Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:20 AM GMT

PDB ID	:	2WOO
Title	:	NUCLEOTIDE-FREE FORM OF S. POMBE GET3
Authors	:	Mateja, A.; Szlachcic, A.; Downing, M.E.; Dobosz, M.; Mariappan, M.; Hegde, R.S.; Keenan, R.J.
Deposited on	:	2009-07-27
Resolution	:	3.01 Å(reported)

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

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

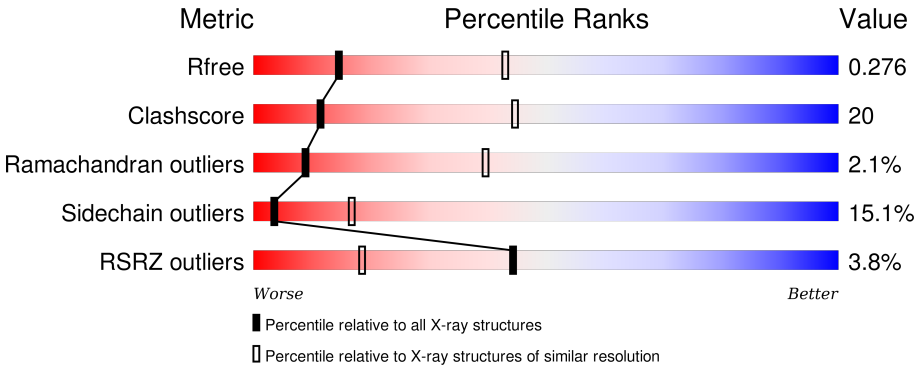
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.01 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	329	59% 26% 6% 8%
1	B	329	5% 57% 29% 6% 8%
1	C	329	2% 58% 27% 7% 8%
1	D	329	2% 58% 28% 6% 8%
1	E	329	4% 57% 27% 9% 8%

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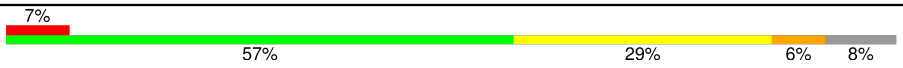
Mol	Chain	Length	Quality of chain
1	F	329	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14115 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 ATPASE GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2352	1494	386	451	21			
1	B	303	Total	C	N	O	S	0	0	0
			2352	1494	386	451	21			
1	C	303	Total	C	N	O	S	0	0	0
			2352	1494	386	451	21			
1	D	303	Total	C	N	O	S	0	0	0
			2352	1494	386	451	21			
1	E	303	Total	C	N	O	S	0	0	0
			2352	1494	386	451	21			
1	F	303	Total	C	N	O	S	0	0	0
			2352	1494	386	451	21			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

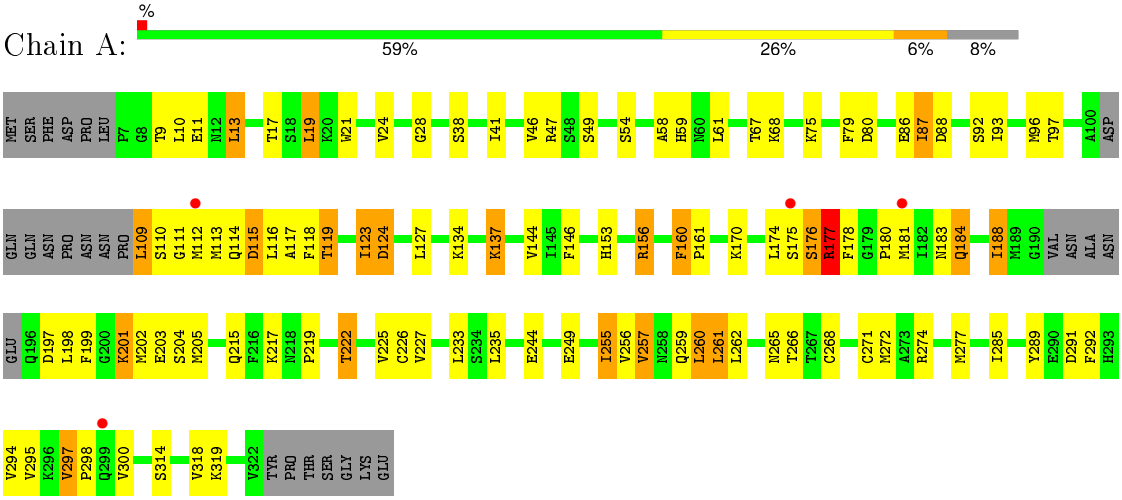
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

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.

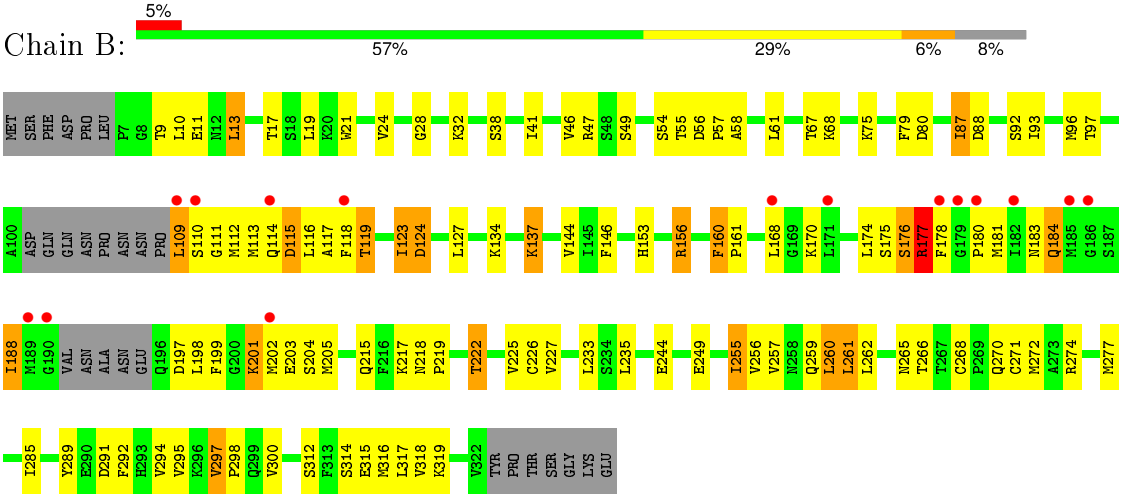
- Molecule 1: ATPASE GET3

Chain A:



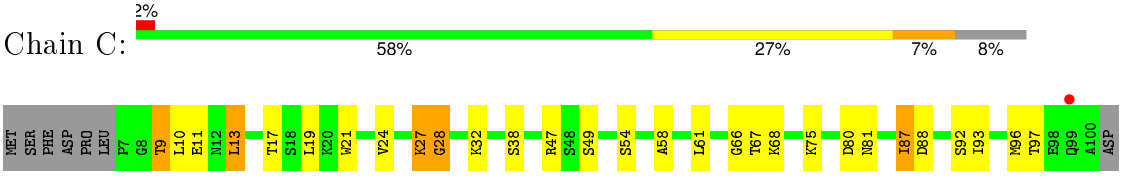
- Molecule 1: ATPASE GET3

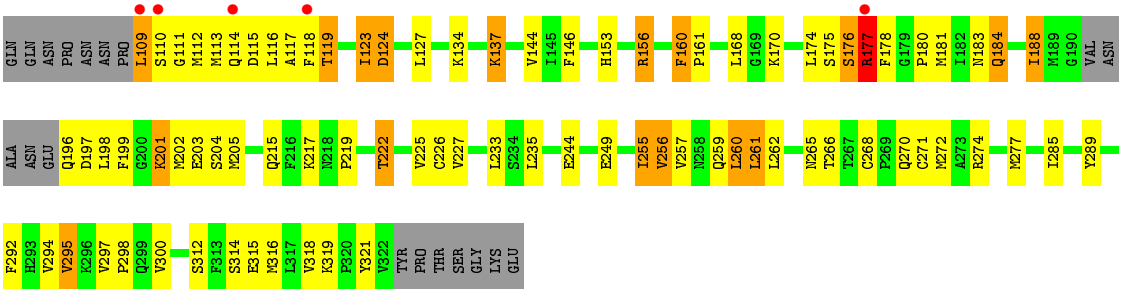
Chain B:



- Molecule 1: ATPASE GET3

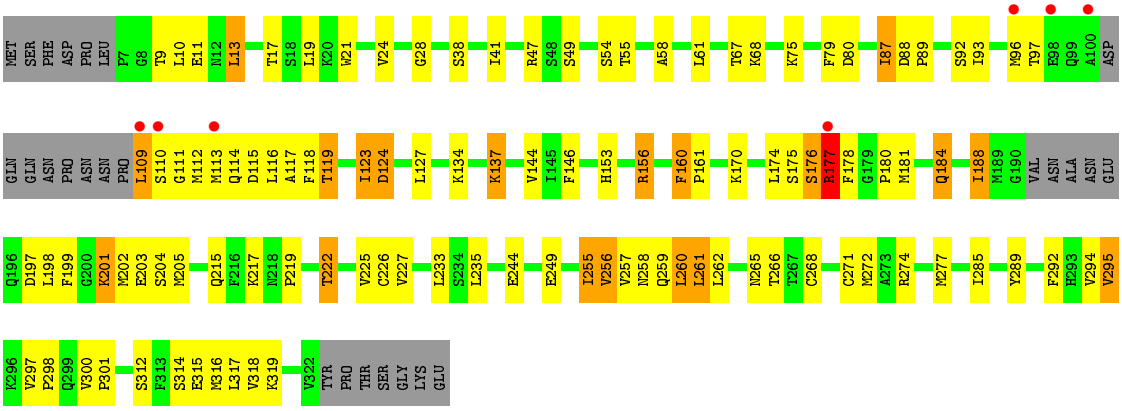
Chain C:





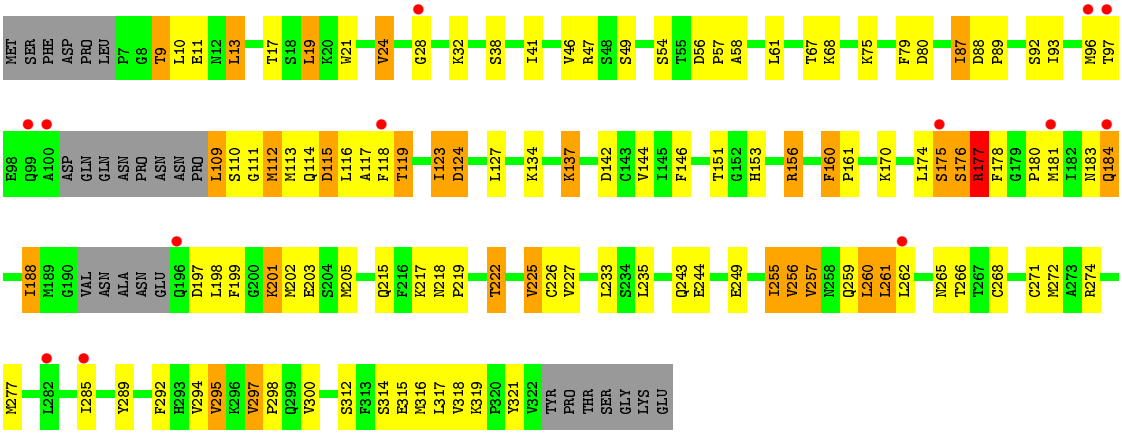
• Molecule 1: ATPASE GET3

Chain D:



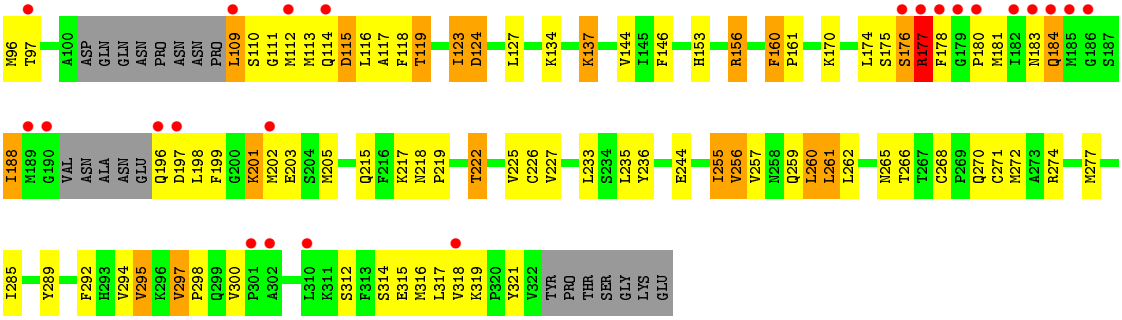
• Molecule 1: ATPASE GET3

Chain E:



• Molecule 1: ATPASE GET3

Chain F:


M96 T97 A100 ASP GLN GLN ASN PRO ASN ASN PRO L109 S110 G111 M112 M113 Q114 D115 L116 A117 F118 T119 I123 D124 L127 K134 K137 V144 I145 F146 H153 R156 F160 P161 K170 L174 S175 S176 R177 F178 G179 P180 M181 I182 N183 Q184 N185 G186 S187
I188 M189 G190 VAL ASN ALA ASN GLU Q196 D197 L198 F199 G200 K201 M202 E203 S204 M205 Q215 F216 K217 N218 P219 T222 V225 C226 V227 L233 S234 L235 Y236 E244 I255 V256 V257 N258 Q259 L260 L261 L262 N265 T266 T267 C268 P269 Q270 C271 M272 A273 R274 M277
I285 Y289 F292 H293 V294 V295 K296 V297 P298 Q299 V300 P301 A302 L310 K311 S312 F313 S314 E315 M316 L317 V318 K319 P320 Y321 V322 TYR PRO THR SER GLY LYS GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.80Å 92.92Å 286.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.69 – 3.01 40.69 – 3.01	Depositor EDS
% Data completeness (in resolution range)	93.8 (40.69-3.01) 93.9 (40.69-3.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.237 , 0.288 0.226 , 0.276	Depositor DCC
R_{free} test set	1889 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	96.1	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 62.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 37729 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14115	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.41	0/2391	0.53	0/3223
1	B	0.38	0/2391	0.53	0/3223
1	C	0.45	0/2391	0.54	0/3223
1	D	0.38	0/2391	0.53	0/3223
1	E	0.38	0/2391	0.53	0/3223
1	F	0.38	0/2391	0.53	0/3223
All	All	0.40	0/14346	0.53	0/19338

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	2352	0	2370	94	0
1	B	2352	0	2370	101	0
1	C	2352	0	2370	122	1
1	D	2352	0	2370	108	0
1	E	2352	0	2370	128	1
1	F	2352	0	2370	108	4
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	F	1	0	0	0	0
All	All	14115	0	14220	580	5

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 20.

All (580) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLN:HG3	1:F:177:ARG:HH21	1.19	1.08
1:A:123:ILE:H	1:A:123:ILE:HD12	1.23	1.02
1:D:123:ILE:HD12	1:D:123:ILE:H	1.25	1.01
1:F:123:ILE:H	1:F:123:ILE:HD12	1.25	0.99
1:F:117:ALA:HA	1:F:123:ILE:HD11	1.45	0.98
1:C:123:ILE:H	1:C:123:ILE:HD12	1.29	0.97
1:E:117:ALA:HA	1:E:123:ILE:HD11	1.46	0.97
1:B:123:ILE:HD12	1:B:123:ILE:H	1.26	0.97
1:E:123:ILE:H	1:E:123:ILE:HD12	1.28	0.95
1:B:117:ALA:HA	1:B:123:ILE:HD11	1.47	0.95
1:C:117:ALA:HA	1:C:123:ILE:HD11	1.46	0.94
1:C:113:MET:HE1	1:E:177:ARG:HD2	1.50	0.94
1:B:118:PHE:HZ	1:E:118:PHE:CZ	1.85	0.93
1:A:117:ALA:HA	1:A:123:ILE:HD11	1.50	0.93
1:D:117:ALA:HA	1:D:123:ILE:HD11	1.49	0.92
1:D:118:PHE:HZ	1:F:118:PHE:CE2	1.88	0.90
1:B:118:PHE:CZ	1:C:118:PHE:HZ	1.90	0.89
1:A:177:ARG:HE	1:D:114:GLN:HG3	1.40	0.86
1:C:114:GLN:HE22	1:E:112:MET:CE	1.89	0.84
1:A:123:ILE:HD12	1:A:123:ILE:N	1.95	0.81
1:A:115:ASP:OD1	1:F:115:ASP:OD1	1.99	0.81
1:D:123:ILE:HD12	1:D:123:ILE:N	1.97	0.80
1:C:113:MET:CE	1:C:124:ASP:HB3	2.12	0.80
1:B:118:PHE:CZ	1:E:118:PHE:CZ	2.69	0.80
1:A:114:GLN:HG3	1:F:177:ARG:NH2	1.96	0.79
1:C:124:ASP:CG	1:E:175:SER:HG	1.85	0.79
1:B:123:ILE:HD12	1:B:123:ILE:N	1.98	0.78
1:E:235:LEU:HD21	1:E:285:ILE:HD11	1.65	0.78
1:B:123:ILE:CD1	1:B:123:ILE:H	1.92	0.78
1:C:114:GLN:HG3	1:E:177:ARG:NH2	1.99	0.77
1:A:115:ASP:CG	1:F:115:ASP:OD1	2.23	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:MET:CE	1:E:124:ASP:HB3	2.15	0.77
1:D:170:LYS:NZ	1:F:118:PHE:HB2	1.99	0.77
1:D:113:MET:CE	1:D:124:ASP:HB3	2.16	0.76
1:C:123:ILE:N	1:C:123:ILE:HD12	2.00	0.76
1:A:113:MET:CE	1:A:124:ASP:HB3	2.16	0.75
1:E:123:ILE:HD12	1:E:123:ILE:N	2.00	0.75
1:A:123:ILE:H	1:A:123:ILE:CD1	1.89	0.75
1:F:123:ILE:N	1:F:123:ILE:HD12	1.99	0.75
1:C:118:PHE:CE2	1:E:115:ASP:HB3	2.21	0.75
1:B:115:ASP:OD1	1:E:115:ASP:OD2	2.04	0.74
1:C:21:TRP:CD1	1:C:146:PHE:HE2	2.05	0.74
1:C:114:GLN:NE2	1:E:112:MET:HE2	2.03	0.73
1:D:21:TRP:HD1	1:D:146:PHE:HE2	1.35	0.73
1:D:21:TRP:CD1	1:D:146:PHE:HE2	2.06	0.73
1:F:235:LEU:HD21	1:F:285:ILE:HD11	1.69	0.73
1:C:123:ILE:H	1:C:123:ILE:CD1	1.92	0.73
1:B:113:MET:CE	1:B:124:ASP:HB3	2.18	0.73
1:B:118:PHE:CZ	1:C:118:PHE:CZ	2.76	0.72
1:E:21:TRP:CD1	1:E:146:PHE:HE2	2.08	0.72
1:C:113:MET:CE	1:E:177:ARG:HD2	2.18	0.72
1:B:235:LEU:HD21	1:B:285:ILE:HD11	1.71	0.72
1:A:21:TRP:CD1	1:A:146:PHE:HE2	2.07	0.71
1:F:21:TRP:CD1	1:F:146:PHE:HE2	2.07	0.71
1:D:110:SER:HA	1:D:113:MET:HB3	1.73	0.71
1:C:110:SER:HA	1:C:113:MET:HB3	1.73	0.71
1:C:114:GLN:HG3	1:E:177:ARG:HH21	1.53	0.71
1:F:123:ILE:H	1:F:123:ILE:CD1	1.93	0.71
1:C:124:ASP:OD2	1:E:177:ARG:HD3	1.91	0.70
1:C:117:ALA:HB3	1:E:178:PHE:CZ	2.26	0.70
1:B:10:LEU:HD22	1:B:13:LEU:HD22	1.73	0.70
1:D:10:LEU:HD22	1:D:13:LEU:HD22	1.73	0.70
1:D:235:LEU:HD21	1:D:285:ILE:HD11	1.74	0.70
1:C:114:GLN:NE2	1:E:112:MET:CE	2.54	0.70
1:D:118:PHE:CZ	1:F:118:PHE:CZ	2.79	0.70
1:D:119:THR:HG21	1:F:118:PHE:CD1	2.27	0.70
1:A:110:SER:HA	1:A:113:MET:HB3	1.74	0.70
1:F:10:LEU:HD22	1:F:13:LEU:HD22	1.72	0.70
1:C:21:TRP:HD1	1:C:146:PHE:HE2	1.40	0.69
1:E:21:TRP:HD1	1:E:146:PHE:HE2	1.39	0.69
1:C:124:ASP:CG	1:E:175:SER:OG	2.30	0.69
1:D:118:PHE:CZ	1:F:118:PHE:CE2	2.78	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:TRP:CD1	1:B:146:PHE:HE2	2.09	0.69
1:C:113:MET:HE3	1:C:124:ASP:HB3	1.75	0.69
1:A:21:TRP:HD1	1:A:146:PHE:HE2	1.40	0.69
1:C:235:LEU:HD21	1:C:285:ILE:HD11	1.74	0.69
1:F:21:TRP:HD1	1:F:146:PHE:HE2	1.40	0.69
1:C:201:LYS:NZ	1:C:201:LYS:HB2	2.07	0.69
1:F:113:MET:CE	1:F:124:ASP:HB3	2.22	0.69
1:A:235:LEU:HD21	1:A:285:ILE:HD11	1.74	0.69
1:A:177:ARG:HE	1:D:114:GLN:CG	2.03	0.69
1:E:110:SER:HA	1:E:113:MET:HB3	1.75	0.69
1:B:118:PHE:HZ	1:E:118:PHE:CE2	2.11	0.68
1:E:113:MET:HE1	1:E:124:ASP:HB3	1.74	0.68
1:D:170:LYS:HZ3	1:F:118:PHE:HB2	1.58	0.68
1:C:117:ALA:HB3	1:E:178:PHE:HZ	1.56	0.68
1:F:201:LYS:NZ	1:F:201:LYS:HB2	2.09	0.68
1:B:21:TRP:HD1	1:B:146:PHE:HE2	1.41	0.67
1:A:201:LYS:NZ	1:A:201:LYS:HB2	2.09	0.67
1:C:114:GLN:HE22	1:E:112:MET:HE3	1.57	0.67
1:B:110:SER:HA	1:B:113:MET:HB3	1.75	0.67
1:C:215:GLN:O	1:C:222:THR:HG23	1.94	0.67
1:D:201:LYS:HB2	1:D:201:LYS:NZ	2.10	0.67
1:F:110:SER:HA	1:F:113:MET:HB3	1.76	0.66
1:B:201:LYS:NZ	1:B:201:LYS:HB2	2.08	0.66
1:A:177:ARG:HH21	1:D:114:GLN:HG3	1.60	0.66
1:D:118:PHE:HZ	1:F:118:PHE:CZ	2.14	0.66
1:E:10:LEU:HD22	1:E:13:LEU:HD22	1.77	0.66
1:E:201:LYS:NZ	1:E:201:LYS:HB2	2.11	0.65
1:D:170:LYS:HE2	1:F:118:PHE:HA	1.79	0.64
1:B:176:SER:O	1:B:177:ARG:HG2	1.97	0.64
1:A:176:SER:O	1:A:177:ARG:HG2	1.98	0.64
1:E:199:PHE:O	1:E:202:MET:HB3	1.98	0.64
1:B:113:MET:HE3	1:B:124:ASP:HB3	1.79	0.64
1:C:176:SER:O	1:C:177:ARG:HG2	1.98	0.64
1:D:123:ILE:H	1:D:123:ILE:CD1	1.90	0.64
1:E:215:GLN:O	1:E:222:THR:HG23	1.98	0.63
1:A:199:PHE:O	1:A:202:MET:HB3	1.98	0.63
1:D:199:PHE:O	1:D:202:MET:HB3	1.98	0.63
1:F:199:PHE:O	1:F:202:MET:HB3	1.98	0.63
1:C:113:MET:CE	1:E:177:ARG:CD	2.76	0.63
1:C:10:LEU:HD22	1:C:13:LEU:HD22	1.81	0.63
1:D:215:GLN:O	1:D:222:THR:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ALA:HA	1:D:123:ILE:CD1	2.27	0.63
1:D:176:SER:O	1:D:177:ARG:HG2	1.99	0.63
1:A:177:ARG:NE	1:D:114:GLN:HG3	2.10	0.62
1:C:110:SER:O	1:E:177:ARG:NH2	2.32	0.62
1:F:215:GLN:O	1:F:222:THR:HG23	1.98	0.62
1:B:153:HIS:O	1:B:156:ARG:HG3	1.99	0.62
1:E:117:ALA:HA	1:E:123:ILE:CD1	2.26	0.62
1:A:10:LEU:HD22	1:A:13:LEU:HD22	1.81	0.62
1:C:124:ASP:OD2	1:E:175:SER:OG	2.17	0.62
1:B:199:PHE:O	1:B:202:MET:HB3	1.99	0.62
1:F:176:SER:O	1:F:177:ARG:HG2	2.00	0.62
1:F:38:SER:HB3	1:F:314:SER:HA	1.81	0.62
1:A:215:GLN:O	1:A:222:THR:HG23	2.00	0.61
1:B:177:ARG:NH1	1:B:177:ARG:HB2	2.15	0.61
1:C:117:ALA:HA	1:C:123:ILE:CD1	2.26	0.61
1:C:38:SER:HB3	1:C:314:SER:HA	1.83	0.61
1:E:176:SER:O	1:E:177:ARG:HG2	2.01	0.60
1:F:153:HIS:O	1:F:156:ARG:HG3	2.01	0.60
1:A:9:THR:HG23	1:A:11:GLU:H	1.65	0.60
1:A:117:ALA:HA	1:A:123:ILE:CD1	2.29	0.60
1:C:199:PHE:O	1:C:202:MET:HB3	1.99	0.60
1:E:38:SER:HB3	1:E:314:SER:HA	1.84	0.60
1:D:177:ARG:HB2	1:D:177:ARG:NH1	2.16	0.60
1:E:153:HIS:O	1:E:156:ARG:HG3	2.01	0.60
1:F:113:MET:HE3	1:F:124:ASP:HB3	1.83	0.60
1:F:117:ALA:HA	1:F:123:ILE:CD1	2.26	0.60
1:A:38:SER:HB3	1:A:314:SER:HA	1.84	0.59
1:E:177:ARG:HB2	1:E:177:ARG:NH1	2.17	0.59
1:F:9:THR:HG23	1:F:11:GLU:H	1.67	0.59
1:C:9:THR:HG23	1:C:11:GLU:H	1.67	0.59
1:D:203:GLU:OE1	1:E:243:GLN:HG2	2.01	0.59
1:D:153:HIS:O	1:D:156:ARG:HG3	2.02	0.59
1:E:9:THR:HG23	1:E:11:GLU:H	1.67	0.59
1:D:9:THR:HG23	1:D:11:GLU:H	1.68	0.59
1:A:153:HIS:O	1:A:156:ARG:HG3	2.02	0.59
1:C:177:ARG:HB2	1:C:177:ARG:NH1	2.18	0.59
1:F:118:PHE:CE1	1:F:119:THR:HG23	2.38	0.59
1:D:127:LEU:HD22	1:D:188:ILE:HD11	1.85	0.59
1:B:9:THR:HG23	1:B:11:GLU:H	1.68	0.59
1:D:38:SER:HB3	1:D:314:SER:HA	1.83	0.59
1:A:177:ARG:HB2	1:A:177:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:LEU:HD22	1:F:261:LEU:H	1.68	0.58
1:F:127:LEU:HD22	1:F:188:ILE:HD11	1.83	0.58
1:F:109:LEU:HD23	1:F:111:GLY:H	1.69	0.58
1:C:109:LEU:HD23	1:C:111:GLY:H	1.69	0.58
1:C:113:MET:HE1	1:E:177:ARG:CD	2.31	0.58
1:B:127:LEU:HD22	1:B:188:ILE:HD11	1.85	0.58
1:B:38:SER:HB3	1:B:314:SER:HA	1.85	0.58
1:F:177:ARG:NH1	1:F:177:ARG:HB2	2.19	0.57
1:A:113:MET:HE3	1:A:124:ASP:HB3	1.86	0.57
1:B:109:LEU:HD23	1:B:111:GLY:H	1.70	0.57
1:C:110:SER:HB2	1:E:177:ARG:NH2	2.20	0.56
1:A:124:ASP:OD2	1:F:177:ARG:HD3	2.05	0.56
1:D:113:MET:HE3	1:D:124:ASP:HB3	1.87	0.56
1:E:151:THR:HB	1:F:236:TYR:CZ	2.40	0.56
1:E:127:LEU:HD22	1:E:188:ILE:HD11	1.87	0.56
1:B:215:GLN:O	1:B:222:THR:HG23	2.05	0.56
1:A:113:MET:HE1	1:A:124:ASP:HB3	1.87	0.55
1:C:153:HIS:O	1:C:156:ARG:HG3	2.06	0.55
1:C:110:SER:HB2	1:E:177:ARG:CZ	2.36	0.55
1:A:177:ARG:HH21	1:D:114:GLN:CG	2.20	0.55
1:B:117:ALA:HA	1:B:123:ILE:CD1	2.28	0.55
1:C:127:LEU:HD22	1:C:188:ILE:HD11	1.88	0.55
1:A:109:LEU:HD23	1:A:111:GLY:H	1.71	0.55
1:D:118:PHE:CE1	1:F:118:PHE:CZ	2.95	0.55
1:C:117:ALA:HB1	1:E:178:PHE:HE1	1.72	0.54
1:C:110:SER:CB	1:E:177:ARG:HH22	2.19	0.54
1:A:127:LEU:HD22	1:A:188:ILE:HD11	1.89	0.54
1:D:113:MET:HE1	1:D:124:ASP:HB3	1.89	0.54
1:C:110:SER:HB2	1:E:177:ARG:NH1	2.23	0.54
1:E:261:LEU:HD23	1:E:261:LEU:O	2.07	0.54
1:B:261:LEU:HD23	1:B:261:LEU:O	2.07	0.54
1:F:261:LEU:O	1:F:261:LEU:HD23	2.08	0.54
1:A:118:PHE:CE1	1:A:119:THR:HG23	2.44	0.53
1:B:114:GLN:HG2	1:C:178:PHE:CZ	2.43	0.53
1:B:134:LYS:HE3	1:B:188:ILE:O	2.08	0.53
1:E:261:LEU:H	1:E:261:LEU:HD22	1.72	0.53
1:C:270:GLN:HE22	1:D:301:PRO:HG3	1.73	0.53
1:B:318:VAL:HG23	1:B:319:LYS:HG3	1.90	0.53
1:D:109:LEU:HD23	1:D:111:GLY:H	1.73	0.53
1:C:134:LYS:HE3	1:C:188:ILE:O	2.09	0.53
1:E:134:LYS:HE3	1:E:188:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:LYS:HZ1	1:C:201:LYS:HB2	1.72	0.53
1:C:113:MET:HE2	1:E:177:ARG:CD	2.39	0.53
1:A:93:ILE:O	1:A:97:THR:HG23	2.09	0.53
1:B:118:PHE:CE1	1:B:119:THR:HG23	2.44	0.53
1:A:177:ARG:NH2	1:D:114:GLN:HG3	2.23	0.52
1:C:117:ALA:HB1	1:E:178:PHE:CE1	2.45	0.52
1:D:201:LYS:O	1:D:205:MET:HG3	2.09	0.52
1:D:119:THR:CG2	1:F:118:PHE:CE1	2.92	0.52
1:A:176:SER:C	1:A:178:PHE:H	2.12	0.52
1:B:261:LEU:H	1:B:261:LEU:HD22	1.75	0.52
1:F:93:ILE:O	1:F:97:THR:HG23	2.09	0.52
1:F:201:LYS:O	1:F:205:MET:HG3	2.10	0.52
1:B:67:THR:HG22	1:B:68:LYS:N	2.25	0.52
1:E:109:LEU:HD23	1:E:111:GLY:H	1.74	0.52
1:E:203:GLU:O	1:E:203:GLU:HG3	2.10	0.52
1:C:174:LEU:HD13	1:C:178:PHE:CE1	2.45	0.51
1:B:93:ILE:O	1:B:97:THR:HG23	2.10	0.51
1:D:201:LYS:HB2	1:D:201:LYS:HZ2	1.74	0.51
1:A:318:VAL:HG23	1:A:319:LYS:HG3	1.92	0.51
1:E:118:PHE:CE1	1:E:119:THR:HG23	2.46	0.51
1:B:176:SER:C	1:B:178:PHE:H	2.13	0.51
1:B:203:GLU:HG3	1:B:203:GLU:O	2.10	0.51
1:A:261:LEU:O	1:A:261:LEU:HD23	2.10	0.51
1:C:67:THR:HG22	1:C:68:LYS:N	2.25	0.51
1:C:261:LEU:HD22	1:C:261:LEU:H	1.74	0.51
1:C:118:PHE:CE1	1:C:119:THR:HG23	2.45	0.51
1:F:176:SER:C	1:F:178:PHE:H	2.14	0.51
1:D:176:SER:C	1:D:178:PHE:H	2.14	0.51
1:D:261:LEU:H	1:D:261:LEU:HD22	1.75	0.51
1:D:170:LYS:CE	1:F:118:PHE:HB2	2.40	0.51
1:F:134:LYS:HE3	1:F:188:ILE:O	2.11	0.51
1:C:75:LYS:HE3	1:C:80:ASP:O	2.11	0.51
1:A:201:LYS:O	1:A:205:MET:HG3	2.11	0.51
1:E:176:SER:C	1:E:178:PHE:H	2.14	0.50
1:E:21:TRP:HB2	1:E:222:THR:HB	1.94	0.50
1:E:318:VAL:HG23	1:E:319:LYS:HG3	1.92	0.50
1:D:67:THR:HG22	1:D:68:LYS:N	2.26	0.50
1:F:75:LYS:HE3	1:F:80:ASP:O	2.11	0.50
1:A:67:THR:HG22	1:A:68:LYS:N	2.26	0.50
1:D:134:LYS:HE3	1:D:188:ILE:O	2.12	0.50
1:E:93:ILE:O	1:E:97:THR:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:SER:C	1:C:178:PHE:H	2.14	0.50
1:D:203:GLU:O	1:D:203:GLU:HG3	2.10	0.50
1:E:201:LYS:O	1:E:205:MET:HG3	2.11	0.50
1:C:203:GLU:O	1:C:203:GLU:HG3	2.11	0.50
1:B:114:GLN:HG2	1:C:178:PHE:HZ	1.76	0.50
1:F:21:TRP:HB2	1:F:222:THR:HB	1.93	0.50
1:F:261:LEU:H	1:F:261:LEU:CD2	2.24	0.50
1:A:75:LYS:HE3	1:A:80:ASP:O	2.12	0.50
1:D:268:CYS:HB3	1:D:271:CYS:HB2	1.92	0.50
1:B:21:TRP:HB2	1:B:222:THR:HB	1.95	0.49
1:B:177:ARG:HH11	1:B:177:ARG:HB2	1.77	0.49
1:E:67:THR:HG22	1:E:68:LYS:N	2.28	0.49
1:E:75:LYS:HE3	1:E:80:ASP:O	2.12	0.49
1:D:118:PHE:CE1	1:D:119:THR:HG23	2.48	0.49
1:C:21:TRP:HD1	1:C:146:PHE:CE2	2.27	0.49
1:D:318:VAL:HG23	1:D:319:LYS:HG3	1.92	0.49
1:D:75:LYS:HE3	1:D:80:ASP:O	2.12	0.49
1:B:180:PRO:O	1:B:184:GLN:HB2	2.13	0.49
1:A:261:LEU:HD22	1:A:261:LEU:H	1.77	0.49
1:D:93:ILE:O	1:D:97:THR:HG23	2.13	0.49
1:C:201:LYS:O	1:C:205:MET:HG3	2.13	0.49
1:E:123:ILE:CD1	1:E:123:ILE:H	1.93	0.48
1:A:21:TRP:HZ2	1:A:137:LYS:HD3	1.78	0.48
1:C:118:PHE:HE1	1:E:118:PHE:HZ	1.60	0.48
1:B:115:ASP:OD1	1:E:115:ASP:CG	2.51	0.48
1:D:21:TRP:HB2	1:D:222:THR:HB	1.95	0.48
1:A:260:LEU:O	1:A:298:PRO:HA	2.13	0.48
1:F:226:CYS:O	1:F:255:ILE:HA	2.13	0.48
1:C:260:LEU:O	1:C:260:LEU:HD12	2.13	0.48
1:C:21:TRP:HZ2	1:C:137:LYS:HD3	1.78	0.48
1:D:21:TRP:HZ2	1:D:137:LYS:HD3	1.78	0.48
1:A:21:TRP:HB2	1:A:222:THR:HB	1.95	0.48
1:A:203:GLU:HG3	1:A:203:GLU:O	2.13	0.48
1:A:201:LYS:HZ1	1:A:201:LYS:HB2	1.78	0.48
1:D:261:LEU:O	1:D:261:LEU:HD23	2.13	0.48
1:B:184:GLN:HA	1:B:184:GLN:NE2	2.28	0.48
1:C:21:TRP:HB2	1:C:222:THR:HB	1.95	0.48
1:F:21:TRP:HD1	1:F:146:PHE:CE2	2.28	0.48
1:A:9:THR:HG23	1:A:11:GLU:HB2	1.94	0.48
1:C:117:ALA:CB	1:E:178:PHE:CZ	2.95	0.48
1:D:21:TRP:HD1	1:D:146:PHE:CE2	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:O	1:C:261:LEU:HD23	2.14	0.48
1:A:118:PHE:HA	1:F:174:LEU:HD21	1.94	0.48
1:F:174:LEU:HD13	1:F:178:PHE:CE1	2.49	0.48
1:D:184:GLN:HA	1:D:184:GLN:NE2	2.28	0.48
1:D:261:LEU:H	1:D:261:LEU:CD2	2.27	0.48
1:C:110:SER:CB	1:E:177:ARG:NH2	2.77	0.48
1:B:261:LEU:H	1:B:261:LEU:CD2	2.27	0.48
1:F:203:GLU:O	1:F:203:GLU:HG3	2.14	0.48
1:C:184:GLN:HA	1:C:184:GLN:NE2	2.29	0.47
1:C:176:SER:O	1:C:177:ARG:CG	2.62	0.47
1:B:176:SER:O	1:B:177:ARG:CG	2.62	0.47
1:B:75:LYS:HE3	1:B:80:ASP:O	2.14	0.47
1:C:174:LEU:HD13	1:C:178:PHE:CZ	2.49	0.47
1:E:226:CYS:O	1:E:255:ILE:HA	2.14	0.47
1:A:180:PRO:O	1:A:184:GLN:HB2	2.14	0.47
1:A:134:LYS:HE3	1:A:188:ILE:O	2.14	0.47
1:D:226:CYS:O	1:D:255:ILE:HA	2.14	0.47
1:F:217:LYS:O	1:F:219:PRO:HD3	2.14	0.47
1:B:289:TYR:HB3	1:B:292:PHE:HB2	1.97	0.47
1:C:318:VAL:HG23	1:C:319:LYS:HG3	1.95	0.47
1:D:177:ARG:HB2	1:D:177:ARG:HH11	1.78	0.47
1:F:318:VAL:HG23	1:F:319:LYS:HG3	1.96	0.47
1:F:218:ASN:OD1	1:F:218:ASN:C	2.53	0.47
1:E:197:ASP:C	1:E:198:LEU:HG	2.35	0.47
1:B:21:TRP:HZ2	1:B:137:LYS:HD3	1.78	0.47
1:B:201:LYS:O	1:B:205:MET:HG3	2.14	0.47
1:C:268:CYS:HB3	1:C:271:CYS:HB2	1.95	0.47
1:E:268:CYS:HB3	1:E:271:CYS:HB2	1.95	0.47
1:C:93:ILE:O	1:C:97:THR:HG23	2.13	0.47
1:E:21:TRP:HZ2	1:E:137:LYS:HD3	1.80	0.47
1:E:17:THR:HA	1:E:47:ARG:NH1	2.30	0.47
1:D:289:TYR:HB3	1:D:292:PHE:HB2	1.96	0.47
1:E:184:GLN:HA	1:E:184:GLN:NE2	2.30	0.47
1:E:260:LEU:HD12	1:E:260:LEU:O	2.15	0.47
1:F:17:THR:HA	1:F:47:ARG:NH1	2.30	0.47
1:D:123:ILE:CD1	1:D:123:ILE:N	2.64	0.47
1:C:215:GLN:O	1:C:222:THR:CG2	2.63	0.47
1:B:174:LEU:HD13	1:B:178:PHE:CE1	2.50	0.47
1:E:9:THR:HG23	1:E:11:GLU:HB2	1.97	0.47
1:B:226:CYS:O	1:B:255:ILE:HA	2.15	0.47
1:A:197:ASP:C	1:A:198:LEU:HG	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:THR:HG22	1:F:68:LYS:N	2.29	0.47
1:C:197:ASP:C	1:C:198:LEU:HG	2.35	0.47
1:A:170:LYS:HD3	1:A:170:LYS:O	2.15	0.46
1:A:176:SER:O	1:A:177:ARG:CG	2.63	0.46
1:B:260:LEU:HD12	1:B:260:LEU:O	2.15	0.46
1:F:289:TYR:HB3	1:F:292:PHE:HB2	1.96	0.46
1:E:54:SER:HB3	1:E:61:LEU:HD22	1.97	0.46
1:F:184:GLN:HA	1:F:184:GLN:NE2	2.29	0.46
1:C:118:PHE:CE1	1:E:118:PHE:HZ	2.32	0.46
1:D:197:ASP:C	1:D:198:LEU:HG	2.35	0.46
1:A:184:GLN:HA	1:A:184:GLN:NE2	2.29	0.46
1:E:217:LYS:O	1:E:219:PRO:HD3	2.16	0.46
1:F:176:SER:O	1:F:177:ARG:CG	2.63	0.46
1:D:176:SER:O	1:D:177:ARG:CG	2.63	0.46
1:C:196:GLN:OE1	1:C:196:GLN:N	2.48	0.46
1:F:256:VAL:HA	1:F:295:VAL:HG13	1.96	0.46
1:A:176:SER:O	1:A:178:PHE:N	2.48	0.46
1:E:177:ARG:HH11	1:E:177:ARG:HB2	1.81	0.46
1:F:38:SER:HB2	1:F:317:LEU:CD2	2.46	0.46
1:A:177:ARG:HB2	1:A:177:ARG:HH11	1.80	0.46
1:C:111:GLY:O	1:C:114:GLN:HB2	2.15	0.46
1:A:41:ILE:HG23	1:A:79:PHE:CE1	2.51	0.46
1:C:21:TRP:CD1	1:C:146:PHE:CE2	2.95	0.46
1:B:87:ILE:HD13	1:B:88:ASP:H	1.79	0.46
1:F:21:TRP:HZ2	1:F:137:LYS:HD3	1.81	0.46
1:C:260:LEU:O	1:C:298:PRO:HA	2.15	0.46
1:D:312:SER:O	1:D:315:GLU:HB2	2.16	0.46
1:D:111:GLY:O	1:D:114:GLN:HB2	2.16	0.46
1:C:177:ARG:HB2	1:C:177:ARG:HH11	1.80	0.46
1:F:180:PRO:O	1:F:184:GLN:HB2	2.15	0.45
1:B:9:THR:HG23	1:B:11:GLU:HB2	1.98	0.45
1:C:270:GLN:NE2	1:D:301:PRO:HG3	2.31	0.45
1:E:180:PRO:O	1:E:184:GLN:HB2	2.16	0.45
1:E:160:PHE:N	1:E:161:PRO:CD	2.79	0.45
1:C:170:LYS:HD3	1:C:170:LYS:O	2.17	0.45
1:B:197:ASP:C	1:B:198:LEU:HG	2.37	0.45
1:F:41:ILE:HG23	1:F:79:PHE:CE1	2.50	0.45
1:B:291:ASP:OD1	1:B:291:ASP:N	2.46	0.45
1:F:92:SER:O	1:F:96:MET:HG2	2.16	0.45
1:C:226:CYS:O	1:C:255:ILE:HA	2.16	0.45
1:C:9:THR:HG23	1:C:11:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:THR:HG23	1:D:11:GLU:HB2	1.99	0.45
1:E:218:ASN:OD1	1:E:218:ASN:C	2.54	0.45
1:F:260:LEU:O	1:F:298:PRO:HA	2.16	0.45
1:D:17:THR:HA	1:D:47:ARG:NH1	2.31	0.45
1:A:177:ARG:NH2	1:D:114:GLN:NE2	2.65	0.45
1:E:174:LEU:HD13	1:E:178:PHE:CE1	2.52	0.45
1:E:261:LEU:CD2	1:E:261:LEU:H	2.30	0.45
1:E:260:LEU:O	1:E:298:PRO:HA	2.16	0.45
1:C:261:LEU:H	1:C:261:LEU:CD2	2.28	0.45
1:E:61:LEU:HD12	1:E:61:LEU:HA	1.85	0.45
1:B:54:SER:HB3	1:B:61:LEU:HD22	1.99	0.45
1:E:151:THR:HG21	1:F:236:TYR:CD1	2.51	0.45
1:B:17:THR:HA	1:B:47:ARG:NH1	2.32	0.45
1:B:170:LYS:O	1:B:170:LYS:HD3	2.17	0.45
1:D:119:THR:CG2	1:F:118:PHE:CD1	2.98	0.45
1:F:38:SER:HB2	1:F:317:LEU:HD22	1.99	0.45
1:E:89:PRO:O	1:E:93:ILE:HG13	2.17	0.45
1:A:226:CYS:O	1:A:255:ILE:HA	2.17	0.45
1:F:177:ARG:HH11	1:F:177:ARG:HB2	1.81	0.44
1:D:109:LEU:N	1:D:184:GLN:HG3	2.32	0.44
1:C:180:PRO:O	1:C:184:GLN:HB2	2.17	0.44
1:A:291:ASP:OD1	1:A:291:ASP:N	2.43	0.44
1:A:217:LYS:O	1:A:219:PRO:HD3	2.17	0.44
1:B:174:LEU:HD13	1:B:178:PHE:CZ	2.52	0.44
1:D:180:PRO:O	1:D:184:GLN:HB2	2.17	0.44
1:E:176:SER:O	1:E:177:ARG:CG	2.66	0.44
1:B:21:TRP:CD1	1:B:146:PHE:CE2	2.99	0.44
1:A:268:CYS:HB3	1:A:271:CYS:HB2	1.98	0.44
1:C:217:LYS:O	1:C:219:PRO:HD3	2.18	0.44
1:D:170:LYS:HE2	1:F:118:PHE:CA	2.44	0.44
1:A:21:TRP:HD1	1:A:146:PHE:CE2	2.28	0.44
1:C:117:ALA:CB	1:E:178:PHE:CE1	3.00	0.44
1:B:114:GLN:O	1:B:117:ALA:N	2.51	0.44
1:F:312:SER:O	1:F:315:GLU:HB2	2.17	0.44
1:F:266:THR:HG23	1:F:272:MET:HG2	2.00	0.44
1:E:256:VAL:HA	1:E:295:VAL:HG13	2.00	0.44
1:C:118:PHE:CE1	1:E:118:PHE:CZ	3.05	0.44
1:D:170:LYS:O	1:D:170:LYS:HD3	2.18	0.44
1:B:127:LEU:HD22	1:B:188:ILE:CD1	2.47	0.44
1:D:217:LYS:O	1:D:219:PRO:HD3	2.17	0.44
1:D:38:SER:HB2	1:D:317:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:SER:O	1:C:114:GLN:N	2.51	0.44
1:E:38:SER:HB2	1:E:317:LEU:CD2	2.48	0.44
1:B:217:LYS:HE3	1:B:249:GLU:HB2	1.99	0.44
1:F:9:THR:HG23	1:F:11:GLU:HB2	2.00	0.44
1:E:87:ILE:HD13	1:E:88:ASP:H	1.82	0.44
1:B:312:SER:O	1:B:315:GLU:HB2	2.18	0.44
1:D:174:LEU:HD13	1:D:178:PHE:CE1	2.53	0.43
1:E:151:THR:HG22	1:F:236:TYR:CD2	2.53	0.43
1:F:87:ILE:HD13	1:F:88:ASP:H	1.83	0.43
1:F:174:LEU:HD13	1:F:178:PHE:CZ	2.53	0.43
1:F:197:ASP:C	1:F:198:LEU:HG	2.39	0.43
1:E:41:ILE:HG23	1:E:79:PHE:CE1	2.53	0.43
1:B:41:ILE:HG23	1:B:79:PHE:CE1	2.53	0.43
1:E:289:TYR:HB3	1:E:292:PHE:HB2	1.99	0.43
1:A:111:GLY:O	1:A:114:GLN:HB2	2.19	0.43
1:A:114:GLN:O	1:A:117:ALA:N	2.51	0.43
1:F:114:GLN:O	1:F:117:ALA:N	2.51	0.43
1:B:46:VAL:O	1:B:46:VAL:HG22	2.18	0.43
1:D:256:VAL:HA	1:D:295:VAL:HG13	1.98	0.43
1:C:184:GLN:HA	1:C:184:GLN:HE21	1.83	0.43
1:A:21:TRP:CZ2	1:A:137:LYS:HD3	2.53	0.43
1:A:21:TRP:CD1	1:A:146:PHE:CE2	2.98	0.43
1:E:298:PRO:HG3	1:E:321:TYR:CD1	2.54	0.43
1:A:266:THR:HG23	1:A:272:MET:HG2	2.01	0.43
1:D:260:LEU:O	1:D:298:PRO:HA	2.18	0.43
1:A:54:SER:HB3	1:A:61:LEU:HD22	2.00	0.43
1:F:170:LYS:HD3	1:F:170:LYS:O	2.17	0.43
1:A:87:ILE:HD13	1:A:88:ASP:H	1.83	0.43
1:A:289:TYR:HB3	1:A:292:PHE:HB2	2.00	0.43
1:B:109:LEU:CD2	1:B:111:GLY:H	2.32	0.43
1:D:21:TRP:CZ2	1:D:137:LYS:HD3	2.53	0.43
1:D:38:SER:CB	1:D:317:LEU:HD22	2.48	0.43
1:D:89:PRO:O	1:D:93:ILE:HG13	2.18	0.43
1:F:15:GLU:O	1:F:17:THR:HG23	2.19	0.43
1:A:217:LYS:HE3	1:A:249:GLU:HB2	2.01	0.43
1:C:17:THR:HA	1:C:47:ARG:NH1	2.34	0.43
1:D:160:PHE:N	1:D:161:PRO:CD	2.82	0.43
1:A:46:VAL:O	1:A:46:VAL:HG22	2.19	0.43
1:C:312:SER:O	1:C:315:GLU:HB2	2.19	0.43
1:E:113:MET:HE3	1:E:124:ASP:HB3	2.00	0.43
1:B:118:PHE:CE2	1:C:118:PHE:HZ	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:SER:CB	1:E:317:LEU:HD22	2.49	0.43
1:A:17:THR:HA	1:A:47:ARG:NH1	2.33	0.43
1:E:92:SER:O	1:E:96:MET:HG2	2.18	0.43
1:C:266:THR:HG23	1:C:272:MET:HG2	1.99	0.43
1:A:184:GLN:HA	1:A:184:GLN:HE21	1.84	0.43
1:F:111:GLY:O	1:F:114:GLN:HB2	2.18	0.43
1:B:110:SER:O	1:B:114:GLN:N	2.51	0.43
1:D:174:LEU:HD13	1:D:178:PHE:CZ	2.53	0.43
1:F:38:SER:CB	1:F:317:LEU:HD22	2.49	0.43
1:B:127:LEU:CD2	1:B:188:ILE:HD11	2.48	0.43
1:C:109:LEU:N	1:C:184:GLN:HG3	2.34	0.43
1:B:160:PHE:N	1:B:161:PRO:CD	2.82	0.43
1:F:54:SER:HB3	1:F:61:LEU:HD22	2.00	0.43
1:D:266:THR:HG23	1:D:272:MET:HG2	2.00	0.43
1:D:61:LEU:HA	1:D:61:LEU:HD12	1.85	0.43
1:F:184:GLN:HA	1:F:184:GLN:HE21	1.84	0.42
1:D:92:SER:O	1:D:96:MET:HG2	2.19	0.42
1:C:160:PHE:N	1:C:161:PRO:CD	2.82	0.42
1:D:114:GLN:O	1:D:117:ALA:N	2.51	0.42
1:D:184:GLN:HE21	1:D:184:GLN:HA	1.85	0.42
1:B:260:LEU:O	1:B:298:PRO:HA	2.19	0.42
1:B:55:THR:HA	1:B:87:ILE:O	2.19	0.42
1:B:21:TRP:HD1	1:B:146:PHE:CE2	2.29	0.42
1:D:55:THR:HA	1:D:87:ILE:O	2.19	0.42
1:B:92:SER:O	1:B:96:MET:HG2	2.19	0.42
1:F:109:LEU:CD2	1:F:111:GLY:H	2.30	0.42
1:F:21:TRP:CD1	1:F:146:PHE:CE2	2.97	0.42
1:C:201:LYS:HA	1:C:204:SER:OG	2.19	0.42
1:B:217:LYS:O	1:B:219:PRO:HD3	2.18	0.42
1:B:266:THR:HG23	1:B:272:MET:HG2	2.02	0.42
1:E:312:SER:O	1:E:315:GLU:HB2	2.20	0.42
1:B:111:GLY:O	1:B:114:GLN:HB2	2.20	0.42
1:F:183:ASN:HA	1:F:201:LYS:HE2	2.01	0.42
1:B:184:GLN:HA	1:B:184:GLN:HE21	1.83	0.42
1:B:218:ASN:C	1:B:218:ASN:OD1	2.57	0.42
1:A:109:LEU:N	1:A:184:GLN:HG3	2.35	0.42
1:A:177:ARG:CZ	1:D:114:GLN:HG3	2.49	0.42
1:B:38:SER:HB2	1:B:317:LEU:CD2	2.50	0.42
1:E:297:VAL:HA	1:E:298:PRO:HD3	1.87	0.42
1:D:217:LYS:HE3	1:D:249:GLU:HB2	2.00	0.42
1:D:54:SER:HB3	1:D:61:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:HA	1:B:168:LEU:HD23	1.87	0.42
1:C:257:VAL:CG2	1:C:257:VAL:O	2.67	0.42
1:D:110:SER:O	1:D:114:GLN:N	2.51	0.42
1:E:127:LEU:HD22	1:E:188:ILE:CD1	2.49	0.42
1:E:271:CYS:SG	1:F:270:GLN:HB2	2.60	0.42
1:C:289:TYR:HB3	1:C:292:PHE:HB2	2.01	0.42
1:C:92:SER:O	1:C:96:MET:HG2	2.19	0.42
1:E:111:GLY:O	1:E:114:GLN:HB2	2.19	0.42
1:B:118:PHE:CD1	1:C:119:THR:HG21	2.55	0.42
1:C:183:ASN:HA	1:C:201:LYS:HE2	2.02	0.42
1:D:176:SER:O	1:D:178:PHE:N	2.51	0.42
1:D:38:SER:HB2	1:D:317:LEU:HD22	2.02	0.42
1:C:257:VAL:HG23	1:C:257:VAL:O	2.20	0.42
1:B:268:CYS:HB3	1:B:271:CYS:HB2	2.02	0.42
1:F:160:PHE:N	1:F:161:PRO:CD	2.82	0.42
1:F:260:LEU:O	1:F:260:LEU:HD12	2.19	0.42
1:A:174:LEU:HD13	1:A:178:PHE:CE1	2.55	0.42
1:C:176:SER:O	1:C:178:PHE:N	2.51	0.42
1:F:127:LEU:HD22	1:F:188:ILE:CD1	2.48	0.42
1:C:160:PHE:CD1	1:C:160:PHE:C	2.94	0.42
1:C:27:LYS:O	1:C:28:GLY:O	2.38	0.42
1:C:87:ILE:HD13	1:C:88:ASP:H	1.85	0.42
1:A:177:ARG:HH21	1:D:114:GLN:CD	2.23	0.41
1:F:110:SER:O	1:F:114:GLN:N	2.52	0.41
1:E:114:GLN:O	1:E:117:ALA:N	2.53	0.41
1:E:183:ASN:HA	1:E:201:LYS:HE2	2.01	0.41
1:B:56:ASP:HA	1:B:57:PRO:HD3	1.88	0.41
1:C:168:LEU:HD23	1:C:168:LEU:HA	1.87	0.41
1:E:266:THR:HG23	1:E:272:MET:HG2	2.02	0.41
1:E:19:LEU:HD12	1:E:19:LEU:HA	1.83	0.41
1:A:92:SER:O	1:A:96:MET:HG2	2.20	0.41
1:F:268:CYS:HB3	1:F:271:CYS:HB2	2.02	0.41
1:C:113:MET:O	1:C:117:ALA:N	2.53	0.41
1:D:235:LEU:HD23	1:D:235:LEU:HA	1.83	0.41
1:E:217:LYS:HE3	1:E:249:GLU:HB2	2.02	0.41
1:F:298:PRO:HG3	1:F:321:TYR:CD1	2.55	0.41
1:C:81:ASN:OD1	1:C:81:ASN:N	2.52	0.41
1:A:257:VAL:HG23	1:A:257:VAL:O	2.19	0.41
1:A:160:PHE:N	1:A:161:PRO:CD	2.82	0.41
1:E:174:LEU:HD13	1:E:178:PHE:CZ	2.55	0.41
1:B:21:TRP:CZ2	1:B:137:LYS:HD3	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:SER:CB	1:B:317:LEU:HD22	2.51	0.41
1:F:55:THR:HA	1:F:87:ILE:O	2.20	0.41
1:F:257:VAL:O	1:F:257:VAL:CG2	2.68	0.41
1:A:109:LEU:CD2	1:A:111:GLY:H	2.33	0.41
1:A:183:ASN:HA	1:A:201:LYS:HE2	2.01	0.41
1:A:261:LEU:CD2	1:A:261:LEU:H	2.33	0.41
1:B:297:VAL:HA	1:B:298:PRO:HD3	1.85	0.41
1:F:61:LEU:HD12	1:F:61:LEU:HA	1.80	0.41
1:E:46:VAL:O	1:E:46:VAL:HG22	2.20	0.41
1:C:54:SER:HB3	1:C:61:LEU:HD22	2.01	0.41
1:C:109:LEU:CD2	1:C:111:GLY:H	2.31	0.41
1:B:118:PHE:CZ	1:E:118:PHE:HZ	2.33	0.41
1:F:197:ASP:HA	1:F:201:LYS:HD2	2.02	0.41
1:F:89:PRO:O	1:F:93:ILE:HG13	2.21	0.41
1:F:297:VAL:HA	1:F:298:PRO:HD3	1.87	0.41
1:D:87:ILE:HD13	1:D:88:ASP:H	1.84	0.41
1:A:59:HIS:HA	1:A:86:GLU:OE1	2.21	0.41
1:E:110:SER:O	1:E:114:GLN:N	2.52	0.41
1:E:38:SER:HB2	1:E:317:LEU:HD22	2.01	0.41
1:A:257:VAL:CG2	1:A:257:VAL:O	2.69	0.41
1:C:256:VAL:HA	1:C:295:VAL:HG13	2.02	0.41
1:E:170:LYS:O	1:E:170:LYS:HD3	2.20	0.41
1:A:19:LEU:HA	1:A:19:LEU:HD12	1.81	0.41
1:B:113:MET:O	1:B:117:ALA:N	2.54	0.41
1:B:170:LYS:HE2	1:E:118:PHE:HB2	2.03	0.41
1:C:21:TRP:CZ2	1:C:137:LYS:HD3	2.54	0.41
1:A:271:CYS:SG	1:B:270:GLN:HB2	2.61	0.41
1:B:257:VAL:O	1:B:257:VAL:HG23	2.20	0.41
1:A:110:SER:O	1:A:114:GLN:N	2.53	0.41
1:E:176:SER:O	1:E:178:PHE:N	2.51	0.41
1:D:21:TRP:CD1	1:D:146:PHE:CE2	2.96	0.41
1:A:201:LYS:HA	1:A:204:SER:OG	2.21	0.41
1:B:197:ASP:HA	1:B:201:LYS:HD2	2.01	0.41
1:B:201:LYS:HA	1:B:204:SER:OG	2.21	0.41
1:F:127:LEU:CD2	1:F:188:ILE:HD11	2.48	0.41
1:E:151:THR:HB	1:F:236:TYR:CE1	2.55	0.41
1:B:67:THR:HG22	1:B:68:LYS:H	1.86	0.41
1:C:298:PRO:HG3	1:C:321:TYR:CD1	2.55	0.41
1:C:61:LEU:HD12	1:C:61:LEU:HA	1.85	0.41
1:B:176:SER:O	1:B:178:PHE:N	2.52	0.41
1:E:257:VAL:O	1:E:257:VAL:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ASN:HA	1:B:201:LYS:HE2	2.02	0.40
1:D:257:VAL:CG2	1:D:257:VAL:O	2.69	0.40
1:E:21:TRP:CZ2	1:E:137:LYS:HD3	2.56	0.40
1:D:201:LYS:HA	1:D:204:SER:OG	2.21	0.40
1:A:297:VAL:HA	1:A:298:PRO:HD3	1.84	0.40
1:D:258:ASN:O	1:D:260:LEU:N	2.54	0.40
1:E:56:ASP:HA	1:E:57:PRO:HD3	1.89	0.40
1:B:235:LEU:HA	1:B:235:LEU:HD23	1.84	0.40
1:E:201:LYS:HZ1	1:E:201:LYS:HB2	1.81	0.40
1:D:41:ILE:HG23	1:D:79:PHE:CE1	2.56	0.40
1:E:184:GLN:HA	1:E:184:GLN:HE21	1.85	0.40
1:C:217:LYS:HE3	1:C:249:GLU:HB2	2.03	0.40
1:D:257:VAL:O	1:D:257:VAL:HG23	2.20	0.40
1:E:24:VAL:HB	1:E:225:VAL:HG13	2.03	0.40
1:F:109:LEU:N	1:F:184:GLN:HG3	2.36	0.40
1:F:127:LEU:HB3	1:F:188:ILE:HD11	2.04	0.40

All (5) 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:F:196:GLN:N	1:F:315:GLU:OE1[3_555]	2.03	0.17
1:C:66:GLY:O	1:E:142:ASP:OD2[4_545]	2.04	0.16
1:F:196:GLN:OE1	1:F:315:GLU:CD[3_555]	2.05	0.15
1:F:196:GLN:OE1	1:F:315:GLU:OE1[3_555]	2.12	0.08
1:F:45:LYS:NZ	1:F:196:GLN:O[3_545]	2.12	0.08

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	297/329 (90%)	271 (91%)	20 (7%)	6 (2%)	9 41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	297/329 (90%)	272 (92%)	19 (6%)	6 (2%)	9	41
1	C	297/329 (90%)	275 (93%)	15 (5%)	7 (2%)	7	35
1	D	297/329 (90%)	273 (92%)	18 (6%)	6 (2%)	9	41
1	E	297/329 (90%)	272 (92%)	19 (6%)	6 (2%)	9	41
1	F	297/329 (90%)	273 (92%)	18 (6%)	6 (2%)	9	41
All	All	1782/1974 (90%)	1636 (92%)	109 (6%)	37 (2%)	9	40

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLY
1	B	28	GLY
1	B	259	GLN
1	C	28	GLY
1	D	28	GLY
1	D	259	GLN
1	E	28	GLY
1	E	259	GLN
1	F	28	GLY
1	F	259	GLN
1	A	176	SER
1	A	259	GLN
1	B	176	SER
1	C	176	SER
1	C	259	GLN
1	D	176	SER
1	E	176	SER
1	F	176	SER
1	C	58	ALA
1	D	58	ALA
1	D	177	ARG
1	F	58	ALA
1	A	58	ALA
1	A	175	SER
1	A	177	ARG
1	B	58	ALA
1	B	177	ARG
1	C	27	LYS
1	C	175	SER
1	C	177	ARG

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Mol	Chain	Res	Type
1	D	175	SER
1	E	58	ALA
1	E	177	ARG
1	F	175	SER
1	F	177	ARG
1	B	175	SER
1	E	175	SER

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	266/290 (92%)	227 (85%)	39 (15%)	4 18
1	B	266/290 (92%)	226 (85%)	40 (15%)	3 17
1	C	266/290 (92%)	225 (85%)	41 (15%)	3 16
1	D	266/290 (92%)	227 (85%)	39 (15%)	4 18
1	E	266/290 (92%)	224 (84%)	42 (16%)	3 15
1	F	266/290 (92%)	226 (85%)	40 (15%)	3 17
All	All	1596/1740 (92%)	1355 (85%)	241 (15%)	3 17

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	19	LEU
1	A	24	VAL
1	A	49	SER
1	A	87	ILE
1	A	109	LEU
1	A	112	MET
1	A	115	ASP
1	A	116	LEU
1	A	119	THR
1	A	123	ILE

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Mol	Chain	Res	Type
1	A	124	ASP
1	A	137	LYS
1	A	144	VAL
1	A	156	ARG
1	A	160	PHE
1	A	177	ARG
1	A	181	MET
1	A	184	GLN
1	A	188	ILE
1	A	201	LYS
1	A	222	THR
1	A	225	VAL
1	A	227	VAL
1	A	233	LEU
1	A	244	GLU
1	A	255	ILE
1	A	256	VAL
1	A	257	VAL
1	A	260	LEU
1	A	261	LEU
1	A	262	LEU
1	A	265	ASN
1	A	274	ARG
1	A	277	MET
1	A	294	VAL
1	A	295	VAL
1	A	297	VAL
1	A	300	VAL
1	B	13	LEU
1	B	19	LEU
1	B	24	VAL
1	B	32	LYS
1	B	49	SER
1	B	87	ILE
1	B	109	LEU
1	B	112	MET
1	B	115	ASP
1	B	116	LEU
1	B	119	THR
1	B	123	ILE
1	B	124	ASP
1	B	137	LYS

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Mol	Chain	Res	Type
1	B	144	VAL
1	B	156	ARG
1	B	160	PHE
1	B	177	ARG
1	B	181	MET
1	B	184	GLN
1	B	188	ILE
1	B	201	LYS
1	B	222	THR
1	B	225	VAL
1	B	227	VAL
1	B	233	LEU
1	B	244	GLU
1	B	255	ILE
1	B	256	VAL
1	B	260	LEU
1	B	261	LEU
1	B	262	LEU
1	B	265	ASN
1	B	274	ARG
1	B	277	MET
1	B	294	VAL
1	B	295	VAL
1	B	297	VAL
1	B	300	VAL
1	B	316	MET
1	C	9	THR
1	C	13	LEU
1	C	19	LEU
1	C	24	VAL
1	C	32	LYS
1	C	49	SER
1	C	87	ILE
1	C	109	LEU
1	C	112	MET
1	C	115	ASP
1	C	116	LEU
1	C	119	THR
1	C	123	ILE
1	C	124	ASP
1	C	137	LYS
1	C	144	VAL

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Mol	Chain	Res	Type
1	C	156	ARG
1	C	160	PHE
1	C	177	ARG
1	C	181	MET
1	C	184	GLN
1	C	188	ILE
1	C	201	LYS
1	C	222	THR
1	C	225	VAL
1	C	227	VAL
1	C	233	LEU
1	C	244	GLU
1	C	255	ILE
1	C	256	VAL
1	C	260	LEU
1	C	261	LEU
1	C	262	LEU
1	C	265	ASN
1	C	274	ARG
1	C	277	MET
1	C	294	VAL
1	C	295	VAL
1	C	297	VAL
1	C	300	VAL
1	C	316	MET
1	D	13	LEU
1	D	19	LEU
1	D	24	VAL
1	D	49	SER
1	D	87	ILE
1	D	109	LEU
1	D	112	MET
1	D	115	ASP
1	D	116	LEU
1	D	119	THR
1	D	123	ILE
1	D	124	ASP
1	D	137	LYS
1	D	144	VAL
1	D	156	ARG
1	D	160	PHE
1	D	177	ARG

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Mol	Chain	Res	Type
1	D	181	MET
1	D	184	GLN
1	D	188	ILE
1	D	201	LYS
1	D	222	THR
1	D	225	VAL
1	D	227	VAL
1	D	233	LEU
1	D	244	GLU
1	D	255	ILE
1	D	256	VAL
1	D	260	LEU
1	D	261	LEU
1	D	262	LEU
1	D	265	ASN
1	D	274	ARG
1	D	277	MET
1	D	294	VAL
1	D	295	VAL
1	D	297	VAL
1	D	300	VAL
1	D	316	MET
1	E	9	THR
1	E	13	LEU
1	E	19	LEU
1	E	24	VAL
1	E	32	LYS
1	E	49	SER
1	E	87	ILE
1	E	109	LEU
1	E	112	MET
1	E	115	ASP
1	E	116	LEU
1	E	119	THR
1	E	123	ILE
1	E	124	ASP
1	E	137	LYS
1	E	144	VAL
1	E	156	ARG
1	E	160	PHE
1	E	177	ARG
1	E	181	MET

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Mol	Chain	Res	Type
1	E	184	GLN
1	E	188	ILE
1	E	201	LYS
1	E	222	THR
1	E	225	VAL
1	E	227	VAL
1	E	233	LEU
1	E	244	GLU
1	E	255	ILE
1	E	256	VAL
1	E	257	VAL
1	E	260	LEU
1	E	261	LEU
1	E	262	LEU
1	E	265	ASN
1	E	274	ARG
1	E	277	MET
1	E	294	VAL
1	E	295	VAL
1	E	297	VAL
1	E	300	VAL
1	E	316	MET
1	F	13	LEU
1	F	19	LEU
1	F	24	VAL
1	F	32	LYS
1	F	49	SER
1	F	87	ILE
1	F	109	LEU
1	F	112	MET
1	F	115	ASP
1	F	116	LEU
1	F	119	THR
1	F	123	ILE
1	F	124	ASP
1	F	137	LYS
1	F	144	VAL
1	F	156	ARG
1	F	160	PHE
1	F	177	ARG
1	F	181	MET
1	F	184	GLN

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Mol	Chain	Res	Type
1	F	188	ILE
1	F	201	LYS
1	F	222	THR
1	F	225	VAL
1	F	227	VAL
1	F	233	LEU
1	F	244	GLU
1	F	255	ILE
1	F	256	VAL
1	F	260	LEU
1	F	261	LEU
1	F	262	LEU
1	F	265	ASN
1	F	274	ARG
1	F	277	MET
1	F	294	VAL
1	F	295	VAL
1	F	297	VAL
1	F	300	VAL
1	F	316	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	59	HIS
1	A	114	GLN
1	A	135	GLN
1	A	184	GLN
1	A	196	GLN
1	A	293	HIS
1	B	12	ASN
1	B	135	GLN
1	B	184	GLN
1	B	196	GLN
1	B	293	HIS
1	C	12	ASN
1	C	59	HIS
1	C	114	GLN
1	C	135	GLN
1	C	184	GLN
1	C	196	GLN

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Mol	Chain	Res	Type
1	C	270	GLN
1	C	293	HIS
1	D	12	ASN
1	D	59	HIS
1	D	114	GLN
1	D	135	GLN
1	D	184	GLN
1	D	196	GLN
1	D	293	HIS
1	E	12	ASN
1	E	59	HIS
1	E	135	GLN
1	E	184	GLN
1	E	196	GLN
1	E	293	HIS
1	F	12	ASN
1	F	59	HIS
1	F	135	GLN
1	F	184	GLN
1	F	293	HIS

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

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	303/329 (92%)	-0.18	4 (1%) 79 53	60, 99, 156, 202	0
1	B	303/329 (92%)	-0.01	15 (4%) 32 13	66, 106, 187, 248	0
1	C	303/329 (92%)	-0.15	6 (1%) 68 39	53, 89, 163, 288	0
1	D	303/329 (92%)	0.03	7 (2%) 64 33	66, 120, 194, 258	0
1	E	303/329 (92%)	0.04	13 (4%) 39 16	72, 121, 191, 240	0
1	F	303/329 (92%)	0.31	24 (7%) 15 5	94, 140, 211, 269	0
All	All	1818/1974 (92%)	0.01	69 (3%) 44 18	53, 113, 193, 288	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	190	GLY	9.1
1	C	110	SER	8.4
1	D	109	LEU	8.1
1	F	196	GLN	8.0
1	C	99	GLN	6.0
1	F	182	ILE	5.8
1	B	110	SER	5.7
1	F	197	ASP	5.6
1	D	110	SER	5.5
1	C	109	LEU	5.4
1	F	178	PHE	5.1
1	F	112	MET	5.1
1	F	186	GLY	5.1
1	D	100	ALA	5.0
1	B	182	ILE	4.8
1	E	97	THR	4.8
1	F	185	MET	4.7
1	F	189	MET	4.6
1	B	185	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	114	GLN	3.9
1	F	179	GLY	3.7
1	F	183	ASN	3.6
1	B	186	GLY	3.6
1	F	301	PRO	3.4
1	D	113	MET	3.4
1	E	181	MET	3.4
1	E	282	LEU	3.3
1	E	100	ALA	3.3
1	D	98	GLU	3.0
1	F	114	GLN	3.0
1	F	177	ARG	3.0
1	F	180	PRO	2.9
1	E	118	PHE	2.9
1	B	179	GLY	2.9
1	B	189	MET	2.9
1	F	176	SER	2.8
1	E	28	GLY	2.8
1	C	118	PHE	2.8
1	E	99	GLN	2.8
1	A	181	MET	2.8
1	E	196	GLN	2.8
1	B	190	GLY	2.8
1	B	202	MET	2.7
1	B	171	LEU	2.7
1	E	96	MET	2.7
1	E	175	SER	2.6
1	B	168	LEU	2.6
1	B	118	PHE	2.6
1	C	177	ARG	2.4
1	E	285	ILE	2.4
1	B	180	PRO	2.4
1	F	310	LEU	2.4
1	F	184	GLN	2.4
1	B	109	LEU	2.3
1	F	10	LEU	2.3
1	F	109	LEU	2.3
1	A	112	MET	2.3
1	E	184	GLN	2.3
1	A	175	SER	2.3
1	B	114	GLN	2.2
1	F	318	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	202	MET	2.1
1	A	299	GLN	2.1
1	F	97	THR	2.1
1	F	302	ALA	2.1
1	D	177	ARG	2.1
1	B	178	PHE	2.0
1	E	262	LEU	2.0
1	D	96	MET	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	C	1323	1/1	0.92	0.17	-0.50	108,108,108,108	0
2	ZN	B	1323	1/1	0.97	0.09	-0.91	113,113,113,113	0
2	ZN	F	1323	1/1	0.60	0.11	-1.36	170,170,170,170	0

6.5 Other polymers (i)

There are no such residues in this entry.