



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:20 AM UTC

PDB ID : 8CNL / pdb_00008cnl
Title : Lymphocytic choriomeningitis virus 3'-5' exonuclease domain of nucleoprotein
Authors : Spiliopoulou, M.; Papageorgiou, N.; Ferron, F.
Deposited on : 2023-02-23
Resolution : 2.80 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

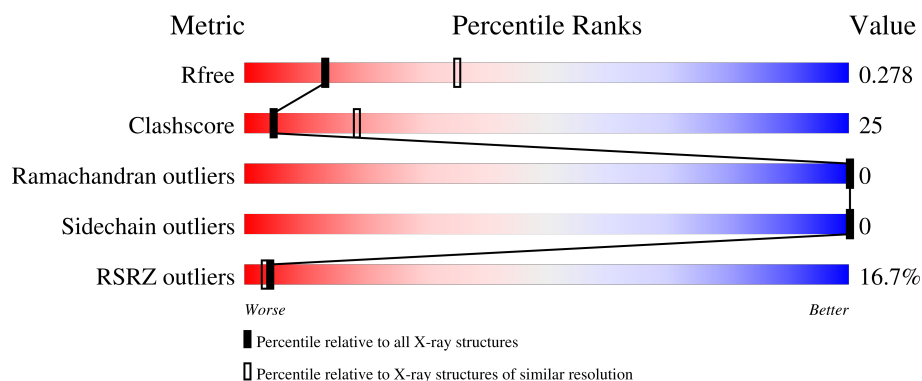
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	218	11% 69% 24% 7%
1	B	218	6% 70% 23% 7%
1	C	218	6% 69% 24% 7%
1	D	218	6% 69% 24% 7%
1	E	218	22% 67% 26% 7%

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Mol	Chain	Length	Quality of chain
1	F	218	22% 67% 26% 7%
1	G	218	26% 67% 26% 7%
1	H	218	24% 67% 26% 7%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12976 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	203	Total	C	N	O	S	0	0	0
			1621	1028	279	303	11			
1	A	203	Total	C	N	O	S	0	0	0
			1621	1028	279	303	11			
1	C	203	Total	C	N	O	S	0	0	0
			1621	1028	279	303	11			
1	D	203	Total	C	N	O	S	0	0	0
			1621	1028	279	303	11			
1	E	203	Total	C	N	O	S	0	0	0
			1621	1028	279	303	11			
1	F	203	Total	C	N	O	S	0	0	0
			1621	1028	279	303	11			
1	G	203	Total	C	N	O	S	0	0	0
			1621	1028	279	303	11			
1	H	203	Total	C	N	O	S	0	0	0
			1621	1028	279	303	11			

- 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	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

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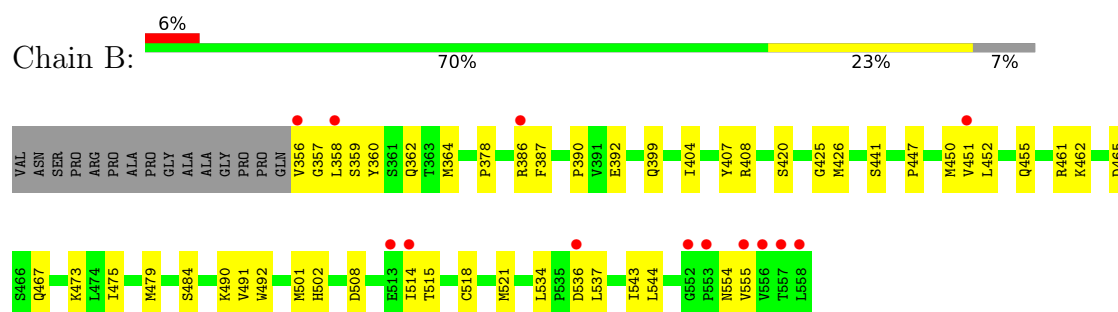
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0

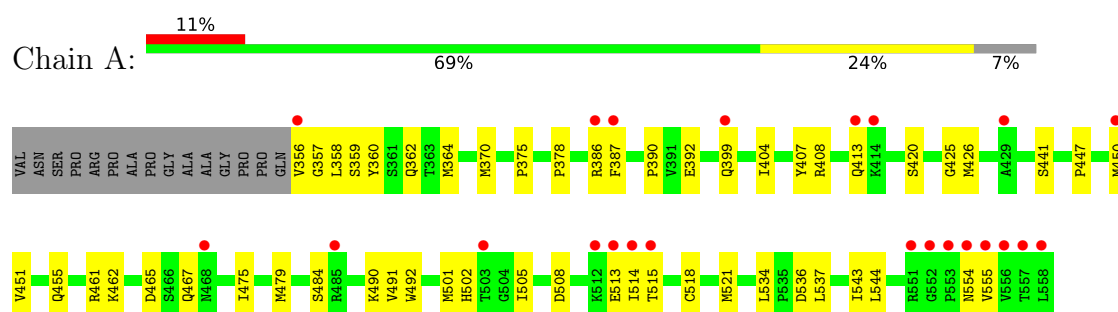
3 Residue-property plots [i](#)

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.

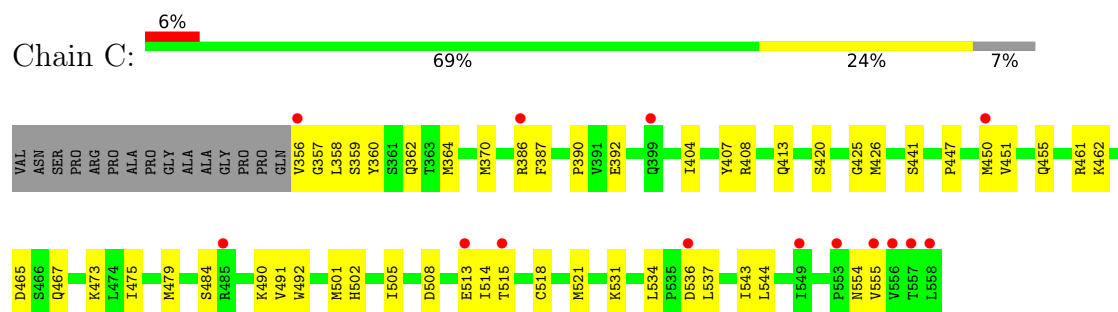
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein

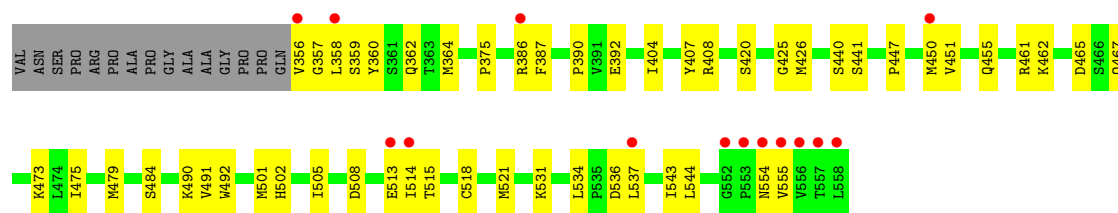


• Molecule 1: Nucleoprotein

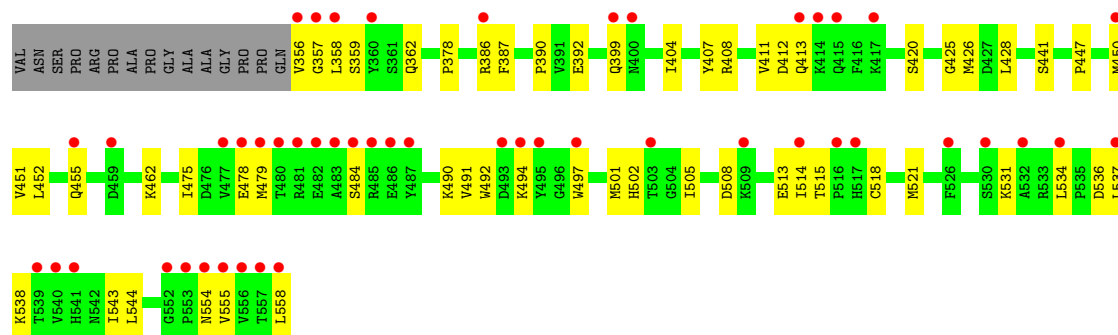


• Molecule 1: Nucleoprotein

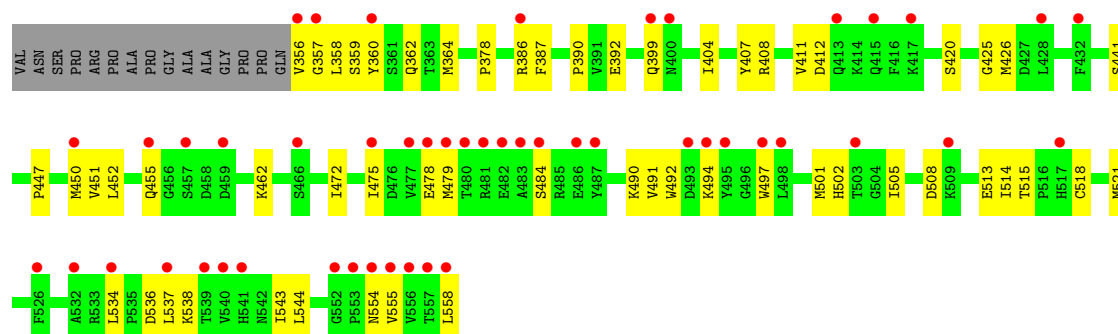




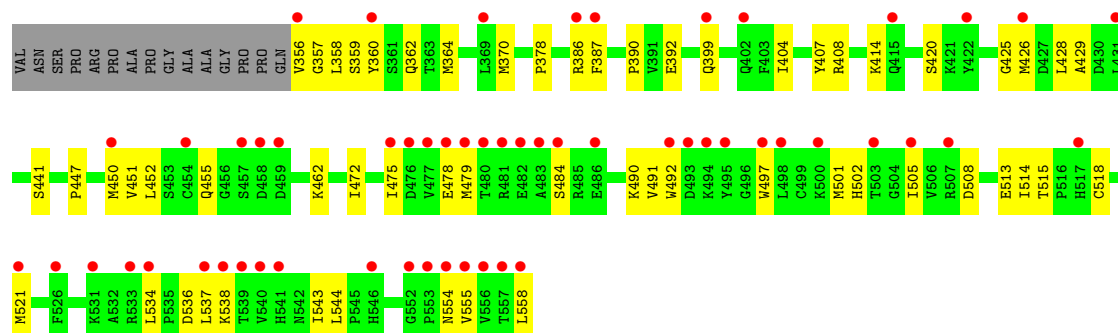
● Molecule 1: Nucleoprotein



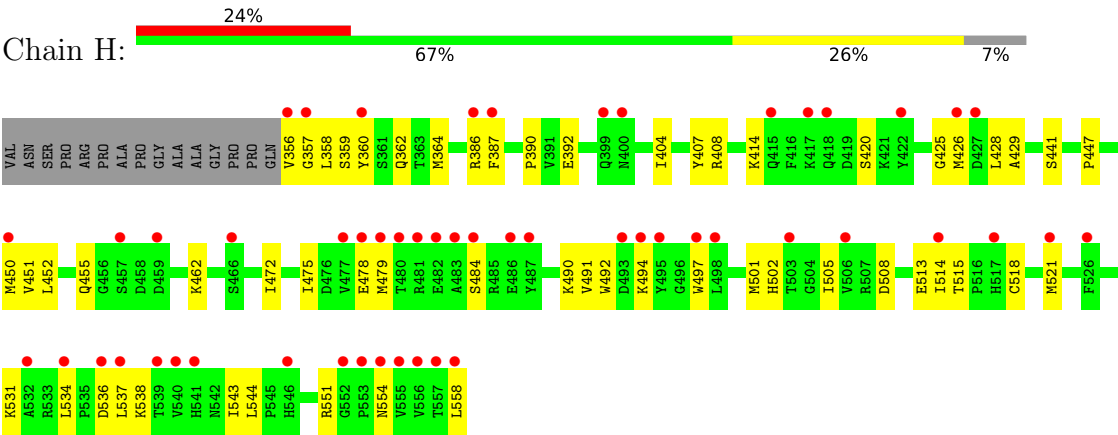
● Molecule 1: Nucleoprotein



● Molecule 1: Nucleoprotein



● Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.08Å 95.07Å 129.13Å 90.00° 97.54° 90.00°	Depositor
Resolution (Å)	81.15 – 2.80 81.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (81.15-2.80) 88.0 (81.15-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 2.82Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.273 , 0.280 0.275 , 0.278	Depositor DCC
R_{free} test set	2000 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12976	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.65	0/1656	0.94	0/2235
1	B	0.65	0/1656	0.95	0/2235
1	C	0.65	0/1656	0.95	0/2235
1	D	0.65	0/1656	0.95	0/2235
1	E	0.65	0/1656	0.94	0/2235
1	F	0.65	0/1656	0.95	0/2235
1	G	0.66	0/1656	0.96	0/2235
1	H	0.65	0/1656	0.95	0/2235
All	All	0.65	0/13248	0.95	0/17880

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1621	0	1615	89	5
1	B	1621	0	1615	79	6
1	C	1621	0	1615	83	7
1	D	1621	0	1615	83	7
1	E	1621	0	1615	93	10

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1621	0	1615	84	11
1	G	1621	0	1613	87	9
1	H	1621	0	1613	86	11
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
All	All	12976	0	12916	658	33

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 25.

All (658) 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:E:413:GLN:NE2	1:E:428:LEU:HD22	1.18	1.49
1:E:413:GLN:CD	1:E:428:LEU:CD2	1.99	1.34
1:E:413:GLN:NE2	1:E:428:LEU:CD2	1.92	1.28
1:E:413:GLN:OE1	1:E:428:LEU:CD2	1.82	1.22
1:E:413:GLN:CD	1:E:428:LEU:HD21	1.61	1.19
1:D:375:PRO:CA	1:D:450:MET:HE1	1.74	1.17
1:D:375:PRO:HA	1:D:450:MET:CE	1.76	1.15
1:C:356:VAL:HG12	1:C:357:GLY:H	1.03	1.14
1:G:356:VAL:HG12	1:G:357:GLY:H	1.03	1.14
1:D:356:VAL:HG12	1:D:357:GLY:H	1.03	1.13
1:F:356:VAL:HG12	1:F:357:GLY:H	1.03	1.13
1:E:413:GLN:OE1	1:E:428:LEU:HD21	0.94	1.10
1:E:356:VAL:HG12	1:E:357:GLY:H	1.03	1.10
1:H:491:VAL:HG12	1:H:521:MET:HE3	1.34	1.10
1:B:356:VAL:HG12	1:B:357:GLY:H	1.03	1.09
1:A:356:VAL:HG12	1:A:357:GLY:H	1.03	1.09
1:D:491:VAL:HG12	1:D:521:MET:HE3	1.35	1.08
1:H:356:VAL:HG12	1:H:357:GLY:H	1.03	1.08
1:E:491:VAL:HG12	1:E:521:MET:HE3	1.35	1.08
1:C:386:ARG:NE	1:C:387:PHE:CD1	2.23	1.07
1:F:386:ARG:NE	1:F:387:PHE:CD1	2.23	1.07
1:F:491:VAL:HG12	1:F:521:MET:HE3	1.35	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ARG:NE	1:B:387:PHE:CD1	2.23	1.06
1:B:491:VAL:HG12	1:B:521:MET:HE3	1.35	1.06
1:E:386:ARG:NE	1:E:387:PHE:CD1	2.23	1.06
1:A:491:VAL:HG12	1:A:521:MET:HE3	1.35	1.06
1:D:386:ARG:NE	1:D:387:PHE:CD1	2.23	1.06
1:A:386:ARG:NE	1:A:387:PHE:CD1	2.23	1.06
1:G:386:ARG:NE	1:G:387:PHE:CD1	2.23	1.06
1:C:491:VAL:HG12	1:C:521:MET:HE3	1.35	1.05
1:H:386:ARG:NE	1:H:387:PHE:CD1	2.23	1.05
1:E:413:GLN:HE22	1:E:428:LEU:CD2	1.62	1.04
1:G:491:VAL:HG12	1:G:521:MET:HE3	1.35	1.04
1:E:492:TRP:HA	1:E:521:MET:HE2	1.40	1.04
1:C:492:TRP:HA	1:C:521:MET:HE2	1.40	1.04
1:F:492:TRP:HA	1:F:521:MET:HE2	1.40	1.04
1:A:491:VAL:HG12	1:A:521:MET:CE	1.88	1.03
1:E:491:VAL:HG12	1:E:521:MET:CE	1.88	1.03
1:A:492:TRP:HA	1:A:521:MET:HE2	1.40	1.03
1:G:492:TRP:HA	1:G:521:MET:HE2	1.40	1.03
1:H:491:VAL:HG12	1:H:521:MET:CE	1.88	1.03
1:C:491:VAL:HG12	1:C:521:MET:CE	1.88	1.02
1:F:491:VAL:HG12	1:F:521:MET:CE	1.88	1.02
1:G:491:VAL:HG12	1:G:521:MET:CE	1.88	1.02
1:H:492:TRP:HA	1:H:521:MET:HE2	1.40	1.02
1:D:492:TRP:HA	1:D:521:MET:HE2	1.40	1.02
1:B:491:VAL:HG12	1:B:521:MET:CE	1.88	1.01
1:D:491:VAL:HG12	1:D:521:MET:CE	1.88	1.01
1:C:447:PRO:HD2	1:C:450:MET:SD	2.01	1.01
1:B:492:TRP:HA	1:B:521:MET:HE2	1.40	1.00
1:C:413:GLN:HE22	1:G:387:PHE:HZ	1.05	1.00
1:A:375:PRO:HA	1:A:450:MET:HE1	1.41	0.99
1:G:356:VAL:HG12	1:G:357:GLY:N	1.77	0.98
1:E:356:VAL:HG12	1:E:357:GLY:N	1.77	0.98
1:C:492:TRP:HA	1:C:521:MET:CE	1.94	0.98
1:A:492:TRP:HA	1:A:521:MET:CE	1.94	0.98
1:E:492:TRP:HA	1:E:521:MET:CE	1.94	0.98
1:H:492:TRP:HA	1:H:521:MET:CE	1.94	0.97
1:G:492:TRP:HA	1:G:521:MET:CE	1.94	0.97
1:B:492:TRP:HA	1:B:521:MET:CE	1.94	0.97
1:D:492:TRP:HA	1:D:521:MET:CE	1.94	0.97
1:F:356:VAL:HG12	1:F:357:GLY:N	1.77	0.96
1:C:356:VAL:HG12	1:C:357:GLY:N	1.77	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:ARG:NE	1:C:387:PHE:CE1	2.33	0.96
1:F:386:ARG:NE	1:F:387:PHE:CE1	2.33	0.96
1:F:492:TRP:HA	1:F:521:MET:CE	1.94	0.96
1:D:386:ARG:NE	1:D:387:PHE:CE1	2.33	0.96
1:E:386:ARG:NE	1:E:387:PHE:CE1	2.33	0.96
1:B:386:ARG:NE	1:B:387:PHE:CE1	2.33	0.96
1:G:386:ARG:NE	1:G:387:PHE:CE1	2.33	0.95
1:B:386:ARG:HH21	1:B:462:LYS:NZ	1.65	0.95
1:D:386:ARG:HH21	1:D:462:LYS:NZ	1.65	0.95
1:E:386:ARG:HH21	1:E:462:LYS:NZ	1.65	0.95
1:B:356:VAL:HG12	1:B:357:GLY:N	1.77	0.95
1:H:386:ARG:NE	1:H:387:PHE:CE1	2.33	0.94
1:F:386:ARG:HH21	1:F:462:LYS:NZ	1.65	0.94
1:C:386:ARG:HH21	1:C:462:LYS:NZ	1.65	0.94
1:E:386:ARG:HE	1:E:387:PHE:HE1	1.11	0.94
1:A:386:ARG:NE	1:A:387:PHE:CE1	2.33	0.94
1:H:386:ARG:HE	1:H:387:PHE:HE1	1.11	0.94
1:H:386:ARG:HH21	1:H:462:LYS:NZ	1.65	0.94
1:A:375:PRO:HA	1:A:450:MET:CE	1.97	0.94
1:G:386:ARG:HE	1:G:387:PHE:HE1	1.11	0.94
1:A:386:ARG:HH21	1:A:462:LYS:NZ	1.64	0.93
1:G:386:ARG:HH21	1:G:462:LYS:NZ	1.65	0.93
1:A:386:ARG:HE	1:A:387:PHE:HE1	1.11	0.93
1:B:386:ARG:HE	1:B:387:PHE:HE1	1.11	0.92
1:D:386:ARG:HE	1:D:387:PHE:HE1	1.11	0.92
1:C:386:ARG:HE	1:C:387:PHE:HE1	1.11	0.92
1:A:356:VAL:HG12	1:A:357:GLY:N	1.77	0.92
1:G:386:ARG:NE	1:G:387:PHE:HD1	1.68	0.91
1:F:386:ARG:HE	1:F:387:PHE:HE1	1.11	0.90
1:D:386:ARG:NE	1:D:387:PHE:HD1	1.68	0.90
1:D:386:ARG:HH22	1:D:462:LYS:HE3	1.37	0.90
1:F:386:ARG:NE	1:F:387:PHE:HD1	1.68	0.90
1:E:386:ARG:HH22	1:E:462:LYS:HE3	1.37	0.90
1:D:356:VAL:HG12	1:D:357:GLY:N	1.77	0.90
1:F:386:ARG:HH22	1:F:462:LYS:HE3	1.37	0.90
1:H:356:VAL:HG12	1:H:357:GLY:N	1.77	0.89
1:B:386:ARG:HH22	1:B:462:LYS:HE3	1.37	0.89
1:A:386:ARG:HH22	1:A:462:LYS:HE3	1.37	0.89
1:C:386:ARG:NE	1:C:387:PHE:HD1	1.68	0.88
1:C:386:ARG:NH2	1:C:462:LYS:HE3	1.89	0.88
1:C:386:ARG:HH22	1:C:462:LYS:HE3	1.37	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:VAL:CG1	1:H:428:LEU:HD23	2.03	0.88
1:G:386:ARG:HH22	1:G:462:LYS:HE3	1.37	0.88
1:D:386:ARG:NH2	1:D:462:LYS:HE3	1.89	0.88
1:H:386:ARG:HH22	1:H:462:LYS:HE3	1.37	0.88
1:H:386:ARG:NE	1:H:387:PHE:HD1	1.68	0.87
1:A:386:ARG:NH2	1:A:462:LYS:HE3	1.89	0.87
1:E:386:ARG:NE	1:E:387:PHE:HD1	1.68	0.87
1:B:386:ARG:NE	1:B:387:PHE:HD1	1.68	0.87
1:H:386:ARG:NH2	1:H:462:LYS:HE3	1.89	0.86
1:E:358:LEU:HD12	1:E:441:SER:OG	1.76	0.86
1:H:358:LEU:HD12	1:H:441:SER:OG	1.76	0.86
1:F:386:ARG:NH2	1:F:462:LYS:HE3	1.89	0.86
1:B:386:ARG:NH2	1:B:462:LYS:HE3	1.89	0.86
1:A:356:VAL:CG1	1:A:357:GLY:H	1.85	0.86
1:E:386:ARG:NH2	1:E:462:LYS:HE3	1.89	0.86
1:G:358:LEU:HD12	1:G:441:SER:OG	1.76	0.86
1:G:386:ARG:NH2	1:G:462:LYS:HE3	1.89	0.86
1:B:358:LEU:HD12	1:B:441:SER:OG	1.76	0.85
1:D:358:LEU:HD12	1:D:441:SER:OG	1.76	0.85
1:C:358:LEU:HD12	1:C:441:SER:OG	1.76	0.85
1:F:358:LEU:HD12	1:F:441:SER:OG	1.76	0.85
1:C:508:ASP:OD2	1:C:514:ILE:HD11	1.77	0.85
1:A:386:ARG:NH2	1:A:462:LYS:NZ	2.25	0.84
1:A:386:ARG:NE	1:A:387:PHE:HD1	1.68	0.84
1:B:386:ARG:HH21	1:B:462:LYS:HZ2	1.25	0.84
1:B:508:ASP:OD2	1:B:514:ILE:HD11	1.77	0.84
1:D:356:VAL:CG1	1:D:357:GLY:H	1.84	0.84
1:E:508:ASP:OD2	1:E:514:ILE:HD11	1.77	0.84
1:H:386:ARG:NH2	1:H:462:LYS:NZ	2.25	0.84
1:D:508:ASP:OD2	1:D:514:ILE:HD11	1.77	0.84
1:A:358:LEU:HD12	1:A:441:SER:OG	1.76	0.84
1:G:508:ASP:OD2	1:G:514:ILE:HD11	1.77	0.84
1:H:508:ASP:OD2	1:H:514:ILE:HD11	1.77	0.84
1:E:386:ARG:NH2	1:E:462:LYS:NZ	2.25	0.84
1:G:386:ARG:NH2	1:G:462:LYS:NZ	2.25	0.84
1:A:508:ASP:OD2	1:A:514:ILE:HD11	1.77	0.83
1:C:386:ARG:NH2	1:C:462:LYS:NZ	2.25	0.83
1:E:356:VAL:CG1	1:E:357:GLY:H	1.85	0.83
1:D:358:LEU:HD12	1:D:441:SER:CB	2.09	0.83
1:D:386:ARG:NH2	1:D:462:LYS:NZ	2.25	0.83
1:E:412:ASP:OD1	1:H:429:ALA:HB2	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:447:PRO:HD2	1:G:450:MET:HE1	1.60	0.83
1:B:356:VAL:CG1	1:B:357:GLY:H	1.85	0.83
1:C:386:ARG:NH2	1:C:462:LYS:CE	2.42	0.83
1:E:386:ARG:NH2	1:E:462:LYS:CE	2.42	0.83
1:F:508:ASP:OD2	1:F:514:ILE:HD11	1.77	0.83
1:B:386:ARG:NH2	1:B:462:LYS:NZ	2.25	0.83
1:A:386:ARG:NH2	1:A:462:LYS:CE	2.42	0.83
1:C:447:PRO:O	1:C:450:MET:HG3	1.79	0.83
1:C:358:LEU:HD12	1:C:441:SER:CB	2.09	0.83
1:D:386:ARG:NH2	1:D:462:LYS:CE	2.42	0.83
1:F:356:VAL:CG1	1:F:357:GLY:H	1.84	0.83
1:A:358:LEU:HD12	1:A:441:SER:CB	2.09	0.83
1:E:358:LEU:HD12	1:E:441:SER:CB	2.09	0.83
1:F:358:LEU:HD12	1:F:441:SER:CB	2.09	0.83
1:F:386:ARG:NH2	1:F:462:LYS:CE	2.42	0.83
1:G:358:LEU:HD12	1:G:441:SER:CB	2.09	0.83
1:H:358:LEU:HD12	1:H:441:SER:CB	2.09	0.83
1:F:386:ARG:NH2	1:F:462:LYS:NZ	2.25	0.82
1:B:386:ARG:NH2	1:B:462:LYS:CE	2.42	0.82
1:A:413:GLN:HE22	1:H:387:PHE:HZ	1.27	0.82
1:H:386:ARG:NH2	1:H:462:LYS:CE	2.42	0.82
1:F:386:ARG:HH21	1:F:462:LYS:HZ2	1.25	0.82
1:G:356:VAL:CG1	1:G:357:GLY:H	1.84	0.82
1:G:447:PRO:HD2	1:G:450:MET:CE	2.09	0.82
1:B:358:LEU:HD12	1:B:441:SER:CB	2.09	0.81
1:G:386:ARG:NH2	1:G:462:LYS:CE	2.42	0.81
1:D:375:PRO:O	1:D:450:MET:SD	2.39	0.81
1:C:447:PRO:CD	1:C:450:MET:SD	2.68	0.80
1:D:386:ARG:HH21	1:D:462:LYS:HZ2	1.31	0.79
1:H:356:VAL:CG1	1:H:357:GLY:H	1.85	0.79
1:A:375:PRO:CA	1:A:450:MET:HE1	2.14	0.78
1:D:447:PRO:HB2	1:D:450:MET:HE2	1.66	0.78
1:C:413:GLN:NE2	1:G:387:PHE:HZ	1.82	0.76
1:C:356:VAL:CG1	1:C:357:GLY:H	1.85	0.75
1:E:491:VAL:C	1:E:521:MET:HE1	2.13	0.74
1:F:491:VAL:C	1:F:521:MET:HE1	2.13	0.74
1:H:491:VAL:C	1:H:521:MET:HE1	2.13	0.74
1:F:411:VAL:CG1	1:G:428:LEU:HD23	2.17	0.74
1:G:491:VAL:C	1:G:521:MET:HE1	2.13	0.74
1:A:491:VAL:C	1:A:521:MET:HE1	2.13	0.74
1:B:492:TRP:CA	1:B:521:MET:HE2	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:492:TRP:CA	1:H:521:MET:HE2	2.18	0.73
1:E:447:PRO:HD2	1:E:450:MET:CE	2.18	0.73
1:B:491:VAL:C	1:B:521:MET:HE1	2.13	0.73
1:D:492:TRP:CA	1:D:521:MET:HE2	2.18	0.73
1:C:491:VAL:C	1:C:521:MET:HE1	2.13	0.72
1:E:492:TRP:CA	1:E:521:MET:HE2	2.18	0.72
1:D:491:VAL:C	1:D:521:MET:HE1	2.13	0.72
1:B:479:MET:HE3	1:B:484:SER:HB2	1.72	0.72
1:A:479:MET:HE3	1:A:484:SER:HB2	1.72	0.72
1:H:447:PRO:HD2	1:H:450:MET:CE	2.20	0.72
1:H:479:MET:HE3	1:H:484:SER:HB2	1.72	0.72
1:C:479:MET:HE3	1:C:484:SER:HB2	1.72	0.72
1:D:479:MET:HE3	1:D:484:SER:HB2	1.72	0.72
1:B:404:ILE:HG12	1:B:543:ILE:HD11	1.69	0.71
1:G:479:MET:HE3	1:G:484:SER:HB2	1.72	0.71
1:C:386:ARG:HH21	1:C:462:LYS:HZ2	1.35	0.71
1:B:492:TRP:CA	1:B:521:MET:CE	2.69	0.71
1:D:492:TRP:CA	1:D:521:MET:CE	2.69	0.71
1:F:492:TRP:CA	1:F:521:MET:HE2	2.18	0.71
1:E:492:TRP:CA	1:E:521:MET:CE	2.69	0.70
1:F:492:TRP:CA	1:F:521:MET:CE	2.69	0.70
1:A:492:TRP:CA	1:A:521:MET:HE2	2.18	0.70
1:E:479:MET:HE3	1:E:484:SER:HB2	1.72	0.70
1:F:479:MET:HE3	1:F:484:SER:HB2	1.72	0.70
1:G:492:TRP:CA	1:G:521:MET:CE	2.69	0.70
1:H:492:TRP:CA	1:H:521:MET:CE	2.69	0.70
1:H:447:PRO:HD2	1:H:450:MET:HE1	1.74	0.69
1:C:492:TRP:CA	1:C:521:MET:CE	2.69	0.69
1:A:492:TRP:CA	1:A:521:MET:CE	2.69	0.69
1:A:386:ARG:HH21	1:A:462:LYS:HZ2	1.39	0.69
1:C:492:TRP:CA	1:C:521:MET:HE2	2.18	0.69
1:D:358:LEU:CD1	1:D:441:SER:CB	2.71	0.69
1:E:358:LEU:CD1	1:E:441:SER:CB	2.71	0.69
1:G:358:LEU:CD1	1:G:441:SER:CB	2.71	0.69
1:B:386:ARG:CZ	1:B:387:PHE:CD1	2.76	0.68
1:C:358:LEU:CD1	1:C:441:SER:CB	2.71	0.68
1:E:386:ARG:CZ	1:E:387:PHE:CD1	2.76	0.68
1:G:492:TRP:CA	1:G:521:MET:HE2	2.18	0.68
1:B:358:LEU:CD1	1:B:441:SER:CB	2.71	0.68
1:F:358:LEU:CD1	1:F:441:SER:CB	2.71	0.68
1:A:386:ARG:CZ	1:A:387:PHE:CD1	2.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:386:ARG:HH21	1:E:462:LYS:HZ2	1.39	0.68
1:G:386:ARG:CZ	1:G:387:PHE:CD1	2.76	0.68
1:H:358:LEU:CD1	1:H:441:SER:CB	2.71	0.68
1:H:386:ARG:CZ	1:H:387:PHE:CD1	2.76	0.68
1:A:375:PRO:C	1:A:450:MET:HE1	2.18	0.68
1:A:375:PRO:O	1:A:450:MET:HE1	1.93	0.68
1:A:358:LEU:CD1	1:A:441:SER:CB	2.71	0.68
1:C:386:ARG:CZ	1:C:387:PHE:CD1	2.76	0.68
1:E:447:PRO:HD2	1:E:450:MET:HE1	1.76	0.68
1:D:386:ARG:CZ	1:D:387:PHE:CD1	2.76	0.67
1:E:518:CYS:HB3	1:E:521:MET:HB2	1.77	0.67
1:D:518:CYS:HB3	1:D:521:MET:HB2	1.76	0.67
1:G:518:CYS:HB3	1:G:521:MET:HB2	1.77	0.67
1:F:518:CYS:HB3	1:F:521:MET:HB2	1.77	0.67
1:F:386:ARG:CZ	1:F:387:PHE:CD1	2.76	0.67
1:H:518:CYS:HB3	1:H:521:MET:HB2	1.77	0.67
1:B:518:CYS:HB3	1:B:521:MET:HB2	1.76	0.67
1:E:411:VAL:HG11	1:H:428:LEU:HD23	1.77	0.66
1:F:447:PRO:HD2	1:F:450:MET:CE	2.25	0.66
1:A:518:CYS:HB3	1:A:521:MET:HB2	1.77	0.66
1:G:356:VAL:CG1	1:G:357:GLY:N	2.52	0.65
1:A:386:ARG:NH2	1:A:462:LYS:HZ1	1.95	0.65
1:E:492:TRP:HA	1:E:521:MET:HE1	1.78	0.65
1:E:450:MET:SD	1:E:452:LEU:HD21	2.37	0.65
1:A:447:PRO:HB2	1:A:450:MET:SD	2.37	0.65
1:C:518:CYS:HB3	1:C:521:MET:HB2	1.77	0.64
1:B:491:VAL:HG12	1:B:521:MET:HE1	1.80	0.64
1:D:492:TRP:HA	1:D:521:MET:HE1	1.78	0.64
1:A:492:TRP:HA	1:A:521:MET:HE1	1.78	0.64
1:F:356:VAL:CG1	1:F:357:GLY:N	2.52	0.64
1:F:447:PRO:HD2	1:F:450:MET:HE1	1.81	0.63
1:D:356:VAL:CG1	1:D:357:GLY:N	2.52	0.63
1:H:492:TRP:HA	1:H:521:MET:HE1	1.79	0.63
1:B:492:TRP:HA	1:B:521:MET:HE1	1.78	0.63
1:A:356:VAL:O	1:H:414:LYS:NZ	2.32	0.63
1:C:447:PRO:HB2	1:C:450:MET:CG	2.30	0.62
1:C:492:TRP:HA	1:C:521:MET:HE1	1.78	0.62
1:G:492:TRP:HA	1:G:521:MET:HE1	1.78	0.62
1:C:386:ARG:CZ	1:C:387:PHE:HD1	2.13	0.62
1:G:491:VAL:HG12	1:G:521:MET:HE1	1.80	0.62
1:A:386:ARG:CZ	1:A:387:PHE:HD1	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:386:ARG:CZ	1:E:387:PHE:HD1	2.13	0.61
1:D:386:ARG:CZ	1:D:387:PHE:HD1	2.13	0.61
1:H:491:VAL:HG12	1:H:521:MET:HE1	1.79	0.61
1:E:386:ARG:HH22	1:E:462:LYS:CE	2.10	0.61
1:H:386:ARG:CZ	1:H:387:PHE:HD1	2.13	0.60
1:B:404:ILE:HG12	1:B:543:ILE:CD1	2.31	0.60
1:F:491:VAL:HG12	1:F:521:MET:HE1	1.79	0.60
1:E:386:ARG:NH2	1:E:462:LYS:HZ1	1.95	0.60
1:C:386:ARG:NH2	1:C:462:LYS:HZ1	1.99	0.60
1:A:491:VAL:HG12	1:A:521:MET:HE1	1.79	0.60
1:F:492:TRP:HA	1:F:521:MET:HE1	1.79	0.60
1:G:386:ARG:CZ	1:G:387:PHE:HD1	2.13	0.60
1:A:356:VAL:CG1	1:A:357:GLY:N	2.52	0.60
1:A:358:LEU:CD1	1:A:441:SER:HB2	2.32	0.60
1:D:358:LEU:CD1	1:D:441:SER:HB2	2.32	0.60
1:F:358:LEU:CD1	1:F:441:SER:HB2	2.32	0.60
1:G:358:LEU:CD1	1:G:441:SER:HB2	2.32	0.59
1:A:508:ASP:HB3	1:A:514:ILE:HD12	1.85	0.59
1:G:508:ASP:HB3	1:G:514:ILE:HD12	1.85	0.59
1:F:508:ASP:HB3	1:F:514:ILE:HD12	1.85	0.59
1:C:358:LEU:CD1	1:C:441:SER:HB2	2.32	0.59
1:D:508:ASP:HB3	1:D:514:ILE:HD12	1.85	0.59
1:E:358:LEU:CD1	1:E:441:SER:HB2	2.32	0.58
1:C:508:ASP:HB3	1:C:514:ILE:HD12	1.85	0.58
1:B:358:LEU:CD1	1:B:441:SER:HB2	2.32	0.58
1:A:375:PRO:O	1:A:450:MET:CE	2.51	0.58
1:C:356:VAL:CG1	1:C:357:GLY:N	2.52	0.58
1:E:508:ASP:HB3	1:E:514:ILE:HD12	1.85	0.58
1:A:359:SER:OG	1:A:362:GLN:HG3	2.04	0.58
1:H:358:LEU:CD1	1:H:441:SER:HB2	2.32	0.58
1:H:508:ASP:HB3	1:H:514:ILE:HD12	1.85	0.58
1:E:412:ASP:OD1	1:H:429:ALA:CB	2.51	0.58
1:B:447:PRO:HD2	1:B:450:MET:CE	2.34	0.58
1:C:491:VAL:HG12	1:C:521:MET:HE1	1.79	0.58
1:B:508:ASP:HB3	1:B:514:ILE:HD12	1.85	0.58
1:F:359:SER:OG	1:F:362:GLN:HG3	2.04	0.58
1:C:359:SER:OG	1:C:362:GLN:HG3	2.04	0.57
1:E:491:VAL:HG12	1:E:521:MET:HE1	1.79	0.57
1:G:359:SER:OG	1:G:362:GLN:HG3	2.03	0.57
1:B:356:VAL:CG1	1:B:357:GLY:N	2.52	0.57
1:B:359:SER:OG	1:B:362:GLN:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:359:SER:OG	1:D:362:GLN:HG3	2.04	0.57
1:H:359:SER:OG	1:H:362:GLN:HG3	2.04	0.57
1:B:386:ARG:CD	1:B:387:PHE:CD1	2.88	0.57
1:G:447:PRO:HD2	1:G:450:MET:HE3	1.85	0.57
1:G:386:ARG:NH2	1:G:462:LYS:HZ1	2.03	0.57
1:D:386:ARG:CD	1:D:387:PHE:CD1	2.88	0.57
1:E:359:SER:OG	1:E:362:GLN:HG3	2.04	0.57
1:F:386:ARG:CD	1:F:387:PHE:CD1	2.88	0.57
1:D:491:VAL:HG12	1:D:521:MET:HE1	1.79	0.57
1:E:386:ARG:CD	1:E:387:PHE:CD1	2.88	0.56
1:A:386:ARG:CD	1:A:387:PHE:CD1	2.88	0.56
1:F:450:MET:SD	1:F:452:LEU:HD21	2.45	0.56
1:G:386:ARG:CD	1:G:387:PHE:CD1	2.88	0.56
1:H:491:VAL:O	1:H:521:MET:HE1	2.06	0.56
1:C:356:VAL:O	1:G:414:LYS:NZ	2.39	0.56
1:E:356:VAL:CG1	1:E:357:GLY:N	2.52	0.56
1:B:386:ARG:CZ	1:B:387:PHE:HD1	2.13	0.56
1:C:386:ARG:CD	1:C:387:PHE:CD1	2.88	0.56
1:G:378:PRO:HD2	1:G:399:GLN:NE2	2.21	0.56
1:D:386:ARG:HH22	1:D:462:LYS:CE	2.10	0.55
1:F:378:PRO:HD2	1:F:399:GLN:NE2	2.21	0.55
1:H:386:ARG:CD	1:H:387:PHE:CD1	2.88	0.55
1:B:451:VAL:CG1	1:B:475:ILE:HD11	2.37	0.55
1:D:386:ARG:NH2	1:D:462:LYS:HZ1	2.03	0.55
1:F:404:ILE:HG23	1:F:544:LEU:HD11	1.88	0.55
1:B:378:PRO:HD2	1:B:399:GLN:NE2	2.21	0.55
1:A:358:LEU:HD11	1:A:441:SER:HB2	1.89	0.55
1:G:491:VAL:O	1:G:521:MET:HE1	2.06	0.55
1:B:386:ARG:HH22	1:B:462:LYS:CE	2.10	0.55
1:E:378:PRO:HD2	1:E:399:GLN:NE2	2.20	0.55
1:A:378:PRO:HD2	1:A:399:GLN:NE2	2.21	0.55
1:A:451:VAL:CG1	1:A:475:ILE:HD11	2.37	0.55
1:D:451:VAL:CG1	1:D:475:ILE:HD11	2.37	0.55
1:F:386:ARG:CZ	1:F:387:PHE:HD1	2.13	0.55
1:G:451:VAL:CG1	1:G:475:ILE:HD11	2.37	0.55
1:C:451:VAL:CG1	1:C:475:ILE:HD11	2.36	0.55
1:C:491:VAL:O	1:C:521:MET:HE1	2.06	0.55
1:E:386:ARG:HH21	1:E:462:LYS:HZ1	1.52	0.55
1:F:451:VAL:CG1	1:F:475:ILE:HD11	2.37	0.55
1:B:404:ILE:HG23	1:B:544:LEU:HD11	1.88	0.55
1:B:447:PRO:HD2	1:B:450:MET:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:VAL:O	1:A:521:MET:HE1	2.06	0.55
1:G:450:MET:SD	1:G:452:LEU:HD21	2.46	0.55
1:C:358:LEU:HD11	1:C:441:SER:HB2	1.89	0.55
1:A:375:PRO:HA	1:A:450:MET:SD	2.47	0.55
1:D:508:ASP:HB3	1:D:514:ILE:CD1	2.37	0.55
1:E:447:PRO:HD2	1:E:450:MET:HE3	1.87	0.55
1:E:451:VAL:CG1	1:E:475:ILE:HD11	2.37	0.55
1:F:491:VAL:O	1:F:521:MET:HE1	2.06	0.55
1:G:404:ILE:HG23	1:G:544:LEU:HD11	1.88	0.55
1:D:375:PRO:HA	1:D:450:MET:HE1	0.80	0.55
1:E:411:VAL:HG12	1:H:428:LEU:HD23	1.87	0.55
1:B:491:VAL:O	1:B:521:MET:HE1	2.06	0.54
1:C:508:ASP:HB3	1:C:514:ILE:CD1	2.38	0.54
1:F:358:LEU:HD11	1:F:441:SER:HB2	1.89	0.54
1:D:358:LEU:HD11	1:D:441:SER:HB2	1.89	0.54
1:D:491:VAL:O	1:D:521:MET:HE1	2.06	0.54
1:E:491:VAL:O	1:E:521:MET:HE1	2.06	0.54
1:B:508:ASP:HB3	1:B:514:ILE:CD1	2.37	0.54
1:E:508:ASP:HB3	1:E:514:ILE:CD1	2.37	0.54
1:G:508:ASP:HB3	1:G:514:ILE:CD1	2.37	0.54
1:H:451:VAL:CG1	1:H:475:ILE:HD11	2.37	0.54
1:E:358:LEU:HD11	1:E:441:SER:HB2	1.89	0.54
1:A:508:ASP:HB3	1:A:514:ILE:CD1	2.38	0.54
1:F:508:ASP:HB3	1:F:514:ILE:CD1	2.38	0.54
1:H:356:VAL:CG1	1:H:357:GLY:N	2.52	0.54
1:H:358:LEU:HD11	1:H:441:SER:HB2	1.89	0.54
1:D:404:ILE:HG23	1:D:544:LEU:HD11	1.88	0.54
1:A:386:ARG:CD	1:A:387:PHE:HD1	2.21	0.54
1:E:404:ILE:HG23	1:E:544:LEU:HD11	1.88	0.54
1:B:358:LEU:HD11	1:B:441:SER:HB2	1.89	0.54
1:A:404:ILE:HG23	1:A:544:LEU:HD11	1.88	0.54
1:H:404:ILE:HG23	1:H:544:LEU:HD11	1.89	0.54
1:H:551:ARG:NH2	1:H:554:ASN:OD1	2.41	0.54
1:C:386:ARG:CD	1:C:387:PHE:HD1	2.21	0.53
1:C:404:ILE:HG23	1:C:544:LEU:HD11	1.89	0.53
1:F:386:ARG:CD	1:F:387:PHE:HD1	2.21	0.53
1:B:386:ARG:CD	1:B:387:PHE:HD1	2.21	0.53
1:G:358:LEU:HD11	1:G:441:SER:HB2	1.89	0.53
1:H:508:ASP:HB3	1:H:514:ILE:CD1	2.38	0.53
1:D:386:ARG:CD	1:D:387:PHE:HD1	2.21	0.53
1:H:426:MET:HE2	1:H:502:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ILE:HG23	1:B:544:LEU:CD1	2.39	0.53
1:C:413:GLN:HB2	1:G:462:LYS:NZ	2.24	0.53
1:D:426:MET:HE2	1:D:502:HIS:CE1	2.44	0.53
1:H:450:MET:SD	1:H:452:LEU:HD21	2.48	0.53
1:B:426:MET:HE2	1:B:502:HIS:CE1	2.44	0.53
1:B:450:MET:SD	1:B:452:LEU:HD21	2.49	0.53
1:A:426:MET:HE2	1:A:502:HIS:CE1	2.44	0.53
1:E:404:ILE:HG23	1:E:544:LEU:CD1	2.39	0.53
1:C:536:ASP:C	1:C:537:LEU:HD23	2.35	0.52
1:E:426:MET:HE2	1:E:502:HIS:CE1	2.44	0.52
1:H:404:ILE:HG23	1:H:544:LEU:CD1	2.39	0.52
1:G:386:ARG:CD	1:G:387:PHE:HD1	2.21	0.52
1:F:536:ASP:C	1:F:537:LEU:HD23	2.34	0.52
1:B:536:ASP:C	1:B:537:LEU:HD23	2.34	0.52
1:C:404:ILE:HG23	1:C:544:LEU:CD1	2.40	0.52
1:C:518:CYS:O	1:C:518:CYS:SG	2.68	0.52
1:E:536:ASP:C	1:E:537:LEU:HD23	2.34	0.52
1:F:426:MET:HE2	1:F:502:HIS:CE1	2.44	0.52
1:A:404:ILE:HG23	1:A:544:LEU:CD1	2.39	0.52
1:A:536:ASP:C	1:A:537:LEU:HD23	2.35	0.52
1:H:536:ASP:C	1:H:537:LEU:HD23	2.34	0.52
1:H:386:ARG:CD	1:H:387:PHE:HD1	2.21	0.52
1:C:426:MET:HE2	1:C:502:HIS:CE1	2.44	0.51
1:C:447:PRO:N	1:C:450:MET:SD	2.83	0.51
1:E:518:CYS:SG	1:E:518:CYS:O	2.68	0.51
1:F:404:ILE:HG23	1:F:544:LEU:CD1	2.39	0.51
1:G:404:ILE:HG23	1:G:544:LEU:CD1	2.39	0.51
1:G:426:MET:HE2	1:G:502:HIS:CE1	2.44	0.51
1:D:518:CYS:SG	1:D:518:CYS:O	2.68	0.51
1:G:536:ASP:C	1:G:537:LEU:HD23	2.34	0.51
1:D:404:ILE:HG23	1:D:544:LEU:CD1	2.39	0.51
1:D:536:ASP:C	1:D:537:LEU:HD23	2.35	0.51
1:H:518:CYS:O	1:H:518:CYS:SG	2.68	0.51
1:F:412:ASP:OD1	1:G:429:ALA:HB2	2.10	0.51
1:F:518:CYS:O	1:F:518:CYS:SG	2.68	0.51
1:A:518:CYS:O	1:A:518:CYS:SG	2.68	0.51
1:G:518:CYS:SG	1:G:518:CYS:O	2.68	0.51
1:B:492:TRP:CG	1:B:521:MET:HE2	2.46	0.50
1:H:492:TRP:CG	1:H:521:MET:HE2	2.46	0.50
1:C:492:TRP:CG	1:C:521:MET:HE2	2.46	0.50
1:E:386:ARG:CD	1:E:387:PHE:HD1	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:CYS:SG	1:B:518:CYS:O	2.68	0.50
1:F:386:ARG:NH2	1:F:462:LYS:HZ1	2.08	0.50
1:G:492:TRP:CG	1:G:521:MET:HE2	2.47	0.50
1:H:386:ARG:NH2	1:H:462:LYS:HZ1	2.10	0.50
1:D:492:TRP:CG	1:D:521:MET:HE2	2.47	0.50
1:A:492:TRP:CG	1:A:521:MET:HE2	2.46	0.50
1:E:492:TRP:CG	1:E:521:MET:HE2	2.46	0.50
1:F:492:TRP:CG	1:F:521:MET:HE2	2.46	0.49
1:F:447:PRO:HD2	1:F:450:MET:HE3	1.95	0.49
1:H:492:TRP:CA	1:H:521:MET:HE1	2.40	0.49
1:B:492:TRP:CA	1:B:521:MET:HE1	2.40	0.48
1:A:492:TRP:CA	1:A:521:MET:HE1	2.40	0.48
1:B:386:ARG:NH2	1:B:462:LYS:HZ1	2.08	0.48
1:D:467:GLN:OE1	1:H:558:LEU:HG	2.14	0.48
1:G:492:TRP:CA	1:G:521:MET:HE1	2.41	0.48
1:H:447:PRO:HD2	1:H:450:MET:HE3	1.95	0.48
1:C:492:TRP:CA	1:C:521:MET:HE1	2.40	0.48
1:A:378:PRO:HD2	1:A:399:GLN:CD	2.39	0.48
1:G:378:PRO:HD2	1:G:399:GLN:CD	2.39	0.48
1:A:375:PRO:CA	1:A:450:MET:SD	3.02	0.47
1:E:378:PRO:HD2	1:E:399:GLN:CD	2.39	0.47
1:D:467:GLN:OE1	1:H:558:LEU:CD1	2.62	0.47
1:D:386:ARG:CZ	1:D:387:PHE:CE1	2.98	0.47
1:D:492:TRP:CA	1:D:521:MET:HE1	2.41	0.47
1:F:378:PRO:HD2	1:F:399:GLN:CD	2.39	0.47
1:B:451:VAL:HG11	1:B:475:ILE:HD11	1.97	0.47
1:A:467:GLN:OE1	1:E:558:LEU:HD12	2.15	0.47
1:F:451:VAL:HG11	1:F:475:ILE:HD11	1.97	0.47
1:C:447:PRO:HB2	1:C:450:MET:SD	2.55	0.47
1:E:413:GLN:HE22	1:E:428:LEU:HD22	0.66	0.47
1:A:467:GLN:OE1	1:E:558:LEU:CD1	2.62	0.46
1:D:451:VAL:HG11	1:D:475:ILE:HD11	1.97	0.46
1:E:451:VAL:HG11	1:E:475:ILE:HD11	1.97	0.46
1:G:451:VAL:HG11	1:G:475:ILE:HD11	1.97	0.46
1:B:378:PRO:HD2	1:B:399:GLN:CD	2.39	0.46
1:E:386:ARG:CZ	1:E:387:PHE:CE1	2.98	0.46
1:G:386:ARG:CZ	1:G:387:PHE:CE1	2.98	0.46
1:C:451:VAL:HG11	1:C:475:ILE:HD11	1.97	0.46
1:F:492:TRP:CA	1:F:521:MET:HE1	2.40	0.46
1:H:451:VAL:HG11	1:H:475:ILE:HD11	1.97	0.46
1:F:411:VAL:HG11	1:G:428:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:ILE:HG12	1:E:543:ILE:HG12	1.98	0.46
1:E:492:TRP:CA	1:E:521:MET:HE1	2.40	0.46
1:C:404:ILE:HG12	1:C:543:ILE:HG12	1.98	0.46
1:A:451:VAL:HG11	1:A:475:ILE:HD11	1.97	0.45
1:D:404:ILE:HG12	1:D:543:ILE:HG12	1.98	0.45
1:F:404:ILE:HG12	1:F:543:ILE:HG12	1.98	0.45
1:C:413:GLN:NE2	1:G:387:PHE:CZ	2.69	0.45
1:D:392:GLU:HB2	1:D:426:MET:HE1	1.98	0.45
1:G:392:GLU:HB2	1:G:426:MET:HE1	1.99	0.45
1:H:392:GLU:HB2	1:H:426:MET:HE1	1.98	0.45
1:B:392:GLU:HB2	1:B:426:MET:HE1	1.99	0.45
1:A:404:ILE:HG12	1:A:543:ILE:HG12	1.98	0.45
1:E:392:GLU:HB2	1:E:426:MET:HE1	1.99	0.45
1:H:404:ILE:HG12	1:H:543:ILE:HG12	1.98	0.45
1:A:386:ARG:CZ	1:A:387:PHE:CE1	2.98	0.45
1:A:392:GLU:HB2	1:A:426:MET:HE1	1.98	0.45
1:E:492:TRP:N	1:E:521:MET:CE	2.80	0.45
1:F:392:GLU:HB2	1:F:426:MET:HE1	1.98	0.45
1:F:492:TRP:N	1:F:521:MET:CE	2.80	0.45
1:G:492:TRP:N	1:G:521:MET:CE	2.80	0.45
1:H:407:TYR:CZ	1:H:501:MET:HG3	2.53	0.44
1:B:407:TYR:CZ	1:B:501:MET:HG3	2.53	0.44
1:A:407:TYR:CZ	1:A:501:MET:HG3	2.53	0.44
1:G:407:TYR:CZ	1:G:501:MET:HG3	2.53	0.44
1:A:358:LEU:HD12	1:A:441:SER:HG	1.79	0.44
1:A:492:TRP:N	1:A:521:MET:HE1	2.33	0.44
1:G:404:ILE:HG12	1:G:543:ILE:HG12	1.98	0.44
1:H:492:TRP:N	1:H:521:MET:CE	2.80	0.44
1:C:386:ARG:CZ	1:C:387:PHE:CE1	2.98	0.44
1:A:447:PRO:O	1:A:450:MET:HG2	2.17	0.44
1:F:450:MET:O	1:F:472:ILE:HG23	2.17	0.44
1:C:392:GLU:HB2	1:C:426:MET:HE1	1.99	0.44
1:D:386:ARG:HG3	1:D:387:PHE:CD1	2.53	0.44
1:B:467:GLN:OE1	1:G:558:LEU:CD1	2.66	0.44
1:A:492:TRP:N	1:A:521:MET:CE	2.80	0.44
1:D:467:GLN:OE1	1:H:558:LEU:HD12	2.17	0.44
1:D:554:ASN:OD1	1:D:555:VAL:N	2.51	0.44
1:F:407:TYR:CZ	1:F:501:MET:HG3	2.53	0.44
1:C:492:TRP:N	1:C:521:MET:CE	2.80	0.43
1:D:407:TYR:CZ	1:D:501:MET:HG3	2.53	0.43
1:F:554:ASN:OD1	1:F:555:VAL:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:514:ILE:HG22	1:H:515:THR:N	2.33	0.43
1:B:386:ARG:HG3	1:B:387:PHE:CD1	2.53	0.43
1:B:492:TRP:N	1:B:521:MET:CE	2.80	0.43
1:A:413:GLN:NE2	1:H:387:PHE:HZ	2.04	0.43
1:C:407:TYR:CZ	1:C:501:MET:HG3	2.53	0.43
1:D:392:GLU:CB	1:D:426:MET:HE1	2.48	0.43
1:D:492:TRP:N	1:D:521:MET:HE1	2.33	0.43
1:F:392:GLU:CB	1:F:426:MET:HE1	2.48	0.43
1:G:514:ILE:HG22	1:G:515:THR:N	2.33	0.43
1:H:386:ARG:CZ	1:H:387:PHE:CE1	2.98	0.43
1:H:492:TRP:N	1:H:521:MET:HE1	2.32	0.43
1:C:492:TRP:N	1:C:521:MET:HE1	2.33	0.43
1:D:492:TRP:N	1:D:521:MET:CE	2.80	0.43
1:E:392:GLU:CB	1:E:426:MET:HE1	2.48	0.43
1:E:407:TYR:CZ	1:E:501:MET:HG3	2.53	0.43
1:A:554:ASN:OD1	1:A:555:VAL:N	2.52	0.43
1:F:492:TRP:N	1:F:521:MET:HE1	2.33	0.43
1:G:370:MET:HE3	1:G:370:MET:HB3	1.76	0.43
1:G:554:ASN:OD1	1:G:555:VAL:N	2.51	0.43
1:B:392:GLU:CB	1:B:426:MET:HE1	2.48	0.43
1:A:386:ARG:HG3	1:A:387:PHE:CD1	2.53	0.43
1:D:514:ILE:HG22	1:D:515:THR:N	2.33	0.43
1:H:386:ARG:HG3	1:H:387:PHE:CD1	2.53	0.43
1:B:554:ASN:OD1	1:B:555:VAL:N	2.51	0.43
1:C:386:ARG:HG3	1:C:387:PHE:CD1	2.53	0.43
1:E:404:ILE:CG2	1:E:544:LEU:HD11	2.49	0.43
1:F:386:ARG:HG3	1:F:387:PHE:CD1	2.53	0.43
1:G:392:GLU:CB	1:G:426:MET:HE1	2.48	0.43
1:B:467:GLN:OE1	1:G:558:LEU:HD12	2.18	0.43
1:C:392:GLU:CB	1:C:426:MET:HE1	2.48	0.43
1:D:404:ILE:CG2	1:D:544:LEU:HD11	2.48	0.43
1:E:531:LYS:HA	1:E:531:LYS:HD3	1.91	0.43
1:B:492:TRP:N	1:B:521:MET:HE1	2.33	0.43
1:B:514:ILE:HG22	1:B:515:THR:N	2.33	0.43
1:C:554:ASN:OD1	1:C:555:VAL:N	2.51	0.43
1:E:386:ARG:HG3	1:E:387:PHE:CD1	2.53	0.43
1:G:386:ARG:HG3	1:G:387:PHE:CD1	2.53	0.43
1:C:467:GLN:OE1	1:F:558:LEU:HD12	2.19	0.42
1:H:390:PRO:O	1:H:408:ARG:HB3	2.19	0.42
1:H:392:GLU:CB	1:H:426:MET:HE1	2.48	0.42
1:A:390:PRO:O	1:A:408:ARG:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:ILE:HG23	1:C:513:GLU:HG3	2.01	0.42
1:D:531:LYS:HA	1:D:531:LYS:HD3	1.91	0.42
1:A:514:ILE:HG22	1:A:515:THR:N	2.33	0.42
1:E:492:TRP:N	1:E:521:MET:HE1	2.33	0.42
1:G:404:ILE:CG2	1:G:544:LEU:HD11	2.49	0.42
1:G:505:ILE:HG23	1:G:513:GLU:HG3	2.02	0.42
1:C:404:ILE:CG2	1:C:544:LEU:HD11	2.49	0.42
1:E:505:ILE:HG23	1:E:513:GLU:HG3	2.02	0.42
1:E:554:ASN:OD1	1:E:555:VAL:N	2.51	0.42
1:G:492:TRP:N	1:G:521:MET:HE1	2.33	0.42
1:A:370:MET:HE3	1:A:370:MET:HB3	1.76	0.42
1:A:392:GLU:CB	1:A:426:MET:HE1	2.48	0.42
1:A:505:ILE:HG23	1:A:513:GLU:HG3	2.01	0.42
1:D:420:SER:O	1:D:425:GLY:HA2	2.20	0.42
1:F:514:ILE:HG22	1:F:515:THR:N	2.34	0.42
1:H:404:ILE:CG2	1:H:544:LEU:HD11	2.49	0.42
1:F:420:SER:O	1:F:425:GLY:HA2	2.20	0.42
1:F:505:ILE:HG23	1:F:513:GLU:HG3	2.02	0.42
1:H:505:ILE:HG23	1:H:513:GLU:HG3	2.02	0.42
1:A:420:SER:O	1:A:425:GLY:HA2	2.20	0.42
1:C:390:PRO:O	1:C:408:ARG:HB3	2.19	0.42
1:C:467:GLN:OE1	1:F:558:LEU:CD1	2.68	0.42
1:F:390:PRO:O	1:F:408:ARG:HB3	2.20	0.42
1:G:390:PRO:O	1:G:408:ARG:HB3	2.19	0.42
1:G:536:ASP:O	1:G:537:LEU:HD23	2.20	0.42
1:A:536:ASP:O	1:A:537:LEU:HD23	2.20	0.42
1:D:536:ASP:O	1:D:537:LEU:HD23	2.20	0.42
1:E:514:ILE:HG22	1:E:515:THR:N	2.34	0.42
1:F:386:ARG:CZ	1:F:387:PHE:CE1	2.98	0.42
1:C:455:GLN:HE21	1:C:479:MET:HB3	1.85	0.42
1:D:390:PRO:O	1:D:408:ARG:HB3	2.19	0.42
1:D:455:GLN:HE21	1:D:479:MET:HB3	1.85	0.42
1:E:455:GLN:HE21	1:E:479:MET:HB3	1.85	0.42
1:F:455:GLN:HE21	1:F:479:MET:HB3	1.85	0.42
1:F:514:ILE:CG2	1:F:515:THR:N	2.83	0.42
1:G:455:GLN:HE21	1:G:479:MET:HB3	1.85	0.42
1:H:420:SER:O	1:H:425:GLY:HA2	2.20	0.42
1:D:505:ILE:HG23	1:D:513:GLU:HG3	2.02	0.41
1:F:536:ASP:O	1:F:537:LEU:HD23	2.20	0.41
1:B:404:ILE:CG2	1:B:544:LEU:HD11	2.48	0.41
1:A:404:ILE:CG2	1:A:544:LEU:HD11	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:GLN:HE21	1:A:479:MET:HB3	1.85	0.41
1:A:490:LYS:HB3	1:A:534:LEU:CD1	2.51	0.41
1:C:514:ILE:HG22	1:C:515:THR:N	2.33	0.41
1:H:450:MET:O	1:H:472:ILE:HG23	2.20	0.41
1:H:514:ILE:CG2	1:H:515:THR:N	2.83	0.41
1:B:386:ARG:CZ	1:B:387:PHE:CE1	2.98	0.41
1:B:536:ASP:O	1:B:537:LEU:HD23	2.20	0.41
1:G:514:ILE:CG2	1:G:515:THR:N	2.83	0.41
1:C:370:MET:HE3	1:C:370:MET:HB3	1.76	0.41
1:D:514:ILE:CG2	1:D:515:THR:N	2.83	0.41
1:E:390:PRO:O	1:E:408:ARG:HB3	2.19	0.41
1:G:420:SER:O	1:G:425:GLY:HA2	2.20	0.41
1:G:450:MET:O	1:G:472:ILE:HG23	2.20	0.41
1:H:536:ASP:O	1:H:537:LEU:HD23	2.20	0.41
1:B:455:GLN:HE21	1:B:479:MET:HB3	1.85	0.41
1:A:514:ILE:CG2	1:A:515:THR:N	2.83	0.41
1:H:531:LYS:HA	1:H:531:LYS:HD3	1.91	0.41
1:B:390:PRO:O	1:B:408:ARG:HB3	2.20	0.41
1:B:491:VAL:CG1	1:B:521:MET:HE3	2.26	0.41
1:C:420:SER:O	1:C:425:GLY:HA2	2.20	0.41
1:D:440:SER:HB3	1:H:558:LEU:H	1.85	0.41
1:D:479:MET:CE	1:D:484:SER:HB2	2.47	0.41
1:E:420:SER:O	1:E:425:GLY:HA2	2.20	0.41
1:E:490:LYS:HB3	1:E:534:LEU:CD1	2.51	0.41
1:E:554:ASN:OD1	1:E:554:ASN:C	2.64	0.41
1:H:455:GLN:HE21	1:H:479:MET:HB3	1.85	0.41
1:B:420:SER:O	1:B:425:GLY:HA2	2.20	0.41
1:B:490:LYS:HB3	1:B:534:LEU:CD1	2.51	0.41
1:E:536:ASP:O	1:E:537:LEU:HD23	2.20	0.41
1:F:404:ILE:CG2	1:F:544:LEU:HD11	2.49	0.41
1:F:479:MET:CE	1:F:484:SER:HB2	2.47	0.41
1:F:490:LYS:HB3	1:F:534:LEU:CD1	2.51	0.41
1:D:375:PRO:HB3	1:D:447:PRO:HB3	2.03	0.41
1:E:386:ARG:HG3	1:E:387:PHE:N	2.36	0.41
1:G:386:ARG:HG3	1:G:387:PHE:N	2.36	0.41
1:B:386:ARG:HG3	1:B:387:PHE:N	2.36	0.41
1:A:360:TYR:O	1:A:364:MET:HG2	2.21	0.41
1:C:490:LYS:HB3	1:C:534:LEU:CD1	2.51	0.41
1:C:536:ASP:O	1:C:537:LEU:HD23	2.20	0.41
1:D:360:TYR:O	1:D:364:MET:HG2	2.21	0.41
1:E:514:ILE:CG2	1:E:515:THR:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:ILE:CG2	1:B:515:THR:N	2.83	0.41
1:A:375:PRO:CA	1:A:450:MET:CE	2.82	0.41
1:D:386:ARG:HG3	1:D:387:PHE:N	2.36	0.41
1:F:386:ARG:HG3	1:F:387:PHE:N	2.36	0.41
1:H:360:TYR:O	1:H:364:MET:HG2	2.21	0.41
1:B:360:TYR:O	1:B:364:MET:HG2	2.21	0.40
1:B:554:ASN:OD1	1:B:554:ASN:C	2.64	0.40
1:G:360:TYR:O	1:G:364:MET:HG2	2.21	0.40
1:G:490:LYS:HB3	1:G:534:LEU:CD1	2.51	0.40
1:H:490:LYS:HB3	1:H:534:LEU:CD1	2.51	0.40
1:C:514:ILE:CG2	1:C:515:THR:N	2.83	0.40
1:D:375:PRO:HB3	1:D:447:PRO:CB	2.51	0.40
1:G:491:VAL:CG1	1:G:521:MET:HE3	2.26	0.40
1:C:360:TYR:O	1:C:364:MET:HG2	2.21	0.40
1:C:531:LYS:HD3	1:C:531:LYS:HA	1.91	0.40
1:D:490:LYS:HB3	1:D:534:LEU:CD1	2.51	0.40
1:F:554:ASN:OD1	1:F:554:ASN:C	2.64	0.40
1:A:386:ARG:HG3	1:A:387:PHE:N	2.36	0.40
1:H:386:ARG:HG3	1:H:387:PHE:N	2.36	0.40
1:F:360:TYR:O	1:F:364:MET:HG2	2.21	0.40
1:F:491:VAL:CG1	1:F:521:MET:HE3	2.26	0.40

All (33) 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:E:478:GLU:OE1	1:G:478:GLU:OE1[1_455]	0.95	1.25
1:F:478:GLU:OE1	1:H:478:GLU:OE1[1_545]	0.98	1.22
1:B:475:ILE:CD1	1:E:497:TRP:CH2[2_546]	1.47	0.73
1:C:475:ILE:CD1	1:F:497:TRP:CH2[2_655]	1.48	0.72
1:D:475:ILE:CD1	1:H:497:TRP:CH2[2_545]	1.52	0.68
1:A:475:ILE:CD1	1:G:497:TRP:CH2[2_656]	1.56	0.64
1:C:461:ARG:NE	1:F:538:LYS:CE[2_655]	1.61	0.59
1:A:461:ARG:NE	1:G:538:LYS:CE[2_656]	1.64	0.56
1:B:461:ARG:NE	1:E:538:LYS:CE[2_546]	1.67	0.53
1:D:461:ARG:NE	1:H:538:LYS:CE[2_545]	1.72	0.48
1:E:478:GLU:CB	1:G:478:GLU:CB[1_455]	1.77	0.43
1:F:478:GLU:CB	1:H:478:GLU:CB[1_545]	1.78	0.42
1:A:465:ASP:OD1	1:G:538:LYS:NZ[2_656]	1.81	0.39
1:C:465:ASP:OD1	1:F:538:LYS:NZ[2_655]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ASP:OD1	1:E:538:LYS:NZ[2_546]	1.84	0.36
1:D:465:ASP:OD1	1:H:538:LYS:NZ[2_545]	1.87	0.33
1:B:475:ILE:CD1	1:E:497:TRP:CZ3[2_546]	1.89	0.31
1:D:475:ILE:CD1	1:H:497:TRP:CZ3[2_545]	1.89	0.31
1:C:475:ILE:CD1	1:F:497:TRP:CZ3[2_655]	1.93	0.27
1:B:473:LYS:CE	1:E:494:LYS:CE[2_546]	1.94	0.26
1:A:475:ILE:CD1	1:G:497:TRP:CZ3[2_656]	1.95	0.25
1:C:461:ARG:CD	1:F:538:LYS:CE[2_655]	2.01	0.19
1:A:461:ARG:CD	1:G:538:LYS:CE[2_656]	2.03	0.17
1:B:461:ARG:CD	1:E:538:LYS:CE[2_546]	2.05	0.15
1:D:461:ARG:CD	1:H:538:LYS:CE[2_545]	2.05	0.15
1:D:473:LYS:NZ	1:H:494:LYS:CE[2_545]	2.05	0.15
1:E:478:GLU:CD	1:G:478:GLU:OE1[1_455]	2.05	0.15
1:F:478:GLU:CD	1:H:478:GLU:OE1[1_545]	2.06	0.14
1:D:473:LYS:CE	1:H:494:LYS:CE[2_545]	2.07	0.13
1:E:478:GLU:OE1	1:G:478:GLU:CD[1_455]	2.13	0.07
1:C:461:ARG:CZ	1:F:538:LYS:CE[2_655]	2.16	0.04
1:C:473:LYS:NZ	1:F:494:LYS:CG[2_655]	2.16	0.04
1:F:478:GLU:OE1	1:H:478:GLU:CD[1_545]	2.16	0.04

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	201/218 (92%)	192 (96%)	9 (4%)	0	100	100
1	B	201/218 (92%)	192 (96%)	9 (4%)	0	100	100
1	C	201/218 (92%)	191 (95%)	10 (5%)	0	100	100
1	D	201/218 (92%)	193 (96%)	8 (4%)	0	100	100
1	E	201/218 (92%)	193 (96%)	8 (4%)	0	100	100
1	F	201/218 (92%)	193 (96%)	8 (4%)	0	100	100
1	G	201/218 (92%)	193 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	201/218 (92%)	193 (96%)	8 (4%)	0	100	100
All	All	1608/1744 (92%)	1540 (96%)	68 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	181/191 (95%)	181 (100%)	0	100	100
1	B	181/191 (95%)	181 (100%)	0	100	100
1	C	181/191 (95%)	181 (100%)	0	100	100
1	D	181/191 (95%)	181 (100%)	0	100	100
1	E	181/191 (95%)	181 (100%)	0	100	100
1	F	181/191 (95%)	181 (100%)	0	100	100
1	G	181/191 (95%)	181 (100%)	0	100	100
1	H	181/191 (95%)	181 (100%)	0	100	100
All	All	1448/1528 (95%)	1448 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	402	GLN
1	B	455	GLN
1	A	402	GLN
1	C	402	GLN
1	D	402	GLN
1	D	455	GLN
1	E	402	GLN
1	F	402	GLN

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Mol	Chain	Res	Type
1	G	402	GLN
1	H	402	GLN
1	H	467	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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, 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	203/218 (93%)	0.83	23 (11%) 10 7	37, 57, 99, 231	0
1	B	203/218 (93%)	0.63	13 (6%) 25 18	34, 57, 97, 230	0
1	C	203/218 (93%)	0.74	14 (6%) 23 16	36, 58, 98, 231	0
1	D	203/218 (93%)	0.69	14 (6%) 23 16	36, 58, 100, 232	0
1	E	203/218 (93%)	1.49	49 (24%) 2 1	43, 65, 111, 236	0
1	F	203/218 (93%)	1.48	49 (24%) 2 1	43, 66, 114, 237	0
1	G	203/218 (93%)	1.61	56 (27%) 1 1	42, 68, 113, 238	0
1	H	203/218 (93%)	1.58	53 (26%) 1 1	45, 69, 114, 239	0
All	All	1624/1744 (93%)	1.13	271 (16%) 4 3	34, 62, 112, 239	0

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	555	VAL	7.9
1	A	557	THR	7.6
1	F	555	VAL	7.5
1	G	557	THR	7.3
1	D	555	VAL	7.3
1	E	555	VAL	7.1
1	F	557	THR	6.8
1	G	495	TYR	6.7
1	B	555	VAL	6.7
1	H	555	VAL	6.7
1	H	483	ALA	6.6
1	H	495	TYR	6.4
1	E	557	THR	6.4
1	C	555	VAL	6.4
1	C	557	THR	6.3
1	G	555	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
1	G	477	VAL	5.9
1	F	495	TYR	5.8
1	B	557	THR	5.8
1	G	541	HIS	5.8
1	E	495	TYR	5.7
1	D	557	THR	5.6
1	E	556	VAL	5.6
1	H	557	THR	5.6
1	H	477	VAL	5.5
1	H	480	THR	5.4
1	A	556	VAL	5.4
1	G	479	MET	5.3
1	C	558	LEU	5.3
1	H	540	VAL	5.3
1	E	497	TRP	5.3
1	A	558	LEU	5.1
1	H	556	VAL	5.1
1	G	483	ALA	5.1
1	F	556	VAL	5.1
1	F	356	VAL	5.0
1	G	556	VAL	5.0
1	E	482	GLU	4.9
1	G	540	VAL	4.8
1	H	497	TRP	4.8
1	F	494	LYS	4.8
1	E	483	ALA	4.8
1	G	558	LEU	4.7
1	A	450	MET	4.7
1	E	477	VAL	4.7
1	H	479	MET	4.6
1	E	480	THR	4.6
1	E	479	MET	4.5
1	F	479	MET	4.5
1	C	356	VAL	4.5
1	F	541	HIS	4.5
1	F	477	VAL	4.5
1	F	540	VAL	4.5
1	B	558	LEU	4.5
1	F	497	TRP	4.4
1	E	486	GLU	4.4
1	G	537	LEU	4.4
1	G	480	THR	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	540	VAL	4.4
1	H	486	GLU	4.4
1	D	558	LEU	4.4
1	F	558	LEU	4.4
1	E	541	HIS	4.4
1	A	553	PRO	4.4
1	F	493	ASP	4.3
1	E	356	VAL	4.3
1	H	541	HIS	4.3
1	B	356	VAL	4.3
1	E	526	PHE	4.2
1	G	494	LYS	4.2
1	G	356	VAL	4.2
1	E	558	LEU	4.2
1	F	480	THR	4.1
1	G	497	TRP	4.1
1	F	537	LEU	4.1
1	B	553	PRO	4.1
1	E	494	LYS	4.1
1	E	537	LEU	4.1
1	H	494	LYS	4.1
1	H	537	LEU	4.0
1	G	517	HIS	4.0
1	H	356	VAL	4.0
1	C	556	VAL	3.9
1	C	553	PRO	3.9
1	G	493	ASP	3.9
1	D	553	PRO	3.9
1	F	526	PHE	3.8
1	H	482	GLU	3.8
1	F	386	ARG	3.8
1	F	553	PRO	3.8
1	A	356	VAL	3.8
1	F	413	GLN	3.7
1	H	558	LEU	3.7
1	F	482	GLU	3.7
1	C	450	MET	3.6
1	E	517	HIS	3.6
1	F	478	GLU	3.6
1	G	478	GLU	3.6
1	F	483	ALA	3.5
1	H	484	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	413	GLN	3.5
1	E	478	GLU	3.5
1	E	493	ASP	3.5
1	F	475	ILE	3.5
1	B	556	VAL	3.4
1	D	356	VAL	3.4
1	H	553	PRO	3.4
1	H	493	ASP	3.4
1	H	459	ASP	3.4
1	E	386	ARG	3.3
1	E	553	PRO	3.3
1	E	534	LEU	3.3
1	D	556	VAL	3.3
1	D	554	ASN	3.2
1	G	386	ARG	3.2
1	G	415	GLN	3.2
1	H	357	GLY	3.2
1	H	386	ARG	3.2
1	D	514	ILE	3.2
1	E	552	GLY	3.2
1	G	457	SER	3.2
1	G	531	LYS	3.1
1	F	486	GLU	3.1
1	B	386	ARG	3.1
1	C	536	ASP	3.1
1	H	426	MET	3.1
1	H	478	GLU	3.1
1	C	386	ARG	3.1
1	H	503	THR	3.1
1	G	459	ASP	3.0
1	G	484	SER	3.0
1	H	399	GLN	3.0
1	H	415	GLN	3.0
1	H	554	ASN	2.9
1	G	486	GLU	2.9
1	G	526	PHE	2.9
1	F	517	HIS	2.9
1	F	534	LEU	2.9
1	H	552	GLY	2.8
1	E	509	LYS	2.8
1	A	386	ARG	2.8
1	E	399	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	414	LYS	2.8
1	H	422	TYR	2.8
1	G	475	ILE	2.8
1	E	530	SER	2.8
1	H	466	SER	2.8
1	G	399	GLN	2.8
1	F	552	GLY	2.8
1	G	482	GLU	2.8
1	A	514	ILE	2.8
1	G	498	LEU	2.8
1	D	450	MET	2.8
1	E	459	ASP	2.8
1	G	503	THR	2.8
1	G	552	GLY	2.8
1	F	415	GLN	2.7
1	G	387	PHE	2.7
1	H	387	PHE	2.7
1	G	554	ASN	2.7
1	C	513	GLU	2.7
1	H	546	HIS	2.7
1	H	400	ASN	2.7
1	H	360	TYR	2.7
1	F	503	THR	2.7
1	F	399	GLN	2.7
1	D	386	ARG	2.7
1	A	552	GLY	2.7
1	H	498	LEU	2.6
1	G	360	TYR	2.6
1	G	534	LEU	2.6
1	H	517	HIS	2.6
1	A	399	GLN	2.6
1	C	399	GLN	2.6
1	A	387	PHE	2.6
1	E	417	LYS	2.6
1	F	509	LYS	2.6
1	F	357	GLY	2.6
1	H	539	THR	2.6
1	E	415	GLN	2.5
1	B	358	LEU	2.5
1	E	357	GLY	2.5
1	H	450	MET	2.5
1	B	514	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	553	PRO	2.5
1	E	503	THR	2.5
1	E	539	THR	2.5
1	G	533	ARG	2.4
1	H	526	PHE	2.4
1	H	532	ALA	2.4
1	A	468	ASN	2.4
1	E	554	ASN	2.4
1	E	358	LEU	2.4
1	E	484	SER	2.4
1	D	358	LEU	2.4
1	F	450	MET	2.4
1	A	554	ASN	2.4
1	E	400	ASN	2.4
1	H	457	SER	2.4
1	E	487	TYR	2.4
1	H	487	TYR	2.4
1	F	532	ALA	2.4
1	F	484	SER	2.4
1	G	492	TRP	2.4
1	C	515	THR	2.4
1	F	455	GLN	2.3
1	F	466	SER	2.3
1	F	487	TYR	2.3
1	F	539	THR	2.3
1	H	536	ASP	2.3
1	G	422	TYR	2.3
1	F	400	ASN	2.3
1	A	429	ALA	2.3
1	F	417	LYS	2.3
1	A	503	THR	2.3
1	H	481	ARG	2.3
1	B	513	GLU	2.2
1	D	513	GLU	2.2
1	A	413	GLN	2.2
1	G	500	LYS	2.2
1	E	481	ARG	2.2
1	E	485	ARG	2.2
1	G	458	ASP	2.2
1	A	414	LYS	2.2
1	E	532	ALA	2.2
1	H	534	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	432	PHE	2.2
1	H	417	LYS	2.2
1	A	485	ARG	2.2
1	F	459	ASP	2.2
1	H	427	ASP	2.2
1	G	521	MET	2.2
1	B	552	GLY	2.2
1	F	360	TYR	2.2
1	A	551	ARG	2.1
1	E	514	ILE	2.1
1	G	426	MET	2.1
1	D	552	GLY	2.1
1	G	402	GLN	2.1
1	E	516	PRO	2.1
1	G	450	MET	2.1
1	G	538	LYS	2.1
1	G	539	THR	2.1
1	F	498	LEU	2.1
1	C	485	ARG	2.1
1	E	360	TYR	2.1
1	G	481	ARG	2.1
1	H	514	ILE	2.1
1	F	554	ASN	2.1
1	H	506	VAL	2.1
1	F	428	LEU	2.1
1	G	431	LEU	2.1
1	F	481	ARG	2.1
1	G	507	ARG	2.1
1	E	455	GLN	2.1
1	H	418	GLN	2.1
1	A	512	LYS	2.1
1	G	546	HIS	2.1
1	H	521	MET	2.1
1	G	369	LEU	2.1
1	G	476	ASP	2.1
1	C	549	ILE	2.1
1	F	457	SER	2.0
1	D	537	LEU	2.0
1	A	515	THR	2.0
1	B	536	ASP	2.0
1	A	513	GLU	2.0
1	G	454	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	505	ILE	2.0
1	E	450	MET	2.0
1	B	451	VAL	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 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(Å ²)	Q<0.9
2	ZN	F	900	1/1	0.95	0.06	57,57,57,57	0
2	ZN	G	900	1/1	0.95	0.10	79,79,79,79	0
2	ZN	D	900	1/1	0.96	0.05	49,49,49,49	0
2	ZN	H	900	1/1	0.96	0.09	75,75,75,75	0
2	ZN	B	900	1/1	0.97	0.05	55,55,55,55	0
2	ZN	E	900	1/1	0.98	0.07	56,56,56,56	0
2	ZN	A	900	1/1	0.98	0.04	48,48,48,48	0
2	ZN	C	900	1/1	0.99	0.02	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.