Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 02:13 PM JST

PDB ID	:	8YQ7
Title	:	Acinetobacter baumannii membrane-bound lytic murein transglycosylase G
Authors	:	Jang, H.S.; Park, H.H.
Deposited on	:	2024-03-19
Resolution	:	2.67 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

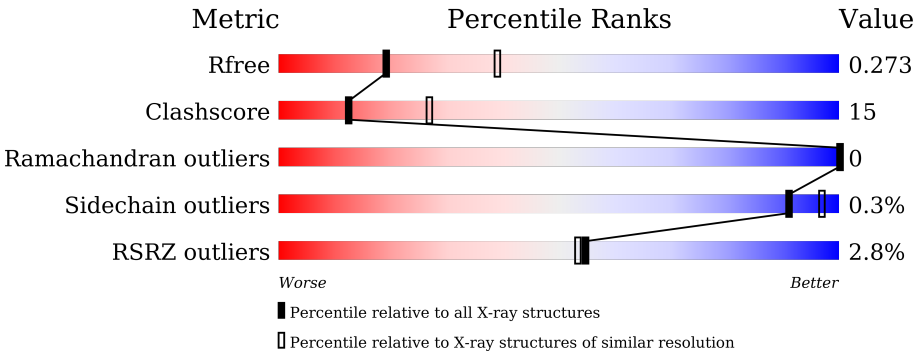
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 2.67 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	4708 (2.70-2.66)
Clashscore	180529	5138 (2.70-2.66)
Ramachandran outliers	177936	5071 (2.70-2.66)
Sidechain outliers	177891	5071 (2.70-2.66)
RSRZ outliers	164620	4708 (2.70-2.66)

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

Mol	Chain	Length	Quality of chain
1	A	269	% 67% 19% 14%
1	B	269	2% 68% 22% 10%
1	C	269	3% 65% 22% • 12%
1	D	269	4% 62% 24% 13%
1	E	269	% 69% 18% 13%
1	F	269	4% 67% 13% • 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10357 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 Endolytic murein transglycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1759	1120	295	338	6			
1	B	241	Total	C	N	O	S	0	0	0
			1813	1150	309	348	6			
1	C	237	Total	C	N	O	S	0	0	0
			1744	1103	295	340	6			
1	D	233	Total	C	N	O	S	0	0	0
			1715	1096	287	327	5			
1	E	233	Total	C	N	O	S	0	0	0
			1741	1105	295	335	6			
1	F	216	Total	C	N	O	S	0	0	0
			1527	962	262	298	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	MET	-	initiating methionine	UNP A0A0D5YEP5
A	288	PRO	LEU	conflict	UNP A0A0D5YEP5
A	357	LEU	-	expression tag	UNP A0A0D5YEP5
A	358	GLU	-	expression tag	UNP A0A0D5YEP5
A	359	HIS	-	expression tag	UNP A0A0D5YEP5
A	360	HIS	-	expression tag	UNP A0A0D5YEP5
A	361	HIS	-	expression tag	UNP A0A0D5YEP5
A	362	HIS	-	expression tag	UNP A0A0D5YEP5
A	363	HIS	-	expression tag	UNP A0A0D5YEP5
A	364	HIS	-	expression tag	UNP A0A0D5YEP5
B	96	MET	-	initiating methionine	UNP A0A0D5YEP5
B	288	PRO	LEU	conflict	UNP A0A0D5YEP5
B	357	LEU	-	expression tag	UNP A0A0D5YEP5
B	358	GLU	-	expression tag	UNP A0A0D5YEP5
B	359	HIS	-	expression tag	UNP A0A0D5YEP5
B	360	HIS	-	expression tag	UNP A0A0D5YEP5
B	361	HIS	-	expression tag	UNP A0A0D5YEP5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	362	HIS	-	expression tag	UNP A0A0D5YEP5
B	363	HIS	-	expression tag	UNP A0A0D5YEP5
B	364	HIS	-	expression tag	UNP A0A0D5YEP5
C	96	MET	-	initiating methionine	UNP A0A0D5YEP5
C	288	PRO	LEU	conflict	UNP A0A0D5YEP5
C	357	LEU	-	expression tag	UNP A0A0D5YEP5
C	358	GLU	-	expression tag	UNP A0A0D5YEP5
C	359	HIS	-	expression tag	UNP A0A0D5YEP5
C	360	HIS	-	expression tag	UNP A0A0D5YEP5
C	361	HIS	-	expression tag	UNP A0A0D5YEP5
C	362	HIS	-	expression tag	UNP A0A0D5YEP5
C	363	HIS	-	expression tag	UNP A0A0D5YEP5
C	364	HIS	-	expression tag	UNP A0A0D5YEP5
D	96	MET	-	initiating methionine	UNP A0A0D5YEP5
D	288	PRO	LEU	conflict	UNP A0A0D5YEP5
D	357	LEU	-	expression tag	UNP A0A0D5YEP5
D	358	GLU	-	expression tag	UNP A0A0D5YEP5
D	359	HIS	-	expression tag	UNP A0A0D5YEP5
D	360	HIS	-	expression tag	UNP A0A0D5YEP5
D	361	HIS	-	expression tag	UNP A0A0D5YEP5
D	362	HIS	-	expression tag	UNP A0A0D5YEP5
D	363	HIS	-	expression tag	UNP A0A0D5YEP5
D	364	HIS	-	expression tag	UNP A0A0D5YEP5
E	96	MET	-	initiating methionine	UNP A0A0D5YEP5
E	288	PRO	LEU	conflict	UNP A0A0D5YEP5
E	357	LEU	-	expression tag	UNP A0A0D5YEP5
E	358	GLU	-	expression tag	UNP A0A0D5YEP5
E	359	HIS	-	expression tag	UNP A0A0D5YEP5
E	360	HIS	-	expression tag	UNP A0A0D5YEP5
E	361	HIS	-	expression tag	UNP A0A0D5YEP5
E	362	HIS	-	expression tag	UNP A0A0D5YEP5
E	363	HIS	-	expression tag	UNP A0A0D5YEP5
E	364	HIS	-	expression tag	UNP A0A0D5YEP5
F	96	MET	-	initiating methionine	UNP A0A0D5YEP5
F	288	PRO	LEU	conflict	UNP A0A0D5YEP5
F	357	LEU	-	expression tag	UNP A0A0D5YEP5
F	358	GLU	-	expression tag	UNP A0A0D5YEP5
F	359	HIS	-	expression tag	UNP A0A0D5YEP5
F	360	HIS	-	expression tag	UNP A0A0D5YEP5
F	361	HIS	-	expression tag	UNP A0A0D5YEP5
F	362	HIS	-	expression tag	UNP A0A0D5YEP5
F	363	HIS	-	expression tag	UNP A0A0D5YEP5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	364	HIS	-	expression tag	UNP A0A0D5YEP5

- Molecule 2 is water.

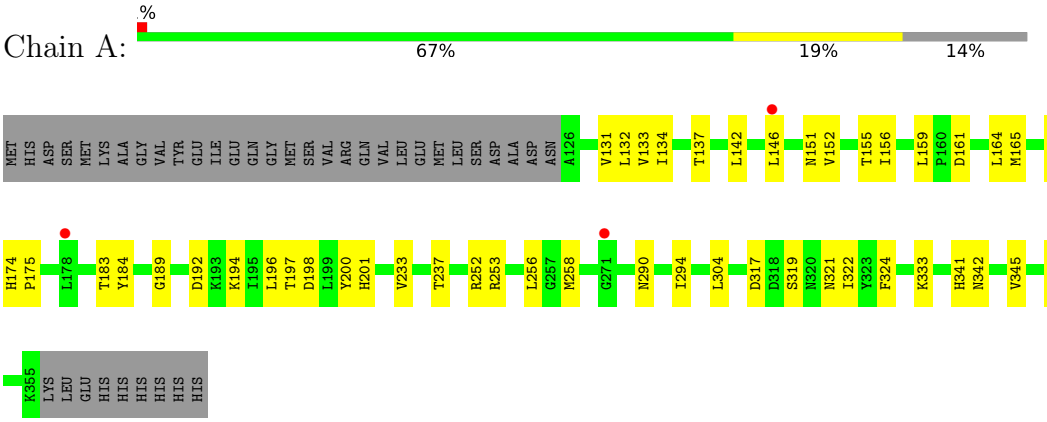
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	13	Total O 13 13	0	0
2	B	13	Total O 13 13	0	0
2	C	12	Total O 12 12	0	0
2	D	5	Total O 5 5	0	0
2	E	7	Total O 7 7	0	0
2	F	8	Total O 8 8	0	0

3 Residue-property plots (i)

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

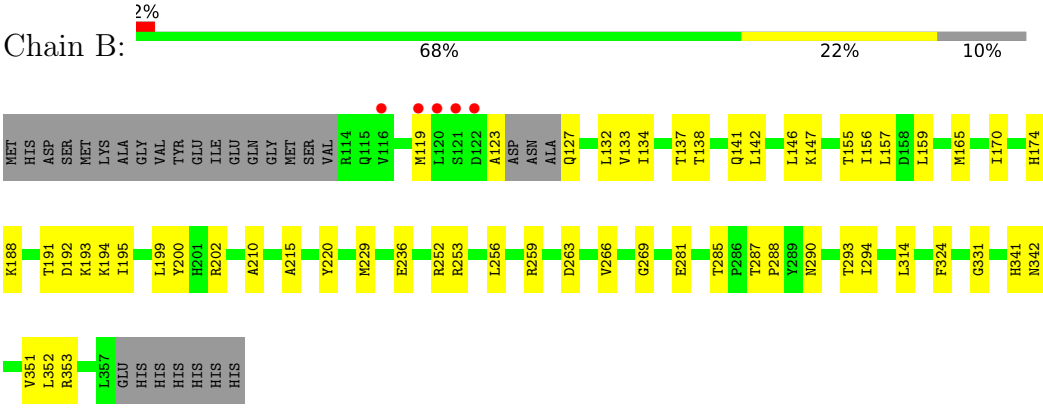
• Molecule 1: Endolytic murein transglycosylase

Chain A:



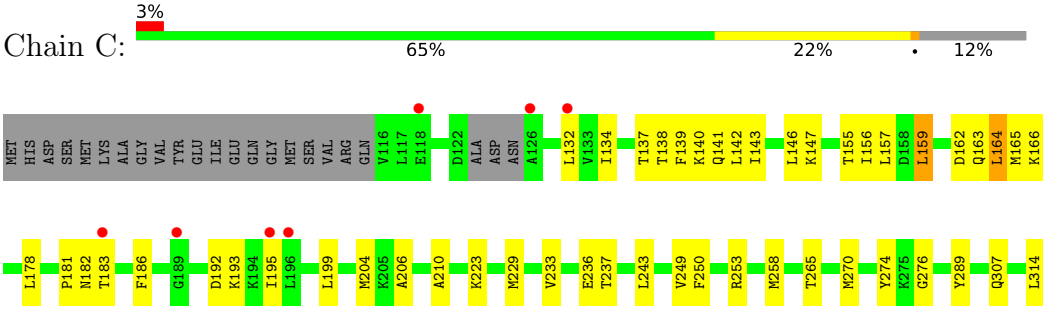
• Molecule 1: Endolytic murein transglycosylase

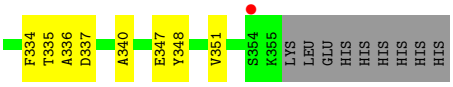
Chain B:



• Molecule 1: Endolytic murein transglycosylase

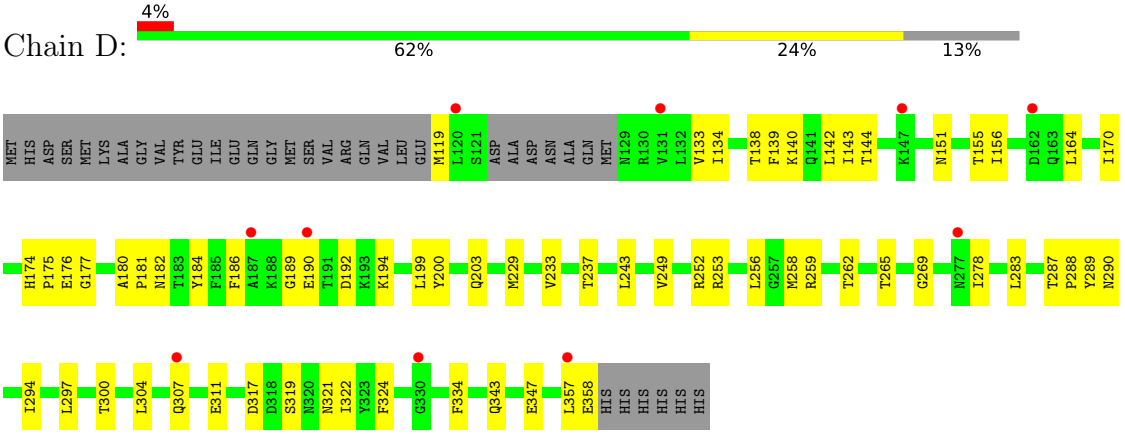
Chain C:





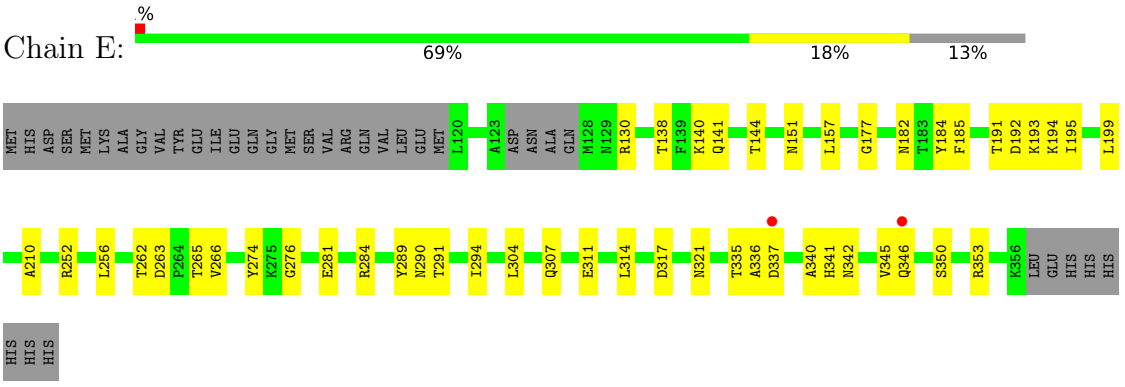
• Molecule 1: Endolytic murein transglycosylase

Chain D:



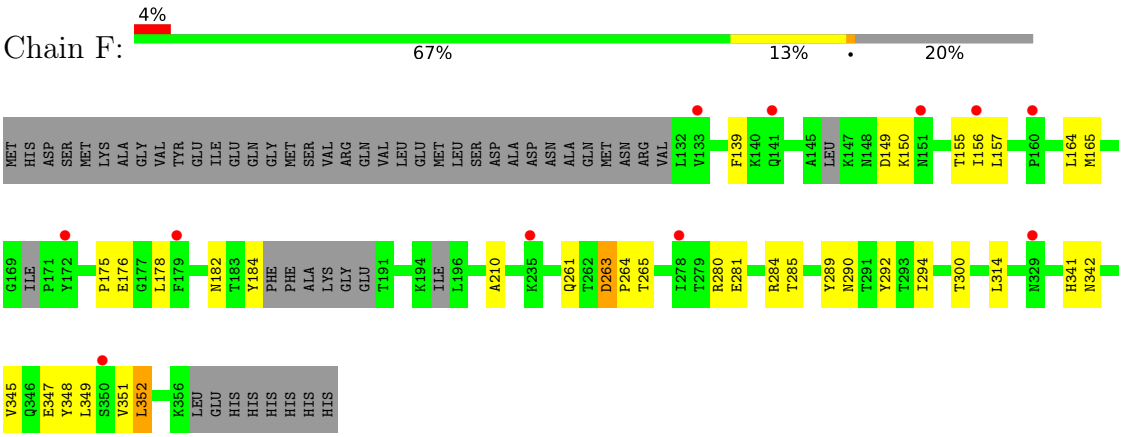
• Molecule 1: Endolytic murein transglycosylase

Chain E:



• Molecule 1: Endolytic murein transglycosylase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.86Å 162.37Å 79.11Å 90.00° 108.96° 90.00°	Depositor
Resolution (Å)	29.47 – 2.67 29.47 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.47-2.67) 99.6 (29.47-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.238 , 0.273 0.240 , 0.273	Depositor DCC
R_{free} test set	2392 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	58.3	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10357	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.36	0/1798	0.56	0/2456
1	B	0.38	0/1850	0.59	0/2522
1	C	0.38	0/1779	0.65	3/2435 (0.1%)
1	D	0.36	0/1753	0.56	0/2400
1	E	0.36	0/1779	0.57	0/2433
1	F	0.37	0/1555	0.61	1/2126 (0.0%)
All	All	0.37	0/10514	0.59	4/14372 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	164	LEU	CB-CG-CD1	8.85	126.04	111.00
1	F	352	LEU	CA-CB-CG	8.09	133.92	115.30
1	C	159	LEU	CB-CG-CD1	-6.57	99.83	111.00
1	C	159	LEU	CB-CG-CD2	5.98	121.16	111.00

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	1759	0	1705	41	0
1	B	1813	0	1717	68	1
1	C	1744	0	1631	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1715	0	1599	57	0
1	E	1741	0	1633	39	1
1	F	1527	0	1356	29	0
2	A	13	0	0	0	0
2	B	13	0	0	4	0
2	C	12	0	0	0	0
2	D	5	0	0	0	0
2	E	7	0	0	1	0
2	F	8	0	0	0	0
All	All	10357	0	9641	301	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (301) 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:159:LEU:HD23	1:C:164:LEU:HA	1.40	1.04
1:C:156:ILE:O	1:C:159:LEU:HD13	1.70	0.91
1:F:182:ASN:HB3	1:F:184:TYR:HD2	1.41	0.86
1:C:140:LYS:HA	1:C:143:ILE:HD13	1.59	0.82
1:B:157:LEU:HD11	1:B:192:ASP:CB	2.08	0.82
1:C:159:LEU:CD2	1:C:164:LEU:HA	2.09	0.82
1:C:159:LEU:HD22	1:C:164:LEU:HD12	1.59	0.82
1:D:133:VAL:HG23	1:D:181:PRO:HA	1.63	0.80
1:A:132:LEU:HD13	1:A:183:THR:HG22	1.64	0.80
1:E:341:HIS:O	1:E:345:VAL:HG13	1.84	0.76
1:B:192:ASP:OD1	1:B:193:LYS:N	2.18	0.76
1:B:285:THR:O	2:B:401:HOH:O	2.03	0.76
1:F:182:ASN:HB3	1:F:184:TYR:CD2	2.21	0.75
1:A:253:ARG:NH1	1:A:322:ILE:O	2.20	0.74
1:B:138:THR:HG23	1:B:141:GLN:H	1.53	0.73
1:C:186:PHE:CB	1:C:195:ILE:HD11	2.19	0.73
1:B:269:GLY:HA3	1:B:287:THR:HG21	1.72	0.72
1:B:191:THR:HG23	1:B:194:LYS:H	1.53	0.72
1:D:287:THR:HG22	1:D:288:PRO:HD2	1.71	0.71
1:F:149:ASP:OD1	1:F:150:LYS:N	2.23	0.71
1:C:139:PHE:CE1	1:C:143:ILE:HD11	2.26	0.71
1:E:138:THR:HG23	1:E:141:GLN:H	1.54	0.71
1:C:159:LEU:HD23	1:C:164:LEU:CA	2.20	0.70
1:B:215:ALA:O	2:B:402:HOH:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:LEU:HA	1:F:352:LEU:HG	1.74	0.70
1:B:342:ASN:O	1:B:345:VAL:HG22	1.92	0.69
1:F:155:THR:O	1:F:156:ILE:HD13	1.93	0.69
1:C:335:THR:HG21	1:C:340:ALA:HB3	1.75	0.69
1:B:157:LEU:CD1	1:B:192:ASP:OD2	2.40	0.68
1:F:341:HIS:O	1:F:345:VAL:HG13	1.93	0.68
1:C:159:LEU:HD22	1:C:164:LEU:CD1	2.22	0.68
1:C:156:ILE:HA	1:C:159:LEU:HD11	1.73	0.68
1:B:155:THR:HG23	1:B:156:ILE:HG23	1.76	0.68
1:B:331:GLY:N	2:B:403:HOH:O	2.26	0.67
1:B:341:HIS:O	1:B:345:VAL:HG13	1.93	0.67
1:B:281:GLU:O	1:B:285:THR:HG23	1.95	0.66
1:D:190:GLU:OE2	1:D:194:LYS:CB	2.43	0.66
1:E:342:ASN:O	1:E:345:VAL:HG22	1.96	0.65
1:A:342:ASN:O	1:A:345:VAL:HG22	1.95	0.65
1:C:156:ILE:CA	1:C:159:LEU:CD1	2.75	0.65
1:B:157:LEU:HD11	1:B:192:ASP:HB2	1.77	0.65
1:B:348:TYR:HA	1:B:351:VAL:HG22	1.79	0.65
1:B:342:ASN:HA	1:B:345:VAL:HG22	1.77	0.65
1:C:159:LEU:CB	1:C:164:LEU:HB2	2.27	0.65
1:C:156:ILE:HA	1:C:159:LEU:CD1	2.27	0.64
1:C:139:PHE:CD1	1:C:143:ILE:HD11	2.32	0.64
1:E:184:TYR:CZ	1:E:199:LEU:HD22	2.33	0.64
1:C:156:ILE:O	1:C:159:LEU:CD1	2.44	0.63
1:C:132:LEU:HD13	1:C:183:THR:HG22	1.81	0.63
1:C:138:THR:HG23	1:C:141:GLN:H	1.62	0.63
1:C:156:ILE:CA	1:C:159:LEU:HD11	2.28	0.63
1:C:162:ASP:OD1	1:C:163:GLN:N	2.31	0.63
1:B:287:THR:HG22	1:B:288:PRO:HD2	1.81	0.62
1:C:192:ASP:OD1	1:C:193:LYS:N	2.33	0.62
1:F:290:ASN:O	1:F:294:ILE:HG12	2.00	0.62
1:B:269:GLY:CA	1:B:287:THR:HG21	2.30	0.62
1:A:134:ILE:HG23	1:A:137:THR:HG23	1.81	0.62
1:E:252:ARG:NH1	1:E:321:ASN:O	2.33	0.61
1:C:335:THR:HG22	1:C:337:ASP:H	1.66	0.61
1:E:335:THR:HG22	1:E:336:ALA:H	1.64	0.61
1:E:191:THR:HG23	1:E:194:LYS:H	1.65	0.60
1:C:233:VAL:O	1:C:237:THR:HG22	2.01	0.60
1:A:341:HIS:O	1:A:345:VAL:HG13	2.02	0.60
1:F:210:ALA:HB1	1:F:314:LEU:HD12	1.84	0.60
1:A:132:LEU:CD1	1:A:183:THR:HG22	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:THR:HG22	1:E:336:ALA:N	2.17	0.59
1:B:263:ASP:O	1:B:266:VAL:HG22	2.02	0.59
1:F:347:GLU:O	1:F:351:VAL:HG23	2.04	0.58
1:E:192:ASP:OD1	1:E:193:LYS:N	2.36	0.58
1:F:342:ASN:O	1:F:345:VAL:HG22	2.04	0.58
1:A:349:LEU:O	1:A:352:LEU:HG	2.04	0.58
1:D:134:ILE:H	1:D:134:ILE:HD12	1.68	0.57
1:A:352:LEU:HD13	1:F:348:TYR:OH	2.04	0.57
1:C:321:ASN:HD22	1:C:334:PHE:CB	2.17	0.57
1:A:252:ARG:NH1	1:A:321:ASN:O	2.38	0.57
1:C:156:ILE:CB	1:C:159:LEU:HD11	2.35	0.57
1:C:147:LYS:HG2	1:C:157:LEU:HD13	1.86	0.57
1:E:291:THR:HA	1:E:294:ILE:HG12	1.86	0.57
1:F:155:THR:C	1:F:156:ILE:HD13	2.26	0.56
1:D:133:VAL:HG12	1:D:142:LEU:HD13	1.86	0.56
1:B:157:LEU:HD11	1:B:192:ASP:HB3	1.87	0.56
1:C:159:LEU:HB3	1:C:164:LEU:HB2	1.88	0.56
1:A:256:LEU:HD13	1:A:258:MET:HE1	1.88	0.56
1:B:132:LEU:HD21	1:B:134:ILE:HG13	1.88	0.55
1:B:155:THR:HG22	1:B:192:ASP:OD1	2.06	0.55
1:C:321:ASN:HD22	1:C:334:PHE:HB3	1.70	0.55
1:D:143:ILE:HG13	1:D:144:THR:N	2.20	0.55
1:D:278:ILE:HG21	1:D:283:LEU:HD21	1.89	0.55
1:C:347:GLU:O	1:C:351:VAL:HG13	2.06	0.55
1:D:134:ILE:HD12	1:D:134:ILE:N	2.21	0.55
1:D:357:LEU:HD12	1:D:358:GLU:CB	2.37	0.55
1:E:252:ARG:NH2	1:E:317:ASP:OD1	2.39	0.55
1:A:348:TYR:OH	1:F:352:LEU:HD13	2.06	0.55
1:B:156:ILE:O	1:B:159:LEU:HD13	2.07	0.55
1:F:164:LEU:C	1:F:164:LEU:HD23	2.28	0.55
1:D:252:ARG:NH2	1:D:317:ASP:OD1	2.36	0.55
1:C:237:THR:HG21	1:C:243:LEU:HD23	1.89	0.54
1:D:252:ARG:NH1	1:D:321:ASN:O	2.41	0.54
1:B:127:GLN:N	1:B:188:LYS:HZ1	2.05	0.54
1:D:177:GLY:O	1:D:203:GLN:NE2	2.39	0.54
1:A:252:ARG:NH2	1:A:317:ASP:OD1	2.40	0.54
1:C:335:THR:HG22	1:C:336:ALA:N	2.22	0.54
1:D:138:THR:HG23	1:D:176:GLU:OE2	2.08	0.54
1:D:229:MET:CE	1:D:297:LEU:HD21	2.38	0.54
1:F:289:TYR:HE2	1:F:300:THR:HG1	1.56	0.54
1:A:134:ILE:HG23	1:A:137:THR:CG2	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:PHE:CZ	1:C:143:ILE:HD11	2.43	0.53
1:B:147:LYS:HG2	1:B:157:LEU:HD23	1.90	0.53
1:B:137:THR:HG23	1:B:141:GLN:HB2	1.91	0.53
1:B:174:HIS:ND1	1:B:175:PRO:HD2	2.23	0.53
1:D:287:THR:HG22	1:D:288:PRO:CD	2.38	0.53
1:D:290:ASN:O	1:D:294:ILE:HG12	2.08	0.53
1:B:342:ASN:HA	1:B:345:VAL:CG2	2.39	0.53
1:C:165:MET:HE2	1:C:165:MET:HA	1.90	0.53
1:D:287:THR:CG2	1:D:288:PRO:HD2	2.39	0.53
1:A:170:ILE:HG23	1:A:200:TYR:CE2	2.44	0.52
1:C:143:ILE:O	1:C:147:LYS:HG3	2.09	0.52
1:B:348:TYR:HA	1:B:351:VAL:CG2	2.39	0.52
1:C:139:PHE:O	1:C:143:ILE:HD12	2.10	0.52
1:D:174:HIS:ND1	1:D:175:PRO:HD2	2.25	0.52
1:E:263:ASP:O	1:E:266:VAL:HG22	2.08	0.52
1:D:324:PHE:HB3	1:D:334:PHE:CD1	2.45	0.52
1:C:134:ILE:HD12	1:C:134:ILE:H	1.75	0.51
1:D:253:ARG:NH1	1:D:259:ARG:O	2.41	0.51
1:D:357:LEU:HD12	1:D:358:GLU:N	2.26	0.51
1:E:157:LEU:CD1	1:E:192:ASP:OD2	2.57	0.51
1:D:156:ILE:O	1:D:164:LEU:HD13	2.11	0.51
1:D:262:THR:O	1:D:265:THR:OG1	2.28	0.51
1:C:229:MET:HE3	1:C:250:PHE:HB3	1.91	0.51
1:C:159:LEU:HB2	1:C:164:LEU:HB2	1.91	0.51
1:F:164:LEU:HD23	1:F:164:LEU:O	2.11	0.51
1:C:335:THR:CG2	1:C:340:ALA:HB3	2.41	0.51
1:A:156:ILE:HD12	1:A:164:LEU:HD12	1.92	0.50
1:F:349:LEU:CA	1:F:352:LEU:HG	2.41	0.50
1:A:133:VAL:HG13	1:A:142:LEU:HD12	1.93	0.50
1:A:349:LEU:HA	1:A:352:LEU:CD2	2.42	0.50
1:B:281:GLU:OE1	1:C:166:LYS:NZ	2.35	0.50
1:C:175:PRO:HA	1:C:178:LEU:HD12	1.93	0.50
1:C:139:PHE:CG	1:C:143:ILE:HD11	2.46	0.50
1:B:134:ILE:H	1:B:134:ILE:HD12	1.76	0.50
1:C:181:PRO:O	1:C:182:ASN:HB2	2.12	0.50
1:E:263:ASP:HA	1:E:266:VAL:HG22	1.93	0.49
1:F:175:PRO:HA	1:F:178:LEU:HD12	1.92	0.49
1:B:195:ILE:O	1:B:199:LEU:HG	2.12	0.49
1:F:265:THR:HB	1:F:289:TYR:O	2.12	0.49
1:B:123:ALA:HB2	1:B:186:PHE:CE2	2.47	0.49
1:C:156:ILE:C	1:C:159:LEU:CD1	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:THR:HG21	1:D:243:LEU:HD23	1.94	0.49
1:E:184:TYR:CE1	1:E:199:LEU:HD22	2.48	0.49
1:E:290:ASN:O	1:E:294:ILE:HG12	2.12	0.49
1:B:133:VAL:HG22	1:B:142:LEU:HD13	1.94	0.49
1:C:348:TYR:O	1:C:351:VAL:HG22	2.13	0.49
1:E:210:ALA:HB1	1:E:314:LEU:HD12	1.93	0.49
1:E:342:ASN:HA	1:E:345:VAL:HG22	1.93	0.49
1:B:170:ILE:HG23	1:B:200:TYR:CE2	2.48	0.49
1:C:335:THR:HG21	1:C:340:ALA:CB	2.43	0.49
1:D:140:LYS:O	1:D:144:THR:HG23	2.13	0.49
1:D:249:VAL:HG11	1:D:324:PHE:HD1	1.78	0.48
1:C:142:LEU:O	1:C:146:LEU:HG	2.13	0.48
1:D:262:THR:HG23	1:D:265:THR:HG23	1.95	0.48
1:B:287:THR:HG22	1:B:288:PRO:CD	2.43	0.48
1:E:263:ASP:O	1:E:266:VAL:CG2	2.62	0.48
1:A:146:LEU:HD23	1:A:152:VAL:HG21	1.96	0.48
1:B:220:TYR:OH	1:B:229:MET:HG2	2.14	0.48
1:B:287:THR:CG2	1:B:288:PRO:HD2	2.44	0.48
1:C:155:THR:OG1	1:C:192:ASP:OD1	2.29	0.48
1:B:290:ASN:OD1	1:B:293:THR:HG23	2.15	0.47
1:C:195:ILE:O	1:C:199:LEU:HD23	2.14	0.47
1:D:170:ILE:HG23	1:D:200:TYR:CE2	2.49	0.47
1:F:281:GLU:O	1:F:285:THR:HG23	2.13	0.47
1:D:229:MET:HE2	1:D:297:LEU:HD21	1.97	0.47
1:C:210:ALA:HB1	1:C:314:LEU:HD12	1.95	0.47
1:D:233:VAL:O	1:D:237:THR:HG22	2.14	0.47
1:D:269:GLY:CA	1:D:287:THR:HG21	2.45	0.47
1:B:119:MET:O	1:B:119:MET:HG3	2.14	0.47
1:B:146:LEU:HB3	1:B:157:LEU:HD21	1.95	0.47
1:E:252:ARG:O	1:E:256:LEU:HD12	2.15	0.47
1:F:349:LEU:HA	1:F:352:LEU:CG	2.44	0.47
1:C:274:TYR:CZ	1:C:276:GLY:HA2	2.49	0.47
1:E:182:ASN:HB3	1:E:184:TYR:CE1	2.50	0.47
1:A:165:MET:HE3	1:A:175:PRO:HB3	1.97	0.47
1:B:138:THR:HG22	1:B:141:GLN:OE1	2.15	0.46
1:E:151:ASN:ND2	2:E:401:HOH:O	2.39	0.46
1:A:174:HIS:CG	1:A:175:PRO:HD2	2.50	0.46
1:D:256:LEU:N	1:D:256:LEU:HD12	2.30	0.46
1:B:119:MET:SD	1:B:202:ARG:NH2	2.87	0.46
1:B:157:LEU:CD1	1:B:192:ASP:CB	2.89	0.46
1:C:164:LEU:O	1:C:164:LEU:HG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ALA:CB	1:B:186:PHE:CD2	2.98	0.46
1:B:348:TYR:O	1:B:351:VAL:HG22	2.15	0.46
1:B:351:VAL:HG23	1:B:352:LEU:N	2.31	0.46
1:D:177:GLY:CA	1:D:304:LEU:HD23	2.46	0.46
1:A:170:ILE:HG23	1:A:200:TYR:CZ	2.50	0.46
1:B:342:ASN:CA	1:B:345:VAL:HG22	2.44	0.46
1:D:138:THR:HG22	1:D:139:PHE:N	2.29	0.46
1:C:229:MET:CE	1:C:250:PHE:HB3	2.45	0.46
1:D:307:GLN:NE2	1:D:311:GLU:OE1	2.48	0.46
1:E:157:LEU:HD12	1:E:192:ASP:OD2	2.15	0.46
1:F:261:GLN:HG2	1:F:292:TYR:CD2	2.50	0.46
1:B:123:ALA:CB	1:B:186:PHE:CE2	2.98	0.46
1:A:131:VAL:HG12	1:A:184:TYR:HB2	1.98	0.46
1:D:262:THR:HG23	1:D:265:THR:CG2	2.46	0.46
1:A:151:ASN:O	1:A:189:GLY:N	2.45	0.46
1:B:252:ARG:O	1:B:256:LEU:HD13	2.15	0.46
1:A:192:ASP:N	1:A:192:ASP:OD1	2.49	0.46
1:A:290:ASN:O	1:A:294:ILE:HG12	2.16	0.46
1:C:206:ALA:HB1	1:C:307:GLN:HG3	1.97	0.46
1:D:343:GLN:O	1:D:347:GLU:HG3	2.16	0.46
1:A:352:LEU:C	1:A:352:LEU:HD12	2.36	0.45
1:B:348:TYR:CA	1:B:351:VAL:HG22	2.45	0.45
1:B:285:THR:OG1	2:B:401:HOH:O	2.18	0.45
1:E:350:SER:HA	1:E:353:ARG:CZ	2.46	0.45
1:C:204:MET:CE	1:C:223:LYS:HE3	2.46	0.45
1:C:249:VAL:HG11	1:C:324:PHE:CD1	2.51	0.45
1:B:210:ALA:HB1	1:B:314:LEU:HD12	1.98	0.45
1:C:253:ARG:HG2	1:C:258:MET:CE	2.46	0.45
1:D:249:VAL:HG11	1:D:324:PHE:CD1	2.52	0.45
1:B:155:THR:HG23	1:B:156:ILE:HG12	1.98	0.45
1:F:157:LEU:N	1:F:157:LEU:HD12	2.32	0.45
1:B:133:VAL:CG2	1:B:142:LEU:HD13	2.46	0.45
1:E:184:TYR:CZ	1:E:199:LEU:CD2	2.99	0.45
1:B:290:ASN:O	1:B:294:ILE:HG12	2.16	0.45
1:E:140:LYS:O	1:E:144:THR:HG23	2.17	0.45
1:F:263:ASP:N	1:F:264:PRO:CD	2.80	0.45
1:C:138:THR:HG22	1:C:141:GLN:OE1	2.16	0.45
1:D:180:ALA:HB2	1:D:203:GLN:HB2	1.99	0.45
1:D:140:LYS:O	1:D:143:ILE:HG12	2.16	0.44
1:A:197:THR:HG22	1:A:201:HIS:CD2	2.52	0.44
1:B:132:LEU:CD2	1:B:134:ILE:HG13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLU:HG2	1:B:324:PHE:HZ	1.83	0.44
1:B:342:ASN:C	1:B:345:VAL:HG22	2.36	0.44
1:A:233:VAL:O	1:A:237:THR:HG22	2.17	0.44
1:A:256:LEU:CD1	1:A:258:MET:HE1	2.46	0.44
1:C:236:GLU:HG2	1:C:324:PHE:HZ	1.82	0.44
1:A:155:THR:OG1	1:A:192:ASP:OD1	2.26	0.44
1:B:132:LEU:C	1:B:132:LEU:HD23	2.38	0.44
1:D:133:VAL:CG1	1:D:142:LEU:HD13	2.48	0.44
1:A:156:ILE:HB	1:A:159:LEU:HD13	2.00	0.43
1:D:289:TYR:HH	1:D:300:THR:HG1	1.52	0.43
1:E:274:TYR:CZ	1:E:276:GLY:HA2	2.52	0.43
1:F:156:ILE:O	1:F:164:LEU:HD12	2.17	0.43
1:D:289:TYR:OH	1:D:300:THR:OG1	2.29	0.43
1:A:352:LEU:CD1	1:F:348:TYR:OH	2.65	0.43
1:B:137:THR:HG22	1:B:138:THR:O	2.19	0.43
1:D:142:LEU:HD12	1:D:142:LEU:O	2.18	0.43
1:D:269:GLY:HA3	1:D:287:THR:HG21	2.01	0.43
1:C:134:ILE:HD12	1:C:134:ILE:N	2.33	0.43
1:F:280:ARG:O	1:F:284:ARG:HG3	2.18	0.43
1:B:165:MET:SD	1:B:175:PRO:HB3	2.59	0.43
1:D:155:THR:HG22	1:D:192:ASP:OD2	2.18	0.43
1:C:165:MET:HE2	1:C:168:LEU:HD12	2.00	0.43
1:C:156:ILE:CB	1:C:159:LEU:CD1	2.96	0.42
1:D:138:THR:HG22	1:D:140:LYS:H	1.83	0.42
1:E:195:ILE:O	1:E:199:LEU:HG	2.19	0.42
1:E:307:GLN:NE2	1:E:311:GLU:OE1	2.51	0.42
1:C:157:LEU:HD23	1:C:157:LEU:HA	1.87	0.42
1:C:204:MET:HE1	1:C:223:LYS:HE3	2.00	0.42
1:E:265:THR:HB	1:E:289:TYR:O	2.19	0.42
1:A:168:LEU:HD21	1:A:196:LEU:HB2	2.01	0.42
1:F:139:PHE:N	1:F:176:GLU:OE1	2.48	0.42
1:C:265:THR:HB	1:C:289:TYR:O	2.19	0.42
1:E:281:GLU:HA	1:E:284:ARG:HB2	2.02	0.42
1:C:249:VAL:HG11	1:C:324:PHE:HD1	1.83	0.42
1:E:130:ARG:HB2	1:E:185:PHE:CE2	2.54	0.42
1:E:262:THR:O	1:E:265:THR:OG1	2.31	0.42
1:E:335:THR:HG21	1:E:337:ASP:OD1	2.20	0.42
1:E:335:THR:HG21	1:E:340:ALA:HB3	2.02	0.42
1:B:157:LEU:HD13	1:B:192:ASP:OD2	2.18	0.42
1:F:164:LEU:HD22	1:F:165:MET:HE2	2.02	0.42
1:A:349:LEU:HA	1:A:352:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:THR:HG22	1:B:141:GLN:HG3	2.02	0.42
1:B:157:LEU:N	1:B:157:LEU:HD12	2.34	0.42
1:A:161:ASP:HB3	1:A:175:PRO:HD3	2.02	0.41
1:C:270:MET:HE3	1:C:270:MET:HB2	1.88	0.41
1:E:177:GLY:H	1:E:304:LEU:HD23	1.85	0.41
1:A:137:THR:O	1:A:304:LEU:HG	2.20	0.41
1:B:157:LEU:HD12	1:B:192:ASP:OD2	2.19	0.41
1:B:159:LEU:N	1:B:159:LEU:HD12	2.35	0.41
1:D:258:MET:CE	1:D:322:ILE:HD12	2.50	0.41
1:E:266:VAL:HG12	1:E:290:ASN:CG	2.40	0.41
1:A:131:VAL:O	1:A:131:VAL:CG1	2.69	0.41
1:D:140:LYS:HA	1:D:143:ILE:HG12	2.03	0.41
1:D:177:GLY:HA2	1:D:304:LEU:HD23	2.02	0.41
1:A:194:LYS:HE3	1:A:198:ASP:OD2	2.21	0.41
1:A:252:ARG:NE	1:A:319:SER:O	2.53	0.41
1:E:345:VAL:HG23	1:E:346:GLN:N	2.35	0.41
1:D:133:VAL:HG23	1:D:182:ASN:H	1.86	0.41
1:D:184:TYR:CZ	1:D:199:LEU:HD22	2.55	0.41
1:A:324:PHE:HA	1:A:333:LYS:O	2.20	0.41
1:C:132:LEU:CD1	1:C:183:THR:HG22	2.49	0.41
1:A:165:MET:HE2	1:A:168:LEU:HD12	2.03	0.41
1:C:147:LYS:HG2	1:C:157:LEU:CD1	2.51	0.41
1:D:184:TYR:CZ	1:D:199:LEU:CD2	3.04	0.41
1:D:181:PRO:O	1:D:182:ASN:HB2	2.21	0.41
1:E:182:ASN:HB3	1:E:184:TYR:CZ	2.55	0.41
1:C:137:THR:HG22	1:C:138:THR:O	2.21	0.40
1:D:155:THR:HG23	1:D:156:ILE:N	2.35	0.40
1:D:252:ARG:NE	1:D:319:SER:O	2.55	0.40
1:D:151:ASN:O	1:D:189:GLY:N	2.51	0.40
1:C:143:ILE:HD12	1:C:143:ILE:H	1.86	0.40
1:B:253:ARG:NH1	1:B:259:ARG:O	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ARG:NH2	1:E:263:ASP:OD2[2_556]	2.05	0.15

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	228/269 (85%)	223 (98%)	5 (2%)	0	100	100
1	B	237/269 (88%)	230 (97%)	7 (3%)	0	100	100
1	C	233/269 (87%)	228 (98%)	5 (2%)	0	100	100
1	D	229/269 (85%)	223 (97%)	6 (3%)	0	100	100
1	E	229/269 (85%)	225 (98%)	4 (2%)	0	100	100
1	F	206/269 (77%)	201 (98%)	5 (2%)	0	100	100
All	All	1362/1614 (84%)	1330 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	184/231 (80%)	184 (100%)	0	100	100
1	B	181/231 (78%)	181 (100%)	0	100	100
1	C	173/231 (75%)	173 (100%)	0	100	100
1	D	166/231 (72%)	164 (99%)	2 (1%)	67	85
1	E	173/231 (75%)	173 (100%)	0	100	100
1	F	138/231 (60%)	137 (99%)	1 (1%)	81	92
All	All	1015/1386 (73%)	1012 (100%)	3 (0%)	91	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	119	MET
1	D	186	PHE
1	F	263	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	C	129	ASN
1	C	321	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 oligosaccharides 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	230/269 (85%)	-0.02	3 (1%)	74	74	38, 55, 85, 110	0
1	B	241/269 (89%)	0.13	5 (2%)	63	62	35, 61, 92, 143	0
1	C	237/269 (88%)	0.37	8 (3%)	48	46	41, 65, 102, 112	0
1	D	233/269 (86%)	0.31	10 (4%)	40	39	33, 66, 106, 116	0
1	E	233/269 (86%)	0.30	2 (0%)	81	80	36, 67, 97, 106	0
1	F	216/269 (80%)	0.65	11 (5%)	34	33	43, 79, 118, 141	0
All	All	1390/1614 (86%)	0.28	39 (2%)	55	53	33, 64, 105, 143	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	LEU	4.6
1	F	278	ILE	4.1
1	F	179	PHE	3.7
1	C	196	LEU	3.7
1	E	346	GLN	3.5
1	B	116	VAL	3.3
1	B	119	MET	3.3
1	C	126	ALA	3.3
1	F	151	ASN	3.3
1	C	354	SER	3.1
1	F	172	TYR	2.9
1	D	131	VAL	2.9
1	C	195	ILE	2.9
1	D	357	LEU	2.8
1	D	162	ASP	2.8
1	D	330	GLY	2.7
1	F	156	ILE	2.6
1	C	189	GLY	2.5
1	B	121	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	132	LEU	2.4
1	D	147	LYS	2.4
1	A	178	LEU	2.3
1	D	187	ALA	2.3
1	A	271	GLY	2.3
1	F	350	SER	2.3
1	D	190	GLU	2.2
1	F	133	VAL	2.2
1	C	183	THR	2.2
1	D	277	ASN	2.2
1	E	337	ASP	2.2
1	D	120	LEU	2.2
1	B	122	ASP	2.2
1	C	118	GLU	2.1
1	D	307	GLN	2.1
1	F	160	PRO	2.1
1	F	235	LYS	2.1
1	F	141	GLN	2.1
1	A	146	LEU	2.0
1	F	329	ASN	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.