



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:24 PM UTC

PDB ID : 7VT2 / pdb_00007vt2
Title : Azumapecten Farreri ferritin
Authors : Zhao, G.; Zhang, C.
Deposited on : 2021-10-27
Resolution : 2.40 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

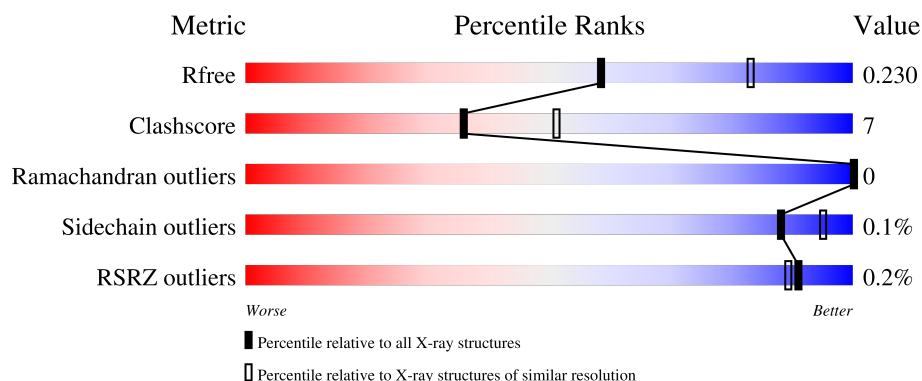
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.



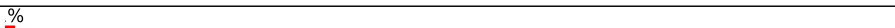
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	171	 81% 17% ..
1	B	171	 80% 19% .
1	C	171	 85% 13% .
1	D	171	 85% 13% ..
1	E	171	 85% 13% .

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Mol	Chain	Length	Quality of chain
1	F	171	 82% 17% .
1	H	171	 78% 20% .
1	I	171	 82% 16% .
1	J	171	 88% 10% ..
1	K	171	 84% 15% .
1	L	171	 87% 12% ..
1	M	171	 78% 20% ..
1	N	171	 88% 10% ..
1	O	171	 85% 13% ..
1	P	171	 81% 17% ..
1	Q	171	 87% 12% .
1	R	171	 78% 20% ..
1	S	171	 84% 14% ..
1	T	171	 84% 15% .
1	U	171	 84% 15% .
1	V	171	 81% 18% ..
1	W	171	 88% 11% .
1	X	171	 80% 19% ..
1	Z	171	 81% 17% ..
1	a	171	 82% 17% .
1	b	171	 81% 18% ..
1	c	171	 88% 11% .
1	d	171	 83% 15% ..
1	e	171	 86% 13% .
1	f	171	 85% 13% ..

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Mol	Chain	Length	Quality of chain
1	g	171	% 85% 14% .
1	h	171	% 81% 16% ..
1	i	171	81% 18% .
1	j	171	84% 14% ..
1	k	171	84% 14% ..
1	l	171	88% 11% .
1	m	171	86% 12% ..
1	n	171	88% 11% ..
1	o	171	82% 16% ..
1	p	171	% 82% 16% ..
1	q	171	89% 9% .
1	r	171	81% 18% .
1	s	171	% 87% 12% .
1	t	171	% 85% 13% ..
1	u	171	% 84% 13% ..
1	v	171	85% 13% ..
1	w	171	78% 20% ..
1	x	171	82% 15% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 73344 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 Ferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	S	169	Total	C	N	O	S	0	0	0
			1297	868	237	185	7			
1	I	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	O	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	V	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	C	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	Q	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	U	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	a	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	c	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	d	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	e	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	f	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	g	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	i	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	j	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	k	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	l	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	m	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	o	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	q	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	w	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	s	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	v	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	B	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	D	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	E	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	F	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	H	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	J	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	K	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	L	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	M	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	N	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	P	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	R	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	T	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	W	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	X	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	Z	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	b	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	h	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	n	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	p	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	r	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	t	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	u	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			
1	x	169	Total	C	N	O	S	0	0	0
			1388	869	237	275	7			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	S	2	Total	Fe	0	0
			2	2		
2	I	2	Total	Fe	0	0
			2	2		
2	O	2	Total	Fe	0	0
			2	2		
2	V	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	Q	2	Total	Fe	0	0
			2	2		
2	U	2	Total	Fe	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	a	2	Total 2	Fe 2	0	0
2	c	2	Total 2	Fe 2	0	0
2	d	2	Total 2	Fe 2	0	0
2	e	2	Total 2	Fe 2	0	0
2	f	2	Total 2	Fe 2	0	0
2	g	2	Total 2	Fe 2	0	0
2	i	2	Total 2	Fe 2	0	0
2	j	2	Total 2	Fe 2	0	0
2	k	2	Total 2	Fe 2	0	0
2	l	2	Total 2	Fe 2	0	0
2	m	2	Total 2	Fe 2	0	0
2	o	2	Total 2	Fe 2	0	0
2	q	2	Total 2	Fe 2	0	0
2	w	2	Total 2	Fe 2	0	0
2	s	2	Total 2	Fe 2	0	0
2	v	2	Total 2	Fe 2	0	0
2	B	2	Total 2	Fe 2	0	0
2	D	2	Total 2	Fe 2	0	0
2	E	2	Total 2	Fe 2	0	0
2	F	2	Total 2	Fe 2	0	0
2	H	2	Total 2	Fe 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	J	2	Total 2	Fe 2	0	0
2	K	2	Total 2	Fe 2	0	0
2	L	2	Total 2	Fe 2	0	0
2	M	2	Total 2	Fe 2	0	0
2	N	2	Total 2	Fe 2	0	0
2	P	2	Total 2	Fe 2	0	0
2	R	2	Total 2	Fe 2	0	0
2	T	2	Total 2	Fe 2	0	0
2	W	2	Total 2	Fe 2	0	0
2	X	1	Total 1	Fe 1	0	0
2	Z	2	Total 2	Fe 2	0	0
2	b	2	Total 2	Fe 2	0	0
2	h	2	Total 2	Fe 2	0	0
2	n	2	Total 2	Fe 2	0	0
2	p	2	Total 2	Fe 2	0	0
2	r	2	Total 2	Fe 2	0	0
2	t	2	Total 2	Fe 2	0	0
2	u	2	Total 2	Fe 2	0	0
2	x	2	Total 2	Fe 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	184	Total O 184 184	0	0
3	S	121	Total O 121 121	0	0
3	I	169	Total O 169 169	0	0
3	O	137	Total O 137 137	0	0
3	V	135	Total O 135 135	0	0
3	C	150	Total O 150 150	0	0
3	Q	127	Total O 127 127	0	0
3	U	122	Total O 122 122	0	0
3	a	126	Total O 126 126	0	0
3	c	166	Total O 166 166	0	0
3	d	164	Total O 164 164	0	0
3	e	136	Total O 136 136	0	0
3	f	164	Total O 164 164	0	0
3	g	189	Total O 189 189	0	0
3	i	114	Total O 114 114	0	0
3	j	171	Total O 171 171	0	0
3	k	164	Total O 164 164	0	0
3	l	142	Total O 142 142	0	0
3	m	142	Total O 142 142	0	0
3	o	129	Total O 129 129	0	0
3	q	144	Total O 144 144	0	0
3	w	113	Total O 113 113	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	s	168	Total O 168 168	0	0
3	v	165	Total O 165 165	0	0
3	B	145	Total O 145 145	0	0
3	D	138	Total O 138 138	0	0
3	E	133	Total O 133 133	0	0
3	F	128	Total O 128 128	0	0
3	H	114	Total O 114 114	0	0
3	J	102	Total O 102 102	0	0
3	K	80	Total O 80 80	0	0
3	L	128	Total O 128 128	0	0
3	M	121	Total O 121 121	0	0
3	N	193	Total O 193 193	0	0
3	P	110	Total O 110 110	0	0
3	R	111	Total O 111 111	0	0
3	T	94	Total O 94 94	0	0
3	W	189	Total O 189 189	0	0
3	X	122	Total O 122 122	0	0
3	Z	138	Total O 138 138	0	0
3	b	151	Total O 151 151	0	0
3	h	119	Total O 119 119	0	0
3	n	123	Total O 123 123	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	p	142	Total 142	O 142	0	0
3	r	157	Total 157	O 157	0	0
3	t	103	Total 103	O 103	0	0
3	u	178	Total 178	O 178	0	0
3	x	155	Total 155	O 155	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: Ferritin

Chain A: 



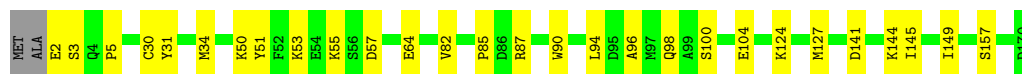
- Molecule 1: Ferritin

Chain S: 



- Molecule 1: Ferritin

Chain I: 



- Molecule 1: Ferritin

Chain O: 



- Molecule 1: Ferritin

Chain V: 



- Molecule 1: Ferritin

Chain C:  85% 13% .



• Molecule 1: Ferritin

Chain Q:  87% 12% .



• Molecule 1: Ferritin

Chain U:  84% 15% .



• Molecule 1: Ferritin

Chain a:  82% 17% .



• Molecule 1: Ferritin

Chain c:  88% 11% .



• Molecule 1: Ferritin

Chain d:  83% 15% ..



• Molecule 1: Ferritin

Chain e:  86% 13% .

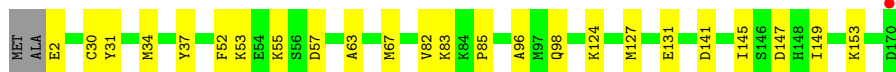
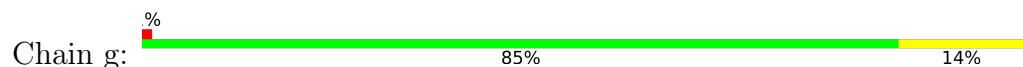


• Molecule 1: Ferritin

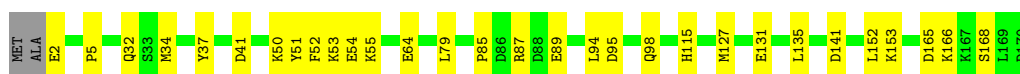
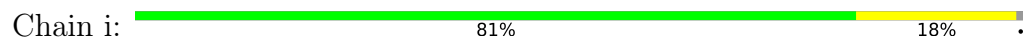
Chain f:  85% 13% ..



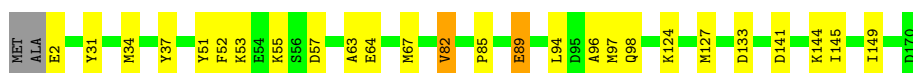
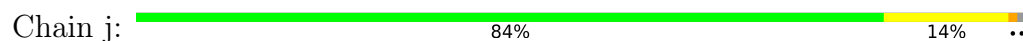
- Molecule 1: Ferritin



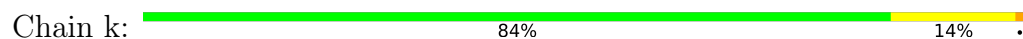
- Molecule 1: Ferritin



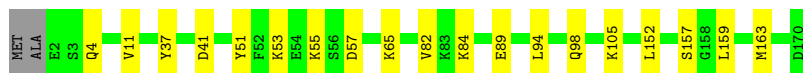
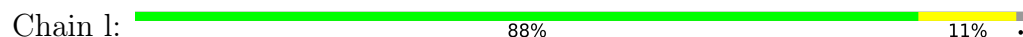
- Molecule 1: Ferritin



- Molecule 1: Ferritin



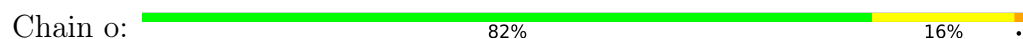
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin





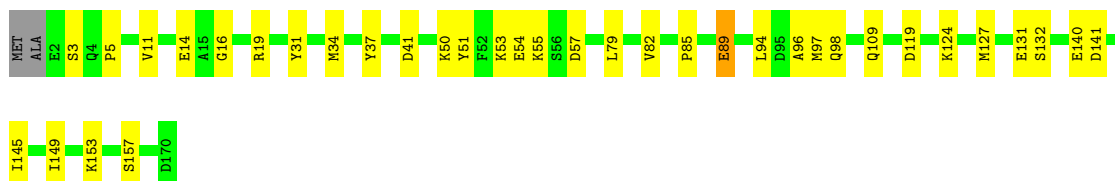
- Molecule 1: Ferritin

Chain q: 89% 9% .



- Molecule 1: Ferritin

Chain w: 78% 20% ..



- Molecule 1: Ferritin

Chain s: 87% 12% .



- Molecule 1: Ferritin

Chain v: 85% 13% ..



- Molecule 1: Ferritin

Chain B: 80% 19% .



- Molecule 1: Ferritin

Chain D: 85% 13% ..



- Molecule 1: Ferritin

Chain E:  85% 13%



• Molecule 1: Ferritin

Chain F:  82% 17%



• Molecule 1: Ferritin

Chain H:  78% 20%



• Molecule 1: Ferritin

Chain J:  88% 10%



• Molecule 1: Ferritin

Chain K:  84% 15%



• Molecule 1: Ferritin

Chain L:  87% 12%



• Molecule 1: Ferritin

Chain M:  78% 20%





- Molecule 1: Ferritin

Chain N: 88% 10% ..



- Molecule 1: Ferritin

Chain P: 81% 17% ..



- Molecule 1: Ferritin

Chain R: 78% 20% ..



- Molecule 1: Ferritin

Chain T: 84% 15% .



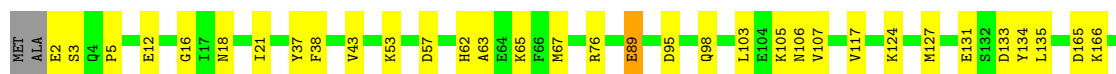
- Molecule 1: Ferritin

Chain W: 88% 11% .

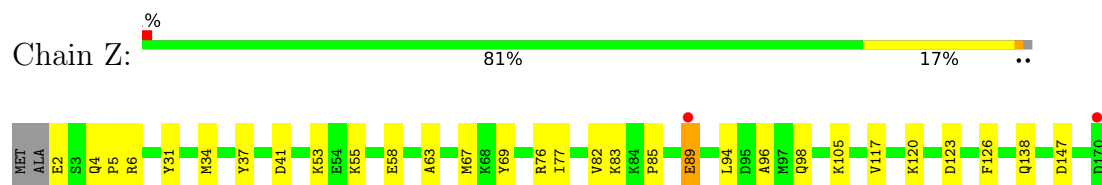


- Molecule 1: Ferritin

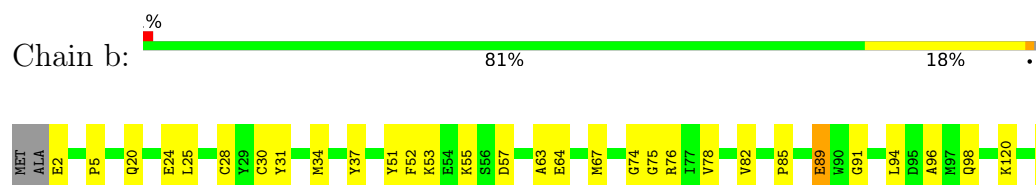
Chain X: 80% 19% ..



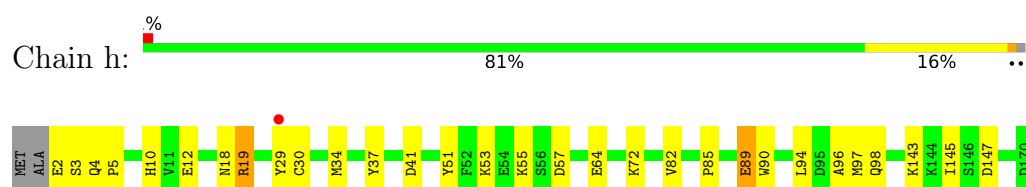
- Molecule 1: Ferritin



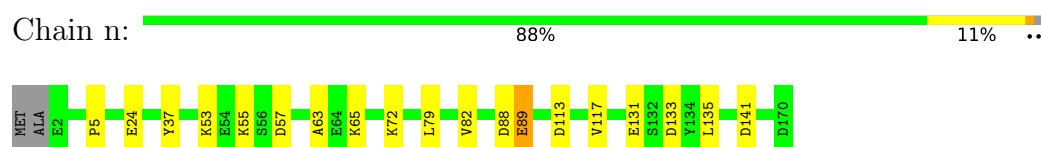
- Molecule 1: Ferritin



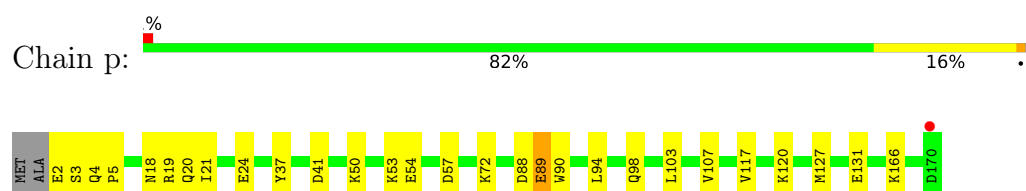
- Molecule 1: Ferritin



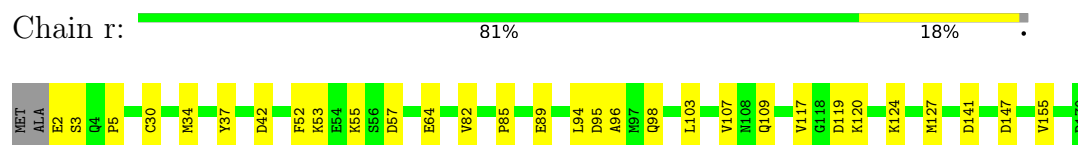
- Molecule 1: Ferritin



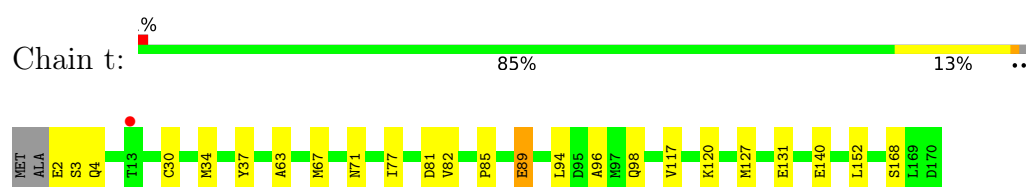
- Molecule 1: Ferritin



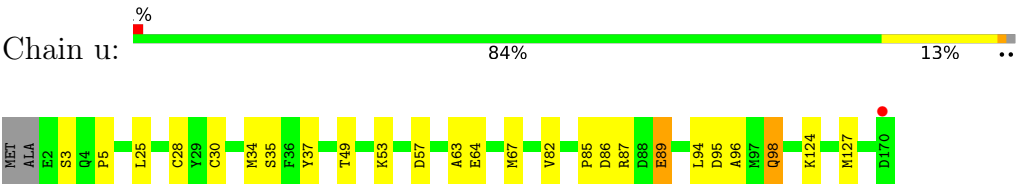
- Molecule 1: Ferritin



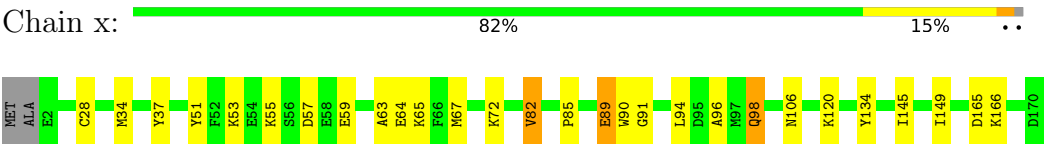
- Molecule 1: Ferritin



● Molecule 1: Ferritin



● Molecule 1: Ferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.53Å 169.58Å 198.37Å 90.00° 95.73° 90.00°	Depositor
Resolution (Å)	29.68 – 2.40 29.68 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.68-2.40) 99.0 (29.68-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.190 , 0.230 0.190 , 0.230	Depositor DCC
R_{free} test set	2000 reflections (0.48%)	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	73344	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5291e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: FE

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	0.39	0/1414	0.58	1/1894 (0.1%)
1	B	0.41	1/1414 (0.1%)	0.62	0/1894
1	C	0.39	0/1414	0.56	0/1894
1	D	0.40	0/1414	0.59	1/1894 (0.1%)
1	E	0.38	0/1414	0.56	0/1894
1	F	0.40	0/1414	0.59	2/1894 (0.1%)
1	H	0.34	0/1414	0.55	1/1894 (0.1%)
1	I	0.39	0/1414	0.57	0/1894
1	J	0.35	0/1414	0.60	1/1894 (0.1%)
1	K	0.31	0/1414	0.54	0/1894
1	L	0.39	0/1414	0.57	1/1894 (0.1%)
1	M	0.41	0/1414	0.62	4/1894 (0.2%)
1	N	0.43	0/1414	0.67	3/1894 (0.2%)
1	O	0.40	0/1414	0.61	1/1894 (0.1%)
1	P	0.39	0/1414	0.60	1/1894 (0.1%)
1	Q	0.34	0/1414	0.60	2/1894 (0.1%)
1	R	0.42	0/1414	0.71	3/1894 (0.2%)
1	S	0.36	0/1323	0.59	0/1715
1	T	0.32	0/1414	0.53	0/1894
1	U	0.36	0/1414	0.55	0/1894
1	V	0.36	0/1414	0.59	1/1894 (0.1%)
1	W	0.38	0/1414	0.57	0/1894
1	X	0.38	0/1414	0.62	2/1894 (0.1%)
1	Z	0.34	0/1414	0.56	1/1894 (0.1%)
1	a	0.38	0/1414	0.55	0/1894
1	b	0.38	0/1414	0.60	1/1894 (0.1%)
1	c	0.36	0/1414	0.58	0/1894
1	d	0.42	0/1414	0.62	0/1894
1	e	0.34	0/1414	0.54	0/1894
1	f	0.36	0/1414	0.58	1/1894 (0.1%)
1	g	0.38	0/1414	0.54	0/1894
1	h	0.42	1/1414 (0.1%)	0.65	3/1894 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	i	0.35	0/1414	0.58	0/1894
1	j	0.39	0/1414	0.56	1/1894 (0.1%)
1	k	0.38	0/1414	0.57	1/1894 (0.1%)
1	l	0.36	0/1414	0.57	1/1894 (0.1%)
1	m	0.39	0/1414	0.60	1/1894 (0.1%)
1	n	0.37	0/1414	0.58	1/1894 (0.1%)
1	o	0.37	0/1414	0.60	1/1894 (0.1%)
1	p	0.38	0/1414	0.62	1/1894 (0.1%)
1	q	0.34	0/1414	0.56	0/1894
1	r	0.37	0/1414	0.57	0/1894
1	s	0.37	0/1414	0.59	1/1894 (0.1%)
1	t	0.41	0/1414	0.60	1/1894 (0.1%)
1	u	0.38	0/1414	0.60	2/1894 (0.1%)
1	v	0.40	0/1414	0.60	1/1894 (0.1%)
1	w	0.35	0/1414	0.55	1/1894 (0.1%)
1	x	0.39	0/1414	0.63	2/1894 (0.1%)
All	All	0.38	2/67781 (0.0%)	0.59	45/90733 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	d	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	61	GLU	CD-OE2	-5.31	1.15	1.25
1	h	19	ARG	CZ-NH1	5.06	1.39	1.32

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	19	ARG	NE-CZ-NH1	-12.61	108.89	121.50
1	R	19	ARG	NE-CZ-NH2	10.14	128.33	119.20
1	N	89	GLU	CA-CB-CG	8.43	130.95	114.10
1	Q	98	GLN	CA-CB-CG	7.59	129.29	114.10
1	m	98	GLN	CA-CB-CG	7.35	128.80	114.10
1	h	89	GLU	CA-CB-CG	6.75	127.59	114.10
1	b	89	GLU	CA-CB-CG	6.73	127.56	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	k	89	GLU	CA-CB-CG	6.50	127.11	114.10
1	Z	89	GLU	CA-CB-CG	6.45	127.00	114.10
1	u	89	GLU	CA-CB-CG	6.45	127.00	114.10
1	p	89	GLU	CA-CB-CG	6.44	126.98	114.10
1	P	89	GLU	CA-CB-CG	6.08	126.25	114.10
1	J	89	GLU	CA-CB-CG	6.06	126.22	114.10
1	A	89	GLU	CA-CB-CG	6.05	126.21	114.10
1	s	98	GLN	CA-CB-CG	5.93	125.97	114.10
1	X	89	GLU	CA-CB-CG	5.92	125.93	114.10
1	R	19	ARG	CB-CG-CD	-5.87	97.80	111.30
1	L	67	MET	CG-SD-CE	5.82	113.70	100.90
1	N	89	GLU	CG-CD-OE2	5.75	131.63	118.40
1	x	89	GLU	CA-CB-CG	5.75	125.59	114.10
1	t	89	GLU	CA-CB-CG	5.74	125.59	114.10
1	X	98	GLN	CA-CB-CG	5.67	125.45	114.10
1	w	89	GLU	CA-CB-CG	5.65	125.41	114.10
1	N	87	ARG	CB-CG-CD	-5.59	98.44	111.30
1	f	89	GLU	CA-CB-CG	5.56	125.22	114.10
1	M	137	GLU	CB-CG-CD	5.51	121.97	112.60
1	j	89	GLU	CA-CB-CG	5.47	125.05	114.10
1	v	89	GLU	CA-CB-CG	5.44	124.98	114.10
1	H	89	GLU	CA-CB-CG	5.42	124.95	114.10
1	n	89	GLU	CA-CB-CG	5.40	124.91	114.10
1	M	89	GLU	CA-CB-CG	5.38	124.85	114.10
1	o	89	GLU	CA-CB-CG	5.29	124.68	114.10
1	V	89	GLU	CA-CB-CG	5.28	124.66	114.10
1	x	98	GLN	CA-CB-CG	5.21	124.53	114.10
1	Q	98	GLN	CB-CA-C	-5.19	102.73	110.88
1	O	131	GLU	CA-CB-CG	5.18	124.47	114.10
1	u	98	GLN	CA-CB-CG	5.18	124.46	114.10
1	M	136	GLU	CA-C-N	5.18	128.18	120.31
1	M	136	GLU	C-N-CA	5.18	128.18	120.31
1	h	18	ASN	CA-C-N	-5.10	112.57	122.06
1	h	18	ASN	C-N-CA	-5.10	112.57	122.06
1	D	89	GLU	CA-CB-CG	5.09	124.27	114.10
1	l	98	GLN	CA-CB-CG	5.07	124.24	114.10
1	F	18	ASN	CA-C-N	-5.03	113.22	121.92
1	F	18	ASN	C-N-CA	-5.03	113.22	121.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	d	82	VAL	Peptide

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	1388	0	1327	29	0
1	B	1388	0	1327	29	0
1	C	1388	0	1327	23	0
1	D	1388	0	1327	18	0
1	E	1388	0	1327	20	0
1	F	1388	0	1327	23	0
1	H	1388	0	1327	31	0
1	I	1388	0	1327	26	0
1	J	1388	0	1327	14	0
1	K	1388	0	1327	21	0
1	L	1388	0	1327	20	0
1	M	1388	0	1327	28	0
1	N	1388	0	1327	17	0
1	O	1388	0	1327	20	0
1	P	1388	0	1327	28	0
1	Q	1388	0	1327	20	0
1	R	1388	0	1327	33	0
1	S	1297	0	1331	20	0
1	T	1388	0	1327	20	0
1	U	1388	0	1327	20	0
1	V	1388	0	1327	25	0
1	W	1388	0	1327	18	0
1	X	1388	0	1327	22	0
1	Z	1388	0	1327	26	0
1	a	1388	0	1327	23	0
1	b	1388	0	1327	28	0
1	c	1388	0	1327	14	0
1	d	1388	0	1327	22	0
1	e	1388	0	1327	17	0
1	f	1388	0	1327	21	0
1	g	1388	0	1327	22	0
1	h	1388	0	1327	27	0
1	i	1388	0	1327	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	j	1388	0	1327	22	0
1	k	1388	0	1327	23	0
1	l	1388	0	1327	16	0
1	m	1388	0	1327	21	0
1	n	1388	0	1327	17	0
1	o	1388	0	1327	26	0
1	p	1388	0	1327	21	0
1	q	1388	0	1327	14	0
1	r	1388	0	1327	27	0
1	s	1388	0	1327	19	0
1	t	1388	0	1327	21	0
1	u	1388	0	1327	19	0
1	v	1388	0	1327	23	0
1	w	1388	0	1327	30	0
1	x	1388	0	1327	22	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
2	M	2	0	0	0	0
2	N	2	0	0	0	0
2	O	2	0	0	0	0
2	P	2	0	0	0	0
2	Q	2	0	0	0	0
2	R	2	0	0	0	0
2	S	2	0	0	0	0
2	T	2	0	0	0	0
2	U	2	0	0	0	0
2	V	2	0	0	0	0
2	W	2	0	0	0	0
2	X	1	0	0	0	0
2	Z	2	0	0	0	0
2	a	2	0	0	0	0
2	b	2	0	0	0	0
2	c	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	d	2	0	0	0	0
2	e	2	0	0	0	0
2	f	2	0	0	0	0
2	g	2	0	0	0	0
2	h	2	0	0	0	0
2	i	2	0	0	0	0
2	j	2	0	0	0	0
2	k	2	0	0	0	0
2	l	2	0	0	0	0
2	m	2	0	0	0	0
2	n	2	0	0	0	0
2	o	2	0	0	0	0
2	p	2	0	0	0	0
2	q	2	0	0	0	0
2	r	2	0	0	0	0
2	s	2	0	0	0	0
2	t	2	0	0	0	0
2	u	2	0	0	0	0
2	v	2	0	0	0	0
2	w	2	0	0	0	0
2	x	2	0	0	0	0
3	A	184	0	0	8	0
3	B	145	0	0	13	0
3	C	150	0	0	8	0
3	D	138	0	0	3	0
3	E	133	0	0	4	0
3	F	128	0	0	6	0
3	H	114	0	0	13	0
3	I	169	0	0	5	0
3	J	102	0	0	4	0
3	K	80	0	0	5	0
3	L	128	0	0	7	0
3	M	121	0	0	8	0
3	N	193	0	0	3	0
3	O	137	0	0	3	0
3	P	110	0	0	10	1
3	Q	127	0	0	2	1
3	R	111	0	0	13	1
3	S	121	0	0	6	0
3	T	94	0	0	4	0
3	U	122	0	0	7	0
3	V	135	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	W	189	0	0	8	0
3	X	122	0	0	9	0
3	Z	138	0	0	12	0
3	a	126	0	0	6	0
3	b	151	0	0	7	0
3	c	166	0	0	7	1
3	d	164	0	0	3	0
3	e	136	0	0	6	0
3	f	164	0	0	5	0
3	g	189	0	0	9	1
3	h	119	0	0	6	0
3	i	114	0	0	6	0
3	j	171	0	0	5	1
3	k	164	0	0	6	0
3	l	142	0	0	7	0
3	m	142	0	0	6	0
3	n	123	0	0	7	0
3	o	129	0	0	10	1
3	p	142	0	0	6	0
3	q	144	0	0	5	0
3	r	157	0	0	9	0
3	s	168	0	0	5	0
3	t	103	0	0	5	0
3	u	178	0	0	3	0
3	v	165	0	0	5	0
3	w	113	0	0	11	0
3	x	155	0	0	3	0
All	All	73344	0	63700	950	4

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 7.

All (950) 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:X:133:ASP:O	3:X:301:HOH:O	1.80	0.99
1:V:133:ASP:OD2	3:V:301:HOH:O	1.82	0.96
1:o:18:ASN:O	3:o:301:HOH:O	1.82	0.96
1:t:81:ASP:OD1	3:t:301:HOH:O	1.84	0.95
1:i:168:SER:O	3:i:301:HOH:O	1.84	0.94
1:e:95:ASP:OD1	3:e:301:HOH:O	1.85	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:12:GLU:OE1	3:c:301:HOH:O	1.86	0.92
1:M:78:VAL:O	3:M:301:HOH:O	1.88	0.91
1:I:157:SER:O	3:I:301:HOH:O	1.87	0.91
1:A:57:ASP:OD2	3:A:301:HOH:O	1.88	0.90
1:S:88:ASP:OD1	3:S:301:HOH:O	1.90	0.90
1:D:120:LYS:O	3:D:301:HOH:O	1.90	0.90
1:Q:2:GLU:N	3:Q:6301:HOH:O	2.02	0.90
1:n:72:LYS:O	3:n:301:HOH:O	1.91	0.88
1:U:161:GLU:OE2	3:U:302:HOH:O	1.91	0.88
1:a:87:ARG:NH1	3:a:301:HOH:O	1.97	0.87
1:w:119:ASP:OD2	3:w:302:HOH:O	1.93	0.86
1:q:153:LYS:NZ	3:q:301:HOH:O	2.09	0.86
1:Z:77:ILE:O	3:Z:301:HOH:O	1.94	0.85
1:V:98:GLN:OE1	3:V:302:HOH:O	1.94	0.85
1:h:10:HIS:HD2	1:h:12:GLU:H	1.25	0.85
1:n:88:ASP:OD1	3:n:302:HOH:O	1.95	0.84
1:S:77:ILE:O	3:S:302:HOH:O	1.95	0.84
1:T:3:SER:HB3	1:T:5:PRO:HD2	1.59	0.84
1:C:2:GLU:N	3:C:301:HOH:O	2.10	0.84
1:B:77:ILE:O	3:B:301:HOH:O	1.96	0.84
1:f:3:SER:HB3	1:f:5:PRO:HD2	1.58	0.84
1:w:14:GLU:OE2	3:w:303:HOH:O	1.95	0.84
1:w:41:ASP:OD1	3:w:304:HOH:O	1.95	0.83
1:r:109:GLN:NE2	3:r:302:HOH:O	1.98	0.83
1:r:147:ASP:OD2	3:r:301:HOH:O	1.96	0.83
1:t:71:ASN:O	3:t:302:HOH:O	1.96	0.83
1:R:2:GLU:N	3:R:306:HOH:O	2.12	0.83
1:H:86:ASP:OD2	3:H:301:HOH:O	1.96	0.82
1:a:2:GLU:N	3:a:302:HOH:O	2.12	0.82
1:p:2:GLU:N	3:p:304:HOH:O	2.13	0.82
1:r:2:GLU:N	3:r:303:HOH:O	2.11	0.82
1:h:12:GLU:OE2	3:h:302:HOH:O	1.97	0.81
1:X:57:ASP:O	3:X:303:HOH:O	1.99	0.81
1:B:42:ASP:OD2	3:B:302:HOH:O	1.97	0.81
1:w:3:SER:HB3	1:w:5:PRO:HD2	1.63	0.80
1:F:116:THR:OG1	3:F:301:HOH:O	1.98	0.80
1:b:120:LYS:NZ	3:b:301:HOH:O	2.10	0.80
1:R:14:GLU:OE2	3:R:301:HOH:O	1.99	0.79
1:D:2:GLU:N	3:D:302:HOH:O	2.16	0.79
1:Q:85:PRO:HG2	3:Q:6327:HOH:O	1.82	0.79
1:C:65:LYS:NZ	3:C:303:HOH:O	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:79:LEU:O	3:L:301:HOH:O	2.00	0.79
1:T:3:SER:O	3:T:301:HOH:O	2.01	0.79
1:M:131:GLU:OE2	3:M:302:HOH:O	2.00	0.79
1:K:3:SER:HB3	1:K:5:PRO:HD2	1.65	0.78
1:X:62:HIS:O	3:X:302:HOH:O	2.02	0.78
1:V:61:GLU:OE1	3:V:303:HOH:O	2.01	0.78
1:P:144:LYS:NZ	3:P:301:HOH:O	2.05	0.78
1:n:113:ASP:OD2	3:n:304:HOH:O	2.01	0.78
1:R:34:MET:SD	3:R:398:HOH:O	2.40	0.78
1:S:88:ASP:OD1	3:S:303:HOH:O	2.01	0.78
1:n:117:VAL:O	3:n:303:HOH:O	2.01	0.77
1:d:4:GLN:OE1	3:d:302:HOH:O	2.00	0.77
1:m:98:GLN:NE2	3:m:303:HOH:O	2.16	0.77
1:h:2:GLU:N	3:h:303:HOH:O	2.17	0.77
1:B:2:GLU:OE1	3:B:303:HOH:O	2.02	0.77
1:g:147:ASP:OD2	3:g:301:HOH:O	2.03	0.77
1:U:86:ASP:OD2	3:U:303:HOH:O	2.03	0.77
1:f:113:ASP:OD2	3:f:301:HOH:O	2.03	0.76
1:o:19:ARG:NH1	3:o:304:HOH:O	2.16	0.76
1:V:156:GLY:O	3:V:304:HOH:O	2.03	0.76
1:i:41:ASP:OD2	1:o:5:PRO:HD3	1.84	0.76
1:I:34:MET:HE3	1:I:96:ALA:HB1	1.67	0.75
1:R:2:GLU:OE2	3:R:302:HOH:O	2.04	0.75
1:b:34:MET:HE3	1:b:96:ALA:HB1	1.69	0.75
1:e:76:ARG:NH2	3:e:302:HOH:O	2.06	0.74
1:I:85:PRO:HG2	3:I:341:HOH:O	1.87	0.74
1:p:3:SER:O	3:p:302:HOH:O	2.05	0.74
1:E:11:VAL:O	3:E:301:HOH:O	2.04	0.74
1:J:77:ILE:O	3:J:301:HOH:O	2.05	0.74
1:H:2:GLU:N	3:H:307:HOH:O	2.20	0.74
1:l:65:LYS:NZ	3:l:303:HOH:O	2.15	0.74
1:M:157:SER:O	3:M:304:HOH:O	2.04	0.73
1:V:85:PRO:HG2	3:V:318:HOH:O	1.89	0.73
1:j:2:GLU:N	3:j:302:HOH:O	2.20	0.73
1:o:98:GLN:OE1	3:o:303:HOH:O	2.07	0.73
1:s:53:LYS:HE2	1:v:64:GLU:OE1	1.89	0.72
1:W:85:PRO:HG2	3:W:318:HOH:O	1.89	0.72
1:R:169:LEU:O	3:R:304:HOH:O	2.08	0.72
1:H:3:SER:HB3	1:H:5:PRO:HD2	1.71	0.72
1:H:65:LYS:NZ	3:H:310:HOH:O	2.22	0.71
1:R:98:GLN:OE1	3:R:305:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:41:ASP:OD2	3:p:303:HOH:O	2.07	0.71
1:o:117:VAL:O	1:o:120:LYS:HG2	1.90	0.71
1:w:85:PRO:HG2	3:w:334:HOH:O	1.89	0.71
1:X:95:ASP:OD2	3:X:304:HOH:O	2.09	0.71
1:e:16:GLY:O	3:e:303:HOH:O	2.08	0.71
1:t:131:GLU:OE2	3:t:303:HOH:O	2.07	0.71
1:V:81:ASP:OD2	3:V:305:HOH:O	2.08	0.71
1:R:58:GLU:O	1:R:62:HIS:ND1	2.24	0.70
1:g:131:GLU:OE2	3:g:302:HOH:O	2.09	0.70
1:o:11:VAL:HG13	3:o:317:HOH:O	1.91	0.70
1:A:2:GLU:N	3:A:304:HOH:O	2.22	0.70
1:j:133:ASP:O	3:j:301:HOH:O	2.08	0.70
1:X:2:GLU:N	3:X:307:HOH:O	2.25	0.70
1:u:95:ASP:OD1	3:u:301:HOH:O	2.10	0.70
1:h:29:TYR:HE2	1:n:79:LEU:HD13	1.57	0.70
1:I:82:VAL:HG13	1:O:82:VAL:HG13	1.74	0.70
1:c:2:GLU:OE2	3:c:302:HOH:O	2.10	0.69
1:Z:147:ASP:OD2	3:Z:302:HOH:O	2.10	0.69
1:C:109:GLN:OE1	3:C:302:HOH:O	2.11	0.69
1:k:34:MET:HE3	1:k:96:ALA:HB1	1.75	0.69
1:m:140:GLU:OE2	3:m:301:HOH:O	2.10	0.69
1:F:139:VAL:O	3:F:302:HOH:O	2.10	0.69
1:d:98:GLN:OE1	3:d:303:HOH:O	2.11	0.69
1:E:53:LYS:NZ	1:E:57:ASP:OD2	2.26	0.69
1:X:106:ASN:OD1	3:X:305:HOH:O	2.10	0.69
1:r:85:PRO:HG2	3:r:347:HOH:O	1.93	0.69
1:P:2:GLU:N	3:P:306:HOH:O	2.26	0.69
1:A:2:GLU:N	3:A:306:HOH:O	2.27	0.68
1:M:95:ASP:OD2	3:M:305:HOH:O	2.11	0.68
1:M:34:MET:HE3	1:M:96:ALA:HB1	1.75	0.68
1:S:128:ASP:OD2	3:S:304:HOH:O	2.12	0.68
1:v:34:MET:SD	3:v:430:HOH:O	2.52	0.68
1:m:12:GLU:O	3:m:302:HOH:O	2.11	0.68
1:U:169:LEU:O	3:U:305:HOH:O	2.12	0.67
1:l:11:VAL:O	3:l:302:HOH:O	2.12	0.67
1:o:87:ARG:NH1	3:o:302:HOH:O	1.97	0.67
1:s:85:PRO:HG2	3:s:335:HOH:O	1.94	0.67
1:b:78:VAL:O	3:b:302:HOH:O	2.12	0.67
1:W:2:GLU:HA	3:W:445:HOH:O	1.94	0.67
1:A:161:GLU:OE2	3:A:302:HOH:O	2.13	0.67
1:I:3:SER:HB3	1:I:5:PRO:HD2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:5:PRO:HD3	1:O:41:ASP:OD2	1.95	0.67
1:l:4:GLN:NE2	3:l:301:HOH:O	1.98	0.67
1:J:2:GLU:N	3:J:306:HOH:O	2.27	0.67
1:I:2:GLU:N	3:I:303:HOH:O	2.28	0.67
1:F:50:LYS:HE2	3:F:359:HOH:O	1.94	0.67
1:W:2:GLU:HG2	3:W:316:HOH:O	1.94	0.67
1:Z:123:ASP:OD1	3:Z:303:HOH:O	2.13	0.67
1:O:2:GLU:OE2	3:O:302:HOH:O	2.12	0.67
1:g:55:LYS:NZ	1:g:141:ASP:OD2	2.26	0.67
1:K:82:VAL:HG13	1:t:82:VAL:HG13	1.76	0.66
1:s:34:MET:HE3	1:s:96:ALA:HB1	1.77	0.66
1:K:91:GLY:O	3:K:302:HOH:O	2.14	0.66
1:U:2:GLU:OE2	3:U:304:HOH:O	2.12	0.66
1:l:41:ASP:OD2	1:m:5:PRO:HD3	1.95	0.66
1:N:2:GLU:N	3:N:304:HOH:O	2.27	0.66
1:T:12:GLU:OE2	3:T:302:HOH:O	2.13	0.66
1:P:95:ASP:OD2	3:P:302:HOH:O	2.13	0.66
1:H:34:MET:HE3	1:H:96:ALA:HB1	1.77	0.66
1:X:3:SER:HB3	1:X:5:PRO:HD2	1.75	0.66
1:D:5:PRO:HD3	1:E:41:ASP:OD2	1.94	0.66
1:b:141:ASP:OD1	3:b:303:HOH:O	2.14	0.66
1:S:168:SER:O	3:S:306:HOH:O	2.13	0.65
1:g:34:MET:HE2	1:g:52:PHE:CE1	2.32	0.65
1:s:12:GLU:OE2	3:s:301:HOH:O	2.14	0.65
1:N:95:ASP:OD1	3:N:302:HOH:O	2.15	0.65
1:R:88:ASP:O	3:R:307:HOH:O	2.15	0.65
1:S:147:ASP:OD2	3:S:307:HOH:O	2.14	0.65
1:c:85:PRO:HG2	3:c:328:HOH:O	1.95	0.65
1:h:2:GLU:N	3:h:307:HOH:O	2.30	0.65
1:u:64:GLU:OE1	1:x:53:LYS:HE2	1.97	0.65
1:a:34:MET:HE3	1:a:96:ALA:HB1	1.79	0.65
1:U:153:LYS:NZ	3:U:301:HOH:O	1.89	0.64
1:o:87:ARG:NH2	3:o:306:HOH:O	2.18	0.64
1:v:64:GLU:OE1	3:v:301:HOH:O	2.14	0.64
1:W:109:GLN:NE2	3:W:303:HOH:O	2.23	0.64
1:J:78:VAL:O	3:J:302:HOH:O	2.15	0.64
1:t:2:GLU:O	3:t:304:HOH:O	2.15	0.64
1:C:123:ASP:OD1	3:C:304:HOH:O	2.15	0.64
1:K:94:LEU:O	1:K:98:GLN:HG2	1.98	0.63
1:F:36:PHE:CD2	1:L:67:MET:HE3	2.32	0.63
1:H:80:GLN:NE2	3:H:303:HOH:O	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:5:PRO:HD3	1:U:41:ASP:OD2	1.98	0.63
1:P:137:GLU:OE2	3:P:303:HOH:O	2.15	0.63
1:P:34:MET:HE3	1:P:96:ALA:HB1	1.81	0.63
1:b:37:TYR:CE1	1:b:89:GLU:HB2	2.34	0.63
1:A:124:LYS:HA	1:A:127:MET:HE3	1.80	0.63
1:O:128:ASP:HA	1:O:131:GLU:HG2	1.81	0.63
1:i:55:LYS:NZ	1:i:141:ASP:OD1	2.31	0.63
1:g:153:LYS:NZ	3:g:303:HOH:O	2.26	0.62
1:j:85:PRO:HG2	3:j:347:HOH:O	1.97	0.62
1:j:124:LYS:HA	1:j:127:MET:HE3	1.81	0.62
1:q:156:GLY:O	3:q:302:HOH:O	2.15	0.62
1:u:87:ARG:NH1	3:u:302:HOH:O	2.16	0.62
1:x:120:LYS:NZ	3:x:302:HOH:O	2.13	0.62
1:L:121:HIS:O	3:L:302:HOH:O	2.16	0.62
1:u:3:SER:HB3	1:u:5:PRO:HD2	1.80	0.62
1:u:82:VAL:HG13	1:x:82:VAL:HG13	1.81	0.62
1:S:3:SER:HB3	1:S:5:PRO:HD2	1.81	0.62
1:v:2:GLU:N	3:v:304:HOH:O	2.33	0.62
1:e:65:LYS:NZ	3:e:309:HOH:O	2.33	0.62
1:f:85:PRO:HG2	3:f:336:HOH:O	1.99	0.62
1:f:153:LYS:NZ	3:f:302:HOH:O	2.04	0.62
1:w:50:LYS:O	1:w:54:GLU:HG3	1.99	0.62
1:H:2:GLU:N	3:H:314:HOH:O	2.33	0.62
1:K:51:TYR:CZ	1:K:55:LYS:HD2	2.35	0.62
1:R:85:PRO:HG2	3:R:352:HOH:O	1.99	0.62
1:h:10:HIS:CD2	1:h:12:GLU:H	2.13	0.62
1:q:85:PRO:HG2	3:q:332:HOH:O	1.99	0.61
1:w:131:GLU:O	3:w:307:HOH:O	2.16	0.61
1:P:81:ASP:HB2	3:P:393:HOH:O	1.99	0.61
1:b:2:GLU:N	3:b:307:HOH:O	2.33	0.61
1:C:5:PRO:HD3	1:Q:41:ASP:OD2	2.00	0.61
1:k:37:TYR:CE1	1:k:89:GLU:HB2	2.36	0.61
1:m:85:PRO:HG2	3:m:322:HOH:O	2.01	0.61
1:q:77:ILE:O	3:q:303:HOH:O	2.16	0.61
1:H:2:GLU:OE2	3:H:304:HOH:O	2.16	0.61
1:a:75:GLY:O	1:a:76:ARG:NH1	2.34	0.61
1:g:85:PRO:HG2	3:g:367:HOH:O	2.01	0.61
1:Z:34:MET:HE3	1:Z:96:ALA:HB1	1.83	0.61
1:g:83:LYS:NZ	3:g:307:HOH:O	2.33	0.60
1:j:34:MET:HE3	1:j:96:ALA:HB1	1.83	0.60
1:Z:105:LYS:NZ	3:Z:311:HOH:O	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:34:MET:HE2	1:L:96:ALA:HB1	1.83	0.60
1:W:2:GLU:OE1	3:W:301:HOH:O	2.16	0.60
1:o:2:GLU:OE2	3:o:305:HOH:O	2.17	0.60
1:w:132:SER:OG	3:w:306:HOH:O	2.16	0.60
1:m:53:LYS:NZ	1:m:57:ASP:OD1	2.34	0.60
1:H:94:LEU:O	1:H:98:GLN:HG2	2.02	0.60
1:L:85:PRO:HG2	3:L:355:HOH:O	2.01	0.60
1:M:63:ALA:O	1:M:67:MET:HG3	2.01	0.60
1:I:141:ASP:HA	1:I:144:LYS:HE3	1.82	0.60
1:f:82:VAL:HG13	1:j:82:VAL:HG13	1.84	0.60
1:t:127:MET:O	1:t:131:GLU:HG3	2.02	0.60
1:f:53:LYS:HE2	1:j:64:GLU:OE1	2.01	0.60
1:h:41:ASP:OD2	1:n:5:PRO:HD3	2.02	0.60
1:L:30:CYS:O	1:L:34:MET:HG3	2.02	0.60
1:O:19:ARG:HD3	1:O:19:ARG:C	2.27	0.59
1:B:3:SER:HB3	1:B:5:PRO:HD2	1.83	0.59
1:P:2:GLU:N	3:P:310:HOH:O	2.35	0.59
1:Z:58:GLU:OE1	3:Z:304:HOH:O	2.16	0.59
1:E:94:LEU:O	1:E:98:GLN:HG2	2.02	0.59
1:V:37:TYR:CE1	1:V:89:GLU:HB2	2.37	0.59
1:V:51:TYR:CZ	1:V:55:LYS:HD2	2.37	0.59
1:C:82:VAL:HG13	1:Q:82:VAL:HG13	1.83	0.59
1:C:3:SER:HB3	1:C:5:PRO:HD2	1.84	0.59
1:f:109:GLN:NE2	3:f:305:HOH:O	2.26	0.59
1:v:3:SER:HB3	1:v:5:PRO:HD2	1.85	0.59
1:a:85:PRO:HG2	3:a:363:HOH:O	2.01	0.59
1:d:51:TYR:CZ	1:d:55:LYS:HD2	2.37	0.59
1:w:124:LYS:HA	1:w:127:MET:HE3	1.85	0.59
1:F:34:MET:HE3	1:F:96:ALA:HB1	1.83	0.59
1:r:95:ASP:OD1	3:r:304:HOH:O	2.17	0.59
1:k:2:GLU:N	3:k:306:HOH:O	2.36	0.58
1:i:87:ARG:NH2	3:i:313:HOH:O	2.35	0.58
1:c:2:GLU:N	3:c:308:HOH:O	2.36	0.58
1:f:94:LEU:O	1:f:98:GLN:HG2	2.03	0.58
1:K:31:TYR:CZ	1:K:55:LYS:HE3	2.39	0.58
1:c:31:TYR:CZ	1:c:55:LYS:HE3	2.38	0.58
1:H:55:LYS:NZ	1:H:141:ASP:OD2	2.36	0.58
1:H:88:ASP:OD2	3:H:305:HOH:O	2.17	0.58
1:P:63:ALA:O	1:P:67:MET:HG3	2.03	0.58
1:B:85:PRO:HG2	3:B:315:HOH:O	2.02	0.58
1:B:124:LYS:HA	1:B:127:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:LEU:O	1:J:98:GLN:HG2	2.04	0.58
1:A:3:SER:HB3	1:A:5:PRO:HD2	1.85	0.58
1:B:34:MET:HE3	1:B:96:ALA:HB1	1.86	0.58
1:r:94:LEU:O	1:r:98:GLN:HG2	2.03	0.58
1:F:53:LYS:HE2	1:L:64:GLU:OE2	2.03	0.57
1:f:34:MET:CE	1:f:96:ALA:HB1	2.35	0.57
1:T:109:GLN:OE1	3:T:303:HOH:O	2.17	0.57
1:d:3:SER:HB3	1:d:5:PRO:HD2	1.86	0.57
1:m:19:ARG:O	3:m:304:HOH:O	2.17	0.57
1:H:4:GLN:HG3	3:H:302:HOH:O	2.04	0.57
1:h:34:MET:CE	1:h:96:ALA:HB1	2.34	0.57
1:x:165:ASP:OD2	1:x:166:LYS:NZ	2.36	0.57
1:F:37:TYR:CE1	1:F:89:GLU:HB2	2.40	0.57
1:A:37:TYR:CE1	1:A:89:GLU:HB2	2.39	0.57
1:O:19:ARG:HH12	1:O:110:ALA:HB1	1.70	0.57
1:x:34:MET:CE	1:x:96:ALA:HB1	2.34	0.57
1:C:85:PRO:HG2	3:C:362:HOH:O	2.05	0.57
1:o:94:LEU:O	1:o:98:GLN:HG2	2.05	0.57
1:T:2:GLU:N	3:T:309:HOH:O	2.38	0.57
1:j:144:LYS:NZ	3:j:303:HOH:O	2.20	0.56
1:l:53:LYS:HE2	1:m:64:GLU:OE1	2.05	0.56
1:X:131:GLU:HA	1:X:135:LEU:HD12	1.85	0.56
1:l:157:SER:O	3:l:305:HOH:O	2.18	0.56
1:E:145:ILE:O	1:E:149:ILE:HG12	2.06	0.56
1:f:19:ARG:HG3	3:f:392:HOH:O	2.04	0.56
1:g:98:GLN:HG3	3:g:328:HOH:O	2.04	0.56
1:k:57:ASP:O	1:k:61:GLU:HG3	2.05	0.56
1:X:37:TYR:CE1	1:X:89:GLU:HB2	2.40	0.56
1:x:94:LEU:O	1:x:98:GLN:HG2	2.05	0.56
1:B:50:LYS:NZ	3:B:317:HOH:O	2.38	0.56
1:F:124:LYS:HA	1:F:127:MET:HE3	1.88	0.56
1:u:37:TYR:CE1	1:u:89:GLU:HB2	2.40	0.56
1:g:34:MET:HE2	1:g:52:PHE:CZ	2.41	0.56
1:B:2:GLU:N	3:B:318:HOH:O	2.39	0.56
1:V:72:LYS:NZ	3:V:306:HOH:O	2.17	0.56
1:w:53:LYS:NZ	1:w:57:ASP:OD1	2.38	0.56
1:N:53:LYS:NZ	1:N:57:ASP:OD1	2.39	0.56
1:u:94:LEU:O	1:u:98:GLN:HG2	2.05	0.56
1:V:94:LEU:O	1:V:98:GLN:HG2	2.06	0.56
1:P:106:ASN:ND2	3:P:311:HOH:O	2.35	0.56
1:n:55:LYS:HE3	1:n:141:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:94:LEU:O	1:U:98:GLN:HG2	2.06	0.55
1:K:4:GLN:NE2	3:K:301:HOH:O	2.12	0.55
1:b:51:TYR:CZ	1:b:55:LYS:HD2	2.41	0.55
1:r:34:MET:HE2	1:r:52:PHE:CE1	2.41	0.55
1:C:34:MET:HE3	1:C:96:ALA:HB1	1.88	0.55
1:a:51:TYR:CZ	1:a:55:LYS:HD2	2.41	0.55
1:o:3:SER:HB3	1:o:5:PRO:HD2	1.88	0.55
1:v:94:LEU:O	1:v:98:GLN:HG2	2.07	0.55
1:N:41:ASP:OD2	1:r:5:PRO:HD3	2.07	0.55
1:p:19:ARG:HG3	1:p:20:GLN:N	2.20	0.55
1:A:50:LYS:NZ	3:A:309:HOH:O	2.39	0.55
1:v:115:HIS:CE1	1:v:127:MET:HE3	2.41	0.55
1:P:77:ILE:O	3:P:304:HOH:O	2.18	0.55
1:Q:53:LYS:NZ	1:Q:57:ASP:OD1	2.38	0.55
1:I:31:TYR:OH	1:I:104:GLU:OE2	2.16	0.55
1:H:34:MET:CE	1:H:96:ALA:HB1	2.37	0.55
1:a:94:LEU:O	1:a:98:GLN:HG2	2.07	0.55
1:R:3:SER:HB3	1:R:5:PRO:HD2	1.89	0.55
1:Z:120:LYS:NZ	3:Z:313:HOH:O	2.39	0.55
1:F:51:TYR:CZ	1:F:55:LYS:HD2	2.42	0.55
1:H:51:TYR:CZ	1:H:55:LYS:HD2	2.43	0.55
1:W:31:TYR:CZ	1:W:55:LYS:HE3	2.42	0.55
1:h:37:TYR:CE1	1:h:89:GLU:HB2	2.42	0.54
1:k:34:MET:CE	1:k:96:ALA:HB1	2.37	0.54
1:E:28:CYS:HB2	1:E:59:GLU:HB2	1.89	0.54
1:p:72:LYS:NZ	3:p:308:HOH:O	2.27	0.54
1:M:34:MET:CE	1:M:96:ALA:HB1	2.37	0.54
1:A:94:LEU:O	1:A:98:GLN:HG2	2.08	0.54
1:e:94:LEU:O	1:e:98:GLN:HG2	2.08	0.54
1:g:82:VAL:HG13	1:k:82:VAL:HG13	1.90	0.54
1:F:32:GLN:HG2	1:L:67:MET:HE1	1.89	0.54
3:c:358:HOH:O	1:q:53:LYS:HD3	2.08	0.54
1:k:30:CYS:O	1:k:34:MET:HG3	2.08	0.54
1:F:30:CYS:SG	1:F:85:PRO:HB3	2.48	0.54
1:N:37:TYR:CE1	1:N:89:GLU:HB3	2.42	0.54
1:D:72:LYS:NZ	3:D:311:HOH:O	2.34	0.54
1:M:30:CYS:SG	1:M:85:PRO:HB3	2.48	0.54
1:k:2:GLU:N	3:k:310:HOH:O	2.41	0.54
1:B:30:CYS:O	1:B:34:MET:HG3	2.08	0.54
1:X:76:ARG:HA	3:X:323:HOH:O	2.07	0.54
1:t:63:ALA:O	1:t:67:MET:HG3	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:50:LYS:O	1:i:54:GLU:HG3	2.08	0.54
1:i:165:ASP:OD2	1:i:166:LYS:NZ	2.40	0.54
1:i:153:LYS:NZ	3:i:302:HOH:O	1.91	0.54
1:L:94:LEU:O	1:L:98:GLN:HG2	2.08	0.54
1:t:94:LEU:O	1:t:98:GLN:HG2	2.08	0.54
1:o:37:TYR:CE1	1:o:89:GLU:HB2	2.43	0.54
1:t:34:MET:CE	1:t:96:ALA:HB1	2.38	0.54
1:Z:37:TYR:CE1	1:Z:89:GLU:HB2	2.43	0.53
1:q:53:LYS:NZ	1:q:57:ASP:OD1	2.41	0.53
1:s:82:VAL:HG13	1:v:82:VAL:HG13	1.90	0.53
1:b:34:MET:CE	1:b:96:ALA:HB1	2.36	0.53
1:d:94:LEU:O	1:d:98:GLN:HG2	2.08	0.53
1:i:53:LYS:HE2	1:o:64:GLU:OE1	2.08	0.53
1:p:53:LYS:NZ	1:p:57:ASP:OD1	2.41	0.53
1:p:94:LEU:O	1:p:98:GLN:HG2	2.08	0.53
1:c:51:TYR:CZ	1:c:55:LYS:HD2	2.43	0.53
1:T:124:LYS:HA	1:T:127:MET:HE3	1.91	0.53
1:h:29:TYR:CE2	1:n:79:LEU:HD13	2.39	0.53
1:Q:31:TYR:CZ	1:Q:55:LYS:HE3	2.44	0.53
1:o:89:GLU:OE1	3:o:306:HOH:O	2.18	0.53
1:w:153:LYS:NZ	3:w:301:HOH:O	1.83	0.53
1:n:53:LYS:NZ	1:n:57:ASP:OD1	2.41	0.53
1:x:85:PRO:HG2	3:x:356:HOH:O	2.07	0.53
1:O:161:GLU:OE2	3:O:303:HOH:O	2.18	0.53
1:g:34:MET:HE3	1:g:96:ALA:HB1	1.90	0.53
1:m:12:GLU:OE1	1:m:121:HIS:NE2	2.32	0.53
1:D:53:LYS:NZ	1:D:57:ASP:OD1	2.42	0.53
1:u:30:CYS:O	1:u:34:MET:HG3	2.08	0.53
1:C:53:LYS:NZ	1:C:57:ASP:OD1	2.42	0.53
1:Q:30:CYS:SG	1:Q:85:PRO:HB3	2.49	0.53
1:P:145:ILE:O	1:P:149:ILE:HG12	2.08	0.53
1:t:30:CYS:O	1:t:34:MET:HG3	2.08	0.53
1:B:11:VAL:HG22	3:B:337:HOH:O	2.08	0.52
1:H:14:GLU:OE2	3:H:306:HOH:O	2.18	0.52
1:X:38:PHE:HA	1:X:43:VAL:HG11	1.90	0.52
1:I:94:LEU:O	1:I:98:GLN:HG2	2.10	0.52
1:C:82:VAL:HG13	1:Q:82:VAL:CG1	2.39	0.52
1:U:30:CYS:SG	1:U:85:PRO:HB3	2.49	0.52
1:P:30:CYS:SG	1:P:85:PRO:HB3	2.49	0.52
1:a:12:GLU:OE2	3:a:303:HOH:O	2.19	0.52
1:a:67:MET:HB3	1:a:77:ILE:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:j:31:TYR:CZ	1:j:55:LYS:HE3	2.44	0.52
1:F:94:LEU:O	1:F:98:GLN:HG2	2.08	0.52
1:W:82:VAL:HG13	1:b:82:VAL:HG13	1.92	0.52
1:a:53:LYS:HE2	1:e:64:GLU:OE1	2.09	0.52
1:L:2:GLU:N	3:L:314:HOH:O	2.42	0.52
1:V:123:ASP:O	1:V:127:MET:HG3	2.09	0.52
1:e:145:ILE:O	1:e:149:ILE:HG12	2.10	0.52
1:k:141:ASP:OD1	3:k:301:HOH:O	2.19	0.52
1:l:82:VAL:HG13	1:m:82:VAL:HG13	1.90	0.52
1:w:94:LEU:O	1:w:98:GLN:HG2	2.09	0.52
1:R:54:GLU:CG	3:R:308:HOH:O	2.57	0.52
1:h:3:SER:HB3	1:h:5:PRO:HD2	1.91	0.52
1:I:145:ILE:O	1:I:149:ILE:HG12	2.10	0.52
1:d:75:GLY:O	1:d:76:ARG:NH1	2.43	0.52
1:K:161:GLU:OE2	3:K:303:HOH:O	2.19	0.52
1:N:53:LYS:HE2	1:r:64:GLU:OE1	2.09	0.52
1:A:34:MET:CE	1:A:96:ALA:HB1	2.40	0.52
1:k:30:CYS:SG	1:k:85:PRO:HB3	2.49	0.52
1:m:87:ARG:HH11	1:m:87:ARG:HG2	1.74	0.52
1:A:95:ASP:OD1	3:A:303:HOH:O	2.18	0.52
1:o:53:LYS:NZ	1:o:57:ASP:OD1	2.42	0.52
1:q:30:CYS:SG	1:q:85:PRO:HB3	2.50	0.52
1:F:64:GLU:OE1	1:L:53:LYS:HE2	2.10	0.52
1:H:53:LYS:NZ	1:H:57:ASP:OD1	2.43	0.52
1:R:94:LEU:O	1:R:98:GLN:HG2	2.10	0.52
1:w:37:TYR:CE1	1:w:89:GLU:HB2	2.44	0.52
1:v:37:TYR:CE1	1:v:89:GLU:HB2	2.44	0.52
1:N:82:VAL:HG13	1:r:82:VAL:HG13	1.91	0.52
1:Z:2:GLU:N	3:Z:317:HOH:O	2.43	0.52
1:r:55:LYS:NZ	1:r:141:ASP:OD2	2.43	0.52
1:S:28:CYS:HB2	1:S:59:GLU:HB2	1.91	0.52
1:f:53:LYS:NZ	1:f:57:ASP:OD1	2.43	0.52
1:i:115:HIS:CE1	1:i:127:MET:HE3	2.45	0.51
1:L:123:ASP:OD1	3:L:303:HOH:O	2.19	0.51
1:R:6:ARG:HD2	3:R:330:HOH:O	2.09	0.51
1:Q:63:ALA:O	1:Q:67:MET:HG3	2.10	0.51
1:w:34:MET:HE2	1:w:96:ALA:HB1	1.93	0.51
1:B:4:GLN:HB2	1:B:5:PRO:HD3	1.92	0.51
1:P:37:TYR:CE1	1:P:89:GLU:HB2	2.45	0.51
1:C:51:TYR:CZ	1:C:55:LYS:HD2	2.46	0.51
1:C:82:VAL:CG1	1:Q:82:VAL:HG13	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:m:55:LYS:NZ	1:m:141:ASP:OD2	2.43	0.51
1:J:53:LYS:NZ	1:J:57:ASP:OD1	2.42	0.51
1:I:82:VAL:CG1	1:O:82:VAL:HG13	2.39	0.51
1:X:105:LYS:NZ	1:t:4:GLN:O	2.43	0.51
1:K:82:VAL:HG13	1:t:82:VAL:CG1	2.40	0.51
1:T:10:HIS:CE1	1:T:12:GLU:HG3	2.45	0.51
1:Z:85:PRO:HG2	3:Z:358:HOH:O	2.09	0.51
1:h:4:GLN:HG3	3:n:347:HOH:O	2.10	0.51
1:V:77:ILE:O	3:V:307:HOH:O	2.19	0.51
1:j:94:LEU:O	1:j:98:GLN:HG2	2.11	0.51
1:Z:34:MET:CE	1:Z:96:ALA:HB1	2.40	0.51
1:x:37:TYR:CE1	1:x:89:GLU:HB2	2.46	0.51
1:v:34:MET:HE3	1:v:96:ALA:HB1	1.92	0.51
1:B:53:LYS:HE2	1:P:64:GLU:OE1	2.10	0.51
1:J:67:MET:HB3	1:J:77:ILE:HD13	1.93	0.51
1:T:34:MET:CE	1:T:96:ALA:HB1	2.40	0.51
1:S:82:VAL:HG13	1:w:82:VAL:CG1	2.41	0.51
1:a:34:MET:CE	1:a:96:ALA:HB1	2.41	0.51
1:c:37:TYR:CE1	1:c:89:GLU:HB2	2.45	0.51
1:g:53:LYS:NZ	1:g:57:ASP:OD1	2.44	0.51
1:i:37:TYR:CE1	1:i:89:GLU:HB2	2.46	0.51
1:F:89:GLU:OE1	1:F:91:GLY:N	2.40	0.51
1:L:14:GLU:OE2	3:L:304:HOH:O	2.20	0.51
1:M:167:LYS:O	1:p:166:LYS:NZ	2.44	0.51
1:r:53:LYS:NZ	1:r:57:ASP:OD1	2.42	0.51
1:S:51:TYR:CZ	1:S:55:LYS:HD2	2.45	0.51
1:e:34:MET:HE3	1:e:96:ALA:HB1	1.93	0.51
1:f:82:VAL:CG1	1:j:82:VAL:HG13	2.41	0.51
1:w:145:ILE:O	1:w:149:ILE:HG12	2.11	0.51
1:w:157:SER:O	3:w:308:HOH:O	2.19	0.51
1:v:34:MET:CE	1:v:96:ALA:HB1	2.40	0.51
1:X:53:LYS:NZ	1:X:57:ASP:OD1	2.44	0.51
1:Z:31:TYR:CZ	1:Z:55:LYS:HE3	2.46	0.51
1:m:51:TYR:CZ	1:m:55:LYS:HD2	2.46	0.50
1:M:81:ASP:O	3:M:307:HOH:O	2.19	0.50
1:a:124:LYS:HE2	3:w:302:HOH:O	2.11	0.50
1:k:51:TYR:CZ	1:k:55:LYS:HD2	2.47	0.50
1:l:82:VAL:HG13	1:m:82:VAL:CG1	2.41	0.50
1:M:94:LEU:O	1:M:98:GLN:HG2	2.11	0.50
1:R:162:TYR:HH	1:t:168:SER:HG	1.56	0.50
1:V:53:LYS:NZ	1:V:57:ASP:OD2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:85:PRO:HG2	3:e:337:HOH:O	2.12	0.50
1:i:2:GLU:N	3:i:322:HOH:O	2.43	0.50
1:F:82:VAL:HG13	1:L:82:VAL:HG13	1.92	0.50
1:I:51:TYR:CZ	1:I:55:LYS:HD2	2.46	0.50
1:d:34:MET:CE	1:d:96:ALA:HB1	2.41	0.50
1:i:5:PRO:O	3:i:303:HOH:O	2.20	0.50
1:F:63:ALA:O	1:F:67:MET:HG3	2.11	0.50
1:u:63:ALA:O	1:u:67:MET:HG3	2.10	0.50
1:A:53:LYS:NZ	1:A:57:ASP:OD1	2.45	0.50
1:K:82:VAL:CG1	1:t:82:VAL:HG13	2.42	0.50
1:K:166:LYS:HD2	1:K:166:LYS:N	2.25	0.50
1:X:103:LEU:O	1:X:107:VAL:HG23	2.11	0.50
1:p:89:GLU:OE1	1:p:90:TRP:N	2.45	0.50
1:c:53:LYS:NZ	1:c:57:ASP:OD1	2.45	0.50
3:l:334:HOH:O	1:m:4:GLN:HG3	2.11	0.50
1:T:63:ALA:O	1:T:67:MET:HG3	2.11	0.50
1:W:12:GLU:CG	3:W:312:HOH:O	2.60	0.50
1:d:117:VAL:O	1:d:120:LYS:HG2	2.11	0.49
1:j:63:ALA:O	1:j:67:MET:HG3	2.12	0.49
1:T:55:LYS:NZ	1:T:141:ASP:OD2	2.44	0.49
1:p:37:TYR:CE1	1:p:89:GLU:HB2	2.46	0.49
1:C:53:LYS:HE2	1:Q:64:GLU:OE1	2.13	0.49
1:k:4:GLN:HB2	1:k:5:PRO:HD3	1.94	0.49
1:w:55:LYS:NZ	1:w:141:ASP:OD2	2.41	0.49
1:K:51:TYR:CE2	1:K:55:LYS:HD2	2.47	0.49
1:S:98:GLN:HB3	1:S:149:ILE:HD12	1.94	0.49
1:c:41:ASP:OD2	1:q:5:PRO:HD3	2.11	0.49
1:c:145:ILE:O	1:c:149:ILE:HG12	2.12	0.49
1:j:53:LYS:NZ	1:j:57:ASP:OD1	2.44	0.49
1:m:98:GLN:HG3	3:m:389:HOH:O	2.12	0.49
1:M:30:CYS:O	1:M:34:MET:HG3	2.13	0.49
1:h:94:LEU:O	1:h:98:GLN:HG2	2.12	0.49
1:v:85:PRO:HG2	3:v:326:HOH:O	2.12	0.49
1:M:82:VAL:HG13	1:R:82:VAL:CG1	2.42	0.49
1:A:81:ASP:OD1	1:d:83:LYS:HD2	2.13	0.49
1:H:84:LYS:NZ	3:H:320:HOH:O	2.46	0.49
1:A:29:TYR:CE2	1:A:84:LYS:HA	2.48	0.49
1:g:145:ILE:O	1:g:149:ILE:HG12	2.13	0.49
1:b:75:GLY:O	1:b:76:ARG:NH1	2.46	0.49
1:K:75:GLY:O	1:K:76:ARG:NH1	2.44	0.49
1:M:64:GLU:OE1	1:R:53:LYS:HE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:r:119:ASP:OD2	3:r:305:HOH:O	2.20	0.49
1:I:30:CYS:SG	1:I:85:PRO:HB3	2.53	0.49
1:Q:51:TYR:CZ	1:Q:55:LYS:HD2	2.47	0.49
1:f:37:TYR:CE1	1:f:89:GLU:HB2	2.48	0.48
1:m:94:LEU:O	1:m:98:GLN:HG2	2.13	0.48
1:w:34:MET:CE	1:w:96:ALA:HB1	2.43	0.48
1:H:40:ARG:HH11	1:H:42:ASP:CG	2.20	0.48
1:N:82:VAL:HG13	1:r:82:VAL:CG1	2.42	0.48
1:R:20:GLN:O	1:R:24:GLU:HG2	2.12	0.48
1:R:31:TYR:OH	1:R:104:GLU:OE2	2.26	0.48
1:h:19:ARG:NE	3:h:314:HOH:O	2.42	0.48
1:f:55:LYS:NZ	1:f:141:ASP:OD2	2.47	0.48
1:B:34:MET:CE	1:B:96:ALA:HB1	2.43	0.48
1:D:115:HIS:CE1	1:D:127:MET:HE3	2.48	0.48
1:F:82:VAL:HG13	1:L:82:VAL:CG1	2.44	0.48
1:u:34:MET:CE	1:u:96:ALA:HB1	2.44	0.48
1:M:37:TYR:CE1	1:M:89:GLU:HB2	2.48	0.48
1:M:145:ILE:O	1:M:149:ILE:HG12	2.13	0.48
1:N:85:PRO:HG2	3:N:311:HOH:O	2.13	0.48
1:T:131:GLU:HA	1:T:135:LEU:HB2	1.95	0.48
1:W:53:LYS:NZ	1:W:57:ASP:OD1	2.46	0.48
1:A:82:VAL:CG1	1:d:82:VAL:HG13	2.44	0.48
1:A:82:VAL:HG13	1:d:82:VAL:HG13	1.96	0.48
1:e:31:TYR:CZ	1:e:55:LYS:HE3	2.48	0.48
1:F:55:LYS:NZ	1:F:141:ASP:OD1	2.44	0.48
1:c:91:GLY:O	3:c:304:HOH:O	2.20	0.48
1:s:34:MET:HE2	1:s:52:PHE:CZ	2.48	0.48
1:D:37:TYR:CE1	1:D:89:GLU:HB2	2.48	0.48
1:D:115:HIS:HE1	1:D:127:MET:HE3	1.79	0.48
1:h:30:CYS:O	1:h:34:MET:HG3	2.14	0.48
1:I:124:LYS:HA	1:I:127:MET:HE3	1.95	0.48
1:a:30:CYS:O	1:a:34:MET:HG3	2.13	0.48
1:M:53:LYS:HE2	1:R:64:GLU:OE1	2.13	0.48
1:S:147:ASP:OD1	1:Q:41:ASP:HA	2.14	0.48
1:a:37:TYR:CE1	1:a:89:GLU:HB2	2.48	0.48
1:i:51:TYR:CZ	1:i:55:LYS:HD2	2.49	0.48
1:s:34:MET:CE	1:s:96:ALA:HB1	2.42	0.48
1:s:144:LYS:HD2	1:s:144:LYS:HA	1.60	0.48
1:F:82:VAL:HA	3:F:313:HOH:O	2.13	0.48
1:J:37:TYR:CE1	1:J:89:GLU:HB2	2.49	0.48
1:E:67:MET:HB3	1:E:77:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:72:LYS:NZ	1:t:140:GLU:OE1	2.27	0.48
1:X:63:ALA:O	1:X:67:MET:HG3	2.14	0.48
1:s:82:VAL:HG13	1:v:82:VAL:CG1	2.44	0.47
1:R:55:LYS:HE2	1:R:141:ASP:OD2	2.14	0.47
1:W:53:LYS:HE2	1:b:64:GLU:OE1	2.13	0.47
1:W:82:VAL:CG1	1:b:82:VAL:HG13	2.44	0.47
1:h:97:MET:HG3	1:h:145:ILE:HG23	1.96	0.47
1:r:34:MET:HE2	1:r:52:PHE:CZ	2.49	0.47
1:A:53:LYS:HE2	1:d:64:GLU:OE1	2.13	0.47
1:g:31:TYR:CZ	1:g:55:LYS:HE3	2.49	0.47
1:v:53:LYS:NZ	1:v:57:ASP:OD1	2.46	0.47
1:L:156:GLY:O	3:L:305:HOH:O	2.20	0.47
1:Z:4:GLN:HB2	1:Z:5:PRO:HD3	1.94	0.47
1:u:82:VAL:CG1	1:x:82:VAL:HG13	2.44	0.47
1:a:64:GLU:OE1	1:e:53:LYS:HE2	2.14	0.47
1:l:82:VAL:CG1	1:m:82:VAL:HG13	2.44	0.47
1:o:55:LYS:NZ	1:o:141:ASP:OD2	2.44	0.47
1:w:16:GLY:HA2	1:w:19:ARG:CZ	2.45	0.47
1:H:53:LYS:HE2	1:J:64:GLU:OE1	2.14	0.47
1:H:166:LYS:NZ	3:H:308:HOH:O	2.21	0.47
1:h:34:MET:HE3	1:h:96:ALA:HB1	1.96	0.47
1:p:50:LYS:O	1:p:54:GLU:HG3	2.14	0.47
1:U:85:PRO:HG2	3:U:323:HOH:O	2.14	0.47
1:U:145:ILE:O	1:U:149:ILE:HG12	2.13	0.47
1:r:155:VAL:O	3:r:306:HOH:O	2.20	0.47
1:U:63:ALA:O	1:U:67:MET:HG3	2.14	0.47
1:w:51:TYR:CZ	1:w:55:LYS:HD2	2.49	0.47
1:N:55:LYS:HB3	1:N:55:LYS:HE3	1.72	0.47
1:S:64:GLU:OE1	1:w:53:LYS:HE2	2.15	0.47
1:d:55:LYS:NZ	1:d:141:ASP:OD2	2.47	0.47
1:B:2:GLU:CD	3:B:303:HOH:O	2.53	0.47
1:N:87:ARG:HD2	1:N:90:TRP:CZ3	2.49	0.47
1:P:140:GLU:OE1	1:h:72:LYS:NZ	2.38	0.47
1:I:82:VAL:HG13	1:O:82:VAL:CG1	2.43	0.47
1:C:145:ILE:O	1:C:149:ILE:HG12	2.13	0.47
1:v:55:LYS:NZ	1:v:141:ASP:OD2	2.47	0.47
1:H:60:ARG:NH2	1:J:57:ASP:OD1	2.43	0.47
1:R:4:GLN:HB2	1:R:5:PRO:HD3	1.97	0.47
1:T:53:LYS:NZ	1:T:57:ASP:OD1	2.45	0.47
1:u:82:VAL:HG13	1:x:82:VAL:CG1	2.44	0.47
1:U:15:ALA:O	1:U:19:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:q:51:TYR:CZ	1:q:55:LYS:HD2	2.50	0.47
1:L:37:TYR:CE1	1:L:89:GLU:HG2	2.50	0.47
1:d:145:ILE:O	1:d:149:ILE:HG12	2.14	0.47
1:D:140:GLU:OE1	1:x:72:LYS:NZ	2.43	0.47
1:H:124:LYS:HA	1:H:127:MET:HE3	1.96	0.47
3:K:325:HOH:O	1:t:3:SER:HA	2.14	0.47
1:O:4:GLN:HB2	1:O:5:PRO:HD3	1.95	0.47
1:a:51:TYR:CE2	1:a:55:LYS:HD2	2.50	0.47
1:f:31:TYR:CZ	1:f:55:LYS:HE3	2.50	0.47
1:s:145:ILE:O	1:s:149:ILE:HG12	2.15	0.47
1:N:124:LYS:HA	1:N:127:MET:HE3	1.96	0.47
1:W:2:GLU:OE2	3:W:302:HOH:O	2.20	0.47
1:h:53:LYS:NZ	1:h:57:ASP:OD1	2.48	0.47
1:I:34:MET:CE	1:I:96:ALA:HB1	2.43	0.46
1:g:2:GLU:N	3:g:314:HOH:O	2.47	0.46
1:l:159:LEU:O	1:l:163:MET:HG2	2.14	0.46
1:E:53:LYS:NZ	1:E:57:ASP:CG	2.73	0.46
1:t:37:TYR:CE1	1:t:89:GLU:HB2	2.50	0.46
1:O:51:TYR:OH	3:O:301:HOH:O	2.05	0.46
1:A:104:GLU:HG3	1:A:145:ILE:CD1	2.46	0.46
1:C:131:GLU:OE2	3:C:305:HOH:O	2.20	0.46
1:k:124:LYS:HA	1:k:127:MET:HE3	1.97	0.46
1:B:145:ILE:O	1:B:149:ILE:HG12	2.16	0.46
1:E:34:MET:HE3	1:E:96:ALA:HB1	1.97	0.46
1:L:51:TYR:CE2	1:L:55:LYS:HD2	2.50	0.46
1:M:29:TYR:CE2	1:M:84:LYS:HA	2.50	0.46
1:R:34:MET:CE	1:R:96:ALA:HB1	2.45	0.46
1:n:37:TYR:CE2	1:n:89:GLU:HB2	2.50	0.46
1:I:50:LYS:HB3	1:I:50:LYS:HE3	1.69	0.46
1:O:53:LYS:NZ	1:O:57:ASP:OD1	2.48	0.46
1:V:145:ILE:O	1:V:149:ILE:HG12	2.16	0.46
1:A:51:TYR:CZ	1:A:55:LYS:HD2	2.51	0.46
1:A:82:VAL:HG13	1:d:82:VAL:CG1	2.45	0.46
1:l:94:LEU:HA	1:l:152:LEU:HD13	1.97	0.46
1:b:89:GLU:OE1	1:b:91:GLY:N	2.47	0.46
1:u:35:SER:O	1:u:49:THR:HG23	2.14	0.46
1:S:82:VAL:HG13	1:w:82:VAL:HG13	1.96	0.46
1:U:82:VAL:HA	3:U:335:HOH:O	2.16	0.46
1:s:82:VAL:CG1	1:v:82:VAL:HG13	2.46	0.46
1:P:97:MET:HB3	1:P:149:ILE:HD13	1.98	0.46
1:F:11:VAL:HG23	3:F:402:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:ARG:O	1:H:64:GLU:HG3	2.16	0.46
1:x:106:ASN:ND2	3:x:318:HOH:O	2.47	0.46
1:a:19:ARG:NH2	3:a:305:HOH:O	2.27	0.46
1:c:64:GLU:OE1	1:q:53:LYS:HE2	2.14	0.46
1:e:30:CYS:SG	1:e:85:PRO:HB3	2.56	0.46
1:B:55:LYS:HB3	1:B:55:LYS:HE3	1.73	0.46
1:B:64:GLU:OE1	1:P:53:LYS:HE2	2.16	0.46
1:M:104:GLU:HG3	1:M:145:ILE:CD1	2.46	0.46
1:C:2:GLU:HG2	3:C:307:HOH:O	2.14	0.46
1:a:138:GLN:NE2	3:a:304:HOH:O	2.20	0.46
1:k:51:TYR:CE2	1:k:55:LYS:HD2	2.51	0.46
1:l:84:LYS:O	3:l:306:HOH:O	2.21	0.46
1:F:28:CYS:HB2	1:F:59:GLU:HB2	1.98	0.46
1:p:103:LEU:O	1:p:107:VAL:HG23	2.15	0.46
1:L:53:LYS:NZ	1:L:57:ASP:OD1	2.48	0.46
1:M:5:PRO:O	3:M:308:HOH:O	2.21	0.46
1:W:145:ILE:O	1:W:149:ILE:HG12	2.16	0.46
1:j:37:TYR:CE1	1:j:89:GLU:HB2	2.51	0.45
1:m:145:ILE:O	1:m:149:ILE:HG12	2.16	0.45
1:o:5:PRO:HG2	1:o:74:GLY:CA	2.46	0.45
1:o:18:ASN:HA	1:o:21:ILE:HD12	1.98	0.45
1:w:97:MET:HB3	1:w:149:ILE:HD13	1.98	0.45
1:J:18:ASN:HA	1:J:21:ILE:HD12	1.98	0.45
1:T:82:VAL:HG13	1:Z:82:VAL:HG13	1.98	0.45
1:h:19:ARG:HD2	3:h:314:HOH:O	2.17	0.45
1:e:29:TYR:CD2	1:e:85:PRO:HD3	2.51	0.45
1:B:25:LEU:O	1:B:28:CYS:HB3	2.16	0.45
1:R:30:CYS:O	1:R:34:MET:HG3	2.17	0.45
1:T:31:TYR:CZ	1:T:55:LYS:HE3	2.51	0.45
1:W:63:ALA:O	1:W:67:MET:HG3	2.16	0.45
1:w:11:VAL:HG13	3:w:350:HOH:O	2.15	0.45
1:D:79:LEU:O	1:E:84:LYS:HD2	2.15	0.45
1:T:104:GLU:HG3	1:T:145:ILE:CD1	2.47	0.45
1:X:18:ASN:HA	1:X:21:ILE:HD12	1.98	0.45
1:Z:63:ALA:O	1:Z:67:MET:HG3	2.16	0.45
1:b:34:MET:HE2	1:b:52:PHE:CZ	2.51	0.45
1:V:34:MET:CE	1:V:96:ALA:HB1	2.46	0.45
1:B:94:LEU:O	1:B:98:GLN:HG2	2.16	0.45
1:K:34:MET:O	1:K:38:PHE:HD2	1.98	0.45
1:T:64:GLU:OE1	1:Z:53:LYS:HE2	2.15	0.45
1:h:29:TYR:CD2	1:h:85:PRO:HD3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:p:88:ASP:O	3:p:306:HOH:O	2.21	0.45
1:U:94:LEU:HA	1:U:152:LEU:HD13	1.99	0.45
1:g:37:TYR:HA	3:g:441:HOH:O	2.15	0.45
1:j:51:TYR:CZ	1:j:55:LYS:HD2	2.51	0.45
1:q:124:LYS:HA	1:q:127:MET:HE3	1.98	0.45
1:w:31:TYR:CZ	1:w:55:LYS:HE3	2.52	0.45
1:P:60:ARG:O	1:P:64:GLU:HG3	2.17	0.45
1:b:53:LYS:NZ	1:b:57:ASP:OD1	2.48	0.45
1:g:82:VAL:HG13	1:k:82:VAL:CG1	2.46	0.45
1:R:54:GLU:HG2	3:R:308:HOH:O	2.17	0.45
1:n:24:GLU:HB2	1:n:63:ALA:HB2	1.99	0.45
1:p:127:MET:O	1:p:131:GLU:HG3	2.16	0.45
1:r:103:LEU:O	1:r:107:VAL:HG23	2.17	0.45
1:I:64:GLU:OE1	1:O:53:LYS:HE2	2.17	0.45
1:f:34:MET:HE2	1:f:96:ALA:HB1	1.97	0.45
1:l:51:TYR:CZ	1:l:55:LYS:HD2	2.52	0.45
1:w:109:GLN:NE2	3:w:305:HOH:O	2.12	0.45
1:W:170:ASP:HB2	3:W:314:HOH:O	2.17	0.45
1:h:2:GLU:OE2	3:h:304:HOH:O	2.21	0.45
1:C:64:GLU:OE1	1:Q:53:LYS:HE2	2.17	0.45
1:g:30:CYS:SG	1:g:85:PRO:HB3	2.57	0.45
1:E:20:GLN:OE1	3:E:302:HOH:O	2.21	0.45
1:E:67:MET:O	1:E:77:ILE:HD11	2.17	0.45
1:b:31:TYR:CZ	1:b:55:LYS:HE3	2.52	0.45
1:r:30:CYS:SG	1:r:85:PRO:HB3	2.57	0.45
1:o:76:ARG:HA	3:o:325:HOH:O	2.17	0.45
1:v:51:TYR:CZ	1:v:55:LYS:HD2	2.51	0.45
1:b:55:LYS:NZ	1:b:141:ASP:OD2	2.50	0.45
1:u:124:LYS:HA	1:u:127:MET:HE3	1.99	0.45
1:O:31:TYR:CZ	1:O:55:LYS:HE3	2.52	0.44
1:a:145:ILE:O	1:a:149:ILE:HG12	2.16	0.44
1:f:64:GLU:OE1	1:j:53:LYS:HE2	2.18	0.44
1:B:82:VAL:CG1	1:P:82:VAL:HG13	2.47	0.44
1:E:117:VAL:O	1:E:120:LYS:HG2	2.18	0.44
1:e:124:LYS:HA	1:e:127:MET:HE3	1.97	0.44
1:s:37:TYR:CE1	1:s:89:GLU:HB2	2.52	0.44
1:Z:94:LEU:O	1:Z:98:GLN:HG2	2.18	0.44
1:x:53:LYS:NZ	1:x:57:ASP:OD1	2.50	0.44
1:A:64:GLU:OE1	1:d:53:LYS:HE2	2.17	0.44
1:O:18:ASN:CG	1:O:78:VAL:H	2.25	0.44
1:g:82:VAL:CG1	1:k:82:VAL:HG13	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:l:53:LYS:NZ	1:l:57:ASP:OD1	2.50	0.44
1:s:63:ALA:O	1:s:67:MET:HG3	2.18	0.44
1:J:19:ARG:NH1	3:J:304:HOH:O	2.21	0.44
1:S:94:LEU:HA	1:S:152:LEU:HD13	1.99	0.44
1:I:55:LYS:NZ	3:I:305:HOH:O	2.34	0.44
1:U:124:LYS:HD2	1:q:115:HIS:CE1	2.52	0.44
1:e:34:MET:HE2	1:e:52:PHE:CZ	2.52	0.44
1:f:145:ILE:O	1:f:149:ILE:HG12	2.18	0.44
1:k:85:PRO:HG2	3:k:344:HOH:O	2.16	0.44
1:K:3:SER:HB2	1:K:6:ARG:HB2	1.99	0.44
1:K:115:HIS:CE1	1:K:127:MET:HE3	2.52	0.44
1:P:104:GLU:HG3	1:P:145:ILE:CD1	2.46	0.44
1:r:2:GLU:OE2	3:r:307:HOH:O	2.21	0.44
1:d:63:ALA:O	1:d:67:MET:HG3	2.18	0.44
1:D:82:VAL:CG1	1:E:82:VAL:HG13	2.47	0.44
1:V:152:LEU:HD23	1:V:152:LEU:HA	1.82	0.44
1:B:41:ASP:OD2	3:B:306:HOH:O	2.21	0.44
1:D:68:LYS:O	1:D:72:LYS:HG3	2.18	0.44
1:b:2:GLU:HA	3:b:412:HOH:O	2.18	0.44
1:a:5:PRO:HG2	1:a:74:GLY:CA	2.48	0.44
1:i:64:GLU:OE1	1:o:53:LYS:HE2	2.18	0.44
1:j:2:GLU:N	3:j:319:HOH:O	2.51	0.44
1:l:37:TYR:CE1	1:l:89:GLU:HB2	2.53	0.44
1:B:50:LYS:CE	3:B:317:HOH:O	2.66	0.44
1:H:166:LYS:HD2	1:H:166:LYS:N	2.33	0.44
1:X:12:GLU:OE1	1:X:117:VAL:HG13	2.18	0.44
1:H:30:CYS:O	1:H:34:MET:HG3	2.18	0.44
1:M:82:VAL:HG13	1:R:82:VAL:HG13	1.99	0.44
1:V:34:MET:HE2	1:V:96:ALA:HB1	1.98	0.44
1:k:63:ALA:O	1:k:67:MET:HG3	2.17	0.44
1:H:148:HIS:HD2	3:H:382:HOH:O	2.00	0.44
1:R:54:GLU:OE2	3:R:308:HOH:O	2.21	0.44
1:t:30:CYS:SG	1:t:85:PRO:HB3	2.58	0.44
1:S:34:MET:HE1	1:S:96:ALA:O	2.17	0.43
1:Q:24:GLU:HB2	1:Q:63:ALA:HB2	2.00	0.43
1:p:117:VAL:O	1:p:120:LYS:HG2	2.18	0.43
1:x:65:LYS:HB3	1:x:134:TYR:OH	2.18	0.43
1:A:63:ALA:O	1:A:67:MET:HG3	2.18	0.43
1:Q:50:LYS:HE2	1:Q:50:LYS:HB3	1.73	0.43
1:B:3:SER:HA	3:B:334:HOH:O	2.18	0.43
1:M:82:VAL:CG1	1:R:82:VAL:HG13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:82:VAL:CG1	1:r:82:VAL:HG13	2.47	0.43
1:P:29:TYR:CD2	1:P:85:PRO:HD3	2.52	0.43
1:P:85:PRO:HG2	3:P:309:HOH:O	2.18	0.43
1:r:34:MET:HE3	1:r:96:ALA:HB1	2.00	0.43
1:u:53:LYS:NZ	1:u:57:ASP:OD1	2.50	0.43
1:S:33:SER:HB2	1:w:79:LEU:CD1	2.49	0.43
1:O:30:CYS:SG	1:O:85:PRO:HB3	2.58	0.43
1:H:145:ILE:O	1:H:149:ILE:HG12	2.17	0.43
1:d:17:ILE:HD11	1:d:126:PHE:CE1	2.53	0.43
1:s:64:GLU:OE1	1:v:53:LYS:HE2	2.18	0.43
1:X:165:ASP:OD2	1:X:166:LYS:NZ	2.49	0.43
1:S:67:MET:HB3	1:S:77:ILE:HD13	2.01	0.43
1:V:4:GLN:O	1:Q:105:LYS:NZ	2.38	0.43
1:f:82:VAL:HG13	1:j:82:VAL:CG1	2.48	0.43
1:i:5:PRO:HD3	1:o:41:ASP:OD2	2.18	0.43
1:m:63:ALA:O	1:m:67:MET:HG3	2.17	0.43
1:j:34:MET:HE2	1:j:52:PHE:CE1	2.54	0.43
1:B:161:GLU:OE2	3:B:307:HOH:O	2.21	0.43
1:D:103:LEU:O	1:D:107:VAL:HG23	2.19	0.43
1:F:82:VAL:CG1	1:L:82:VAL:HG13	2.48	0.43
1:M:75:GLY:O	1:M:76:ARG:NH1	2.51	0.43
1:N:51:TYR:O	1:N:55:LYS:HG3	2.18	0.43
1:r:37:TYR:CE1	1:r:89:GLU:HB2	2.53	0.43
1:g:63:ALA:O	1:g:67:MET:HG3	2.19	0.43
1:i:94:LEU:HA	1:i:152:LEU:HD13	2.01	0.43
1:B:117:VAL:O	1:B:120:LYS:HG2	2.19	0.43
1:O:94:LEU:O	1:O:98:GLN:HG2	2.19	0.43
1:C:34:MET:CE	1:C:96:ALA:HB1	2.48	0.43
1:B:80:GLN:NE2	3:B:305:HOH:O	2.18	0.43
1:t:67:MET:HB3	1:t:77:ILE:HD13	2.00	0.43
1:x:89:GLU:OE1	1:x:90:TRP:N	2.52	0.43
1:S:169:LEU:HD13	1:S:169:LEU:HA	1.85	0.43
1:I:53:LYS:HE2	1:O:64:GLU:OE1	2.19	0.43
1:f:37:TYR:CD1	1:f:40:ARG:HD3	2.54	0.43
1:q:6:ARG:HD2	3:q:347:HOH:O	2.19	0.43
1:D:94:LEU:O	1:D:98:GLN:HG2	2.19	0.43
1:R:83:LYS:NZ	3:R:303:HOH:O	2.07	0.43
1:b:5:PRO:HG2	1:b:74:GLY:CA	2.48	0.43
1:h:64:GLU:OE1	1:n:53:LYS:HE2	2.19	0.43
1:r:124:LYS:HA	1:r:127:MET:HE3	2.00	0.43
1:A:50:LYS:CE	3:A:309:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:HD2	1:d:79:LEU:O	2.18	0.42
1:D:82:VAL:HG13	1:E:82:VAL:CG1	2.49	0.42
1:I:100:SER:O	1:I:104:GLU:HG2	2.19	0.42
1:V:64:GLU:OE1	1:U:53:LYS:HE2	2.19	0.42
1:U:115:HIS:CE1	1:U:127:MET:HG2	2.55	0.42
1:E:34:MET:HE2	1:E:52:PHE:CZ	2.54	0.42
1:K:4:GLN:HG3	3:t:328:HOH:O	2.18	0.42
1:T:82:VAL:CG1	1:Z:82:VAL:HG13	2.48	0.42
1:X:134:TYR:OH	3:X:302:HOH:O	1.92	0.42
1:b:63:ALA:O	1:b:67:MET:HG3	2.19	0.42
1:r:42:ASP:OD2	3:r:308:HOH:O	2.21	0.42
1:S:35:SER:OG	1:S:49:THR:O	2.37	0.42
1:V:63:ALA:O	1:V:67:MET:HG3	2.19	0.42
1:s:62:HIS:NE2	3:s:303:HOH:O	2.36	0.42
1:P:67:MET:O	1:P:77:ILE:HD11	2.19	0.42
1:A:81:ASP:CG	1:d:83:LYS:HD2	2.44	0.42
1:E:34:MET:HE2	1:E:52:PHE:CE1	2.54	0.42
1:J:55:LYS:NZ	1:J:141:ASP:OD2	2.51	0.42
1:J:67:MET:HB3	1:J:77:ILE:CD1	2.49	0.42
1:N:24:GLU:HB2	1:N:63:ALA:HB2	2.01	0.42
1:Z:83:LYS:HG2	3:Z:305:HOH:O	2.19	0.42
1:b:5:PRO:HG2	1:b:74:GLY:HA3	2.01	0.42
1:d:97:MET:HB3	1:d:149:ILE:HD13	2.01	0.42
1:i:34:MET:HE2	1:i:52:PHE:CZ	2.55	0.42
1:k:94:LEU:O	1:k:98:GLN:HG2	2.18	0.42
1:v:83:LYS:NZ	3:v:309:HOH:O	2.48	0.42
1:K:63:ALA:O	1:K:67:MET:HG3	2.19	0.42
1:b:25:LEU:O	1:b:28:CYS:HB3	2.20	0.42
1:h:51:TYR:CZ	1:h:55:LYS:HD2	2.55	0.42
1:n:113:ASP:HA	3:n:304:HOH:O	2.19	0.42
1:u:86:ASP:HA	3:u:378:HOH:O	2.20	0.42
1:x:63:ALA:O	1:x:67:MET:HG3	2.19	0.42
1:i:32:GLN:OE1	1:o:67:MET:HE1	2.20	0.42
1:s:19:ARG:HD2	3:s:421:HOH:O	2.19	0.42
1:F:122:GLY:HA2	3:F:337:HOH:O	2.19	0.42
1:u:53:LYS:HE2	1:x:64:GLU:OE1	2.20	0.42
1:V:34:MET:O	1:V:38:PHE:HD2	2.01	0.42
1:o:85:PRO:HG2	3:o:349:HOH:O	2.19	0.42
1:q:155:VAL:O	1:q:160:GLY:HA3	2.19	0.42
1:v:24:GLU:HB2	1:v:63:ALA:HB2	2.02	0.42
1:P:51:TYR:CZ	1:P:55:LYS:HD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:79:LEU:HA	3:P:328:HOH:O	2.18	0.42
1:C:94:LEU:O	1:C:98:GLN:HG2	2.20	0.42
1:o:37:TYR:CD1	1:o:40:ARG:HD3	2.55	0.42
1:R:59:GLU:O	1:R:62:HIS:HB2	2.20	0.42
1:b:91:GLY:O	3:b:304:HOH:O	2.21	0.42
1:p:4:GLN:HB2	1:p:5:PRO:HD3	2.01	0.42
1:p:117:VAL:HA	1:p:120:LYS:HE3	2.02	0.42
1:Q:5:PRO:HG2	1:Q:74:GLY:CA	2.50	0.42
1:D:4:GLN:HB2	1:D:5:PRO:HD3	2.02	0.42
1:E:84:LYS:NZ	3:E:307:HOH:O	2.28	0.42
1:O:55:LYS:NZ	1:O:141:ASP:OD2	2.53	0.42
1:a:114:LEU:HD12	1:a:114:LEU:HA	1.89	0.42
1:k:18:ASN:O	3:k:302:HOH:O	2.22	0.42
1:o:145:ILE:O	1:o:149:ILE:HG12	2.19	0.42
1:T:101:LEU:HD11	1:T:142:ILE:HG23	2.01	0.42
1:n:37:TYR:HA	3:n:400:HOH:O	2.20	0.42
1:I:141:ASP:HA	1:I:144:LYS:CE	2.49	0.41
1:C:34:MET:HE2	1:C:52:PHE:CZ	2.55	0.41
1:V:82:VAL:CG1	1:U:82:VAL:HG13	2.50	0.41
1:k:109:GLN:NE2	3:k:304:HOH:O	2.30	0.41
1:v:130:LEU:HD23	1:v:130:LEU:HA	1.92	0.41
1:K:104:GLU:HG3	1:K:145:ILE:CD1	2.49	0.41
1:X:124:LYS:HA	1:X:127:MET:HE3	2.00	0.41
1:Z:69:TYR:CE1	1:Z:126:PHE:HD1	2.39	0.41
1:A:145:ILE:O	1:A:149:ILE:HG12	2.21	0.41
1:g:124:LYS:HA	1:g:127:MET:HE3	2.02	0.41
1:k:75:GLY:O	1:k:76:ARG:NH1	2.53	0.41
1:w:89:GLU:OE1	1:w:89:GLU:C	2.63	0.41
1:Z:6:ARG:HD2	3:Z:316:HOH:O	2.20	0.41
1:b:30:CYS:SG	1:b:85:PRO:HB3	2.60	0.41
1:t:117:VAL:O	1:t:120:LYS:HG2	2.20	0.41
1:x:28:CYS:HB2	1:x:59:GLU:HB2	2.02	0.41
1:i:94:LEU:O	1:i:98:GLN:HG2	2.20	0.41
1:E:21:ILE:HG13	1:E:66:PHE:HB3	2.01	0.41
1:P:34:MET:HE2	1:P:52:PHE:CZ	2.55	0.41
1:R:117:VAL:O	1:R:120:LYS:HG2	2.20	0.41
1:T:5:PRO:HD3	1:Z:41:ASP:OD2	2.21	0.41
1:W:37:TYR:CE1	1:W:89:GLU:HB2	2.56	0.41
1:Z:117:VAL:O	1:Z:120:LYS:HG2	2.20	0.41
1:i:95:ASP:O	1:i:98:GLN:HB2	2.20	0.41
1:B:34:MET:HE2	1:B:52:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:TYR:CZ	1:D:55:LYS:HD2	2.56	0.41
1:H:38:PHE:HA	1:H:43:VAL:HG11	2.02	0.41
1:p:98:GLN:NE2	3:p:316:HOH:O	2.41	0.41
1:c:124:LYS:HA	1:c:127:MET:HE3	2.03	0.41
1:j:97:MET:HB3	1:j:149:ILE:HD13	2.03	0.41
1:j:145:ILE:O	1:j:149:ILE:HG12	2.20	0.41
1:b:94:LEU:O	1:b:98:GLN:HG2	2.21	0.41
1:r:3:SER:HB2	1:r:5:PRO:HD2	2.03	0.41
1:t:152:LEU:HD23	1:t:152:LEU:HA	1.95	0.41
1:I:87:ARG:NH2	3:I:307:HOH:O	2.49	0.41
1:i:85:PRO:HG2	3:i:344:HOH:O	2.20	0.41
1:i:131:GLU:HA	1:i:135:LEU:HB2	2.03	0.41
1:H:141:ASP:O	1:H:145:ILE:HG13	2.21	0.41
1:K:70:GLN:OE1	1:K:75:GLY:HA3	2.20	0.41
1:K:144:LYS:HG3	3:K:321:HOH:O	2.20	0.41
1:x:34:MET:HE3	1:x:96:ALA:HB1	2.00	0.41
1:x:89:GLU:OE1	1:x:91:GLY:N	2.54	0.41
1:a:72:LYS:NZ	1:w:140:GLU:OE1	2.48	0.41
1:B:51:TYR:O	1:B:55:LYS:HG3	2.21	0.41
1:M:87:ARG:HD2	3:M:328:HOH:O	2.19	0.41
1:M:117:VAL:O	1:M:120:LYS:HG2	2.21	0.41
1:N:64:GLU:OE1	1:r:53:LYS:HE2	2.21	0.41
1:P:51:TYR:CE2	1:P:55:LYS:HD2	2.56	0.41
1:b:85:PRO:HG2	3:b:325:HOH:O	2.20	0.41
1:A:29:TYR:HE2	1:A:84:LYS:HA	1.85	0.41
1:I:53:LYS:NZ	1:I:57:ASP:OD1	2.54	0.41
1:O:83:LYS:HE3	1:O:83:LYS:HB3	1.86	0.41
1:C:41:ASP:OD2	1:Q:5:PRO:HD3	2.20	0.41
1:d:85:PRO:HG2	3:d:318:HOH:O	2.21	0.41
1:g:2:GLU:HG2	3:g:405:HOH:O	2.21	0.41
1:j:55:LYS:NZ	1:j:141:ASP:OD2	2.54	0.41
1:k:4:GLN:O	1:m:105:LYS:NZ	2.51	0.41
1:s:41:ASP:OD2	1:v:5:PRO:HD3	2.21	0.41
1:s:130:LEU:HD23	1:s:130:LEU:HA	1.85	0.41
1:v:115:HIS:HE1	1:v:127:MET:HE3	1.84	0.41
1:W:37:TYR:CD1	1:W:40:ARG:HD3	2.54	0.41
1:Z:37:TYR:HA	3:Z:408:HOH:O	2.21	0.41
1:Z:76:ARG:HA	1:Z:76:ARG:HD3	1.88	0.41
1:r:117:VAL:O	1:r:120:LYS:HG2	2.21	0.41
1:u:25:LEU:O	1:u:28:CYS:HB3	2.21	0.41
1:u:30:CYS:SG	1:u:85:PRO:HB3	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:84:LYS:HB3	1:e:80:GLN:C	2.46	0.41
1:H:105:LYS:NZ	1:T:4:GLN:O	2.48	0.41
1:M:18:ASN:HA	1:M:21:ILE:HD12	2.03	0.41
1:h:143:LYS:NZ	1:h:147:ASP:OD1	2.46	0.41
1:p:19:ARG:CG	1:p:20:GLN:N	2.82	0.41
1:p:20:GLN:O	1:p:24:GLU:HG2	2.20	0.41
1:A:29:TYR:CD2	1:A:85:PRO:HD3	2.56	0.40
1:V:53:LYS:HE2	1:U:64:GLU:OE1	2.21	0.40
1:Q:55:LYS:NZ	1:Q:141:ASP:OD2	2.49	0.40
1:f:135:LEU:HD23	1:f:135:LEU:HA	1.85	0.40
1:i:79:LEU:HB3	1:o:29:TYR:OH	2.21	0.40
1:s:84:LYS:NZ	3:s:313:HOH:O	2.53	0.40
1:H:6:ARG:HD2	3:H:354:HOH:O	2.21	0.40
1:Z:138:GLN:NE2	3:Z:323:HOH:O	2.53	0.40
1:b:20:GLN:O	1:b:24:GLU:HG2	2.20	0.40
1:x:51:TYR:CZ	1:x:55:LYS:HD2	2.56	0.40
1:e:81:ASP:HB2	3:e:426:HOH:O	2.21	0.40
1:N:63:ALA:O	1:N:67:MET:HG3	2.21	0.40
1:R:19:ARG:HH11	1:R:19:ARG:HD3	1.31	0.40
1:W:64:GLU:OE1	1:b:53:LYS:HE2	2.22	0.40
1:n:131:GLU:HA	1:n:135:LEU:HB2	2.03	0.40
1:I:34:MET:HG2	1:I:90:TRP:CD2	2.56	0.40
1:U:34:MET:CE	1:U:96:ALA:HB1	2.52	0.40
1:c:153:LYS:NZ	3:c:309:HOH:O	2.38	0.40
1:l:105:LYS:NZ	3:l:323:HOH:O	2.54	0.40
1:J:145:ILE:O	1:J:149:ILE:HG12	2.22	0.40
1:P:29:TYR:CE2	1:P:84:LYS:HA	2.56	0.40
1:X:12:GLU:O	1:X:16:GLY:N	2.53	0.40
1:h:82:VAL:CG1	1:n:82:VAL:HG13	2.51	0.40
1:x:145:ILE:O	1:x:149:ILE:HG12	2.21	0.40
1:R:53:LYS:NZ	1:R:57:ASP:OD1	2.54	0.40
1:R:145:ILE:O	1:R:149:ILE:HG12	2.21	0.40
1:X:65:LYS:HB3	3:X:302:HOH:O	2.20	0.40
1:h:89:GLU:OE1	1:h:90:TRP:N	2.55	0.40
1:p:18:ASN:HA	1:p:21:ILE:HD12	2.04	0.40
1:A:170:ASP:HB2	3:A:309:HOH:O	2.21	0.40
1:V:75:GLY:O	1:V:76:ARG:NH1	2.55	0.40
1:C:19:ARG:HB3	3:C:433:HOH:O	2.20	0.40
1:D:20:GLN:O	1:D:24:GLU:HG2	2.21	0.40
1:E:42:ASP:HB3	3:E:401:HOH:O	2.20	0.40
1:M:168:SER:O	3:M:309:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:65:LYS:NZ	1:n:133:ASP:HB3	2.37	0.40

All (4) 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)
3:Q:6410:HOH:O	3:R:397:HOH:O[1_645]	2.03	0.17
3:j:451:HOH:O	3:j:451:HOH:O[2_656]	2.11	0.09
3:o:400:HOH:O	3:P:358:HOH:O[2_545]	2.12	0.08
3:c:383:HOH:O	3:g:359:HOH:O[2_555]	2.18	0.02

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	167/171 (98%)	165 (99%)	2 (1%)	0	100	100
1	B	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	C	167/171 (98%)	162 (97%)	5 (3%)	0	100	100
1	D	167/171 (98%)	165 (99%)	2 (1%)	0	100	100
1	E	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	F	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	H	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	I	167/171 (98%)	165 (99%)	2 (1%)	0	100	100
1	J	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	K	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	L	167/171 (98%)	162 (97%)	5 (3%)	0	100	100
1	M	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	N	167/171 (98%)	162 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	167/171 (98%)	165 (99%)	2 (1%)	0	100	100
1	P	167/171 (98%)	165 (99%)	2 (1%)	0	100	100
1	Q	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	R	167/171 (98%)	162 (97%)	5 (3%)	0	100	100
1	S	167/171 (98%)	162 (97%)	5 (3%)	0	100	100
1	T	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	U	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	V	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	W	167/171 (98%)	165 (99%)	2 (1%)	0	100	100
1	X	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	Z	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	a	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	b	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	c	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	d	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	e	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	f	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	g	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	h	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	i	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	j	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	k	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	l	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	m	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	n	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	o	167/171 (98%)	162 (97%)	5 (3%)	0	100	100
1	p	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	q	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	r	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	s	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	t	167/171 (98%)	162 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	167/171 (98%)	164 (98%)	3 (2%)	0	100	100
1	v	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	w	167/171 (98%)	163 (98%)	4 (2%)	0	100	100
1	x	167/171 (98%)	162 (97%)	5 (3%)	0	100	100
All	All	8016/8208 (98%)	7847 (98%)	169 (2%)	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	151/152 (99%)	151 (100%)	0	100	100
1	B	151/152 (99%)	151 (100%)	0	100	100
1	C	151/152 (99%)	151 (100%)	0	100	100
1	D	151/152 (99%)	151 (100%)	0	100	100
1	E	151/152 (99%)	151 (100%)	0	100	100
1	F	151/152 (99%)	151 (100%)	0	100	100
1	H	151/152 (99%)	151 (100%)	0	100	100
1	I	151/152 (99%)	151 (100%)	0	100	100
1	J	151/152 (99%)	151 (100%)	0	100	100
1	K	151/152 (99%)	151 (100%)	0	100	100
1	L	151/152 (99%)	151 (100%)	0	100	100
1	M	151/152 (99%)	151 (100%)	0	100	100
1	N	151/152 (99%)	151 (100%)	0	100	100
1	O	151/152 (99%)	150 (99%)	1 (1%)	76	88
1	P	151/152 (99%)	151 (100%)	0	100	100
1	Q	151/152 (99%)	151 (100%)	0	100	100
1	R	151/152 (99%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	S	150/152 (99%)	146 (97%)	4 (3%)	39	62
1	T	151/152 (99%)	151 (100%)	0	100	100
1	U	151/152 (99%)	151 (100%)	0	100	100
1	V	151/152 (99%)	151 (100%)	0	100	100
1	W	151/152 (99%)	151 (100%)	0	100	100
1	X	151/152 (99%)	151 (100%)	0	100	100
1	Z	151/152 (99%)	151 (100%)	0	100	100
1	a	151/152 (99%)	151 (100%)	0	100	100
1	b	151/152 (99%)	151 (100%)	0	100	100
1	c	151/152 (99%)	151 (100%)	0	100	100
1	d	151/152 (99%)	151 (100%)	0	100	100
1	e	151/152 (99%)	151 (100%)	0	100	100
1	f	151/152 (99%)	151 (100%)	0	100	100
1	g	151/152 (99%)	151 (100%)	0	100	100
1	h	151/152 (99%)	151 (100%)	0	100	100
1	i	151/152 (99%)	151 (100%)	0	100	100
1	j	151/152 (99%)	150 (99%)	1 (1%)	76	88
1	k	151/152 (99%)	151 (100%)	0	100	100
1	l	151/152 (99%)	151 (100%)	0	100	100
1	m	151/152 (99%)	151 (100%)	0	100	100
1	n	151/152 (99%)	151 (100%)	0	100	100
1	o	151/152 (99%)	151 (100%)	0	100	100
1	p	151/152 (99%)	151 (100%)	0	100	100
1	q	151/152 (99%)	151 (100%)	0	100	100
1	r	151/152 (99%)	151 (100%)	0	100	100
1	s	151/152 (99%)	151 (100%)	0	100	100
1	t	151/152 (99%)	151 (100%)	0	100	100
1	u	151/152 (99%)	151 (100%)	0	100	100
1	v	151/152 (99%)	151 (100%)	0	100	100
1	w	151/152 (99%)	151 (100%)	0	100	100
1	x	151/152 (99%)	150 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7247/7296 (99%)	7240 (100%)	7 (0%)	88 95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	19	ARG
1	S	28	CYS
1	S	132	SER
1	S	169	LEU
1	O	82	VAL
1	j	82	VAL
1	x	82	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	S	138	GLN
1	S	151	ASN
1	I	70	GLN
1	C	108	ASN
1	C	109	GLN
1	Q	32	GLN
1	Q	62	HIS
1	U	98	GLN
1	a	108	ASN
1	a	109	GLN
1	a	148	HIS
1	c	22	ASN
1	d	4	GLN
1	f	7	GLN
1	f	32	GLN
1	f	138	GLN
1	g	108	ASN
1	i	7	GLN
1	i	70	GLN
1	k	106	ASN
1	k	108	ASN
1	l	4	GLN
1	l	108	ASN
1	m	32	GLN

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Mol	Chain	Res	Type
1	o	106	ASN
1	q	22	ASN
1	s	106	ASN
1	v	32	GLN
1	v	108	ASN
1	B	4	GLN
1	B	108	ASN
1	D	7	GLN
1	D	106	ASN
1	D	115	HIS
1	E	108	ASN
1	F	7	GLN
1	F	22	ASN
1	H	148	HIS
1	H	151	ASN
1	K	7	GLN
1	L	98	GLN
1	L	106	ASN
1	L	108	ASN
1	N	70	GLN
1	P	22	ASN
1	P	32	GLN
1	P	106	ASN
1	R	108	ASN
1	R	151	ASN
1	T	22	ASN
1	T	108	ASN
1	T	109	GLN
1	T	121	HIS
1	T	138	GLN
1	W	108	ASN
1	X	106	ASN
1	X	138	GLN
1	Z	32	GLN
1	b	7	GLN
1	h	10	HIS
1	n	7	GLN
1	n	106	ASN
1	n	108	ASN
1	p	7	GLN
1	r	138	GLN
1	t	121	HIS

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Mol	Chain	Res	Type
1	u	109	GLN
1	x	106	ASN

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 95 ligands modelled in this entry, 95 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	169/171 (98%)	-0.47	0 100 100	18, 24, 34, 56	0
1	B	169/171 (98%)	-0.16	1 (0%) 85 83	23, 28, 37, 58	0
1	C	169/171 (98%)	-0.55	0 100 100	17, 26, 35, 56	0
1	D	169/171 (98%)	-0.05	0 100 100	21, 29, 38, 63	0
1	E	169/171 (98%)	-0.04	0 100 100	25, 31, 39, 60	0
1	F	169/171 (98%)	-0.00	0 100 100	21, 31, 38, 61	0
1	H	169/171 (98%)	-0.30	0 100 100	23, 31, 39, 57	0
1	I	169/171 (98%)	-0.33	0 100 100	20, 26, 36, 61	0
1	J	169/171 (98%)	0.01	2 (1%) 76 73	28, 34, 41, 64	0
1	K	169/171 (98%)	0.05	1 (0%) 85 83	29, 35, 42, 65	0
1	L	169/171 (98%)	-0.02	0 100 100	24, 31, 41, 59	0
1	M	169/171 (98%)	0.09	2 (1%) 76 73	24, 33, 41, 53	0
1	N	169/171 (98%)	-0.69	0 100 100	15, 21, 31, 53	0
1	O	169/171 (98%)	-0.30	0 100 100	20, 27, 35, 60	0
1	P	169/171 (98%)	-0.12	0 100 100	21, 30, 38, 56	0
1	Q	169/171 (98%)	-0.26	0 100 100	23, 30, 39, 59	0
1	R	169/171 (98%)	0.06	0 100 100	25, 33, 41, 58	0
1	S	169/171 (98%)	0.14	1 (0%) 85 83	22, 31, 39, 56	0
1	T	169/171 (98%)	-0.34	0 100 100	22, 31, 41, 64	0
1	U	169/171 (98%)	-0.07	0 100 100	25, 31, 41, 63	0
1	V	169/171 (98%)	-0.16	0 100 100	22, 29, 39, 57	0
1	W	169/171 (98%)	-0.60	1 (0%) 85 83	16, 23, 32, 57	0
1	X	169/171 (98%)	0.15	0 100 100	27, 35, 43, 64	0
1	Z	169/171 (98%)	-0.34	2 (1%) 76 73	19, 30, 38, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	a	169/171 (98%)	-0.09	0 100 100	24, 31, 40, 59	0
1	b	169/171 (98%)	-0.41	1 (0%) 85 83	18, 26, 37, 62	0
1	c	169/171 (98%)	-0.67	1 (0%) 85 83	14, 22, 31, 57	0
1	d	169/171 (98%)	-0.37	1 (0%) 85 83	20, 25, 35, 62	0
1	e	169/171 (98%)	-0.25	0 100 100	25, 30, 38, 57	0
1	f	169/171 (98%)	-0.60	1 (0%) 85 83	18, 25, 34, 63	0
1	g	169/171 (98%)	-0.61	1 (0%) 85 83	15, 22, 30, 62	0
1	h	169/171 (98%)	0.01	1 (0%) 85 83	28, 33, 42, 62	0
1	i	169/171 (98%)	0.00	0 100 100	28, 33, 43, 63	0
1	j	169/171 (98%)	-0.61	0 100 100	15, 24, 33, 57	0
1	k	169/171 (98%)	-0.47	0 100 100	17, 25, 34, 59	0
1	l	169/171 (98%)	-0.31	0 100 100	23, 28, 37, 57	0
1	m	169/171 (98%)	-0.32	0 100 100	19, 28, 37, 56	0
1	n	169/171 (98%)	-0.10	0 100 100	21, 31, 39, 64	0
1	o	169/171 (98%)	-0.11	0 100 100	23, 31, 40, 60	0
1	p	169/171 (98%)	-0.04	1 (0%) 85 83	24, 30, 41, 62	0
1	q	169/171 (98%)	-0.42	0 100 100	19, 27, 34, 61	0
1	r	169/171 (98%)	-0.41	0 100 100	20, 26, 35, 60	0
1	s	169/171 (98%)	-0.56	1 (0%) 85 83	17, 23, 33, 60	0
1	t	169/171 (98%)	0.24	1 (0%) 85 83	28, 36, 45, 65	0
1	u	169/171 (98%)	-0.47	1 (0%) 85 83	18, 24, 32, 63	0
1	v	169/171 (98%)	-0.41	0 100 100	19, 24, 35, 58	0
1	w	169/171 (98%)	-0.11	0 100 100	25, 32, 41, 63	0
1	x	169/171 (98%)	-0.30	0 100 100	21, 26, 37, 59	0
All	All	8112/8208 (98%)	-0.24	20 (0%) 91 89	14, 29, 39, 65	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	S	169	LEU	3.9
1	b	170	ASP	2.9
1	c	170	ASP	2.6
1	d	170	ASP	2.6
1	f	170	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	h	29	TYR	2.5
1	Z	89	GLU	2.4
1	u	170	ASP	2.4
1	K	96	ALA	2.3
1	W	170	ASP	2.2
1	Z	170	ASP	2.2
1	J	170	ASP	2.1
1	p	170	ASP	2.1
1	M	118	GLY	2.1
1	s	170	ASP	2.1
1	t	13	THR	2.1
1	J	89	GLU	2.1
1	g	170	ASP	2.1
1	M	89	GLU	2.1
1	B	3	SER	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($\text{\AA}^2$)	Q<0.9
2	FE	U	202	1/1	0.68	0.16	86,86,86,86	0
2	FE	S	202	1/1	0.73	0.15	95,95,95,95	0
2	FE	p	202	1/1	0.77	0.14	90,90,90,90	0
2	FE	J	202	1/1	0.80	0.15	86,86,86,86	0
2	FE	R	202	1/1	0.81	0.17	96,96,96,96	0
2	FE	l	202	1/1	0.81	0.13	86,86,86,86	0
2	FE	Q	202	1/1	0.83	0.14	94,94,94,94	0
2	FE	t	202	1/1	0.83	0.17	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	j	202	1/1	0.84	0.14	74,74,74,74	0
2	FE	w	202	1/1	0.84	0.14	86,86,86,86	0
2	FE	a	202	1/1	0.85	0.13	83,83,83,83	0
2	FE	E	202	1/1	0.85	0.16	81,81,81,81	0
2	FE	V	202	1/1	0.86	0.10	90,90,90,90	0
2	FE	D	202	1/1	0.86	0.14	86,86,86,86	0
2	FE	b	202	1/1	0.86	0.11	84,84,84,84	0
2	FE	m	202	1/1	0.86	0.11	78,78,78,78	0
2	FE	F	202	1/1	0.86	0.12	80,80,80,80	0
2	FE	o	202	1/1	0.87	0.12	85,85,85,85	0
2	FE	v	202	1/1	0.87	0.14	85,85,85,85	0
2	FE	x	202	1/1	0.87	0.14	82,82,82,82	0
2	FE	e	202	1/1	0.88	0.14	84,84,84,84	0
2	FE	u	202	1/1	0.88	0.12	77,77,77,77	0
2	FE	I	202	1/1	0.88	0.17	84,84,84,84	0
2	FE	k	202	1/1	0.89	0.10	85,85,85,85	0
2	FE	L	202	1/1	0.89	0.14	88,88,88,88	0
2	FE	M	202	1/1	0.89	0.12	80,80,80,80	0
2	FE	U	201	1/1	0.90	0.09	67,67,67,67	0
2	FE	g	202	1/1	0.90	0.11	72,72,72,72	0
2	FE	i	202	1/1	0.90	0.14	89,89,89,89	0
2	FE	h	202	1/1	0.90	0.13	82,82,82,82	0
2	FE	n	202	1/1	0.91	0.09	80,80,80,80	0
2	FE	q	202	1/1	0.91	0.09	73,73,73,73	0
2	FE	r	202	1/1	0.91	0.10	75,75,75,75	0
2	FE	K	201	1/1	0.91	0.07	70,70,70,70	0
2	FE	f	202	1/1	0.91	0.12	75,75,75,75	0
2	FE	M	201	1/1	0.91	0.08	63,63,63,63	0
2	FE	Z	202	1/1	0.92	0.10	74,74,74,74	0
2	FE	B	202	1/1	0.92	0.10	78,78,78,78	0
2	FE	H	202	1/1	0.92	0.09	79,79,79,79	0
2	FE	C	202	1/1	0.93	0.09	69,69,69,69	0
2	FE	N	202	1/1	0.93	0.10	68,68,68,68	0
2	FE	P	202	1/1	0.93	0.09	76,76,76,76	0
2	FE	c	202	1/1	0.93	0.10	67,67,67,67	0
2	FE	t	201	1/1	0.93	0.09	69,69,69,69	0
2	FE	W	202	1/1	0.93	0.10	73,73,73,73	0
2	FE	d	202	1/1	0.93	0.15	74,74,74,74	0
2	FE	A	202	1/1	0.93	0.11	75,75,75,75	0
2	FE	T	202	1/1	0.94	0.11	77,77,77,77	0
2	FE	s	201	1/1	0.94	0.06	54,54,54,54	0
2	FE	n	201	1/1	0.94	0.06	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	X	201	1/1	0.94	0.07	69,69,69,69	0
2	FE	s	202	1/1	0.94	0.09	78,78,78,78	0
2	FE	K	202	1/1	0.95	0.07	83,83,83,83	0
2	FE	L	201	1/1	0.95	0.06	58,58,58,58	0
2	FE	p	201	1/1	0.95	0.06	60,60,60,60	0
2	FE	F	201	1/1	0.95	0.07	63,63,63,63	0
2	FE	i	201	1/1	0.95	0.06	60,60,60,60	0
2	FE	O	202	1/1	0.95	0.10	75,75,75,75	0
2	FE	E	201	1/1	0.95	0.08	63,63,63,63	0
2	FE	h	201	1/1	0.95	0.06	59,59,59,59	0
2	FE	o	201	1/1	0.95	0.06	63,63,63,63	0
2	FE	V	201	1/1	0.96	0.05	58,58,58,58	0
2	FE	P	201	1/1	0.96	0.07	57,57,57,57	0
2	FE	w	201	1/1	0.96	0.08	63,63,63,63	0
2	FE	l	201	1/1	0.96	0.04	57,57,57,57	0
2	FE	e	201	1/1	0.96	0.05	63,63,63,63	0
2	FE	A	201	1/1	0.97	0.06	52,52,52,52	0
2	FE	d	201	1/1	0.97	0.07	53,53,53,53	0
2	FE	C	201	1/1	0.97	0.04	55,55,55,55	0
2	FE	v	201	1/1	0.97	0.04	57,57,57,57	0
2	FE	H	201	1/1	0.97	0.07	63,63,63,63	0
2	FE	O	201	1/1	0.97	0.04	50,50,50,50	0
2	FE	R	201	1/1	0.97	0.07	60,60,60,60	0
2	FE	B	201	1/1	0.97	0.05	57,57,57,57	0
2	FE	r	201	1/1	0.97	0.05	56,56,56,56	0
2	FE	T	201	1/1	0.97	0.04	54,54,54,54	0
2	FE	a	201	1/1	0.97	0.06	59,59,59,59	0
2	FE	D	201	1/1	0.97	0.04	56,56,56,56	0
2	FE	u	201	1/1	0.97	0.05	54,54,54,54	0
2	FE	Q	201	1/1	0.97	0.04	61,61,61,61	0
2	FE	Z	201	1/1	0.97	0.04	52,52,52,52	0
2	FE	S	201	1/1	0.98	0.05	55,55,55,55	0
2	FE	j	201	1/1	0.98	0.04	49,49,49,49	0
2	FE	q	201	1/1	0.98	0.05	52,52,52,52	0
2	FE	c	201	1/1	0.98	0.04	44,44,44,44	0
2	FE	k	201	1/1	0.98	0.03	47,47,47,47	0
2	FE	J	201	1/1	0.98	0.04	58,58,58,58	0
2	FE	x	201	1/1	0.98	0.04	57,57,57,57	0
2	FE	b	201	1/1	0.98	0.07	52,52,52,52	0
2	FE	N	201	1/1	0.99	0.02	46,46,46,46	0
2	FE	I	201	1/1	0.99	0.04	51,51,51,51	0
2	FE	g	201	1/1	0.99	0.04	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	W	201	1/1	0.99	0.04	46,46,46,46	0
2	FE	m	201	1/1	0.99	0.05	51,51,51,51	0
2	FE	f	201	1/1	0.99	0.04	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.