



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:02 PM UTC

PDB ID : 2WOO / pdb_00002woo
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

<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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

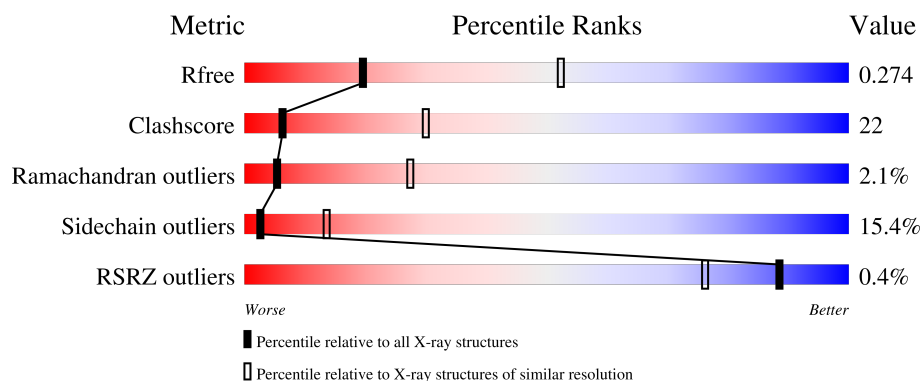
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	329	
1	B	329	
1	C	329	
1	D	329	
1	E	329	

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Mol	Chain	Length	Quality of chain
1	F	329	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (55%), yellow (29%), orange (9%), and grey (8%).

2 Entry composition

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.

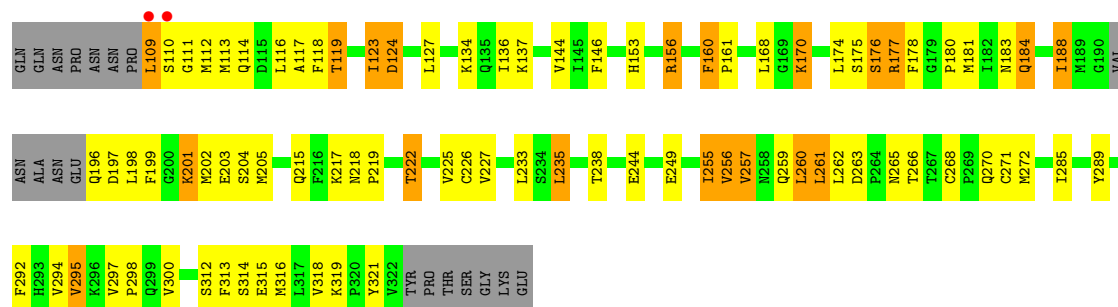
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2352	1494	386	451	21			
1	B	303	Total	C	N	O	S	0	0	0
			2352	1494	386	451	21			
1	C	303	Total	C	N	O	S	0	0	0
			2352	1494	386	451	21			
1	D	303	Total	C	N	O	S	0	0	0
			2352	1494	386	451	21			
1	E	303	Total	C	N	O	S	0	0	0
			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 (CCD ID: ZN) (formula: Zn).

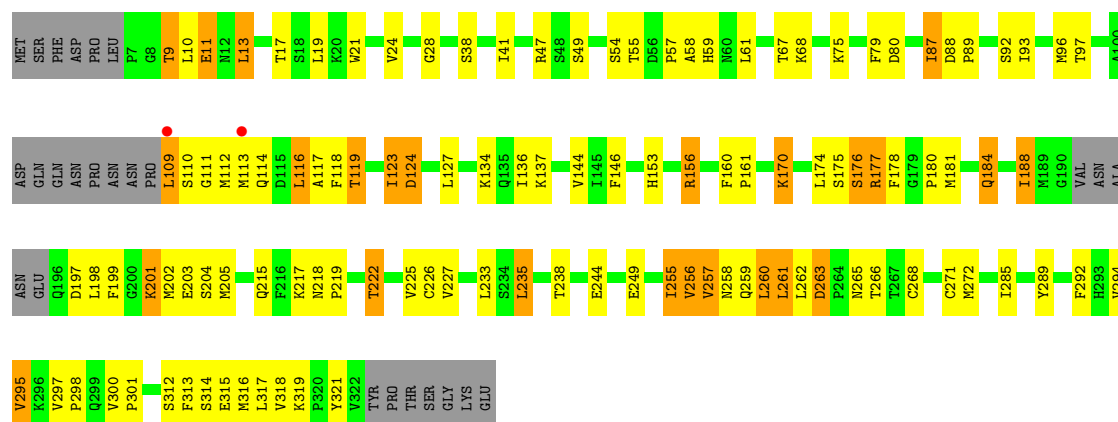
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 1: ATPASE GET3

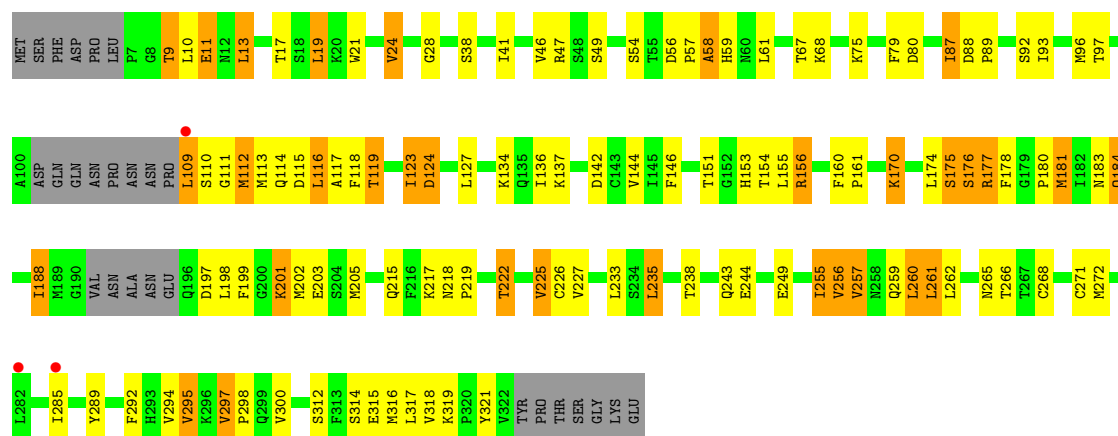




• Molecule 1: ATPASE GET3

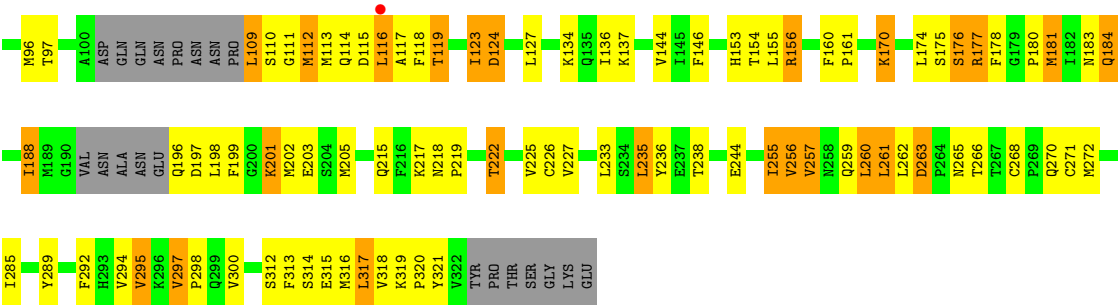


• Molecule 1: ATPASE GET3



• Molecule 1: ATPASE GET3





4 Data and refinement statistics

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) 93.8 (40.69-3.01)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.237 , 0.288 0.230 , 0.274	Depositor DCC
R_{free} test set	1892 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	96.1	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 78.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

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

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	0.52	0/2391	0.83	0/3223
1	B	0.50	0/2391	0.84	2/3223 (0.1%)
1	C	0.60	0/2391	0.83	0/3223
1	D	0.48	0/2391	0.83	2/3223 (0.1%)
1	E	0.48	0/2391	0.83	0/3223
1	F	0.45	0/2391	0.83	2/3223 (0.1%)
All	All	0.51	0/14346	0.83	6/19338 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	263	ASP	CA-C-N	5.24	125.29	119.32
1	F	263	ASP	C-N-CA	5.24	125.29	119.32
1	B	263	ASP	CA-C-N	5.22	125.28	119.32
1	B	263	ASP	C-N-CA	5.22	125.28	119.32
1	D	263	ASP	CA-C-N	5.01	125.03	119.32
1	D	263	ASP	C-N-CA	5.01	125.03	119.32

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	104	0
1	B	2352	0	2370	110	0
1	C	2352	0	2370	130	1
1	D	2352	0	2370	116	0
1	E	2352	0	2370	136	1
1	F	2352	0	2370	119	4
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	F	1	0	0	0	0
All	All	14115	0	14220	629	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 22.

All (629) 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:C:113:MET:HE2	1:E:177:ARG:CD	1.85	1.06
1:A:123:ILE:HD12	1:A:123:ILE:H	1.23	1.02
1:D:123:ILE:HD12	1:D:123:ILE:H	1.25	1.01
1:F:123:ILE:HD12	1:F:123:ILE:H	1.25	0.99
1:F:117:ALA:HA	1:F:123:ILE:HD11	1.45	0.98
1:C:123:ILE:HD12	1:C:123:ILE:H	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:113:MET:HE2	1:E:177:ARG:HD2	1.48	0.95
1:C:117:ALA:HA	1:C:123:ILE:HD11	1.46	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:D:170:LYS:HZ3	1:F:118:PHE:HB2	1.42	0.85
1:C:114:GLN:HE22	1:E:112:MET:CE	1.89	0.84
1:C:124:ASP:CG	1:E:175:SER:HG	1.85	0.83
1:C:114:GLN:HE22	1:E:112:MET:HE3	1.43	0.82
1:A:115:ASP:CG	1:F:115:ASP:OD1	2.23	0.82
1:A:123:ILE:HD12	1:A:123:ILE:N	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H	1:B:123:ILE:CD1	1.92	0.78
1:C:114:GLN:HG3	1:E:177:ARG:NH2	1.99	0.77
1:D:170:LYS:NZ	1:F:118:PHE:HB2	1.99	0.77
1:E:113:MET:CE	1:E:124:ASP:HB3	2.15	0.77
1:D:113:MET:CE	1:D:124:ASP:HB3	2.16	0.76
1:C:123:ILE:HD12	1:C:123:ILE:N	2.00	0.76
1:E:113:MET:HE3	1:E:124:ASP:HB3	1.68	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:C:118:PHE:CE2	1:E:115:ASP:HB3	2.21	0.75
1:F:123:ILE:HD12	1:F:123:ILE:N	1.99	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:124:ASP:CG	1:E:175:SER:OG	2.30	0.74
1:A:113:MET:HE3	1:A:124:ASP:HB3	1.69	0.74
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:C:110:SER:HA	1:C:113:MET:HB3	1.73	0.71
1:D:110:SER:HA	1:D:113:MET:HB3	1.73	0.71
1:C:114:GLN:HG3	1:E:177:ARG:HH21	1.53	0.71
1:C:113:MET:HE3	1:C:124:ASP:HB3	1.73	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:B:10:LEU:HD22	1:B:13:LEU:HD22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ALA:HB3	1:E:178:PHE:CZ	2.26	0.70
1:D:113:MET:HE3	1:D:124:ASP:HB3	1.72	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:114:GLN:NE2	1:E:112:MET:HE3	2.06	0.69
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:B:21:TRP:CD1	1:B:146:PHE:HE2	2.09	0.69
1:D:118:PHE:CZ	1:F:118:PHE:CE2	2.78	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:C:201:LYS:HB2	1:C:201:LYS:NZ	2.07	0.69
1:F:21:TRP:HD1	1:F:146:PHE:HE2	1.40	0.69
1:B:113:MET:HE3	1:B:124:ASP:HB3	1.72	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:F:113:MET:HE3	1:F:124:ASP:HB3	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:C:117:ALA:HB3	1:E:178:PHE:HZ	1.56	0.68
1:F:201:LYS:HB2	1:F:201:LYS:NZ	2.09	0.68
1:B:21:TRP:HD1	1:B:146:PHE:HE2	1.41	0.67
1:A:201:LYS:HB2	1:A:201:LYS:NZ	2.09	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:HB2	1:B:201:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:PHE:O	1:E:202:MET:HB3	1.98	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: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:E:215:GLN:O	1:E:222:THR:HG23	1.98	0.63
1:F:199:PHE:O	1:F:202:MET:HB3	1.98	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
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:B:153:HIS:O	1:B:156:ARG:HG3	1.99	0.62
1:F:215:GLN:O	1:F:222:THR:HG23	1.98	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:B:199:PHE:O	1:B:202:MET:HB3	1.99	0.62
1:C:124:ASP:OD2	1:E:175:SER:OG	2.17	0.62
1:F:38:SER:HB3	1:F:314:SER:HA	1.81	0.62
1:F:176:SER:O	1:F:177:ARG:HG2	2.00	0.62
1:A:215:GLN:O	1:A:222:THR:HG23	2.00	0.61
1:B:177:ARG:HB2	1:B:177:ARG:NH1	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:A:9:THR:HG23	1:A:11:GLU:H	1.65	0.60
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: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: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:NH1	1:E:177:ARG:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:HIS:O	1:A:156:ARG:HG3	2.02	0.59
1:D:9:THR:HG23	1:D:11:GLU:H	1.68	0.59
1:C:177:ARG:NH1	1:C:177:ARG:HB2	2.18	0.59
1:D:127:LEU:HD22	1:D:188:ILE:HD11	1.85	0.59
1:F:118:PHE:CE1	1:F:119:THR:HG23	2.38	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:NH1	1:A:177:ARG:HB2	2.18	0.58
1:F:261:LEU:H	1:F:261:LEU:HD22	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:B:127:LEU:HD22	1:B:188:ILE:HD11	1.85	0.58
1:A:176:SER:C	1:A:178:PHE:H	2.12	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:B:109:LEU:HD23	1:B:111:GLY:H	1.70	0.57
1:C:201:LYS:HB2	1:C:201:LYS:HZ2	1.68	0.56
1:C:110:SER:HB2	1:E:177:ARG:NH2	2.20	0.56
1:B:176:SER:C	1:B:178:PHE:H	2.13	0.56
1:A:124:ASP:OD2	1:F:177:ARG:HD3	2.05	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:D:176:SER:C	1:D:178:PHE:H	2.14	0.56
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:E:176:SER:C	1:E:178:PHE:H	2.14	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:C:176:SER:C	1:C:178:PHE:H	2.14	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:A:127:LEU:HD22	1:A:188:ILE:HD11	1.89	0.54
1:C:110:SER:CB	1:E:177:ARG:HH22	2.19	0.54
1:C:117:ALA:HB1	1:E:178:PHE:HE1	1.72	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:F:176:SER:C	1:F:178:PHE:H	2.14	0.54
1:B:261:LEU:HD23	1:B:261:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:LEU:HD23	1:F:261:LEU:O	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:C:113:MET:HE2	1:E:177:ARG:NE	2.23	0.53
1:B:134:LYS:HE3	1:B:188:ILE:O	2.08	0.53
1:B:318:VAL:HG23	1:B:319:LYS:HG3	1.90	0.53
1:C:270:GLN:HE22	1:D:301:PRO:HG3	1.73	0.53
1:E:261:LEU:HD22	1:E:261:LEU:H	1.72	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:B:115:ASP:OD1	1:E:115:ASP:CG	2.51	0.53
1:E:134:LYS:HE3	1:E:188:ILE:O	2.09	0.53
1:C:113:MET:HE2	1:E:177:ARG:HD3	1.83	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:D:201:LYS:HB2	1:D:201:LYS:HZ2	1.73	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:E:197:ASP:C	1:E:198:LEU:HG	2.35	0.52
1:F:218:ASN:C	1:F:218:ASN:OD1	2.53	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:B:67:THR:HG22	1:B:68:LYS:N	2.25	0.52
1:D:197:ASP:C	1:D:198:LEU:HG	2.35	0.52
1:F:201:LYS:O	1:F:205:MET:HG3	2.10	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:B:93:ILE:O	1:B:97:THR:HG23	2.10	0.51
1:C:174:LEU:HD13	1:C:178:PHE:CE1	2.45	0.51
1:A:197:ASP:C	1:A:198:LEU:HG	2.34	0.51
1:A:318:VAL:HG23	1:A:319:LYS:HG3	1.92	0.51
1:C:197:ASP:C	1:C:198:LEU:HG	2.35	0.51
1:A:261:LEU:HD23	1:A:261:LEU:O	2.10	0.51
1:B:203:GLU:HG3	1:B:203:GLU:O	2.10	0.51
1:C:67:THR:HG22	1:C:68:LYS:N	2.25	0.51
1:E:118:PHE:CE1	1:E:119:THR:HG23	2.46	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:D:261:LEU:H	1:D:261:LEU:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LYS:HE3	1:C:80:ASP:O	2.11	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:A:201:LYS:O	1:A:205:MET:HG3	2.11	0.51
1:F:201:LYS:HB2	1:F:201:LYS:HZ1	1.75	0.51
1:D:67:THR:HG22	1:D:68:LYS:N	2.26	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:A:67:THR:HG22	1:A:68:LYS:N	2.26	0.50
1:C:114:GLN:NE2	1:E:112:MET:HE2	2.26	0.50
1:F:75:LYS:HE3	1:F:80:ASP:O	2.11	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
1:B:197:ASP:C	1:B:198:LEU:HG	2.37	0.50
1:D:203:GLU:HG3	1:D:203:GLU:O	2.10	0.50
1:C:203:GLU:O	1:C:203:GLU:HG3	2.11	0.50
1:E:201:LYS:O	1:E:205:MET: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: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:F:261:LEU:H	1:F:261:LEU:CD2	2.24	0.50
1:B:21:TRP:HB2	1:B:222:THR:HB	1.95	0.49
1:B:177:ARG:HB2	1:B:177:ARG:HH11	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:C:21:TRP:HD1	1:C:146:PHE:CE2	2.27	0.49
1:D:118:PHE:CE1	1:D:119:THR:HG23	2.48	0.49
1:D:318:VAL:HG23	1:D:319:LYS:HG3	1.92	0.49
1:B:180:PRO:O	1:B:184:GLN:HB2	2.13	0.49
1:D:75:LYS:HE3	1:D:80:ASP:O	2.12	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:218:ASN:OD1	1:E:218:ASN:C	2.54	0.49
1:A:21:TRP:HZ2	1:A:137:LYS:HD3	1.78	0.48
1:E:123:ILE:H	1:E:123:ILE:CD1	1.93	0.48
1:A:260:LEU:O	1:A:298:PRO:HA	2.13	0.48
1:C:118:PHE:HE1	1:E:118:PHE:HZ	1.60	0.48
1:C:260:LEU:HD12	1:C:260:LEU:O	2.13	0.48
1:D:21:TRP:HB2	1:D:222:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:226:CYS:O	1:F:255:ILE:HA	2.13	0.48
1:A:21:TRP:HB2	1:A:222:THR:HB	1.95	0.48
1:A:203:GLU:O	1:A:203:GLU:HG3	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:201:LYS:HB2	1:A:201:LYS:HZ2	1.78	0.48
1:B:184:GLN:HA	1:B:184:GLN:NE2	2.28	0.48
1:D:261:LEU:HD23	1:D:261:LEU:O	2.13	0.48
1:F:197:ASP:C	1:F:198:LEU:HG	2.39	0.48
1:C:21:TRP:HB2	1:C:222:THR:HB	1.95	0.48
1:A:9:THR:HG23	1:A:11:GLU:HB2	1.94	0.48
1:F:21:TRP:HD1	1:F:146:PHE:CE2	2.28	0.48
1:C:117:ALA:CB	1:E:178:PHE:CZ	2.95	0.48
1:C:261:LEU:O	1:C:261:LEU:HD23	2.14	0.48
1:D:21:TRP:HD1	1:D:146:PHE:CE2	2.24	0.48
1:A:118:PHE:HA	1:F:174:LEU:HD21	1.94	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:F:174:LEU:HD13	1:F:178:PHE:CE1	2.49	0.48
1:B:261:LEU:H	1:B:261:LEU:CD2	2.27	0.48
1:C:110:SER:CB	1:E:177:ARG:NH2	2.77	0.48
1:F:203:GLU:O	1:F:203:GLU:HG3	2.14	0.48
1:B:75:LYS:HE3	1:B:80:ASP:O	2.14	0.47
1:B:176:SER:O	1:B:177:ARG:CG	2.62	0.47
1:C:176:SER:O	1:C:177:ARG:CG	2.62	0.47
1:C:184:GLN:NE2	1:C:184:GLN:HA	2.29	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: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: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: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: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:93:ILE:O	1:C:97:THR:HG23	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASN:OD1	1:B:218:ASN:C	2.57	0.47
1:D:289:TYR:HB3	1:D:292:PHE:HB2	1.96	0.47
1:E:17:THR:HA	1:E:47:ARG:NH1	2.30	0.47
1:E:21:TRP:HZ2	1:E:137:LYS:HD3	1.80	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:N	1:D:123:ILE:CD1	2.64	0.47
1:B:174:LEU:HD13	1:B:178:PHE:CE1	2.50	0.47
1:B:226:CYS:O	1:B:255:ILE:HA	2.15	0.47
1:C:215:GLN:O	1:C:222:THR:CG2	2.63	0.47
1:E:9:THR:HG23	1:E:11:GLU:HB2	1.97	0.47
1:F:67:THR:HG22	1:F:68:LYS:N	2.29	0.47
1:A:170:LYS:O	1:A:170:LYS:HD3	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:C:160:PHE:CD1	1:C:160:PHE:C	2.94	0.46
1:E:54:SER:HB3	1:E:61:LEU:HD22	1.97	0.46
1:F:289:TYR:HB3	1:F:292:PHE:HB2	1.96	0.46
1:A:177:ARG:HH21	1:D:114:GLN:CD	2.23	0.46
1:C:118:PHE:CE1	1:E:118:PHE:HZ	2.32	0.46
1:F:184:GLN:HA	1:F:184:GLN:NE2	2.29	0.46
1:A:184:GLN:NE2	1:A:184:GLN:HA	2.29	0.46
1:E:217:LYS:O	1:E:219:PRO:HD3	2.16	0.46
1:C:196:GLN:N	1:C:196:GLN:OE1	2.48	0.46
1:D:176:SER:O	1:D:177:ARG:CG	2.63	0.46
1:F:176:SER:O	1:F:177:ARG:CG	2.63	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:HB2	1:E:177:ARG:HH11	1.81	0.46
1:F:38:SER:HB2	1:F:317:LEU:CD2	2.46	0.46
1:A:41:ILE:HG23	1:A:79:PHE:CE1	2.51	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:B:87:ILE:HD13	1:B:88:ASP:H	1.79	0.46
1:C:21:TRP:CD1	1:C:146:PHE:CE2	2.95	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:F:21:TRP:HZ2	1:F:137:LYS:HD3	1.81	0.46
1:C:177:ARG:HB2	1:C:177:ARG:HH11	1.80	0.46
1:D:111:GLY:O	1:D:114:GLN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:THR:HG23	1:B:11:GLU:HB2	1.98	0.45
1:C:170:LYS:O	1:C:170:LYS:HD3	2.17	0.45
1:C:270:GLN:NE2	1:D:301:PRO:HG3	2.31	0.45
1:E:160:PHE:N	1:E:161:PRO:CD	2.79	0.45
1:E:180:PRO:O	1:E:184:GLN:HB2	2.16	0.45
1:F:180:PRO:O	1:F:184:GLN:HB2	2.15	0.45
1:B:291:ASP:OD1	1:B:291:ASP:N	2.46	0.45
1:C:226:CYS:O	1:C:255:ILE:HA	2.16	0.45
1:F:41:ILE:HG23	1:F:79:PHE:CE1	2.50	0.45
1:F:92:SER:O	1:F:96:MET:HG2	2.16	0.45
1:C:9:THR:HG23	1:C:11:GLU:HB2	1.98	0.45
1:D:9:THR:HG23	1:D:11:GLU:HB2	1.99	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:260:LEU:O	1:E:298:PRO:HA	2.16	0.45
1:E:261:LEU:H	1:E:261:LEU:CD2	2.30	0.45
1:B:54:SER:HB3	1:B:61:LEU:HD22	1.99	0.45
1:C:57:PRO:C	1:C:59:HIS:H	2.24	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:17:THR:HA	1:B:47:ARG:NH1	2.32	0.45
1:E:151:THR:HG21	1:F:236:TYR:CD1	2.51	0.45
1:A:226:CYS:O	1:A:255:ILE:HA	2.17	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:E:89:PRO:O	1:E:93:ILE:HG13	2.17	0.45
1:F:38:SER:HB2	1:F:317:LEU:HD22	1.99	0.45
1:A:217:LYS:O	1:A:219:PRO:HD3	2.17	0.44
1:A:291:ASP:OD1	1:A:291:ASP:N	2.43	0.44
1:C:180:PRO:O	1:C:184:GLN:HB2	2.17	0.44
1:D:109:LEU:N	1:D:184:GLN:HG3	2.32	0.44
1:F:177:ARG:HB2	1:F:177:ARG:HH11	1.81	0.44
1:B:174:LEU:HD13	1:B:178:PHE:CZ	2.52	0.44
1:D:57:PRO:C	1:D:59:HIS:H	2.25	0.44
1:A:268:CYS:HB3	1:A:271:CYS:HB2	1.98	0.44
1:B:21:TRP:CD1	1:B:146:PHE:CE2	2.99	0.44
1:C:217:LYS:O	1:C:219:PRO:HD3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:HD1	1:A:146:PHE:CE2	2.28	0.44
1:A:57:PRO:C	1:A:59:HIS:H	2.25	0.44
1:D:170:LYS:HE2	1:F:118:PHE:CA	2.44	0.44
1:B:114:GLN:O	1:B:117:ALA:N	2.51	0.44
1:C:117:ALA:CB	1:E:178:PHE:CE1	3.00	0.44
1:E:256:VAL:HA	1:E:295:VAL:HG13	2.00	0.44
1:F:57:PRO:C	1:F:59:HIS:H	2.25	0.44
1:F:266:THR:HG23	1:F:272:MET:HG2	2.00	0.44
1:F:312:SER:O	1:F:315:GLU:HB2	2.17	0.44
1:B:127:LEU:HD22	1:B:188:ILE:CD1	2.47	0.44
1:C:118:PHE:CE1	1:E:118:PHE:CZ	3.05	0.44
1:D:170:LYS:HD3	1:D:170:LYS:O	2.18	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
1:E:57:PRO:C	1:E:59:HIS:H	2.25	0.44
1:B:217:LYS:HE3	1:B:249:GLU:HB2	1.99	0.44
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:312:SER:O	1:B:315:GLU:HB2	2.18	0.44
1:E:87:ILE:HD13	1:E:88:ASP:H	1.82	0.44
1:F:9:THR:HG23	1:F:11:GLU:HB2	2.00	0.44
1:B:57:PRO:C	1:B:59:HIS:H	2.26	0.43
1:D:174:LEU:HD13	1:D:178:PHE:CE1	2.53	0.43
1:D:263:ASP:OD2	1:D:263:ASP:C	2.61	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:A:114:GLN:C	1:A:117:ALA:H	2.27	0.43
1:B:41:ILE:HG23	1:B:79:PHE:CE1	2.53	0.43
1:E:41:ILE:HG23	1:E:79:PHE:CE1	2.53	0.43
1:E:289:TYR:HB3	1:E:292:PHE:HB2	1.99	0.43
1:F:174:LEU:HD13	1:F:178:PHE:CZ	2.53	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:B:46:VAL:HG22	1:B:46:VAL:O	2.18	0.43
1:D:256:VAL:HA	1:D:295:VAL:HG13	1.98	0.43
1:F:114:GLN:O	1:F:117:ALA:N	2.51	0.43
1:A:21:TRP:CD1	1:A:146:PHE:CE2	2.98	0.43
1:A:21:TRP:CZ2	1:A:137:LYS:HD3	2.53	0.43
1:A:54:SER:HB3	1:A:61:LEU:HD22	2.00	0.43
1:A:87:ILE:HD13	1:A:88:ASP:H	1.83	0.43
1:A:266:THR:HG23	1:A:272:MET:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:GLN:HA	1:C:184:GLN:HE21	1.83	0.43
1:D:260:LEU:O	1:D:298:PRO:HA	2.18	0.43
1:E:298:PRO:HG3	1:E:321:TYR:CD1	2.54	0.43
1:F:170:LYS:O	1:F:170:LYS:HD3	2.17	0.43
1:A:289:TYR:HB3	1:A:292:PHE:HB2	2.00	0.43
1:A:46:VAL:HG22	1:A:46:VAL:O	2.19	0.43
1:A:217:LYS:HE3	1:A:249:GLU:HB2	2.01	0.43
1:B:109:LEU:CD2	1:B:111:GLY:H	2.32	0.43
1:C:17:THR:HA	1:C:47:ARG:NH1	2.34	0.43
1:C:312:SER:O	1:C:315:GLU:HB2	2.19	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:D:160:PHE:N	1:D:161:PRO:CD	2.82	0.43
1:F:15:GLU:O	1:F:17:THR:HG23	2.19	0.43
1:A:17:THR:HA	1:A:47:ARG:NH1	2.33	0.43
1:B:118:PHE:CE2	1:C:118:PHE:HZ	2.31	0.43
1:C:266:THR:HG23	1:C:272:MET:HG2	1.99	0.43
1:E:38:SER:CB	1:E:317:LEU:HD22	2.49	0.43
1:E:92:SER:O	1:E:96:MET:HG2	2.18	0.43
1:F:114:GLN:C	1:F:116:LEU:N	2.76	0.43
1:A:184:GLN:HA	1:A:184:GLN:HE21	1.84	0.43
1:B:110:SER:O	1:B:114:GLN:N	2.51	0.43
1:B:127:LEU:CD2	1:B:188:ILE:HD11	2.48	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:F:111:GLY:O	1:F:114:GLN:HB2	2.18	0.43
1:B:160:PHE:N	1:B:161:PRO:CD	2.82	0.43
1:C:109:LEU:N	1:C:184:GLN:HG3	2.34	0.43
1:D:61:LEU:HD12	1:D:61:LEU:HA	1.85	0.43
1:D:266:THR:HG23	1:D:272:MET:HG2	2.00	0.43
1:F:54:SER:HB3	1:F:61:LEU:HD22	2.00	0.43
1:F:313:PHE:C	1:F:315:GLU:N	2.77	0.43
1:C:160:PHE:N	1:C:161:PRO:CD	2.82	0.42
1:D:92:SER:O	1:D:96:MET:HG2	2.19	0.42
1:F:184:GLN:HA	1:F:184:GLN:HE21	1.84	0.42
1:B:55:THR:HA	1:B:87:ILE:O	2.19	0.42
1:B:260:LEU:O	1:B:298:PRO:HA	2.19	0.42
1:C:110:SER:C	1:E:177:ARG:NH2	2.77	0.42
1:C:114:GLN:CD	1:E:112:MET:HE3	2.43	0.42
1:D:114:GLN:O	1:D:117:ALA:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:GLN:HA	1:D:184:GLN:HE21	1.85	0.42
1:B:21:TRP:HD1	1:B:146:PHE:CE2	2.29	0.42
1:B:92:SER:O	1:B:96:MET:HG2	2.19	0.42
1:B:114:GLN:C	1:B:116:LEU:N	2.76	0.42
1:D:55:THR:HA	1:D:87:ILE:O	2.19	0.42
1:D:218:ASN:OD1	1:D:218:ASN:C	2.62	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:C:201:LYS:HA	1:C:204:SER:OG	2.19	0.42
1:C:218:ASN:OD1	1:C:218:ASN:C	2.63	0.42
1:E:312:SER:O	1:E:315:GLU:HB2	2.20	0.42
1:F:21:TRP:CD1	1:F:146:PHE:CE2	2.97	0.42
1:F:109:LEU:CD2	1:F:111:GLY:H	2.30	0.42
1:F:114:GLN:C	1:F:117:ALA:H	2.27	0.42
1:B:111:GLY:O	1:B:114:GLN:HB2	2.20	0.42
1:B:160:PHE:CD1	1:B:160:PHE:C	2.98	0.42
1:B:184:GLN:HA	1:B:184:GLN:HE21	1.83	0.42
1:F:183:ASN:HA	1:F:201:LYS:HE2	2.01	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:B:168:LEU:HD23	1:B:168:LEU:HA	1.87	0.42
1:C:257:VAL:O	1:C:257:VAL:CG2	2.67	0.42
1:D:54:SER:HB3	1:D:61:LEU:HD22	2.02	0.42
1:D:217:LYS:HE3	1:D:249:GLU:HB2	2.00	0.42
1:E:297:VAL:HA	1:E:298:PRO:HD3	1.87	0.42
1:A:176:SER:C	1:A:178:PHE:N	2.77	0.42
1:C:92:SER:O	1:C:96:MET:HG2	2.19	0.42
1:C:263:ASP:C	1:C:263:ASP:OD2	2.62	0.42
1:C:289:TYR:HB3	1:C:292:PHE:HB2	2.01	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:B:118:PHE:CD1	1:C:119:THR:HG21	2.55	0.42
1:B:268:CYS:HB3	1:B:271:CYS:HB2	2.02	0.42
1:C:183:ASN:HA	1:C:201:LYS:HE2	2.02	0.42
1:C:257:VAL:O	1:C:257:VAL:HG23	2.20	0.42
1:D:38:SER:HB2	1:D:317:LEU:HD22	2.02	0.42
1:D:176:SER:O	1:D:178:PHE:N	2.51	0.42
1:E:111:GLY:O	1:E:114:GLN:HB2	2.19	0.42
1:F:160:PHE:N	1:F:161:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:ASP:OD2	1:F:263:ASP:C	2.63	0.42
1:D:160:PHE:CD1	1:D:160:PHE:C	2.97	0.42
1:E:114:GLN:C	1:E:116:LEU:N	2.78	0.42
1:F:260:LEU:O	1:F:260:LEU:HD12	2.19	0.42
1:A:114:GLN:HE22	1:F:112:MET:HE3	1.85	0.42
1:A:174:LEU:HD13	1:A:178:PHE:CE1	2.55	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: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: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: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:E:266:THR:HG23	1:E:272:MET:HG2	2.02	0.41
1:F:110:SER:O	1:F:114:GLN:N	2.52	0.41
1:A:92:SER:O	1:A:96:MET:HG2	2.20	0.41
1:A:218:ASN:OD1	1:A:218:ASN:C	2.63	0.41
1:E:19:LEU:HD12	1:E:19:LEU:HA	1.83	0.41
1:E:58:ALA:O	1:E:59:HIS:C	2.63	0.41
1:F:268:CYS:HB3	1:F:271:CYS:HB2	2.02	0.41
1:A:160:PHE:N	1:A:161:PRO:CD	2.82	0.41
1:A:257:VAL:O	1:A:257:VAL:HG23	2.19	0.41
1:C:81:ASN:OD1	1:C:81:ASN:N	2.52	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:B:21:TRP:CZ2	1:B:137:LYS:HD3	2.54	0.41
1:B:38:SER:CB	1:B:317:LEU:HD22	2.51	0.41
1:E:174:LEU:HD13	1:E:178:PHE:CZ	2.55	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:H	1:A:261:LEU:CD2	2.33	0.41
1:B:297:VAL:HA	1:B:298:PRO:HD3	1.85	0.41
1:C:54:SER:HB3	1:C:61:LEU:HD22	2.01	0.41
1:E:46:VAL:O	1:E:46:VAL:HG22	2.20	0.41
1:E:114:GLN:C	1:E:117:ALA:H	2.27	0.41
1:F:61:LEU:HA	1:F:61:LEU:HD12	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:HIS:HA	1:A:86:GLU:OE1	2.21	0.41
1:A:321:TYR:CD1	1:A:321:TYR:C	2.99	0.41
1:B:118:PHE:CZ	1:E:118:PHE:HZ	2.33	0.41
1:C:58:ALA:O	1:C:59:HIS:C	2.64	0.41
1:C:109:LEU:CD2	1:C:111:GLY:H	2.31	0.41
1:D:87:ILE:HD13	1:D:88:ASP:H	1.84	0.41
1:D:114:GLN:C	1:D:117:ALA:H	2.28	0.41
1:D:321:TYR:CD1	1:D:321:TYR:C	2.98	0.41
1:F:89:PRO:O	1:F:93:ILE:HG13	2.21	0.41
1:F:197:ASP:HA	1:F:201:LYS:HD2	2.02	0.41
1:F:297:VAL:HA	1:F:298:PRO:HD3	1.87	0.41
1:A:19:LEU:HA	1:A:19:LEU:HD12	1.81	0.41
1:A:257:VAL:O	1:A:257:VAL:CG2	2.69	0.41
1:B:114:GLN:C	1:B:117:ALA:H	2.28	0.41
1:C:256:VAL:HA	1:C:295:VAL:HG13	2.02	0.41
1:C:313:PHE:C	1:C:315:GLU:N	2.78	0.41
1:E:38:SER:HB2	1:E:317:LEU:HD22	2.01	0.41
1:E:110:SER:O	1:E:114:GLN:N	2.52	0.41
1:E:154:THR:C	1:E:155:LEU:HD12	2.46	0.41
1:E:170:LYS:O	1:E:170:LYS:HD3	2.20	0.41
1:E:181:MET:HE3	1:E:181:MET:HB2	1.93	0.41
1:A:181:MET:HE3	1:A:181:MET:HB2	1.95	0.41
1:A:271:CYS:SG	1:B:270:GLN:HB2	2.61	0.41
1:B:58:ALA:O	1:B:59:HIS:C	2.64	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:B:257:VAL:O	1:B:257:VAL:HG23	2.20	0.41
1:C:21:TRP:CZ2	1:C:137:LYS:HD3	2.54	0.41
1:F:321:TYR:CD1	1:F:321:TYR:C	2.98	0.41
1:A:110:SER:O	1:A:114:GLN:N	2.53	0.41
1:A:177:ARG:NH2	1:D:114:GLN:CD	2.79	0.41
1:A:201:LYS:HA	1:A:204:SER:OG	2.21	0.41
1:B:67:THR:HG22	1:B:68:LYS:H	1.86	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:C:61:LEU:HD12	1:C:61:LEU:HA	1.85	0.41
1:C:298:PRO:HG3	1:C:321:TYR:CD1	2.55	0.41
1:D:21:TRP:CD1	1:D:146:PHE:CE2	2.96	0.41
1:D:114:GLN:C	1:D:116:LEU:N	2.77	0.41
1:D:313:PHE:C	1:D:315:GLU:N	2.78	0.41
1:E:151:THR:HB	1:F:236:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:SER:O	1:E:178:PHE:N	2.51	0.41
1:F:127:LEU:CD2	1:F:188:ILE:HD11	2.48	0.41
1:F:181:MET:HE3	1:F:181:MET:HB2	1.94	0.41
1:B:176:SER:O	1:B:178:PHE:N	2.52	0.41
1:B:176:SER:C	1:B:178:PHE:N	2.79	0.41
1:B:182:ILE:O	1:B:205:MET:HE1	2.21	0.41
1:E:257:VAL:O	1:E:257:VAL:CG2	2.69	0.41
1:A:73:ALA:HB2	1:A:85:MET:HE2	2.03	0.40
1:A:263:ASP:OD2	1:A:263:ASP:C	2.63	0.40
1:B:183:ASN:HA	1:B:201:LYS:HE2	2.02	0.40
1:B:263:ASP:OD2	1:B:263:ASP:C	2.63	0.40
1:D:257:VAL:O	1:D:257:VAL:CG2	2.69	0.40
1:A:160:PHE:CD1	1:A:160:PHE:C	2.99	0.40
1:A:297:VAL:HA	1:A:298:PRO:HD3	1.84	0.40
1:B:319:LYS:O	1:B:320:PRO:C	2.65	0.40
1:D:201:LYS:HA	1:D:204:SER:OG	2.21	0.40
1:D:258:ASN:O	1:D:260:LEU:N	2.54	0.40
1:E:21:TRP:CZ2	1:E:137:LYS:HD3	2.56	0.40
1:E:56:ASP:HA	1:E:57:PRO:HD3	1.89	0.40
1:B:235:LEU:HD23	1:B:235:LEU:HA	1.84	0.40
1:D:41:ILE:HG23	1:D:79:PHE:CE1	2.56	0.40
1:E:201:LYS:HB2	1:E:201:LYS:HZ1	1.81	0.40
1:F:319:LYS:O	1:F:320:PRO:C	2.64	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:E:184:GLN:HA	1:E:184:GLN:HE21	1.85	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
1:F:154:THR:C	1:F:155:LEU:HD12	2.46	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:45:LYS:NZ	1:F:196:GLN:O[3_545]	2.12	0.08
1:F:196:GLN:OE1	1:F:315:GLU:OE1[3_555]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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%)	6	28
1	B	297/329 (90%)	272 (92%)	19 (6%)	6 (2%)	6	28
1	C	297/329 (90%)	275 (93%)	15 (5%)	7 (2%)	4	24
1	D	297/329 (90%)	273 (92%)	18 (6%)	6 (2%)	6	28
1	E	297/329 (90%)	272 (92%)	19 (6%)	6 (2%)	6	28
1	F	297/329 (90%)	273 (92%)	18 (6%)	6 (2%)	6	28
All	All	1782/1974 (90%)	1636 (92%)	109 (6%)	37 (2%)	5	27

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

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Mol	Chain	Res	Type
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
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%)	225 (85%)	41 (15%)	2	13
1	B	266/290 (92%)	225 (85%)	41 (15%)	2	13
1	C	266/290 (92%)	224 (84%)	42 (16%)	2	13
1	D	266/290 (92%)	226 (85%)	40 (15%)	3	14
1	E	266/290 (92%)	226 (85%)	40 (15%)	3	14
1	F	266/290 (92%)	224 (84%)	42 (16%)	2	13
All	All	1596/1740 (92%)	1350 (85%)	246 (15%)	2	13

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR

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Mol	Chain	Res	Type
1	A	11	GLU
1	A	13	LEU
1	A	19	LEU
1	A	24	VAL
1	A	49	SER
1	A	53	ILE
1	A	87	ILE
1	A	109	LEU
1	A	112	MET
1	A	116	LEU
1	A	119	THR
1	A	123	ILE
1	A	124	ASP
1	A	136	ILE
1	A	144	VAL
1	A	156	ARG
1	A	170	LYS
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	235	LEU
1	A	238	THR
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	294	VAL
1	A	295	VAL
1	A	297	VAL
1	A	300	VAL
1	A	316	MET
1	B	9	THR
1	B	11	GLU

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Mol	Chain	Res	Type
1	B	13	LEU
1	B	19	LEU
1	B	24	VAL
1	B	49	SER
1	B	87	ILE
1	B	109	LEU
1	B	112	MET
1	B	116	LEU
1	B	119	THR
1	B	123	ILE
1	B	124	ASP
1	B	136	ILE
1	B	144	VAL
1	B	156	ARG
1	B	170	LYS
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	235	LEU
1	B	238	THR
1	B	244	GLU
1	B	255	ILE
1	B	256	VAL
1	B	257	VAL
1	B	260	LEU
1	B	261	LEU
1	B	262	LEU
1	B	265	ASN
1	B	294	VAL
1	B	295	VAL
1	B	297	VAL
1	B	300	VAL
1	B	316	MET
1	B	317	LEU
1	C	9	THR
1	C	11	GLU
1	C	13	LEU

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Mol	Chain	Res	Type
1	C	19	LEU
1	C	24	VAL
1	C	49	SER
1	C	53	ILE
1	C	87	ILE
1	C	109	LEU
1	C	112	MET
1	C	116	LEU
1	C	119	THR
1	C	123	ILE
1	C	124	ASP
1	C	136	ILE
1	C	144	VAL
1	C	156	ARG
1	C	160	PHE
1	C	170	LYS
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	235	LEU
1	C	238	THR
1	C	244	GLU
1	C	255	ILE
1	C	256	VAL
1	C	257	VAL
1	C	260	LEU
1	C	261	LEU
1	C	262	LEU
1	C	265	ASN
1	C	294	VAL
1	C	295	VAL
1	C	297	VAL
1	C	300	VAL
1	C	316	MET
1	D	9	THR
1	D	11	GLU
1	D	13	LEU

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Mol	Chain	Res	Type
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	116	LEU
1	D	119	THR
1	D	123	ILE
1	D	124	ASP
1	D	136	ILE
1	D	144	VAL
1	D	156	ARG
1	D	170	LYS
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	235	LEU
1	D	238	THR
1	D	244	GLU
1	D	255	ILE
1	D	256	VAL
1	D	257	VAL
1	D	260	LEU
1	D	261	LEU
1	D	262	LEU
1	D	265	ASN
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	11	GLU
1	E	13	LEU
1	E	19	LEU
1	E	24	VAL

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Mol	Chain	Res	Type
1	E	49	SER
1	E	87	ILE
1	E	109	LEU
1	E	112	MET
1	E	116	LEU
1	E	119	THR
1	E	123	ILE
1	E	124	ASP
1	E	136	ILE
1	E	144	VAL
1	E	156	ARG
1	E	170	LYS
1	E	181	MET
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	235	LEU
1	E	238	THR
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	294	VAL
1	E	295	VAL
1	E	297	VAL
1	E	300	VAL
1	E	316	MET
1	F	9	THR
1	F	11	GLU
1	F	13	LEU
1	F	19	LEU
1	F	24	VAL
1	F	49	SER
1	F	53	ILE

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Mol	Chain	Res	Type
1	F	87	ILE
1	F	109	LEU
1	F	112	MET
1	F	116	LEU
1	F	119	THR
1	F	123	ILE
1	F	124	ASP
1	F	136	ILE
1	F	144	VAL
1	F	156	ARG
1	F	170	LYS
1	F	181	MET
1	F	184	GLN
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	235	LEU
1	F	238	THR
1	F	244	GLU
1	F	255	ILE
1	F	256	VAL
1	F	257	VAL
1	F	260	LEU
1	F	261	LEU
1	F	262	LEU
1	F	265	ASN
1	F	294	VAL
1	F	295	VAL
1	F	297	VAL
1	F	300	VAL
1	F	316	MET
1	F	317	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	59	HIS
1	A	114	GLN

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Mol	Chain	Res	Type
1	A	135	GLN
1	A	159	ASN
1	A	184	GLN
1	A	196	GLN
1	A	293	HIS
1	A	299	GLN
1	B	12	ASN
1	B	135	GLN
1	B	159	ASN
1	B	184	GLN
1	B	196	GLN
1	B	293	HIS
1	C	59	HIS
1	C	114	GLN
1	C	135	GLN
1	C	184	GLN
1	C	196	GLN
1	C	253	HIS
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	159	ASN
1	D	184	GLN
1	D	196	GLN
1	D	293	HIS
1	D	299	GLN
1	E	12	ASN
1	E	42	GLN
1	E	59	HIS
1	E	114	GLN
1	E	135	GLN
1	E	159	ASN
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	159	ASN

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Mol	Chain	Res	Type
1	F	184	GLN
1	F	293	HIS

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](#)

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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	303/329 (92%)	-0.53	0	100 100	60, 99, 156, 202	0
1	B	303/329 (92%)	-0.42	0	100 100	66, 106, 187, 248	0
1	C	303/329 (92%)	-0.37	2 (0%)	84 66	53, 89, 163, 288	0
1	D	303/329 (92%)	-0.37	2 (0%)	84 66	66, 120, 194, 258	0
1	E	303/329 (92%)	-0.25	3 (0%)	79 59	72, 121, 191, 240	0
1	F	303/329 (92%)	-0.33	1 (0%)	90 79	94, 140, 211, 269	0
All	All	1818/1974 (92%)	-0.38	8 (0%)	88 76	53, 113, 193, 288	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	110	SER	3.8
1	D	109	LEU	3.3
1	C	109	LEU	3.2
1	E	109	LEU	2.7
1	D	113	MET	2.5
1	E	282	LEU	2.3
1	F	116	LEU	2.2
1	E	285	ILE	2.1

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	F	1323	1/1	0.95	0.06	170,170,170,170	0
2	ZN	C	1323	1/1	0.97	0.06	108,108,108,108	0
2	ZN	B	1323	1/1	0.97	0.04	113,113,113,113	0

6.5 Other polymers [i](#)

There are no such residues in this entry.