135:LEU:CD1	2.40	0.51
1:E:14:ILE:HD11	1:F:39:PHE:HE1	1.75	0.51
1:E:178:ASN:HD22	1:E:178:ASN:N	2.08	0.51
1:F:116:LEU:HD23	1:G:144:HIS:CE1	2.45	0.51
1:D:264:ASN:C	1:D:264:ASN:ND2	2.62	0.51
1:C:178:ASN:N	1:C:178:ASN:ND2	2.57	0.51
1:E:116:LEU:HD13	1:E:116:LEU:C	2.30	0.51
1:E:74:ASN:O	1:E:259:HIS:HA	2.10	0.51
1:F:125:THR:HG22	1:F:126:GLY:N	2.25	0.51
1:B:101:TYR:OH	1:C:60:THR:CG2	2.59	0.51
1:A:1:ALA:HB3	1:A:4:ASP:OD1	2.11	0.50
1:A:248:ILE:HD12	1:A:248:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:TYR:OH	1:C:60:THR:HG22	2.11	0.50
1:F:202:GLY:HA3	1:F:204:MET:CE	2.41	0.50
1:F:123:ASN:OD1	1:G:135:LEU:HD11	2.11	0.50
1:C:170:ILE:HD12	1:C:170:ILE:O	2.10	0.50
1:B:85:LYS:HD2	1:B:250:GLU:OE1	2.11	0.50
1:B:10:GLY:HA2	1:B:13:ASP:OD2	2.11	0.50
1:C:58:LYS:HA	1:C:226:PRO:O	2.11	0.50
1:C:144:HIS:CD2	1:C:144:HIS:C	2.84	0.50
1:E:191:TYR:CE1	1:E:200:ARG:HB3	2.47	0.49
1:F:52:LEU:HD23	1:F:233:THR:HG22	1.94	0.49
1:A:40:TYR:CE1	1:A:291:MET:HB2	2.47	0.49
1:A:123:ASN:ND2	1:B:135:LEU:HD11	2.27	0.49
1:D:178:ASN:HD22	1:D:178:ASN:N	2.08	0.49
1:A:24:ASP:O	1:A:25:LEU:HD13	2.11	0.49
1:D:111:GLU:OE1	1:E:147:LYS:HE3	2.13	0.49
1:E:184:ARG:HD2	1:E:254:ASP:OD2	2.13	0.49
1:C:110:LYS:HD3	1:D:175:VAL:HG23	1.94	0.49
1:E:195:LEU:HD13	1:E:196:PHE:CE2	2.47	0.49
1:A:39:PHE:CE1	1:G:14:ILE:HD11	2.40	0.49
1:F:141:SER:C	1:F:142:ILE:HD12	2.32	0.49
1:B:141:SER:C	1:B:142:ILE:HD12	2.33	0.49
1:D:56:ARG:NH2	2:D:298:HOH:O	2.46	0.49
1:E:199:THR:OG1	1:E:204:MET:HE3	2.12	0.48
1:G:178:ASN:ND2	1:G:178:ASN:N	2.60	0.48
1:D:177:GLN:O	1:D:179:TRP:HD1	1.96	0.48
1:F:178:ASN:ND2	1:F:178:ASN:N	2.57	0.48
1:C:101:TYR:OH	1:D:60:THR:CG2	2.62	0.48
1:E:191:TYR:CZ	1:E:200:ARG:HD3	2.49	0.48
1:B:184:ARG:HD2	1:B:254:ASP:OD2	2.13	0.48
1:B:195:LEU:HD13	1:B:196:PHE:CE2	2.48	0.48
1:B:169:VAL:HG21	1:B:224:PHE:CZ	2.48	0.48
1:A:193:ASN:OD1	1:A:195:LEU:HB2	2.13	0.48
1:C:177:GLN:O	1:C:179:TRP:HD1	1.96	0.48
1:B:282:TYR:CD1	1:B:293:ASN:HB3	2.48	0.48
1:D:260:TRP:NE1	1:D:262:SER:HA	2.29	0.48
1:A:125:THR:HG22	1:A:126:GLY:N	2.28	0.48
1:G:193:ASN:OD1	1:G:195:LEU:HB2	2.14	0.48
1:D:169:VAL:HG21	1:D:224:PHE:CZ	2.49	0.48
1:G:123:ASN:HD22	1:G:135:LEU:HB3	1.79	0.48
1:E:161:THR:HG22	1:F:28:TYR:CZ	2.48	0.48
1:A:51:LYS:HG3	1:A:236:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:HIS:CE1	1:G:116:LEU:HB3	2.49	0.48
1:E:261:THR:O	1:E:262:SER:HB2	2.14	0.48
1:B:49:ASN:O	1:B:50:LYS:HG3	2.13	0.47
1:E:37:LYS:HD2	1:E:37:LYS:C	2.34	0.47
1:B:23:GLY:HA3	1:B:40:TYR:CZ	2.49	0.47
1:G:32:ASN:O	1:G:251:ARG:NH1	2.43	0.47
1:C:204:MET:HE1	1:C:265:TRP:HE1	1.79	0.47
1:B:50:LYS:NZ	2:B:325:HOH:O	2.47	0.47
1:A:50:LYS:NZ	2:A:303:HOH:O	2.48	0.47
1:D:273:LYS:HD2	1:D:274:TRP:CE2	2.50	0.47
1:D:118:TYR:HA	1:D:139:ASN:O	2.15	0.47
1:B:74:ASN:O	1:B:259:HIS:HA	2.15	0.47
1:C:37:LYS:HD2	1:C:38:VAL:N	2.29	0.47
1:F:169:VAL:HG21	1:F:224:PHE:CZ	2.49	0.47
1:D:177:GLN:O	1:D:179:TRP:CD1	2.68	0.47
1:E:118:TYR:O	1:F:141:SER:HB2	2.14	0.47
1:F:23:GLY:HA3	1:F:40:TYR:CZ	2.50	0.47
1:A:113:PHE:O	1:A:144:HIS:HA	2.14	0.47
1:B:248:ILE:N	1:B:248:ILE:HD12	2.29	0.47
1:A:123:ASN:CG	1:B:135:LEU:HD11	2.34	0.47
1:F:98:ILE:HD12	1:F:164:LYS:N	2.30	0.47
1:D:23:GLY:HA3	1:D:40:TYR:CZ	2.50	0.47
1:F:193:ASN:OD1	1:F:195:LEU:HB2	2.15	0.47
1:B:161:THR:HG22	1:C:28:TYR:CZ	2.50	0.47
1:F:101:TYR:OH	1:G:60:THR:CG2	2.63	0.47
1:C:32:ASN:O	1:C:251:ARG:NH1	2.46	0.46
1:F:14:ILE:HD11	1:G:39:PHE:HE1	1.79	0.46
1:E:111:GLU:HG2	1:F:149:VAL:HG22	1.98	0.46
1:F:65:TYR:CE2	1:F:78:LEU:HD21	2.51	0.46
1:E:179:TRP:CD1	1:E:179:TRP:N	2.81	0.46
1:B:198:LYS:HB3	1:B:209:ASN:ND2	2.31	0.46
1:G:123:ASN:HD22	1:G:135:LEU:CB	2.28	0.46
1:A:148:TYR:CD1	1:A:148:TYR:N	2.83	0.46
1:A:148:TYR:OH	1:B:178:ASN:CG	2.54	0.46
1:E:179:TRP:HZ3	1:E:200:ARG:NH2	2.13	0.46
1:D:89:GLN:HG3	1:D:164:LYS:HB3	1.97	0.46
1:G:113:PHE:O	1:G:144:HIS:HA	2.15	0.46
1:D:191:TYR:CE2	1:D:200:ARG:HB3	2.50	0.46
1:G:14:ILE:HD13	1:G:52:LEU:HD11	1.98	0.46
1:B:288:LYS:HB2	1:B:290:GLU:HG2	1.98	0.46
1:F:260:TRP:CZ3	1:F:264:ASN:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:TYR:N	1:C:148:TYR:CD1	2.83	0.46
1:D:158:GLU:O	1:D:160:PRO:HD3	2.16	0.46
1:G:58:LYS:HA	1:G:226:PRO:O	2.16	0.46
1:F:123:ASN:CG	1:G:135:LEU:HD11	2.35	0.46
1:A:184:ARG:HD2	1:A:254:ASP:OD2	2.16	0.46
1:E:116:LEU:HD11	1:E:118:TYR:CZ	2.51	0.46
1:B:65:TYR:CE2	1:B:78:LEU:HD21	2.51	0.46
1:D:178:ASN:N	1:D:178:ASN:ND2	2.64	0.46
1:A:66:ARG:C	1:A:78:LEU:HD12	2.37	0.46
1:D:247:VAL:C	1:D:248:ILE:HD12	2.37	0.46
1:G:37:LYS:HD2	1:G:37:LYS:C	2.36	0.46
1:F:63:GLY:O	1:F:64:GLN:HB2	2.16	0.45
1:A:151:PRO:HA	1:G:109:THR:HG22	1.98	0.45
1:D:63:GLY:O	1:D:64:GLN:HB2	2.16	0.45
1:G:98:ILE:HD12	1:G:164:LYS:N	2.31	0.45
1:B:40:TYR:CE1	1:B:291:MET:HB3	2.50	0.45
1:A:178:ASN:CG	1:G:148:TYR:OH	2.54	0.45
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.78	0.45
1:D:204:MET:HB2	2:D:317:HOH:O	2.15	0.45
1:F:157:LEU:O	1:G:222:SER:HB3	2.16	0.45
1:G:288:LYS:HE2	1:G:290:GLU:CD	2.37	0.45
1:D:202:GLY:HA3	1:D:204:MET:HE3	1.98	0.45
1:D:37:LYS:C	1:D:37:LYS:HD2	2.37	0.45
1:F:50:LYS:NZ	2:F:325:HOH:O	2.48	0.45
1:A:169:VAL:HG21	1:A:224:PHE:CZ	2.52	0.45
1:F:101:TYR:OH	1:G:60:THR:HG22	2.17	0.45
1:D:160:PRO:HB3	1:D:165:VAL:HG23	1.98	0.44
1:A:32:ASN:O	1:A:251:ARG:NH1	2.48	0.44
1:A:282:TYR:CD1	1:A:293:ASN:HB3	2.52	0.44
1:B:37:LYS:HD2	1:B:37:LYS:C	2.38	0.44
1:A:139:ASN:HB3	1:G:121:ASN:CB	2.47	0.44
1:F:116:LEU:HD23	1:G:144:HIS:HE1	1.83	0.44
1:A:123:ASN:HD21	1:B:135:LEU:HD11	1.82	0.44
1:A:37:LYS:HD2	1:A:37:LYS:C	2.37	0.44
1:D:260:TRP:CZ3	1:D:264:ASN:HA	2.53	0.44
1:A:139:ASN:HB3	1:G:121:ASN:HB2	2.00	0.44
1:A:109:THR:HG22	1:B:151:PRO:HA	2.00	0.44
1:E:158:GLU:O	1:E:160:PRO:HD3	2.17	0.44
1:A:195:LEU:HD13	1:A:196:PHE:CE2	2.53	0.44
1:B:63:GLY:O	1:B:64:GLN:HB2	2.18	0.44
1:B:94:GLU:O	1:B:163:LYS:NZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:TYR:CD1	1:F:148:TYR:N	2.86	0.43
1:G:273:LYS:HD3	1:G:274:TRP:CZ2	2.53	0.43
1:C:50:LYS:NZ	2:C:315:HOH:O	2.51	0.43
1:G:261:THR:O	1:G:262:SER:HB3	2.18	0.43
1:C:139:ASN:HD22	1:C:139:ASN:H	1.64	0.43
1:G:259:HIS:CE1	1:G:266:LYS:HB3	2.53	0.43
1:D:111:GLU:HG2	1:E:149:VAL:HG22	2.00	0.43
1:B:237:LYS:O	1:B:238:ALA:C	2.57	0.43
1:C:195:LEU:HD13	1:C:196:PHE:CE2	2.54	0.43
1:B:126:GLY:HA2	1:B:131:LYS:O	2.19	0.43
1:D:65:TYR:CE2	1:D:78:LEU:HD21	2.54	0.43
1:F:161:THR:HG22	1:G:28:TYR:CZ	2.54	0.43
1:E:282:TYR:CD1	1:E:293:ASN:HB3	2.53	0.43
1:E:14:ILE:CG2	1:E:15:GLY:N	2.81	0.43
1:B:66:ARG:HG3	1:B:66:ARG:HH11	1.84	0.43
1:C:191:TYR:CE2	1:C:200:ARG:HB3	2.53	0.43
1:D:177:GLN:O	1:D:178:ASN:HB2	2.19	0.43
1:D:288:LYS:HB2	1:D:290:GLU:HG2	2.00	0.43
1:B:232:ILE:HD12	1:B:232:ILE:N	2.33	0.43
1:B:32:ASN:O	1:B:251:ARG:NH1	2.41	0.42
1:G:176:ASN:OD1	1:G:177:GLN:HG3	2.19	0.42
1:G:12:THR:CG2	1:G:12:THR:O	2.67	0.42
1:B:52:LEU:HD21	1:B:233:THR:HG22	1.96	0.42
1:C:212:ASP:OD1	1:C:213:PRO:HD2	2.18	0.42
1:D:51:LYS:O	1:D:52:LEU:HD23	2.19	0.42
1:E:148:TYR:CD1	1:E:148:TYR:N	2.87	0.42
1:D:14:ILE:HG22	1:D:15:GLY:N	2.34	0.42
1:F:52:LEU:HD21	1:F:233:THR:HG22	1.99	0.42
1:C:123:ASN:HB3	1:C:135:LEU:HD23	2.01	0.42
1:B:204:MET:HE3	1:B:209:ASN:HB2	2.01	0.42
1:D:293:ASN:CG	1:D:293:ASN:O	2.58	0.42
1:E:58:LYS:HA	1:E:226:PRO:O	2.20	0.42
1:B:24:ASP:C	1:B:25:LEU:HD22	2.40	0.42
1:D:248:ILE:N	1:D:248:ILE:HD12	2.34	0.42
1:C:98:ILE:HD13	1:C:165:VAL:HG12	2.01	0.42
1:D:88:LEU:HD13	1:D:230:THR:HG21	2.00	0.42
1:F:1:ALA:O	1:F:4:ASP:HB2	2.20	0.42
1:D:240:LYS:HE3	1:D:242:GLN:HE21	1.83	0.42
1:E:23:GLY:HA3	1:E:40:TYR:CZ	2.55	0.42
1:E:178:ASN:ND2	1:E:178:ASN:N	2.66	0.42
1:B:127:ASP:C	1:B:129:THR:H	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:THR:HG22	1:C:126:GLY:N	2.34	0.42
1:G:112:TYR:OH	1:G:144:HIS:CD2	2.73	0.42
1:F:81:PRO:CG	1:F:220:LEU:HA	2.50	0.42
1:C:122:GLY:HA2	1:C:135:LEU:O	2.20	0.41
1:B:261:THR:C	1:B:263:THR:H	2.22	0.41
1:D:46:LYS:HA	1:D:46:LYS:HD3	1.88	0.41
1:D:188:ASN:OD1	1:D:190:VAL:N	2.51	0.41
1:B:142:ILE:HD12	1:B:142:ILE:N	2.35	0.41
1:F:109:THR:HG22	1:G:151:PRO:HA	2.01	0.41
1:G:100:ASP:N	1:G:231:VAL:HG13	2.34	0.41
1:D:240:LYS:HD2	1:D:242:GLN:HE22	1.81	0.41
1:C:52:LEU:HD21	1:C:233:THR:CG2	2.49	0.41
1:A:74:ASN:O	1:A:259:HIS:HA	2.21	0.41
1:D:23:GLY:HA3	1:D:40:TYR:CE1	2.55	0.41
1:A:158:GLU:O	1:A:160:PRO:HD3	2.19	0.41
1:F:199:THR:OG1	1:F:204:MET:HE3	2.19	0.41
1:C:139:ASN:ND2	1:C:139:ASN:N	2.68	0.41
1:G:165:VAL:HG22	1:G:166:GLY:N	2.36	0.41
1:A:250:GLU:OE2	1:A:277:ARG:HD2	2.20	0.41
1:D:242:GLN:HE21	1:D:242:GLN:HB2	1.72	0.41
1:C:88:LEU:HB3	1:C:245:ILE:HD11	2.03	0.41
1:E:188:ASN:HA	1:E:189:PRO:HD3	1.94	0.41
1:C:14:ILE:CD1	1:D:39:PHE:HE1	2.30	0.41
1:E:14:ILE:HG22	1:E:15:GLY:N	2.35	0.41
1:C:65:TYR:CE2	1:C:78:LEU:HD21	2.56	0.41
1:F:14:ILE:CD1	1:F:48:HIS:CE1	3.02	0.41
1:D:257:GLN:HB2	1:D:268:THR:HG22	2.02	0.41
1:G:240:LYS:CB	1:G:240:LYS:NZ	2.83	0.41
1:D:154:LYS:O	1:D:169:VAL:HA	2.20	0.41
1:G:201:ASN:HD22	1:G:264:ASN:HB3	1.85	0.41
1:A:123:ASN:O	1:A:134:GLY:HA2	2.21	0.41
1:G:117:THR:CG2	1:G:141:SER:HB3	2.48	0.41
1:F:80:TRP:CE2	1:F:254:ASP:HB2	2.56	0.41
1:B:64:GLN:NE2	1:B:251:ARG:CZ	2.84	0.41
1:F:255:ASP:HB3	1:F:270:THR:HB	2.03	0.40
1:E:260:TRP:CZ3	1:E:264:ASN:HA	2.56	0.40
1:D:40:TYR:HB2	1:D:53:LEU:HD11	2.02	0.40
1:F:177:GLN:O	1:F:178:ASN:HB2	2.21	0.40
1:G:88:LEU:HD12	1:G:88:LEU:N	2.37	0.40
1:F:206:ALA:C	1:F:208:ASP:H	2.25	0.40
1:F:183:ASP:HB2	2:F:339:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:LEU:HD13	1:G:196:PHE:CE2	2.57	0.40
1:E:160:PRO:HB3	1:E:165:VAL:HG23	2.03	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	291/294 (99%)	273 (94%)	16 (6%)	2 (1%)	26 21
1	B	291/294 (99%)	272 (94%)	19 (6%)	0	100 100
1	C	291/294 (99%)	274 (94%)	16 (6%)	1 (0%)	46 45
1	D	291/294 (99%)	277 (95%)	13 (4%)	1 (0%)	46 45
1	E	291/294 (99%)	276 (95%)	15 (5%)	0	100 100
1	F	291/294 (99%)	276 (95%)	14 (5%)	1 (0%)	46 45
1	G	291/294 (99%)	276 (95%)	14 (5%)	1 (0%)	46 45
All	All	2037/2058 (99%)	1924 (94%)	107 (5%)	6 (0%)	46 45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	SER
1	C	262	SER
1	G	123	ASN
1	F	262	SER
1	A	128	ASP
1	D	202	GLY

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	258/260 (99%)	246 (95%)	12 (5%)	32	30
1	B	259/260 (100%)	253 (98%)	6 (2%)	58	62
1	C	259/260 (100%)	247 (95%)	12 (5%)	33	31
1	D	259/260 (100%)	249 (96%)	10 (4%)	39	39
1	E	259/260 (100%)	248 (96%)	11 (4%)	36	35
1	F	259/260 (100%)	250 (96%)	9 (4%)	43	44
1	G	259/260 (100%)	249 (96%)	10 (4%)	39	39
All	All	1812/1820 (100%)	1742 (96%)	70 (4%)	39	39

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	25	LEU
1	A	37	LYS
1	A	52	LEU
1	A	60	THR
1	A	101	TYR
1	A	148	TYR
1	A	178	ASN
1	A	195	LEU
1	A	204	MET
1	A	231	VAL
1	A	283	LYS
1	B	101	TYR
1	B	144	HIS
1	B	178	ASN
1	B	195	LEU
1	B	204	MET
1	B	242	GLN
1	C	25	LEU
1	C	60	THR

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Mol	Chain	Res	Type
1	C	101	TYR
1	C	108	ASP
1	C	139	ASN
1	C	144	HIS
1	C	148	TYR
1	C	178	ASN
1	C	195	LEU
1	C	204	MET
1	C	242	GLN
1	C	273	LYS
1	D	24	ASP
1	D	25	LEU
1	D	60	THR
1	D	95	VAL
1	D	101	TYR
1	D	195	LEU
1	D	204	MET
1	D	231	VAL
1	D	242	GLN
1	D	264	ASN
1	E	24	ASP
1	E	25	LEU
1	E	66	ARG
1	E	67	VAL
1	E	101	TYR
1	E	108	ASP
1	E	117	THR
1	E	195	LEU
1	E	204	MET
1	E	234	MET
1	E	283	LYS
1	F	24	ASP
1	F	101	TYR
1	F	120	PHE
1	F	148	TYR
1	F	178	ASN
1	F	195	LEU
1	F	204	MET
1	F	208	ASP
1	F	291	MET
1	G	12	THR
1	G	25	LEU

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Mol	Chain	Res	Type
1	G	60	THR
1	G	101	TYR
1	G	178	ASN
1	G	179	TRP
1	G	195	LEU
1	G	204	MET
1	G	234	MET
1	G	240	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	47	ASN
1	A	64	GLN
1	A	74	ASN
1	A	144	HIS
1	A	178	ASN
1	A	242	GLN
1	A	259	HIS
1	B	17	ASN
1	B	64	GLN
1	B	74	ASN
1	B	89	GLN
1	B	144	HIS
1	B	178	ASN
1	B	209	ASN
1	B	242	GLN
1	B	259	HIS
1	C	64	GLN
1	C	74	ASN
1	C	139	ASN
1	C	144	HIS
1	C	178	ASN
1	C	242	GLN
1	C	259	HIS
1	D	64	GLN
1	D	74	ASN
1	D	178	ASN
1	D	242	GLN
1	D	244	ASN
1	D	257	GLN

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Mol	Chain	Res	Type
1	D	259	HIS
1	D	264	ASN
1	E	64	GLN
1	E	74	ASN
1	E	178	ASN
1	F	64	GLN
1	F	74	ASN
1	F	89	GLN
1	F	178	ASN
1	F	242	GLN
1	F	259	HIS
1	G	17	ASN
1	G	64	GLN
1	G	74	ASN
1	G	89	GLN
1	G	123	ASN
1	G	144	HIS
1	G	178	ASN
1	G	201	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	293/294 (99%)	0.91	43 (14%) 3 5	20, 34, 66, 84	13 (4%)
1	B	292/294 (99%)	0.70	38 (13%) 5 6	18, 33, 68, 80	12 (4%)
1	C	293/294 (99%)	0.43	29 (9%) 9 13	20, 32, 67, 86	16 (5%)
1	D	292/294 (99%)	0.40	18 (6%) 24 32	18, 32, 65, 75	19 (6%)
1	E	293/294 (99%)	0.68	25 (8%) 13 18	19, 33, 67, 79	17 (5%)
1	F	293/294 (99%)	0.62	32 (10%) 7 10	19, 33, 66, 81	19 (6%)
1	G	292/294 (99%)	0.32	19 (6%) 22 29	20, 33, 62, 81	16 (5%)
All	All	2048/2058 (99%)	0.58	204 (9%) 9 13	18, 33, 67, 86	112 (5%)

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	179	TRP	7.4
1	B	260	TRP	6.4
1	F	262	SER	6.2
1	E	179	TRP	6.2
1	A	179	TRP	6.1
1	E	262	SER	6.1
1	A	129	THR	6.1
1	D	179	TRP	6.1
1	C	179	TRP	5.9
1	G	179	TRP	5.8
1	F	73	ALA	5.7
1	B	133	GLY	5.7
1	A	261	THR	5.6
1	B	71	GLU	5.6
1	F	126	GLY	5.4
1	A	133	GLY	5.3
1	F	133	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	133	GLY	5.2
1	B	134	GLY	5.1
1	A	144	HIS	5.1
1	F	75	LYS	5.0
1	A	260	TRP	5.0
1	G	134	GLY	4.9
1	B	72	GLY	4.8
1	C	132	ILE	4.7
1	A	148	TYR	4.7
1	A	132	ILE	4.7
1	C	263	THR	4.7
1	D	133	GLY	4.7
1	B	73	ALA	4.7
1	F	72	GLY	4.7
1	E	68	TYR	4.6
1	B	179	TRP	4.6
1	F	260	TRP	4.5
1	F	135	LEU	4.4
1	B	262	SER	4.4
1	C	126	GLY	4.4
1	A	264	ASN	4.3
1	B	70	GLU	4.3
1	B	203	SER	4.2
1	A	72	GLY	4.2
1	C	125	THR	4.1
1	G	144	HIS	4.1
1	A	128	ASP	4.0
1	E	130	GLY	4.0
1	B	118	TYR	3.9
1	B	259	HIS	3.9
1	C	73	ALA	3.9
1	A	203	SER	3.9
1	B	148	TYR	3.9
1	B	74	ASN	3.9
1	F	148	TYR	3.8
1	F	74	ASN	3.8
1	A	130	GLY	3.8
1	F	261	THR	3.8
1	F	134	GLY	3.8
1	F	125	THR	3.8
1	A	134	GLY	3.8
1	A	66	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	132	ILE	3.7
1	D	263	THR	3.7
1	G	261	THR	3.7
1	C	130	GLY	3.7
1	B	201	ASN	3.6
1	G	137	GLY	3.6
1	E	260	TRP	3.6
1	F	207	ALA	3.6
1	B	132	ILE	3.6
1	B	125	THR	3.6
1	E	191	TYR	3.6
1	G	148	TYR	3.6
1	F	274	TRP	3.6
1	C	135	LEU	3.5
1	C	68	TYR	3.5
1	C	144	HIS	3.5
1	A	118	TYR	3.5
1	A	74	ASN	3.5
1	D	262	SER	3.4
1	E	203	SER	3.4
1	D	125	THR	3.4
1	F	77	GLY	3.4
1	C	75	LYS	3.4
1	A	188	ASN	3.4
1	F	259	HIS	3.3
1	A	73	ALA	3.3
1	A	71	GLU	3.3
1	E	131	LYS	3.3
1	E	118	TYR	3.3
1	G	263	THR	3.3
1	B	187	TRP	3.3
1	E	187	TRP	3.2
1	E	1	ALA	3.2
1	A	190	VAL	3.2
1	C	262	SER	3.2
1	A	259	HIS	3.2
1	B	144	HIS	3.1
1	F	118	TYR	3.1
1	G	136	ILE	3.1
1	B	265	TRP	3.1
1	A	125	THR	3.1
1	A	75	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	68	TYR	3.1
1	C	190	VAL	3.1
1	B	261	THR	3.0
1	A	77	GLY	3.0
1	A	70	GLU	3.0
1	B	68	TYR	3.0
1	B	126	GLY	2.9
1	A	69	SER	2.9
1	B	200	ARG	2.9
1	D	130	GLY	2.9
1	A	191	TYR	2.9
1	E	67	VAL	2.8
1	F	123	ASN	2.8
1	C	131	LYS	2.8
1	E	266	LYS	2.8
1	C	191	TYR	2.8
1	C	264	ASN	2.8
1	D	260	TRP	2.8
1	A	262	SER	2.8
1	F	122	GLY	2.8
1	E	148	TYR	2.8
1	G	203	SER	2.8
1	B	263	THR	2.7
1	E	259	HIS	2.7
1	D	72	GLY	2.7
1	G	191	TYR	2.7
1	E	31	GLU	2.7
1	E	71	GLU	2.7
1	F	263	THR	2.7
1	A	127	ASP	2.7
1	A	131	LYS	2.7
1	F	258	LEU	2.7
1	B	190	VAL	2.7
1	A	207	ALA	2.6
1	A	263	THR	2.6
1	F	121	ASN	2.6
1	F	264	ASN	2.6
1	F	69	SER	2.6
1	C	72	GLY	2.6
1	B	127	ASP	2.6
1	G	260	TRP	2.5
1	B	135	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	203	SER	2.5
1	B	264	ASN	2.5
1	D	148	TYR	2.5
1	E	72	GLY	2.5
1	E	132	ILE	2.5
1	C	71	GLU	2.5
1	D	200	ARG	2.5
1	A	126	GLY	2.5
1	D	93	ASN	2.5
1	C	201	ASN	2.4
1	C	148	TYR	2.4
1	G	187	TRP	2.4
1	E	75	LYS	2.4
1	D	126	GLY	2.4
1	A	53	LEU	2.4
1	C	74	ASN	2.4
1	A	124	VAL	2.3
1	C	200	ARG	2.3
1	F	129	THR	2.3
1	B	258	LEU	2.3
1	B	191	TYR	2.3
1	E	189	PRO	2.3
1	A	202	GLY	2.3
1	D	132	ILE	2.3
1	E	190	VAL	2.3
1	E	263	THR	2.3
1	C	139	ASN	2.3
1	G	262	SER	2.2
1	A	200	ARG	2.2
1	C	69	SER	2.2
1	A	136	ILE	2.2
1	C	260	TRP	2.2
1	F	92	ASP	2.2
1	C	259	HIS	2.2
1	G	264	ASN	2.2
1	E	129	THR	2.2
1	A	52	LEU	2.2
1	G	122	GLY	2.2
1	A	258	LEU	2.1
1	C	261	THR	2.1
1	G	190	VAL	2.1
1	B	266	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	134	GLY	2.1
1	G	130	GLY	2.1
1	D	74	ASN	2.1
1	G	201	ASN	2.1
1	A	135	LEU	2.1
1	D	1	ALA	2.1
1	A	68	TYR	2.1
1	B	77	GLY	2.1
1	B	188	ASN	2.1
1	F	76	SER	2.1
1	D	92	ASP	2.1
1	E	74	ASN	2.1
1	B	130	GLY	2.0
1	C	129	THR	2.0
1	D	261	THR	2.0
1	B	137	GLY	2.0
1	G	135	LEU	2.0
1	B	31	GLU	2.0
1	B	142	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.