



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 03:43 PM EDT

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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

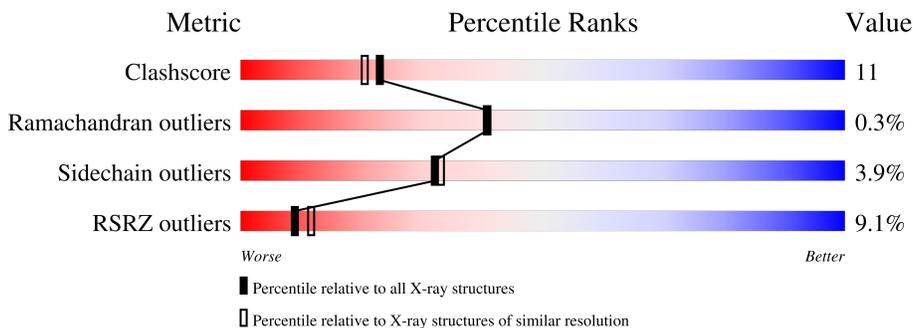
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	294	 14% 79% 18%
1	B	294	 11% 74% 23%
1	C	294	 10% 79% 18%
1	D	294	 5% 73% 24%
1	E	294	 8% 78% 21%
1	F	294	 11% 75% 22%

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Mol	Chain	Length	Quality of chain
1	G	294	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a small red segment on the left labeled '6%', a large green segment in the middle labeled '78%', and a yellow segment on the right labeled '20%'. A small black dot is visible at the far right end of the bar.</p>

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

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 mutation	UNP P09616
B	0	MET	-	initiating methionine	UNP P09616
B	113	PHE	MET	engineered mutation	UNP P09616
C	0	MET	-	initiating methionine	UNP P09616
C	113	PHE	MET	engineered mutation	UNP P09616
D	0	MET	-	initiating methionine	UNP P09616
D	113	PHE	MET	engineered mutation	UNP P09616
E	0	MET	-	initiating methionine	UNP P09616
E	113	PHE	MET	engineered mutation	UNP P09616
F	0	MET	-	initiating methionine	UNP P09616
F	113	PHE	MET	engineered mutation	UNP P09616
G	0	MET	-	initiating methionine	UNP P09616
G	113	PHE	MET	engineered mutation	UNP P09616

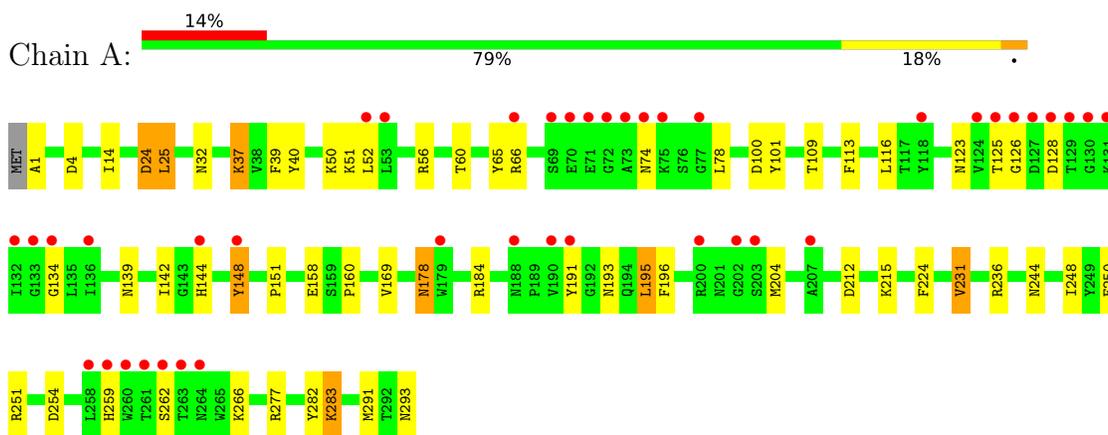
- Molecule 2 is water.

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

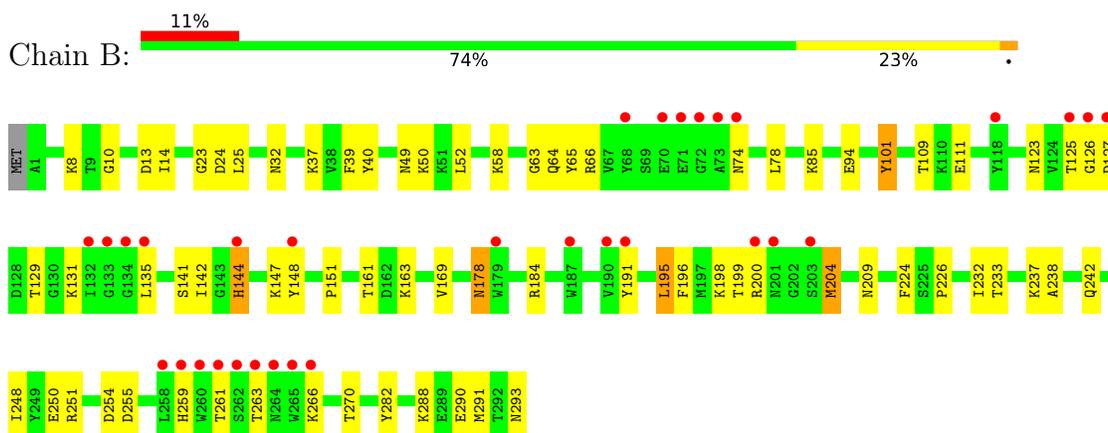
3 Residue-property plots

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

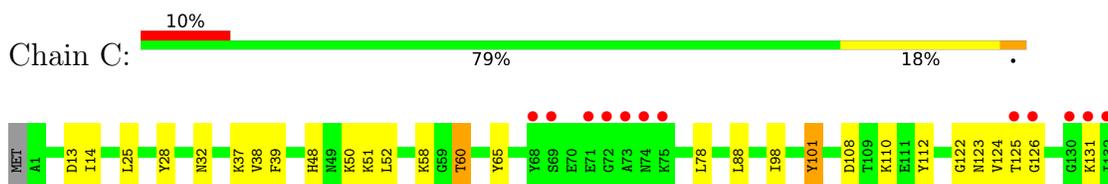
- Molecule 1: Alpha-hemolysin

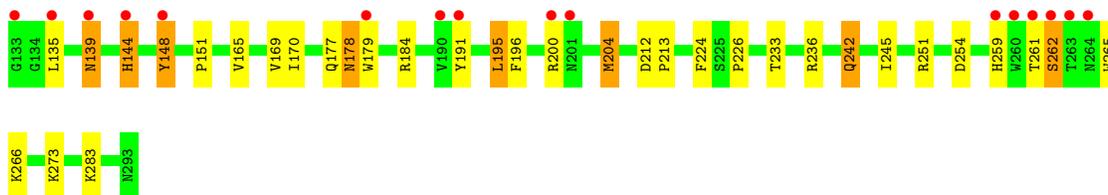


- Molecule 1: Alpha-hemolysin

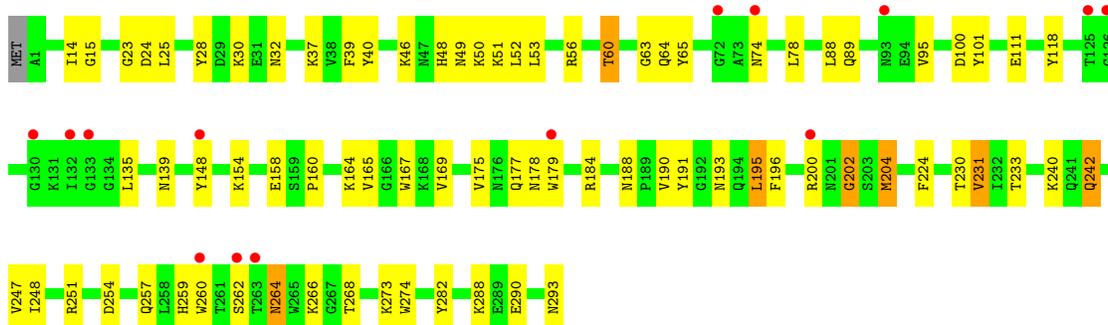


- Molecule 1: Alpha-hemolysin

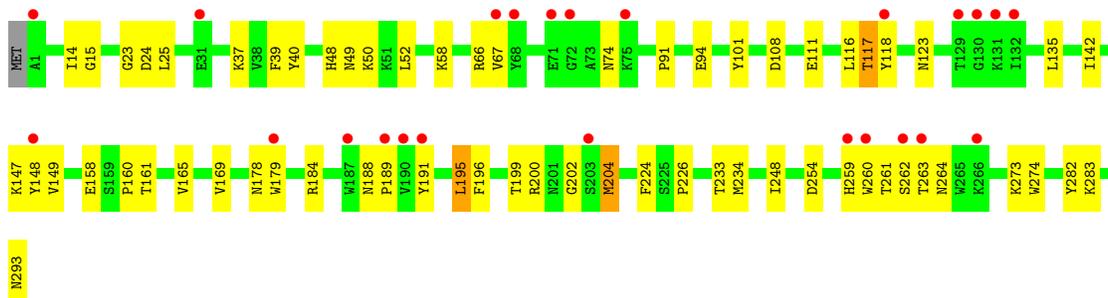
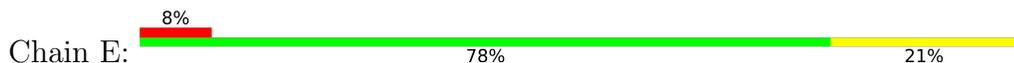




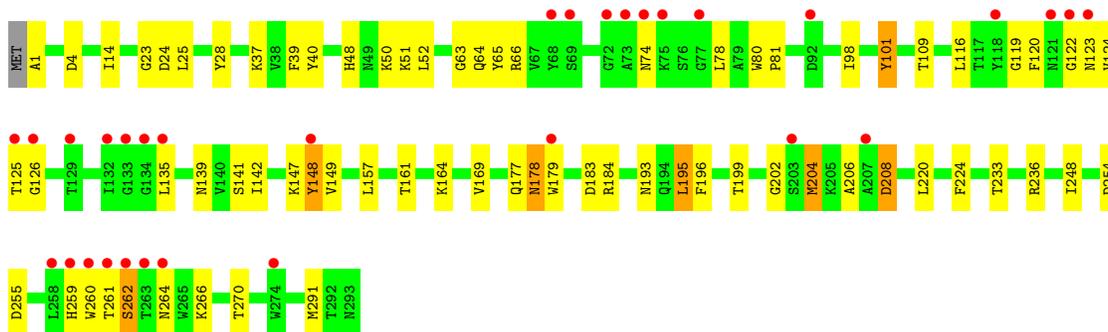
- Molecule 1: Alpha-hemolysin



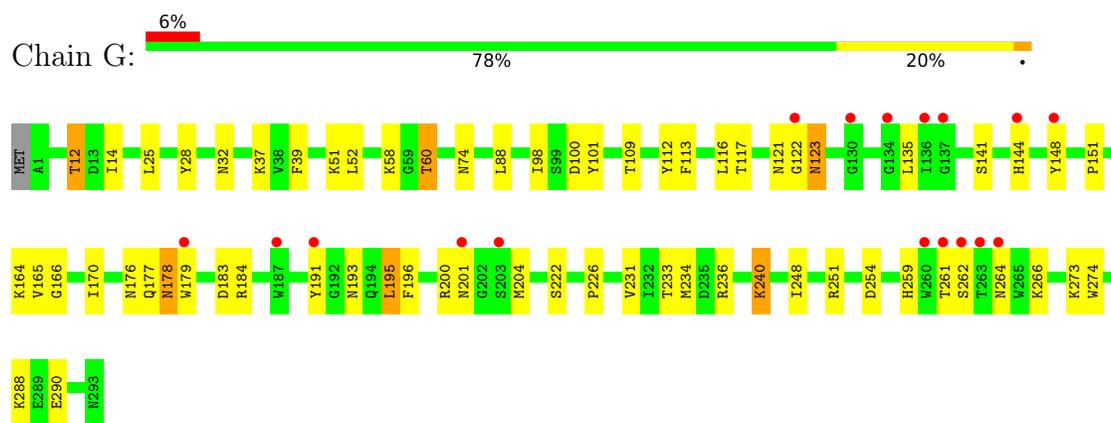
- Molecule 1: Alpha-hemolysin



- Molecule 1: Alpha-hemolysin



- Molecule 1: Alpha-hemolysin



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
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.10Å)	Xtrriage
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.	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtrriage
Anisotropy	0.331	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:N	1:B:178:ASN:HD22	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:N	1:A:178:ASN:HD22	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:E:91:PRO:HD2	1:E:94:GLU:HG3	1.69	0.74
1:F:123:ASN:HD21	1:G:135:LEU:HD11	1.52	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:N	1:C:178:ASN:HD22	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:C:14:ILE:HD11	1:C:48:HIS:CE1	2.29	0.67
1:E:52:LEU:CD2	1:E:233:THR:HG22	2.23	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:N	1:G:178:ASN:HD22	1.97	0.62
1:B:111:GLU:OE1	1:B:147:LYS:HD3	2.00	0.62
1:E:116:LEU:HD13	1:E:117:THR:N	2.15	0.62
1:A:100:ASP:HB3	1:A:231:VAL:HG13	1.83	0.61
1:B:144:HIS:C	1:B:144:HIS:CD2	2.73	0.61
1:B:259:HIS:CE1	1:B:266:LYS:HB3	2.36	0.61
1:D:240:LYS:HD2	1:D:242:GLN:NE2	2.16	0.61
1:C:14:ILE:HD11	1:D:39:PHE:HE1	1.65	0.60
1:F:177:GLN:O	1:F:179:TRP:HD1	1.84	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:N	1:A:178:ASN:ND2	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:A:244:ASN:OD1	1:A:283:LYS:HE2	2.05	0.57
1:F:74:ASN:O	1:F:259:HIS:HA	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:116:LEU:HD13	1:A:142:ILE:CD1	2.35	0.56
1:A:178:ASN:ND2	1:G:148:TYR:OH	2.38	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:HD2	1:C:37:LYS:C	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:C:259:HIS:CE1	1:C:266:LYS:HB3	2.41	0.56
1:D:240:LYS:CE	1:D:242:GLN:HE21	2.19	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:37:LYS:HD2	1:F:37:LYS:C	2.27	0.55
1:F:259:HIS:CE1	1:F:266:LYS:HB3	2.40	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: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
1:D:193:ASN:OD1	1:D:195:LEU:HB2	2.08	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:C:184:ARG:HD2	1:C:254:ASP:OD2	2.08	0.53
1:F:51:LYS:HG3	1:F:236:ARG:HG2	1.89	0.53
1:G:122:GLY:O	1:G:123:ASN:HB2	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:A:191:TYR:O	1:A:266:LYS:HA	2.09	0.53
1:B:125:THR:HG22	1:C:135:LEU:HD13	1.91	0.53
1:E:169:VAL:HG21	1:E:224:PHE:CZ	2.44	0.53
1:C:126:GLY:HA2	1:C:131:LYS:O	2.08	0.53
1:D:32:ASN:O	1:D:251:ARG:NH2	2.35	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:F:261:THR:O	1:F:262:SER:HB2	2.08	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:D:28:TYR:CE1	1:D:30:LYS:HG2	2.46	0.51
1:F:122:GLY:O	1:F:123:ASN:HB2	2.09	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:N	1:E:178:ASN:HD22	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:74:ASN:O	1:E:259:HIS:HA	2.10	0.51
1:E:116:LEU:HD13	1:E:116:LEU:C	2.30	0.51
1:B:101:TYR:OH	1:C:60:THR:CG2	2.59	0.51
1:F:125:THR:HG22	1:F:126:GLY:N	2.25	0.51
1:A:1:ALA:HB3	1:A:4:ASP:OD1	2.11	0.50
1:A:248:ILE:N	1:A:248:ILE:HD12	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:B:85:LYS:HD2	1:B:250:GLU:OE1	2.11	0.50
1:C:170:ILE:O	1:C:170:ILE:HD12	2.10	0.50
1:F:123:ASN:OD1	1:G:135:LEU:HD11	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:C	1:C:144:HIS:CD2	2.84	0.50
1:E:191:TYR:CE1	1:E:200:ARG:HB3	2.47	0.49
1:A:40:TYR:CE1	1:A:291:MET:HB2	2.47	0.49
1:F:52:LEU:HD23	1:F:233:THR:HG22	1.94	0.49
1:A:123:ASN:ND2	1:B:135:LEU:HD11	2.27	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:D:178:ASN:HD22	1:D:178:ASN:N	2.08	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:B:141:SER:C	1:B:142:ILE:HD12	2.33	0.49
1:F:141:SER:C	1:F:142:ILE:HD12	2.32	0.49
1:D:56:ARG:NH2	2:D:298:HOH:O	2.46	0.49
1:D:177:GLN:O	1:D:179:TRP:HD1	1.96	0.48
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: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:F:178:ASN:N	1:F:178:ASN:ND2	2.57	0.48
1:B:169:VAL:HG21	1:B:224:PHE:CZ	2.48	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:A:193:ASN:OD1	1:A:195:LEU:HB2	2.13	0.48
1:B:282:TYR:CD1	1:B:293:ASN:HB3	2.48	0.48
1:C:177:GLN:O	1:C:179:TRP:HD1	1.96	0.48
1:A:125:THR:HG22	1:A:126:GLY:N	2.28	0.48
1:D:169:VAL:HG21	1:D:224:PHE:CZ	2.49	0.48
1:D:260:TRP:NE1	1:D:262:SER:HA	2.29	0.48
1:G:193:ASN:OD1	1:G:195:LEU:HB2	2.14	0.48
1:E:161:THR:HG22	1:F:28:TYR:CZ	2.48	0.48
1:G:123:ASN:HD22	1:G:135:LEU:HB3	1.79	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:C:204:MET:HE1	1:C:265:TRP:HE1	1.79	0.47
1:G:32:ASN:O	1:G:251:ARG:NH1	2.43	0.47
1:A:50:LYS:NZ	2:A:303:HOH:O	2.48	0.47
1:B:50:LYS:NZ	2:B:325:HOH:O	2.47	0.47
1:D:118:TYR:HA	1:D:139:ASN:O	2.15	0.47
1:D:273:LYS:HD2	1:D:274:TRP:CE2	2.50	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:A:113:PHE:O	1:A:144:HIS:HA	2.14	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:B:248:ILE:HD12	1:B:248:ILE:N	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: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:F:193:ASN:OD1	1:F:195:LEU:HB2	2.15	0.47
1:C:32:ASN:O	1:C:251:ARG:NH1	2.46	0.46
1:E:111:GLU:HG2	1:F:149:VAL:HG22	1.98	0.46
1:E:179:TRP:CD1	1:E:179:TRP:N	2.81	0.46
1:F:14:ILE:HD11	1:G:39:PHE:HE1	1.79	0.46
1:F:65:TYR:CE2	1:F:78:LEU:HD21	2.51	0.46
1:A:148:TYR:OH	1:B:178:ASN:CG	2.54	0.46
1:A:148:TYR:CD1	1:A:148:TYR:N	2.83	0.46
1:B:198:LYS:HB3	1:B:209:ASN:ND2	2.31	0.46
1:D:89:GLN:HG3	1:D:164:LYS:HB3	1.97	0.46
1:E:179:TRP:HZ3	1:E:200:ARG:NH2	2.13	0.46
1:G:123:ASN:HD22	1:G:135:LEU:CB	2.28	0.46
1:D:191:TYR:CE2	1:D:200:ARG:HB3	2.50	0.46
1:G:113:PHE:O	1:G:144:HIS:HA	2.15	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
1:G:14:ILE:HD13	1:G:52:LEU:HD11	1.98	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:A:184:ARG:HD2	1:A:254:ASP:OD2	2.16	0.46
1:F:123:ASN:CG	1:G:135:LEU:HD11	2.35	0.46
1:B:65:TYR:CE2	1:B:78:LEU:HD21	2.51	0.46
1:E:116:LEU:HD11	1:E:118:TYR:CZ	2.51	0.46
1:A:66:ARG:C	1:A:78:LEU:HD12	2.37	0.46
1:D:178:ASN:ND2	1:D:178:ASN:N	2.64	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: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:F:63:GLY:O	1:F: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:37:LYS:C	1:D:37:LYS:HD2	2.37	0.45
1:D:202:GLY:HA3	1:D:204:MET:HE3	1.98	0.45
1:A:169:VAL:HG21	1:A:224:PHE:CZ	2.52	0.45
1:F:50:LYS:NZ	2:F:325:HOH:O	2.48	0.45
1:F:101:TYR:OH	1:G:60:THR:HG22	2.17	0.45
1:A:32:ASN:O	1:A:251:ARG:NH1	2.48	0.44
1:A:139:ASN:HB3	1:G:121:ASN:CB	2.47	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:D:160:PRO:HB3	1:D:165:VAL:HG23	1.98	0.44
1:F:116:LEU:HD23	1:G:144:HIS:HE1	1.83	0.44
1:A:37:LYS:HD2	1:A:37:LYS:C	2.37	0.44
1:A:123:ASN:HD21	1:B:135:LEU:HD11	1.82	0.44
1:A:139:ASN:HB3	1:G:121:ASN:HB2	2.00	0.44
1:D:260:TRP:CZ3	1:D:264:ASN:HA	2.53	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:C:50:LYS:NZ	2:C:315:HOH:O	2.51	0.43
1:F:148:TYR:N	1:F:148:TYR:CD1	2.86	0.43
1:G:273:LYS:HD3	1:G:274:TRP:CZ2	2.53	0.43
1:G:261:THR:O	1:G:262:SER:HB3	2.18	0.43
1:B:237:LYS:O	1:B:238:ALA:C	2.57	0.43
1:C:139:ASN:HD22	1:C:139:ASN:H	1.64	0.43
1:D:111:GLU:HG2	1:E:149:VAL:HG22	2.00	0.43
1:G:259:HIS:CE1	1:G:266:LYS:HB3	2.53	0.43
1:B:126:GLY:HA2	1:B:131:LYS:O	2.19	0.43
1:C:195:LEU:HD13	1:C:196:PHE:CE2	2.54	0.43
1:D:65:TYR:CE2	1:D:78:LEU:HD21	2.54	0.43
1:E:282:TYR:CD1	1:E:293:ASN:HB3	2.53	0.43
1:F:161:THR:HG22	1:G:28:TYR:CZ	2.54	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:E:14:ILE:CG2	1:E:15:GLY:N	2.81	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:N	1:B:232:ILE:HD12	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: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:G:12:THR:O	1:G:12:THR:CG2	2.67	0.42
1:D:14:ILE:HG22	1:D:15:GLY:N	2.34	0.42
1:D:51:LYS:O	1:D:52:LEU:HD23	2.19	0.42
1:E:148:TYR:N	1:E:148:TYR:CD1	2.87	0.42
1:F:52:LEU:HD21	1:F:233:THR:HG22	1.99	0.42
1:B:204:MET:HE3	1:B:209:ASN:HB2	2.01	0.42
1:C:123:ASN:HB3	1:C:135:LEU:HD23	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:C:98:ILE:HD13	1:C:165:VAL:HG12	2.01	0.42
1:D:248:ILE:HD12	1:D:248:ILE:N	2.34	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:F:81:PRO:CG	1:F:220:LEU:HA	2.50	0.42
1:G:112:TYR:OH	1:G:144:HIS:CD2	2.73	0.42
1:B:261:THR:C	1:B:263:THR:H	2.22	0.41
1:C:122:GLY:HA2	1:C:135:LEU:O	2.20	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:A:74:ASN:O	1:A:259:HIS:HA	2.21	0.41
1:C:52:LEU:HD21	1:C:233:THR:CG2	2.49	0.41
1:D:240:LYS:HD2	1:D:242:GLN:HE22	1.81	0.41
1:G:100:ASP:N	1:G:231:VAL:HG13	2.34	0.41
1:A:158:GLU:O	1:A:160:PRO:HD3	2.19	0.41
1:D:23:GLY:HA3	1:D:40:TYR:CE1	2.55	0.41
1:F:199:THR:OG1	1:F:204:MET:HE3	2.19	0.41
1:A:250:GLU:OE2	1:A:277:ARG:HD2	2.20	0.41
1:C:139:ASN:N	1:C:139:ASN:ND2	2.68	0.41
1:G:165:VAL:HG22	1:G:166:GLY:N	2.36	0.41
1:C:88:LEU:HB3	1:C:245:ILE:HD11	2.03	0.41
1:D:242:GLN:HE21	1:D:242:GLN:HB2	1.72	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:C:65:TYR:CE2	1:C:78:LEU:HD21	2.56	0.41
1:E:14:ILE:HG22	1:E:15:GLY:N	2.35	0.41
1:D:154:LYS:O	1:D:169:VAL:HA	2.20	0.41
1:D:257:GLN:HB2	1:D:268:THR:HG22	2.02	0.41
1:F:14:ILE:CD1	1:F:48:HIS:CE1	3.02	0.41
1:G:201:ASN:HD22	1:G:264:ASN:HB3	1.85	0.41
1:G:240:LYS:NZ	1:G:240:LYS:CB	2.83	0.41
1:A:123:ASN:O	1:A:134:GLY:HA2	2.21	0.41
1:B:64:GLN:NE2	1:B:251:ARG:CZ	2.84	0.41
1:F:80:TRP:CE2	1:F:254:ASP:HB2	2.56	0.41
1:G:117:THR:CG2	1:G:141:SER:HB3	2.48	0.41
1:F:255:ASP:HB3	1:F:270:THR:HB	2.03	0.40
1:D:40:TYR:HB2	1:D:53:LEU:HD11	2.02	0.40
1:E:260:TRP:CZ3	1:E:264:ASN:HA	2.56	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:183:ASP:HB2	2:F:339:HOH:O	2.21	0.40
1:F:206:ALA:C	1:F:208:ASP:H	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:PRO:HB3	1:E:165:VAL:HG23	2.03	0.40
1:G:195:LEU:HD13	1:G:196:PHE:CE2	2.57	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%)	22 18
1	B	291/294 (99%)	272 (94%)	19 (6%)	0	100 100
1	C	291/294 (99%)	274 (94%)	16 (6%)	1 (0%)	41 41
1	D	291/294 (99%)	277 (95%)	13 (4%)	1 (0%)	41 41
1	E	291/294 (99%)	276 (95%)	15 (5%)	0	100 100
1	F	291/294 (99%)	276 (95%)	14 (5%)	1 (0%)	41 41
1	G	291/294 (99%)	276 (95%)	14 (5%)	1 (0%)	41 41
All	All	2037/2058 (99%)	1924 (94%)	107 (5%)	6 (0%)	41 41

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

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%)	26	25
1	B	259/260 (100%)	253 (98%)	6 (2%)	50	55
1	C	259/260 (100%)	247 (95%)	12 (5%)	27	26
1	D	259/260 (100%)	249 (96%)	10 (4%)	32	33
1	E	259/260 (100%)	248 (96%)	11 (4%)	30	30
1	F	259/260 (100%)	250 (96%)	9 (4%)	36	38
1	G	259/260 (100%)	249 (96%)	10 (4%)	32	33
All	All	1812/1820 (100%)	1742 (96%)	70 (4%)	32	33

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

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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%)	0.83	41 (13%) 2 3	20, 34, 66, 84	13 (4%)
1	B	292/294 (99%)	0.62	32 (10%) 5 7	18, 33, 68, 80	12 (4%)
1	C	293/294 (99%)	0.36	28 (9%) 8 10	20, 32, 67, 86	16 (5%)
1	D	292/294 (99%)	0.34	14 (4%) 30 36	18, 32, 65, 75	19 (6%)
1	E	293/294 (99%)	0.61	24 (8%) 11 15	19, 33, 67, 79	17 (5%)
1	F	293/294 (99%)	0.54	31 (10%) 6 7	19, 33, 66, 81	19 (6%)
1	G	292/294 (99%)	0.26	17 (5%) 23 28	20, 33, 62, 81	16 (5%)
All	All	2048/2058 (99%)	0.51	187 (9%) 9 12	18, 33, 67, 86	112 (5%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	179	TRP	7.0
1	B	260	TRP	6.0
1	F	262	SER	5.9
1	A	179	TRP	5.9
1	E	262	SER	5.9
1	E	179	TRP	5.9
1	A	129	THR	5.8
1	D	179	TRP	5.8
1	C	179	TRP	5.6
1	G	179	TRP	5.6
1	B	133	GLY	5.4
1	F	73	ALA	5.4
1	B	71	GLU	5.4
1	A	261	THR	5.3
1	F	126	GLY	5.2
1	A	133	GLY	5.1
1	F	133	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	144	HIS	4.9
1	C	133	GLY	4.9
1	B	134	GLY	4.9
1	F	75	LYS	4.9
1	G	134	GLY	4.8
1	A	260	TRP	4.7
1	B	72	GLY	4.6
1	A	148	TYR	4.6
1	F	72	GLY	4.5
1	C	132	ILE	4.5
1	C	263	THR	4.5
1	D	133	GLY	4.5
1	A	132	ILE	4.4
1	B	73	ALA	4.4
1	E	68	TYR	4.4
1	B	179	TRP	4.3
1	F	135	LEU	4.3
1	F	260	TRP	4.2
1	A	264	ASN	4.2
1	B	262	SER	4.2
1	B	70	GLU	4.2
1	C	126	GLY	4.2
1	B	203	SER	4.1
1	A	72	GLY	4.0
1	G	144	HIS	3.9
1	C	125	THR	3.9
1	A	128	ASP	3.9
1	B	259	HIS	3.8
1	B	118	TYR	3.8
1	B	148	TYR	3.7
1	B	74	ASN	3.7
1	E	130	GLY	3.7
1	A	203	SER	3.7
1	F	148	TYR	3.7
1	F	74	ASN	3.7
1	C	73	ALA	3.6
1	A	130	GLY	3.6
1	A	134	GLY	3.6
1	A	66	ARG	3.6
1	F	134	GLY	3.6
1	F	125	THR	3.6
1	F	261	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	130	GLY	3.5
1	B	201	ASN	3.5
1	F	132	ILE	3.5
1	G	148	TYR	3.5
1	G	137	GLY	3.5
1	D	263	THR	3.5
1	G	261	THR	3.5
1	E	191	TYR	3.5
1	E	260	TRP	3.4
1	F	207	ALA	3.4
1	C	144	HIS	3.4
1	C	68	TYR	3.4
1	B	125	THR	3.4
1	F	274	TRP	3.4
1	B	132	ILE	3.4
1	A	118	TYR	3.4
1	C	135	LEU	3.4
1	A	74	ASN	3.3
1	E	203	SER	3.3
1	C	75	LYS	3.3
1	F	259	HIS	3.2
1	A	188	ASN	3.2
1	D	262	SER	3.2
1	D	125	THR	3.2
1	F	77	GLY	3.2
1	A	71	GLU	3.2
1	A	73	ALA	3.2
1	E	118	TYR	3.2
1	E	131	LYS	3.2
1	G	263	THR	3.1
1	B	187	TRP	3.1
1	A	259	HIS	3.0
1	B	144	HIS	3.0
1	E	187	TRP	3.0
1	A	190	VAL	3.0
1	E	1	ALA	3.0
1	F	118	TYR	3.0
1	C	262	SER	3.0
1	A	75	LYS	3.0
1	A	125	THR	2.9
1	B	265	TRP	2.9
1	A	77	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	68	TYR	2.9
1	B	261	THR	2.9
1	G	136	ILE	2.9
1	C	190	VAL	2.9
1	A	70	GLU	2.9
1	B	68	TYR	2.9
1	B	200	ARG	2.8
1	A	69	SER	2.8
1	A	191	TYR	2.7
1	B	126	GLY	2.7
1	E	266	LYS	2.7
1	F	123	ASN	2.7
1	C	191	TYR	2.7
1	C	131	LYS	2.7
1	C	264	ASN	2.7
1	D	130	GLY	2.7
1	F	122	GLY	2.7
1	E	148	TYR	2.6
1	E	67	VAL	2.6
1	E	71	GLU	2.6
1	E	259	HIS	2.6
1	A	262	SER	2.6
1	G	203	SER	2.6
1	D	260	TRP	2.6
1	D	72	GLY	2.6
1	G	191	TYR	2.6
1	B	263	THR	2.6
1	A	127	ASP	2.6
1	A	131	LYS	2.6
1	E	31	GLU	2.6
1	F	258	LEU	2.6
1	A	207	ALA	2.5
1	F	121	ASN	2.5
1	F	263	THR	2.5
1	A	263	THR	2.5
1	B	190	VAL	2.5
1	F	264	ASN	2.5
1	B	127	ASP	2.5
1	B	264	ASN	2.4
1	C	72	GLY	2.4
1	D	148	TYR	2.4
1	B	135	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	203	SER	2.4
1	D	200	ARG	2.4
1	G	260	TRP	2.4
1	F	69	SER	2.4
1	C	71	GLU	2.4
1	E	72	GLY	2.4
1	A	126	GLY	2.3
1	C	201	ASN	2.3
1	E	132	ILE	2.3
1	C	148	TYR	2.3
1	D	93	ASN	2.3
1	E	75	LYS	2.3
1	D	126	GLY	2.3
1	C	74	ASN	2.3
1	G	187	TRP	2.3
1	C	200	ARG	2.3
1	B	191	TYR	2.2
1	F	129	THR	2.2
1	A	53	LEU	2.2
1	A	202	GLY	2.2
1	B	258	LEU	2.2
1	E	189	PRO	2.2
1	C	139	ASN	2.2
1	A	200	ARG	2.2
1	E	190	VAL	2.1
1	E	263	THR	2.1
1	C	259	HIS	2.1
1	D	132	ILE	2.1
1	A	124	VAL	2.1
1	C	69	SER	2.1
1	G	262	SER	2.1
1	G	264	ASN	2.1
1	E	129	THR	2.1
1	C	260	TRP	2.1
1	F	92	ASP	2.1
1	B	266	LYS	2.1
1	G	122	GLY	2.1
1	A	136	ILE	2.0
1	A	258	LEU	2.0
1	D	74	ASN	2.0
1	G	201	ASN	2.0
1	A	52	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	130	GLY	2.0
1	C	261	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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.