



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:08 PM UTC

PDB ID : 6U7M / pdb_00006u7m
EMDB ID : EMD-20673
Title : Cryo-EM Structure of Helical Lipoprotein Lipase
Authors : Gunn, K.H.; Wang, F.; Egelman, E.H.; Neher, S.B.
Deposited on : 2019-09-03
Resolution : 3.80 Å(reported)
Based on initial model : 6E7K

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

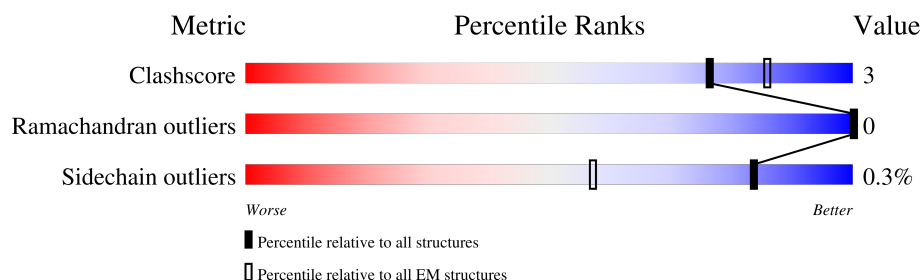
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



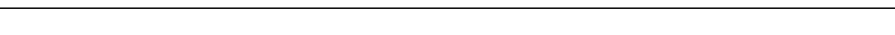
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	478	78% 9% 13%
1	B	478	79% 8% 13%
1	C	478	79% 8% 13%
1	D	478	78% 9% 13%
1	E	478	80% 8% 13%
1	F	478	79% 8% 13%
1	G	478	78% 9% 13%
1	H	478	79% 9% 13%
1	I	478	79% 8% 13%

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Mol	Chain	Length	Quality of chain
1	J	478	
1	K	478	
1	L	478	
1	M	478	
1	N	478	
1	O	478	
1	P	478	
1	Q	478	
1	R	478	
1	S	478	
1	T	478	
1	U	478	
1	a	478	
1	b	478	
1	c	478	
1	d	478	
1	e	478	
1	f	478	
1	g	478	
1	h	478	
1	i	478	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 99420 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Lipoprotein lipase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	B	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	C	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	D	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	E	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	F	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	G	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	H	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	I	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	J	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	K	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	L	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	M	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	N	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	O	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	P	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	Q	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		

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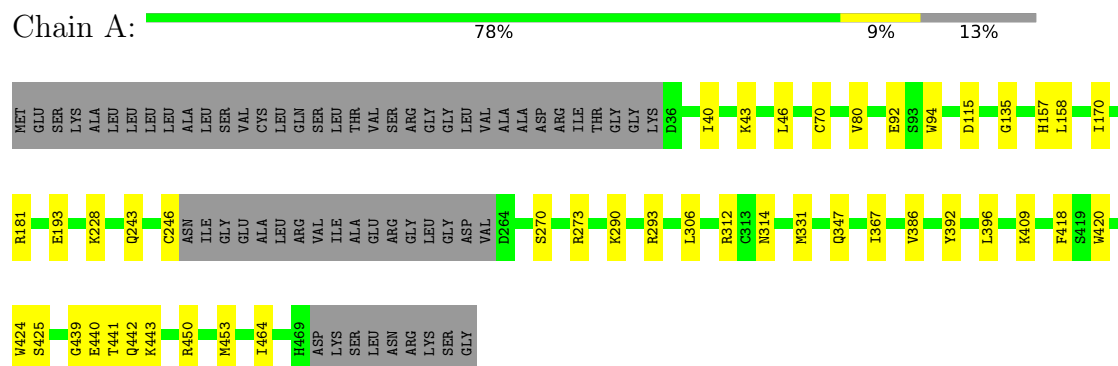
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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	S	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	T	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	U	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	a	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	b	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	c	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	d	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	e	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	f	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	g	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	h	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		
1	i	417	Total	C	N	O	S	0	0
			3314	2114	568	614	18		

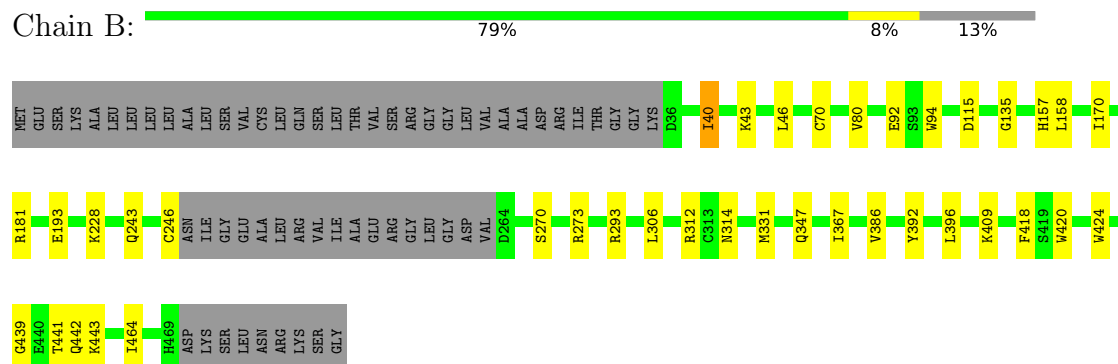
3 Residue-property plots [i](#)

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. 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. 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.

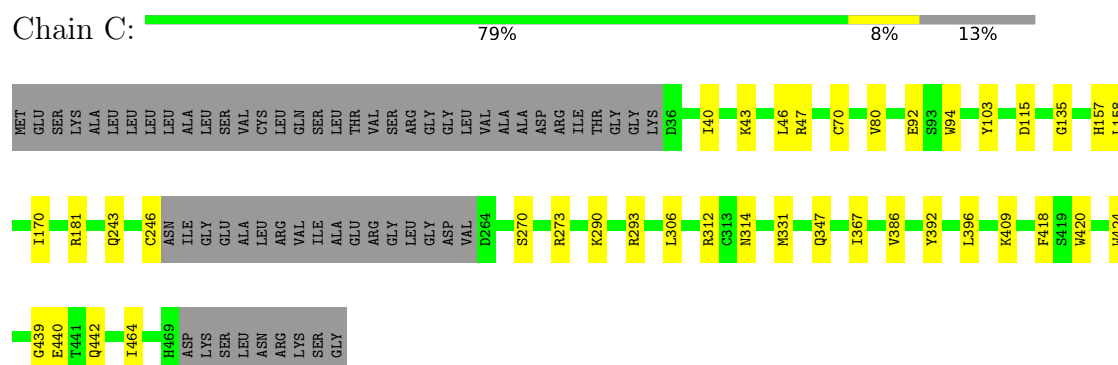
- Molecule 1: Lipoprotein lipase



- Molecule 1: Lipoprotein lipase



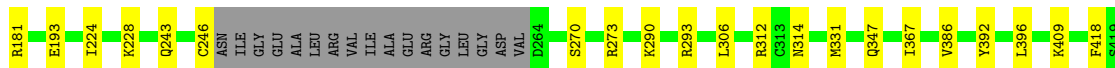
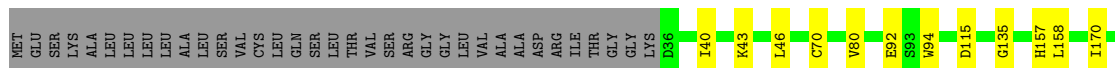
- Molecule 1: Lipoprotein lipase





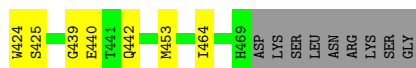
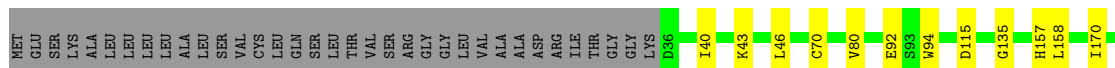
• Molecule 1: Lipoprotein lipase

Chain H:  79% 9% 13%



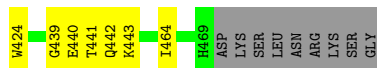
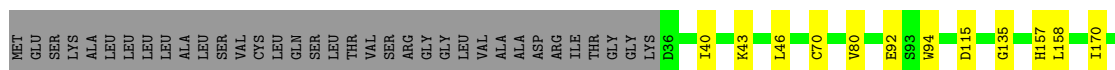
• Molecule 1: Lipoprotein lipase

Chain I:  79% 8% 13%



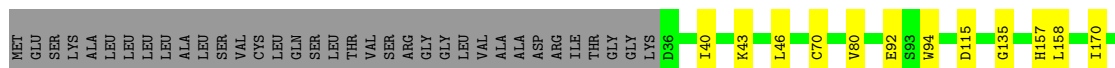
• Molecule 1: Lipoprotein lipase

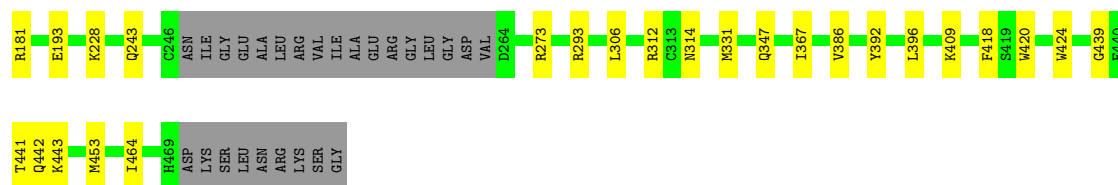
Chain J:  79% 8% 13%



• Molecule 1: Lipoprotein lipase

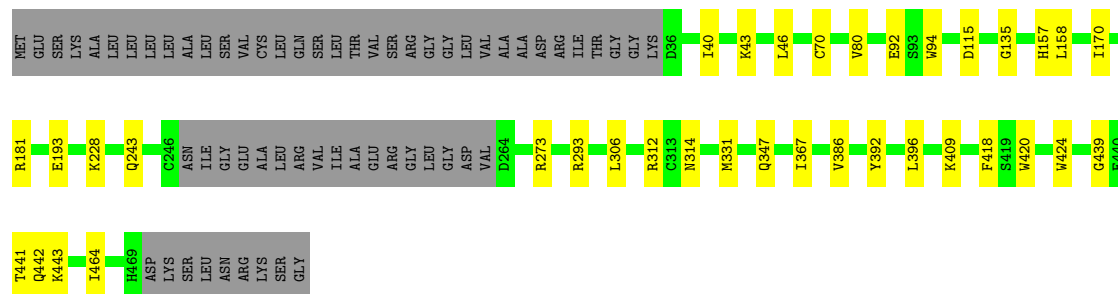
Chain K:  79% 8% 13%





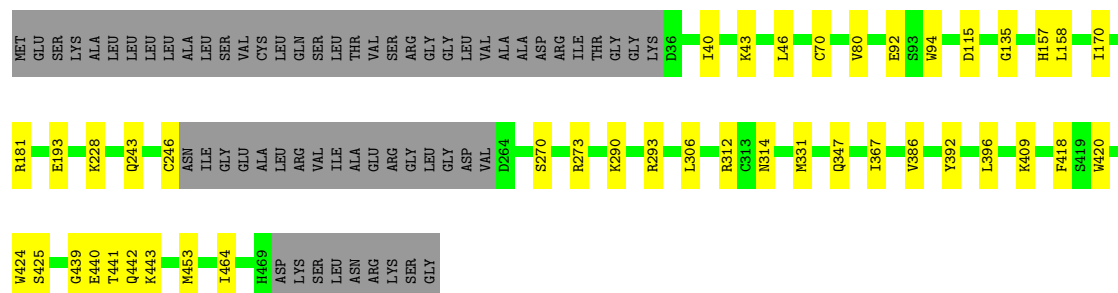
- Molecule 1: Lipoprotein lipase

Chain L: 80% 8% 13%



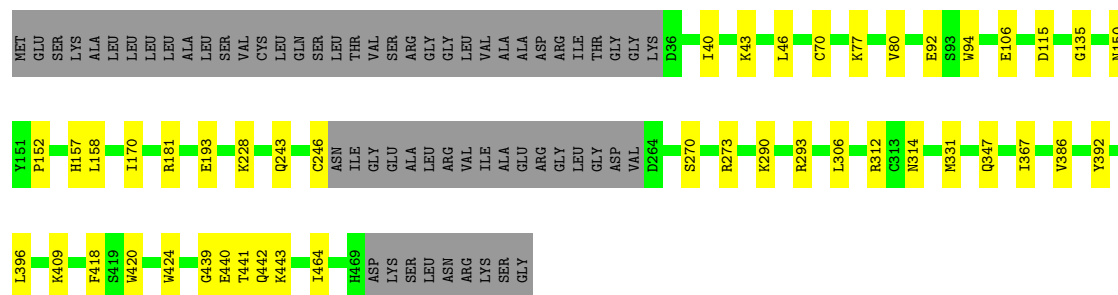
- Molecule 1: Lipoprotein lipase

Chain M: 78% 9% 13%



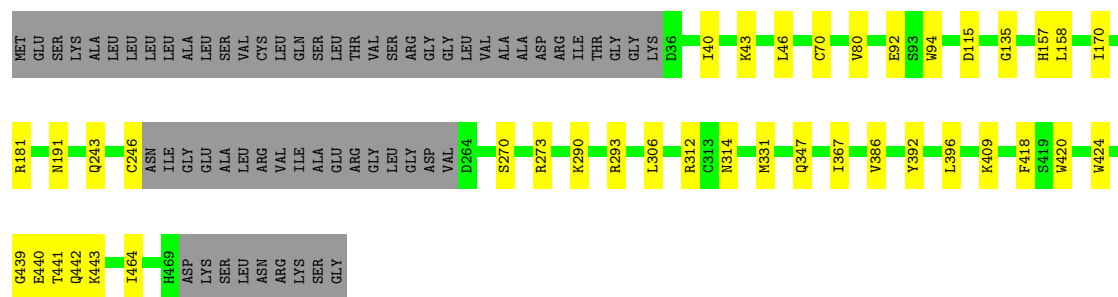
- Molecule 1: Lipoprotein lipase

Chain N: 78% 9% 13%



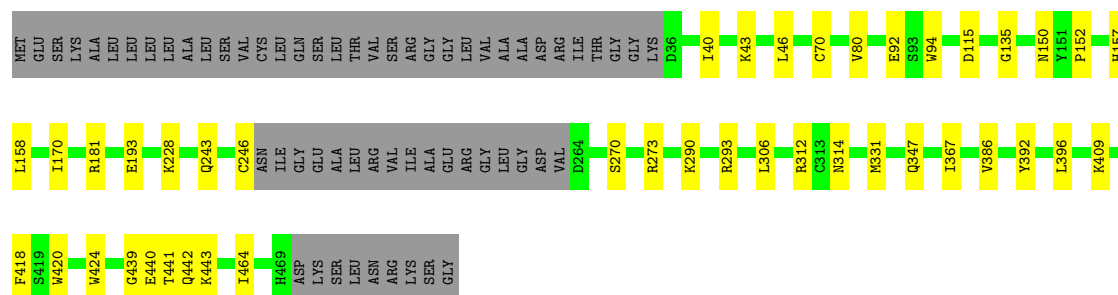
- Molecule 1: Lipoprotein lipase

Chain O: 79% 8% 13%



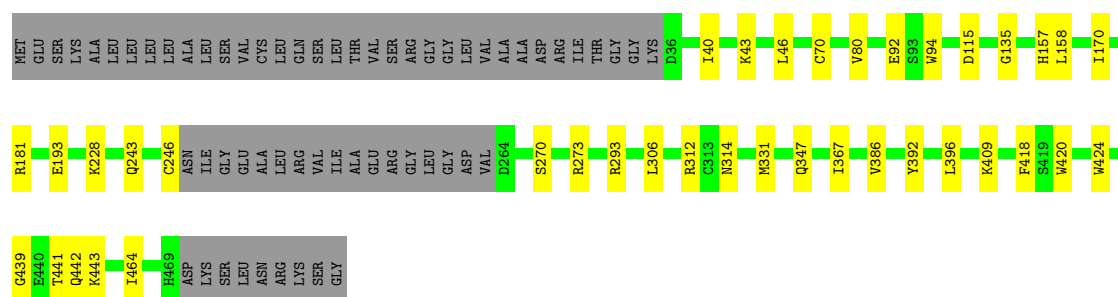
- Molecule 1: Lipoprotein lipase

Chain P: 78% 9% 13%



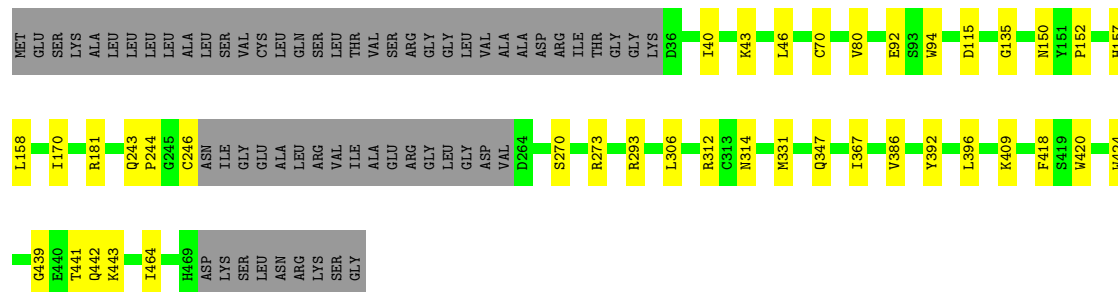
- Molecule 1: Lipoprotein lipase

Chain Q: 79% 8% 13%



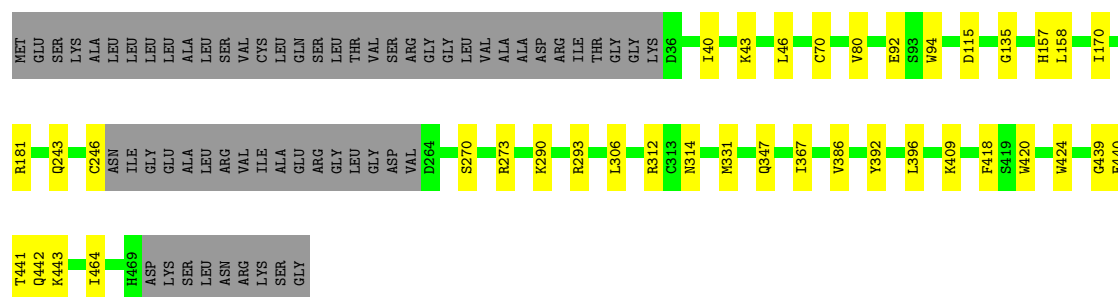
- Molecule 1: Lipoprotein lipase

Chain R: 79% 8% 13%



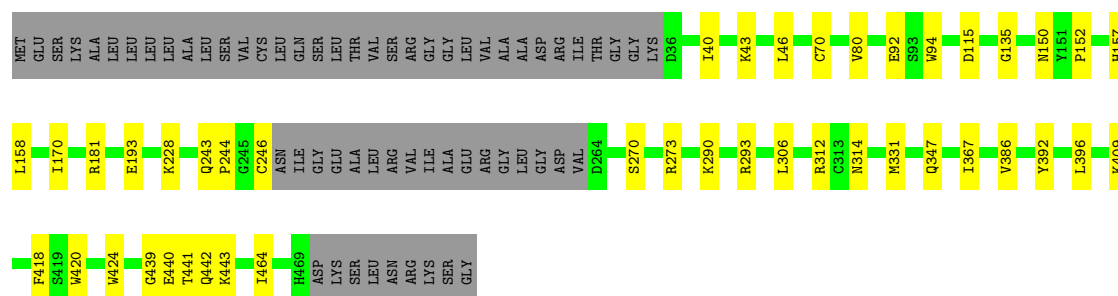
- Molecule 1: Lipoprotein lipase

Chain S:  79% 8% 13%



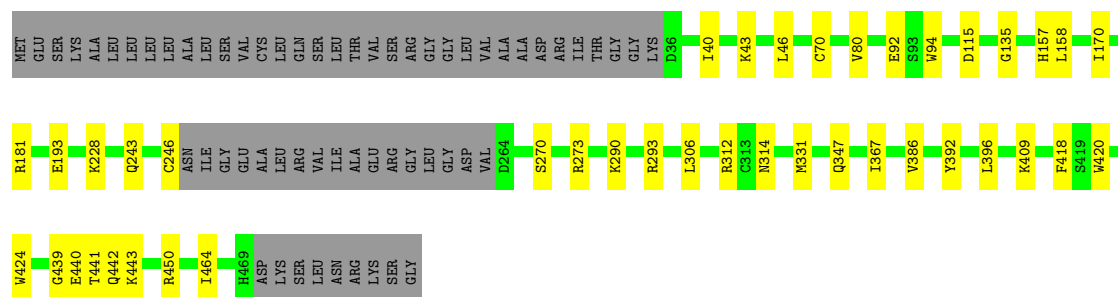
• Molecule 1: Lipoprotein lipase

Chain T:  78% 9% 13%



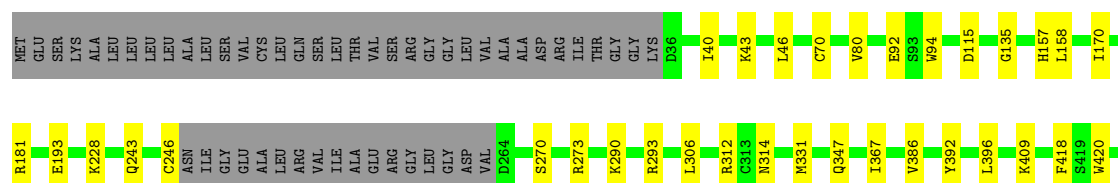
• Molecule 1: Lipoprotein lipase

Chain U:  79% 9% 13%



• Molecule 1: Lipoprotein lipase

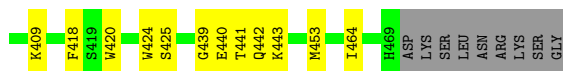
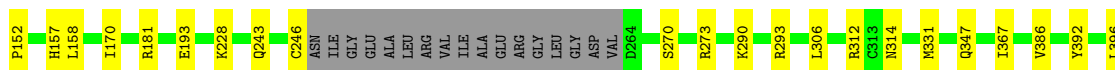
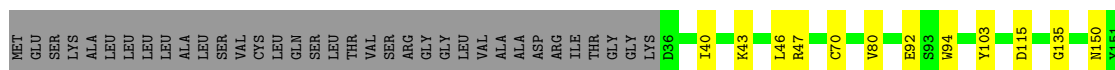
Chain a:  79% 8% 13%





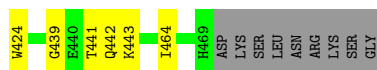
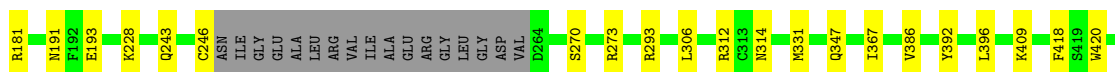
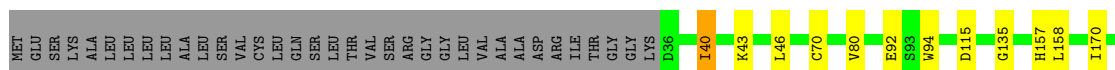
• Molecule 1: Lipoprotein lipase

Chain b: 78% 10% 13%



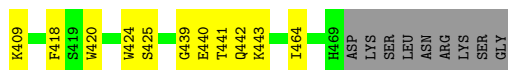
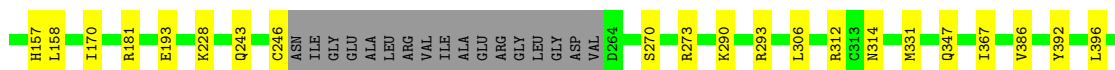
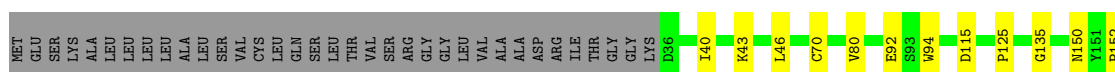
• Molecule 1: Lipoprotein lipase

Chain c: 79% 8% 13%



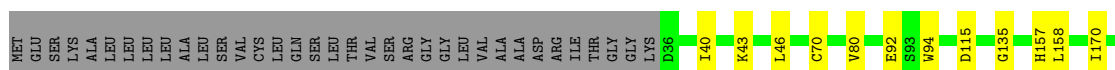
• Molecule 1: Lipoprotein lipase

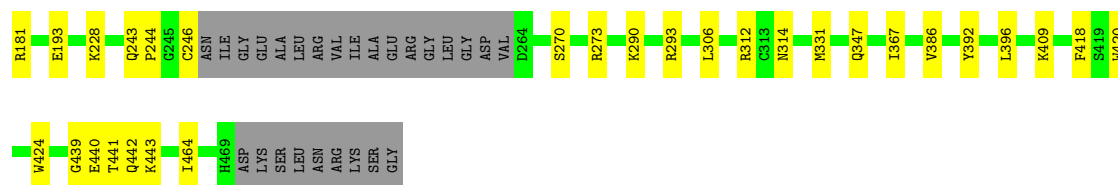
Chain d: 78% 9% 13%



• Molecule 1: Lipoprotein lipase

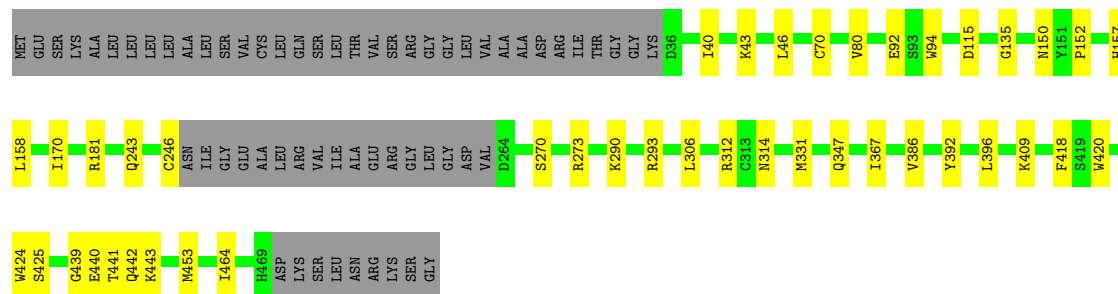
Chain e: 79% 9% 13%





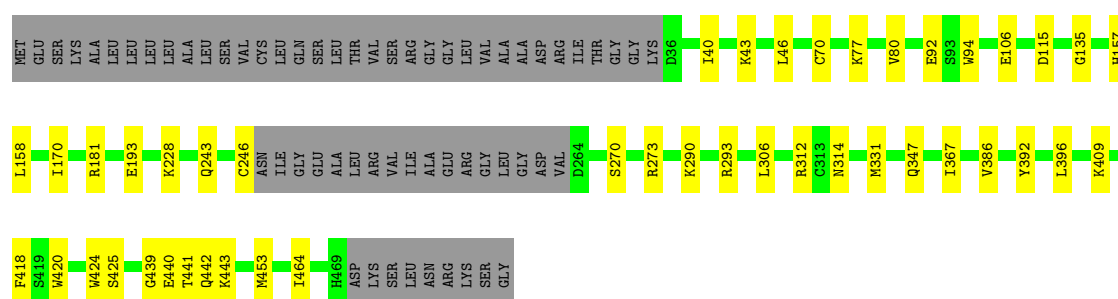
• Molecule 1: Lipoprotein lipase

Chain f: 78% 9% 13%



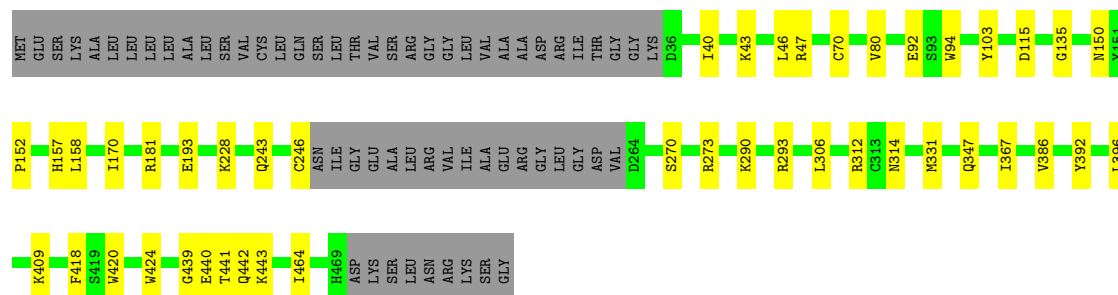
• Molecule 1: Lipoprotein lipase

Chain g: 78% 9% 13%



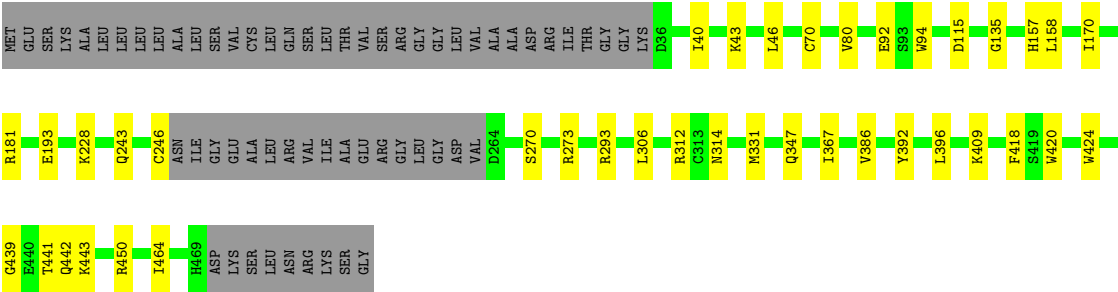
• Molecule 1: Lipoprotein lipase

Chain h: 78% 9% 13%



• Molecule 1: Lipoprotein lipase

Chain i: 79% 8% 13%



4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=130.05°, rise=10.88 Å, axial sym=C1	Depositor
Number of segments used	108911	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	46.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	45000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.19	0/3402	0.47	1/4607 (0.0%)
1	B	0.19	0/3402	0.47	1/4607 (0.0%)
1	C	0.19	0/3402	0.47	1/4607 (0.0%)
1	D	0.19	0/3402	0.47	1/4607 (0.0%)
1	E	0.19	0/3402	0.47	1/4607 (0.0%)
1	F	0.19	0/3402	0.47	1/4607 (0.0%)
1	G	0.19	0/3402	0.47	1/4607 (0.0%)
1	H	0.19	0/3402	0.47	1/4607 (0.0%)
1	I	0.19	0/3402	0.47	1/4607 (0.0%)
1	J	0.19	0/3402	0.47	1/4607 (0.0%)
1	K	0.19	0/3402	0.47	1/4607 (0.0%)
1	L	0.19	0/3402	0.47	1/4607 (0.0%)
1	M	0.19	0/3402	0.47	1/4607 (0.0%)
1	N	0.19	0/3402	0.47	1/4607 (0.0%)
1	O	0.19	0/3402	0.47	1/4607 (0.0%)
1	P	0.19	0/3402	0.47	1/4607 (0.0%)
1	Q	0.19	0/3402	0.47	1/4607 (0.0%)
1	R	0.19	0/3402	0.47	1/4607 (0.0%)
1	S	0.19	0/3402	0.47	1/4607 (0.0%)
1	T	0.19	0/3402	0.47	1/4607 (0.0%)
1	U	0.19	0/3402	0.47	1/4607 (0.0%)
1	a	0.19	0/3402	0.47	1/4607 (0.0%)
1	b	0.19	0/3402	0.47	1/4607 (0.0%)
1	c	0.19	0/3402	0.47	1/4607 (0.0%)
1	d	0.19	0/3402	0.47	1/4607 (0.0%)
1	e	0.19	0/3402	0.47	1/4607 (0.0%)
1	f	0.19	0/3402	0.47	1/4607 (0.0%)
1	g	0.19	0/3402	0.47	1/4607 (0.0%)
1	h	0.19	0/3402	0.47	1/4607 (0.0%)
1	i	0.19	0/3402	0.47	1/4607 (0.0%)
All	All	0.19	0/102060	0.47	30/138210 (0.0%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	424	TRP	CA-CB-CG	5.24	123.55	113.60
1	J	424	TRP	CA-CB-CG	5.24	123.55	113.60
1	L	424	TRP	CA-CB-CG	5.23	123.53	113.60
1	g	424	TRP	CA-CB-CG	5.22	123.53	113.60
1	d	424	TRP	CA-CB-CG	5.22	123.52	113.60
1	G	424	TRP	CA-CB-CG	5.22	123.51	113.60
1	M	424	TRP	CA-CB-CG	5.22	123.51	113.60
1	A	424	TRP	CA-CB-CG	5.21	123.50	113.60
1	D	424	TRP	CA-CB-CG	5.21	123.50	113.60
1	R	424	TRP	CA-CB-CG	5.21	123.50	113.60
1	U	424	TRP	CA-CB-CG	5.21	123.50	113.60
1	S	424	TRP	CA-CB-CG	5.21	123.49	113.60
1	e	424	TRP	CA-CB-CG	5.21	123.49	113.60
1	F	424	TRP	CA-CB-CG	5.20	123.48	113.60
1	I	424	TRP	CA-CB-CG	5.20	123.49	113.60
1	Q	424	TRP	CA-CB-CG	5.20	123.48	113.60
1	a	424	TRP	CA-CB-CG	5.20	123.48	113.60
1	h	424	TRP	CA-CB-CG	5.20	123.48	113.60
1	T	424	TRP	CA-CB-CG	5.20	123.47	113.60
1	c	424	TRP	CA-CB-CG	5.20	123.48	113.60
1	i	424	TRP	CA-CB-CG	5.20	123.47	113.60
1	E	424	TRP	CA-CB-CG	5.20	123.47	113.60
1	N	424	TRP	CA-CB-CG	5.19	123.47	113.60
1	f	424	TRP	CA-CB-CG	5.19	123.47	113.60
1	H	424	TRP	CA-CB-CG	5.19	123.46	113.60
1	C	424	TRP	CA-CB-CG	5.19	123.46	113.60
1	P	424	TRP	CA-CB-CG	5.19	123.46	113.60
1	B	424	TRP	CA-CB-CG	5.18	123.45	113.60
1	K	424	TRP	CA-CB-CG	5.18	123.45	113.60
1	b	424	TRP	CA-CB-CG	5.18	123.44	113.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3314	0	3229	22	0
1	B	3314	0	3229	19	0
1	C	3314	0	3229	18	0
1	D	3314	0	3229	20	0
1	E	3314	0	3229	17	0
1	F	3314	0	3229	19	0
1	G	3314	0	3229	21	0
1	H	3314	0	3229	20	0
1	I	3314	0	3229	20	0
1	J	3314	0	3229	19	0
1	K	3314	0	3229	18	0
1	L	3314	0	3229	17	0
1	M	3314	0	3229	21	0
1	N	3314	0	3229	22	0
1	O	3314	0	3229	19	0
1	P	3314	0	3229	21	0
1	Q	3314	0	3229	18	0
1	R	3314	0	3229	20	0
1	S	3314	0	3229	18	0
1	T	3314	0	3229	22	0
1	U	3314	0	3229	20	0
1	a	3314	0	3229	20	0
1	b	3314	0	3229	24	0
1	c	3314	0	3229	22	0
1	d	3314	0	3229	23	0
1	e	3314	0	3229	20	0
1	f	3314	0	3229	22	0
1	g	3314	0	3229	22	0
1	h	3314	0	3229	22	0
1	i	3314	0	3229	21	0
All	All	99420	0	96870	584	0

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 3.

All (584) 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:T:150:ASN:HD22	1:b:152:PRO:HG3	1.57	0.69
1:R:152:PRO:HG3	1:d:150:ASN:HD22	1.59	0.66
1:T:152:PRO:HG3	1:b:150:ASN:HD22	1.63	0.64
1:G:425:SER:HB2	1:a:453:MET:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:150:ASN:HD22	1:f:152:PRO:HG3	1.73	0.54
1:R:150:ASN:HD22	1:d:152:PRO:HG3	1.74	0.53
1:N:152:PRO:HG3	1:h:150:ASN:HD22	1.73	0.53
1:I:439:GLY:O	1:I:442:GLN:NE2	2.42	0.53
1:N:439:GLY:O	1:N:442:GLN:NE2	2.42	0.53
1:O:439:GLY:O	1:O:442:GLN:NE2	2.42	0.53
1:N:150:ASN:HD22	1:h:152:PRO:HG3	1.73	0.53
1:g:439:GLY:O	1:g:442:GLN:NE2	2.42	0.53
1:T:439:GLY:O	1:T:442:GLN:NE2	2.42	0.53
1:f:439:GLY:O	1:f:442:GLN:NE2	2.42	0.53
1:E:439:GLY:O	1:E:442:GLN:NE2	2.42	0.52
1:R:439:GLY:O	1:R:442:GLN:NE2	2.42	0.52
1:S:439:GLY:O	1:S:442:GLN:NE2	2.42	0.52
1:a:439:GLY:O	1:a:442:GLN:NE2	2.42	0.52
1:H:439:GLY:O	1:H:442:GLN:NE2	2.42	0.52
1:J:439:GLY:O	1:J:442:GLN:NE2	2.42	0.52
1:M:439:GLY:O	1:M:442:GLN:NE2	2.42	0.52
1:C:439:GLY:O	1:C:442:GLN:NE2	2.42	0.52
1:G:439:GLY:O	1:G:442:GLN:NE2	2.42	0.52
1:K:439:GLY:O	1:K:442:GLN:NE2	2.42	0.52
1:d:439:GLY:O	1:d:442:GLN:NE2	2.42	0.52
1:A:439:GLY:O	1:A:442:GLN:NE2	2.42	0.52
1:P:439:GLY:O	1:P:442:GLN:NE2	2.42	0.52
1:i:439:GLY:O	1:i:442:GLN:NE2	2.42	0.52
1:D:439:GLY:O	1:D:442:GLN:NE2	2.42	0.52
1:U:439:GLY:O	1:U:442:GLN:NE2	2.42	0.52
1:e:439:GLY:O	1:e:442:GLN:NE2	2.42	0.52
1:F:439:GLY:O	1:F:442:GLN:NE2	2.42	0.52
1:L:439:GLY:O	1:L:442:GLN:NE2	2.42	0.52
1:M:425:SER:HB2	1:f:453:MET:HG2	1.92	0.52
1:c:439:GLY:O	1:c:442:GLN:NE2	2.42	0.52
1:B:439:GLY:O	1:B:442:GLN:NE2	2.42	0.52
1:b:439:GLY:O	1:b:442:GLN:NE2	2.42	0.52
1:h:439:GLY:O	1:h:442:GLN:NE2	2.42	0.52
1:Q:439:GLY:O	1:Q:442:GLN:NE2	2.42	0.52
1:A:425:SER:HB2	1:g:453:MET:HG2	1.92	0.51
1:c:191:ASN:HD22	1:i:450:ARG:NH1	2.08	0.51
1:h:246:CYS:SG	1:h:270:SER:OG	2.67	0.51
1:A:306:LEU:HD12	1:A:347:GLN:HB2	1.93	0.51
1:G:306:LEU:HD12	1:G:347:GLN:HB2	1.93	0.51
1:M:92:GLU:OE1	1:M:94:TRP:NE1	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:306:LEU:HD12	1:P:347:GLN:HB2	1.93	0.51
1:e:306:LEU:HD12	1:e:347:GLN:HB2	1.93	0.51
1:e:246:CYS:SG	1:e:270:SER:OG	2.67	0.51
1:f:306:LEU:HD12	1:f:347:GLN:HB2	1.93	0.51
1:D:306:LEU:HD12	1:D:347:GLN:HB2	1.93	0.50
1:J:306:LEU:HD12	1:J:347:GLN:HB2	1.93	0.50
1:S:306:LEU:HD12	1:S:347:GLN:HB2	1.93	0.50
1:f:293:ARG:HD3	1:f:312:ARG:HG2	1.93	0.50
1:M:306:LEU:HD12	1:M:347:GLN:HB2	1.93	0.50
1:O:306:LEU:HD12	1:O:347:GLN:HB2	1.93	0.50
1:P:92:GLU:OE1	1:P:94:TRP:NE1	2.38	0.50
1:P:293:ARG:HD3	1:P:312:ARG:HG2	1.93	0.50
1:U:306:LEU:HD12	1:U:347:GLN:HB2	1.93	0.50
1:b:306:LEU:HD12	1:b:347:GLN:HB2	1.93	0.50
1:d:306:LEU:HD12	1:d:347:GLN:HB2	1.93	0.50
1:E:92:GLU:OE1	1:E:94:TRP:NE1	2.38	0.50
1:S:293:ARG:HD3	1:S:312:ARG:HG2	1.93	0.50
1:I:92:GLU:OE1	1:I:94:TRP:NE1	2.38	0.50
1:a:306:LEU:HD12	1:a:347:GLN:HB2	1.93	0.50
1:A:293:ARG:HD3	1:A:312:ARG:HG2	1.93	0.50
1:B:293:ARG:HD3	1:B:312:ARG:HG2	1.93	0.50
1:F:306:LEU:HD12	1:F:347:GLN:HB2	1.93	0.50
1:Q:306:LEU:HD12	1:Q:347:GLN:HB2	1.93	0.50
1:c:293:ARG:HD3	1:c:312:ARG:HG2	1.93	0.50
1:c:306:LEU:HD12	1:c:347:GLN:HB2	1.93	0.50
1:h:306:LEU:HD12	1:h:347:GLN:HB2	1.93	0.50
1:A:453:MET:HG2	1:g:425:SER:HB2	1.92	0.50
1:C:293:ARG:HD3	1:C:312:ARG:HG2	1.93	0.50
1:G:293:ARG:HD3	1:G:312:ARG:HG2	1.93	0.50
1:I:306:LEU:HD12	1:I:347:GLN:HB2	1.93	0.50
1:R:306:LEU:HD12	1:R:347:GLN:HB2	1.93	0.50
1:C:306:LEU:HD12	1:C:347:GLN:HB2	1.93	0.50
1:E:293:ARG:HD3	1:E:312:ARG:HG2	1.93	0.50
1:D:293:ARG:HD3	1:D:312:ARG:HG2	1.93	0.50
1:J:293:ARG:HD3	1:J:312:ARG:HG2	1.93	0.50
1:i:293:ARG:HD3	1:i:312:ARG:HG2	1.93	0.50
1:H:293:ARG:HD3	1:H:312:ARG:HG2	1.93	0.49
1:L:306:LEU:HD12	1:L:347:GLN:HB2	1.93	0.49
1:N:193:GLU:OE2	1:N:228:LYS:NZ	2.44	0.49
1:R:293:ARG:HD3	1:R:312:ARG:HG2	1.93	0.49
1:T:306:LEU:HD12	1:T:347:GLN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:293:ARG:HD3	1:d:312:ARG:HG2	1.93	0.49
1:K:293:ARG:HD3	1:K:312:ARG:HG2	1.93	0.49
1:b:293:ARG:HD3	1:b:312:ARG:HG2	1.93	0.49
1:K:306:LEU:HD12	1:K:347:GLN:HB2	1.93	0.49
1:L:293:ARG:HD3	1:L:312:ARG:HG2	1.93	0.49
1:T:293:ARG:HD3	1:T:312:ARG:HG2	1.93	0.49
1:U:293:ARG:HD3	1:U:312:ARG:HG2	1.93	0.49
1:i:306:LEU:HD12	1:i:347:GLN:HB2	1.93	0.49
1:G:92:GLU:OE1	1:G:94:TRP:NE1	2.38	0.49
1:H:306:LEU:HD12	1:H:347:GLN:HB2	1.93	0.49
1:M:293:ARG:HD3	1:M:312:ARG:HG2	1.93	0.49
1:N:306:LEU:HD12	1:N:347:GLN:HB2	1.93	0.49
1:O:293:ARG:HD3	1:O:312:ARG:HG2	1.93	0.49
1:a:293:ARG:HD3	1:a:312:ARG:HG2	1.93	0.49
1:g:306:LEU:HD12	1:g:347:GLN:HB2	1.93	0.49
1:G:453:MET:HG2	1:a:425:SER:HB2	1.92	0.49
1:I:193:GLU:OE2	1:I:228:LYS:NZ	2.44	0.49
1:N:293:ARG:HD3	1:N:312:ARG:HG2	1.93	0.49
1:g:293:ARG:HD3	1:g:312:ARG:HG2	1.93	0.49
1:I:293:ARG:HD3	1:I:312:ARG:HG2	1.93	0.49
1:T:193:GLU:OE2	1:T:228:LYS:NZ	2.44	0.49
1:h:293:ARG:HD3	1:h:312:ARG:HG2	1.93	0.49
1:B:306:LEU:HD12	1:B:347:GLN:HB2	1.93	0.49
1:D:193:GLU:OE2	1:D:228:LYS:NZ	2.45	0.49
1:E:306:LEU:HD12	1:E:347:GLN:HB2	1.93	0.49
1:Q:293:ARG:HD3	1:Q:312:ARG:HG2	1.93	0.49
1:T:92:GLU:OE1	1:T:94:TRP:NE1	2.38	0.49
1:h:193:GLU:OE2	1:h:228:LYS:NZ	2.44	0.49
1:E:193:GLU:OE2	1:E:228:LYS:NZ	2.44	0.49
1:e:293:ARG:HD3	1:e:312:ARG:HG2	1.93	0.49
1:F:293:ARG:HD3	1:F:312:ARG:HG2	1.93	0.48
1:J:193:GLU:OE2	1:J:228:LYS:NZ	2.45	0.48
1:c:92:GLU:OE1	1:c:94:TRP:NE1	2.38	0.48
1:M:193:GLU:OE2	1:M:228:LYS:NZ	2.45	0.48
1:i:193:GLU:OE2	1:i:228:LYS:NZ	2.44	0.48
1:K:193:GLU:OE2	1:K:228:LYS:NZ	2.44	0.48
1:P:193:GLU:OE2	1:P:228:LYS:NZ	2.44	0.48
1:c:157:HIS:CE1	1:c:181:ARG:HD3	2.49	0.48
1:g:92:GLU:OE1	1:g:94:TRP:NE1	2.38	0.48
1:i:157:HIS:CE1	1:i:181:ARG:HD3	2.49	0.48
1:A:92:GLU:OE1	1:A:94:TRP:NE1	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:HIS:CE1	1:F:181:ARG:HD3	2.49	0.48
1:L:157:HIS:CE1	1:L:181:ARG:HD3	2.49	0.48
1:P:157:HIS:CE1	1:P:181:ARG:HD3	2.49	0.48
1:R:157:HIS:CE1	1:R:181:ARG:HD3	2.49	0.48
1:F:246:CYS:SG	1:F:270:SER:OG	2.67	0.47
1:G:193:GLU:OE2	1:G:228:LYS:NZ	2.44	0.47
1:e:92:GLU:OE1	1:e:94:TRP:NE1	2.38	0.47
1:A:157:HIS:CE1	1:A:181:ARG:HD3	2.49	0.47
1:E:157:HIS:CE1	1:E:181:ARG:HD3	2.49	0.47
1:K:157:HIS:CE1	1:K:181:ARG:HD3	2.49	0.47
1:Q:157:HIS:CE1	1:Q:181:ARG:HD3	2.49	0.47
1:Q:246:CYS:SG	1:Q:270:SER:OG	2.67	0.47
1:d:157:HIS:CE1	1:d:181:ARG:HD3	2.49	0.47
1:e:157:HIS:CE1	1:e:181:ARG:HD3	2.49	0.47
1:B:157:HIS:CE1	1:B:181:ARG:HD3	2.49	0.47
1:D:77:LYS:NZ	1:D:106:GLU:OE1	2.39	0.47
1:J:157:HIS:CE1	1:J:181:ARG:HD3	2.49	0.47
1:U:157:HIS:CE1	1:U:181:ARG:HD3	2.49	0.47
1:i:92:GLU:OE1	1:i:94:TRP:NE1	2.38	0.47
1:G:157:HIS:CE1	1:G:181:ARG:HD3	2.49	0.47
1:b:157:HIS:CE1	1:b:181:ARG:HD3	2.49	0.47
1:h:157:HIS:CE1	1:h:181:ARG:HD3	2.49	0.47
1:T:157:HIS:CE1	1:T:181:ARG:HD3	2.49	0.47
1:g:157:HIS:CE1	1:g:181:ARG:HD3	2.49	0.47
1:B:92:GLU:OE1	1:B:94:TRP:NE1	2.38	0.47
1:C:92:GLU:OE1	1:C:94:TRP:NE1	2.38	0.47
1:H:157:HIS:CE1	1:H:181:ARG:HD3	2.49	0.47
1:N:157:HIS:CE1	1:N:181:ARG:HD3	2.49	0.47
1:O:157:HIS:CE1	1:O:181:ARG:HD3	2.49	0.47
1:a:193:GLU:OE2	1:a:228:LYS:NZ	2.45	0.47
1:e:193:GLU:OE2	1:e:228:LYS:NZ	2.44	0.47
1:A:193:GLU:OE2	1:A:228:LYS:NZ	2.45	0.47
1:D:157:HIS:CE1	1:D:181:ARG:HD3	2.49	0.47
1:L:193:GLU:OE2	1:L:228:LYS:NZ	2.44	0.47
1:a:157:HIS:CE1	1:a:181:ARG:HD3	2.49	0.47
1:I:246:CYS:SG	1:I:270:SER:OG	2.67	0.47
1:N:246:CYS:SG	1:N:270:SER:OG	2.67	0.47
1:g:246:CYS:SG	1:g:270:SER:OG	2.67	0.47
1:T:246:CYS:SG	1:T:270:SER:OG	2.67	0.47
1:I:453:MET:HG2	1:b:425:SER:HB2	1.96	0.46
1:F:193:GLU:OE2	1:F:228:LYS:NZ	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:191:ASN:HD22	1:i:450:ARG:HH12	1.63	0.46
1:f:157:HIS:CE1	1:f:181:ARG:HD3	2.49	0.46
1:C:246:CYS:SG	1:C:270:SER:OG	2.67	0.46
1:M:157:HIS:CE1	1:M:181:ARG:HD3	2.49	0.46
1:S:157:HIS:CE1	1:S:181:ARG:HD3	2.49	0.46
1:C:157:HIS:CE1	1:C:181:ARG:HD3	2.49	0.46
1:Q:193:GLU:OE2	1:Q:228:LYS:NZ	2.45	0.46
1:b:193:GLU:OE2	1:b:228:LYS:NZ	2.45	0.46
1:I:157:HIS:CE1	1:I:181:ARG:HD3	2.49	0.46
1:M:453:MET:HG2	1:f:425:SER:HB2	1.96	0.46
1:a:246:CYS:SG	1:a:270:SER:OG	2.67	0.46
1:O:246:CYS:SG	1:O:270:SER:OG	2.67	0.46
1:U:92:GLU:OE1	1:U:94:TRP:NE1	2.38	0.46
1:b:92:GLU:OE1	1:b:94:TRP:NE1	2.38	0.46
1:F:92:GLU:OE1	1:F:94:TRP:NE1	2.38	0.46
1:A:246:CYS:SG	1:A:270:SER:OG	2.67	0.45
1:Q:135:GLY:HA3	1:Q:170:ILE:HG23	1.98	0.45
1:d:92:GLU:OE1	1:d:94:TRP:NE1	2.38	0.45
1:H:246:CYS:SG	1:H:270:SER:OG	2.67	0.45
1:h:135:GLY:HA3	1:h:170:ILE:HG23	1.98	0.45
1:K:135:GLY:HA3	1:K:170:ILE:HG23	1.98	0.45
1:b:135:GLY:HA3	1:b:170:ILE:HG23	1.98	0.45
1:i:135:GLY:HA3	1:i:170:ILE:HG23	1.98	0.45
1:I:135:GLY:HA3	1:I:170:ILE:HG23	1.98	0.45
1:T:135:GLY:HA3	1:T:170:ILE:HG23	1.98	0.45
1:U:246:CYS:SG	1:U:270:SER:OG	2.67	0.45
1:d:246:CYS:SG	1:d:270:SER:OG	2.67	0.45
1:F:135:GLY:HA3	1:F:170:ILE:HG23	1.98	0.45
1:O:135:GLY:HA3	1:O:170:ILE:HG23	1.98	0.45
1:A:135:GLY:HA3	1:A:170:ILE:HG23	1.98	0.45
1:H:92:GLU:OE1	1:H:94:TRP:NE1	2.38	0.45
1:L:135:GLY:HA3	1:L:170:ILE:HG23	1.98	0.45
1:P:135:GLY:HA3	1:P:170:ILE:HG23	1.98	0.45
1:c:464:ILE:HD13	1:d:125:PRO:HB2	1.99	0.45
1:E:135:GLY:HA3	1:E:170:ILE:HG23	1.98	0.45
1:N:135:GLY:HA3	1:N:170:ILE:HG23	1.98	0.45
1:R:135:GLY:HA3	1:R:170:ILE:HG23	1.98	0.45
1:e:135:GLY:HA3	1:e:170:ILE:HG23	1.98	0.45
1:C:135:GLY:HA3	1:C:170:ILE:HG23	1.98	0.45
1:G:135:GLY:HA3	1:G:170:ILE:HG23	1.98	0.45
1:c:135:GLY:HA3	1:c:170:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:CYS:SG	1:B:270:SER:OG	2.67	0.45
1:a:135:GLY:HA3	1:a:170:ILE:HG23	1.98	0.45
1:F:43:LYS:NZ	1:F:115:ASP:OD2	2.51	0.45
1:I:425:SER:HB2	1:b:453:MET:HG2	1.98	0.45
1:S:135:GLY:HA3	1:S:170:ILE:HG23	1.98	0.45
1:b:246:CYS:SG	1:b:270:SER:OG	2.67	0.45
1:K:43:LYS:NZ	1:K:115:ASP:OD2	2.51	0.44
1:P:246:CYS:SG	1:P:270:SER:OG	2.67	0.44
1:T:43:LYS:NZ	1:T:115:ASP:OD2	2.51	0.44
1:U:135:GLY:HA3	1:U:170:ILE:HG23	1.98	0.44
1:b:43:LYS:NZ	1:b:115:ASP:OD2	2.51	0.44
1:c:43:LYS:NZ	1:c:115:ASP:OD2	2.51	0.44
1:d:135:GLY:HA3	1:d:170:ILE:HG23	1.98	0.44
1:A:450:ARG:NH1	1:F:191:ASN:HD22	2.15	0.44
1:B:43:LYS:NZ	1:B:115:ASP:OD2	2.50	0.44
1:B:193:GLU:OE2	1:B:228:LYS:NZ	2.45	0.44
1:D:43:LYS:NZ	1:D:115:ASP:OD2	2.51	0.44
1:G:43:LYS:NZ	1:G:115:ASP:OD2	2.51	0.44
1:I:43:LYS:NZ	1:I:115:ASP:OD2	2.50	0.44
1:M:135:GLY:HA3	1:M:170:ILE:HG23	1.98	0.44
1:R:43:LYS:NZ	1:R:115:ASP:OD2	2.51	0.44
1:f:135:GLY:HA3	1:f:170:ILE:HG23	1.98	0.44
1:H:43:LYS:NZ	1:H:115:ASP:OD2	2.51	0.44
1:a:43:LYS:NZ	1:a:115:ASP:OD2	2.51	0.44
1:a:92:GLU:OE1	1:a:94:TRP:NE1	2.38	0.44
1:B:135:GLY:HA3	1:B:170:ILE:HG23	1.98	0.44
1:D:243:GLN:HG3	1:D:273:ARG:HG3	2.00	0.44
1:E:409:LYS:HG2	1:E:464:ILE:HG12	2.00	0.44
1:J:135:GLY:HA3	1:J:170:ILE:HG23	1.98	0.44
1:O:409:LYS:HG2	1:O:464:ILE:HG12	2.00	0.44
1:g:135:GLY:HA3	1:g:170:ILE:HG23	1.98	0.44
1:G:418:PHE:HB3	1:G:420:TRP:HE3	1.83	0.44
1:J:43:LYS:NZ	1:J:115:ASP:OD2	2.51	0.44
1:O:43:LYS:NZ	1:O:115:ASP:OD2	2.51	0.44
1:O:386:VAL:HA	1:O:392:TYR:HE2	1.83	0.44
1:P:418:PHE:HB3	1:P:420:TRP:HE3	1.83	0.44
1:c:409:LYS:HG2	1:c:464:ILE:HG12	2.00	0.44
1:f:43:LYS:NZ	1:f:115:ASP:OD2	2.51	0.44
1:i:409:LYS:HG2	1:i:464:ILE:HG12	2.00	0.44
1:D:135:GLY:HA3	1:D:170:ILE:HG23	1.98	0.44
1:G:246:CYS:SG	1:G:270:SER:OG	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:243:GLN:HG3	1:H:273:ARG:HG3	2.00	0.44
1:M:43:LYS:NZ	1:M:115:ASP:OD2	2.51	0.44
1:N:386:VAL:HA	1:N:392:TYR:HE2	1.83	0.44
1:O:243:GLN:HG3	1:O:273:ARG:HG3	2.00	0.44
1:S:43:LYS:NZ	1:S:115:ASP:OD2	2.51	0.44
1:T:243:GLN:HG3	1:T:273:ARG:HG3	2.00	0.44
1:U:43:LYS:NZ	1:U:115:ASP:OD2	2.51	0.44
1:c:193:GLU:OE2	1:c:228:LYS:NZ	2.44	0.44
1:f:418:PHE:HB3	1:f:420:TRP:HE3	1.83	0.44
1:g:43:LYS:NZ	1:g:115:ASP:OD2	2.50	0.44
1:g:243:GLN:HG3	1:g:273:ARG:HG3	2.00	0.44
1:i:386:VAL:HA	1:i:392:TYR:HE2	1.83	0.44
1:B:409:LYS:HG2	1:B:464:ILE:HG12	2.00	0.44
1:E:386:VAL:HA	1:E:392:TYR:HE2	1.83	0.44
1:H:135:GLY:HA3	1:H:170:ILE:HG23	1.98	0.44
1:I:243:GLN:HG3	1:I:273:ARG:HG3	2.00	0.44
1:I:409:LYS:HG2	1:I:464:ILE:HG12	2.00	0.44
1:L:386:VAL:HA	1:L:392:TYR:HE2	1.83	0.44
1:M:243:GLN:HG3	1:M:273:ARG:HG3	2.00	0.44
1:N:409:LYS:HG2	1:N:464:ILE:HG12	2.00	0.44
1:P:43:LYS:NZ	1:P:115:ASP:OD2	2.51	0.44
1:Q:386:VAL:HA	1:Q:392:TYR:HE2	1.83	0.44
1:S:418:PHE:HB3	1:S:420:TRP:HE3	1.83	0.44
1:d:43:LYS:NZ	1:d:115:ASP:OD2	2.51	0.44
1:C:43:LYS:NZ	1:C:115:ASP:OD2	2.51	0.44
1:H:409:LYS:HG2	1:H:464:ILE:HG12	2.00	0.44
1:R:409:LYS:HG2	1:R:464:ILE:HG12	2.00	0.44
1:h:386:VAL:HA	1:h:392:TYR:HE2	1.83	0.44
1:C:409:LYS:HG2	1:C:464:ILE:HG12	2.00	0.44
1:K:409:LYS:HG2	1:K:464:ILE:HG12	2.00	0.44
1:L:409:LYS:HG2	1:L:464:ILE:HG12	2.00	0.44
1:O:92:GLU:OE1	1:O:94:TRP:NE1	2.38	0.44
1:T:409:LYS:HG2	1:T:464:ILE:HG12	2.00	0.44
1:T:418:PHE:HB3	1:T:420:TRP:HE3	1.83	0.44
1:a:243:GLN:HG3	1:a:273:ARG:HG3	2.00	0.44
1:a:386:VAL:HA	1:a:392:TYR:HE2	1.83	0.44
1:g:409:LYS:HG2	1:g:464:ILE:HG12	2.00	0.44
1:B:243:GLN:HG3	1:B:273:ARG:HG3	2.00	0.43
1:B:386:VAL:HA	1:B:392:TYR:HE2	1.83	0.43
1:F:409:LYS:HG2	1:F:464:ILE:HG12	2.00	0.43
1:N:43:LYS:NZ	1:N:115:ASP:OD2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:409:LYS:HG2	1:U:464:ILE:HG12	2.00	0.43
1:c:243:GLN:HG3	1:c:273:ARG:HG3	2.00	0.43
1:d:409:LYS:HG2	1:d:464:ILE:HG12	2.00	0.43
1:h:43:LYS:NZ	1:h:115:ASP:OD2	2.51	0.43
1:E:43:LYS:NZ	1:E:115:ASP:OD2	2.51	0.43
1:Q:43:LYS:NZ	1:Q:115:ASP:OD2	2.51	0.43
1:S:243:GLN:HG3	1:S:273:ARG:HG3	2.00	0.43
1:e:418:PHE:HB3	1:e:420:TRP:HE3	1.83	0.43
1:g:386:VAL:HA	1:g:392:TYR:HE2	1.83	0.43
1:i:43:LYS:NZ	1:i:115:ASP:OD2	2.51	0.43
1:A:43:LYS:NZ	1:A:115:ASP:OD2	2.51	0.43
1:C:386:VAL:HA	1:C:392:TYR:HE2	1.83	0.43
1:C:418:PHE:HB3	1:C:420:TRP:HE3	1.83	0.43
1:D:92:GLU:OE1	1:D:94:TRP:NE1	2.38	0.43
1:D:386:VAL:HA	1:D:392:TYR:HE2	1.83	0.43
1:D:418:PHE:HB3	1:D:420:TRP:HE3	1.83	0.43
1:J:246:CYS:SG	1:J:270:SER:OG	2.67	0.43
1:J:418:PHE:HB3	1:J:420:TRP:HE3	1.83	0.43
1:P:386:VAL:HA	1:P:392:TYR:HE2	1.83	0.43
1:Q:92:GLU:OE1	1:Q:94:TRP:NE1	2.38	0.43
1:b:418:PHE:HB3	1:b:420:TRP:HE3	1.83	0.43
1:f:243:GLN:HG3	1:f:273:ARG:HG3	2.00	0.43
1:F:418:PHE:HB3	1:F:420:TRP:HE3	1.83	0.43
1:H:193:GLU:OE2	1:H:228:LYS:NZ	2.45	0.43
1:I:386:VAL:HA	1:I:392:TYR:HE2	1.83	0.43
1:J:243:GLN:HG3	1:J:273:ARG:HG3	2.00	0.43
1:K:243:GLN:HG3	1:K:273:ARG:HG3	2.00	0.43
1:L:43:LYS:NZ	1:L:115:ASP:OD2	2.50	0.43
1:O:191:ASN:HD22	1:U:450:ARG:NH1	2.15	0.43
1:Q:409:LYS:HG2	1:Q:464:ILE:HG12	2.00	0.43
1:R:418:PHE:HB3	1:R:420:TRP:HE3	1.83	0.43
1:U:193:GLU:OE2	1:U:228:LYS:NZ	2.45	0.43
1:c:386:VAL:HA	1:c:392:TYR:HE2	1.83	0.43
1:e:43:LYS:NZ	1:e:115:ASP:OD2	2.51	0.43
1:e:243:GLN:HG3	1:e:273:ARG:HG3	2.00	0.43
1:g:418:PHE:HB3	1:g:420:TRP:HE3	1.83	0.43
1:J:386:VAL:HA	1:J:392:TYR:HE2	1.83	0.43
1:M:386:VAL:HA	1:M:392:TYR:HE2	1.83	0.43
1:T:386:VAL:HA	1:T:392:TYR:HE2	1.83	0.43
1:c:246:CYS:SG	1:c:270:SER:OG	2.67	0.43
1:h:409:LYS:HG2	1:h:464:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:418:PHE:HB3	1:i:420:TRP:HE3	1.83	0.43
1:A:386:VAL:HA	1:A:392:TYR:HE2	1.83	0.43
1:A:409:LYS:HG2	1:A:464:ILE:HG12	2.00	0.43
1:B:418:PHE:HB3	1:B:420:TRP:HE3	1.83	0.43
1:H:418:PHE:HB3	1:H:420:TRP:HE3	1.83	0.43
1:a:409:LYS:HG2	1:a:464:ILE:HG12	2.00	0.43
1:b:409:LYS:HG2	1:b:464:ILE:HG12	2.00	0.43
1:d:386:VAL:HA	1:d:392:TYR:HE2	1.83	0.43
1:e:386:VAL:HA	1:e:392:TYR:HE2	1.83	0.43
1:C:243:GLN:HG3	1:C:273:ARG:HG3	2.00	0.43
1:D:409:LYS:HG2	1:D:464:ILE:HG12	2.00	0.43
1:E:246:CYS:SG	1:E:270:SER:OG	2.67	0.43
1:F:243:GLN:HG3	1:F:273:ARG:HG3	2.00	0.43
1:H:386:VAL:HA	1:H:392:TYR:HE2	1.83	0.43
1:P:243:GLN:HG3	1:P:273:ARG:HG3	2.00	0.43
1:R:243:GLN:HG3	1:R:273:ARG:HG3	2.00	0.43
1:S:386:VAL:HA	1:S:392:TYR:HE2	1.83	0.43
1:S:409:LYS:HG2	1:S:464:ILE:HG12	2.00	0.43
1:T:314:ASN:HD22	1:T:331:MET:HE1	1.84	0.43
1:U:386:VAL:HA	1:U:392:TYR:HE2	1.83	0.43
1:c:418:PHE:HB3	1:c:420:TRP:HE3	1.83	0.43
1:i:243:GLN:HG3	1:i:273:ARG:HG3	2.00	0.43
1:D:246:CYS:SG	1:D:270:SER:OG	2.67	0.43
1:G:386:VAL:HA	1:G:392:TYR:HE2	1.83	0.43
1:I:314:ASN:HD22	1:I:331:MET:HE1	1.84	0.43
1:L:314:ASN:HD22	1:L:331:MET:HE1	1.84	0.43
1:P:314:ASN:HD22	1:P:331:MET:HE1	1.84	0.43
1:Q:243:GLN:HG3	1:Q:273:ARG:HG3	2.00	0.43
1:a:314:ASN:HD22	1:a:331:MET:HE1	1.84	0.43
1:e:409:LYS:HG2	1:e:464:ILE:HG12	2.00	0.43
1:f:386:VAL:HA	1:f:392:TYR:HE2	1.83	0.43
1:D:314:ASN:HD22	1:D:331:MET:HE1	1.84	0.43
1:E:243:GLN:HG3	1:E:273:ARG:HG3	2.00	0.43
1:G:409:LYS:HG2	1:G:464:ILE:HG12	2.00	0.43
1:M:246:CYS:SG	1:M:270:SER:OG	2.67	0.43
1:M:314:ASN:HD22	1:M:331:MET:HE1	1.84	0.43
1:M:409:LYS:HG2	1:M:464:ILE:HG12	2.00	0.43
1:P:80:VAL:HB	1:P:158:LEU:HD23	2.01	0.43
1:Q:418:PHE:HB3	1:Q:420:TRP:HE3	1.83	0.43
1:R:386:VAL:HA	1:R:392:TYR:HE2	1.83	0.43
1:c:80:VAL:HB	1:c:158:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:193:GLU:OE2	1:d:228:LYS:NZ	2.45	0.43
1:f:409:LYS:HG2	1:f:464:ILE:HG12	2.00	0.43
1:h:92:GLU:OE1	1:h:94:TRP:NE1	2.38	0.43
1:i:314:ASN:HD22	1:i:331:MET:HE1	1.84	0.43
1:E:314:ASN:HD22	1:E:331:MET:HE1	1.84	0.43
1:F:386:VAL:HA	1:F:392:TYR:HE2	1.83	0.43
1:L:80:VAL:HB	1:L:158:LEU:HD23	2.01	0.43
1:L:418:PHE:HB3	1:L:420:TRP:HE3	1.83	0.43
1:N:243:GLN:HG3	1:N:273:ARG:HG3	2.00	0.43
1:N:418:PHE:HB3	1:N:420:TRP:HE3	1.83	0.43
1:Q:314:ASN:HD22	1:Q:331:MET:HE1	1.84	0.43
1:a:418:PHE:HB3	1:a:420:TRP:HE3	1.83	0.43
1:e:80:VAL:HB	1:e:158:LEU:HD23	2.01	0.43
1:h:314:ASN:HD22	1:h:331:MET:HE1	1.84	0.43
1:A:243:GLN:HG3	1:A:273:ARG:HG3	2.00	0.42
1:E:80:VAL:HB	1:E:158:LEU:HD23	2.01	0.42
1:G:243:GLN:HG3	1:G:273:ARG:HG3	2.00	0.42
1:K:80:VAL:HB	1:K:158:LEU:HD23	2.01	0.42
1:P:152:PRO:HG3	1:f:150:ASN:HD22	1.84	0.42
1:P:409:LYS:HG2	1:P:464:ILE:HG12	2.00	0.42
1:b:80:VAL:HB	1:b:158:LEU:HD23	2.01	0.42
1:d:243:GLN:HG3	1:d:273:ARG:HG3	2.00	0.42
1:h:243:GLN:HG3	1:h:273:ARG:HG3	2.00	0.42
1:h:418:PHE:HB3	1:h:420:TRP:HE3	1.83	0.42
1:i:80:VAL:HB	1:i:158:LEU:HD23	2.01	0.42
1:A:80:VAL:HB	1:A:158:LEU:HD23	2.01	0.42
1:B:80:VAL:HB	1:B:158:LEU:HD23	2.01	0.42
1:F:80:VAL:HB	1:F:158:LEU:HD23	2.01	0.42
1:H:314:ASN:HD22	1:H:331:MET:HE1	1.84	0.42
1:J:80:VAL:HB	1:J:158:LEU:HD23	2.01	0.42
1:J:409:LYS:HG2	1:J:464:ILE:HG12	2.00	0.42
1:K:386:VAL:HA	1:K:392:TYR:HE2	1.83	0.42
1:O:418:PHE:HB3	1:O:420:TRP:HE3	1.83	0.42
1:R:80:VAL:HB	1:R:158:LEU:HD23	2.01	0.42
1:U:243:GLN:HG3	1:U:273:ARG:HG3	2.00	0.42
1:e:314:ASN:HD22	1:e:331:MET:HE1	1.84	0.42
1:E:418:PHE:HB3	1:E:420:TRP:HE3	1.83	0.42
1:F:314:ASN:HD22	1:F:331:MET:HE1	1.84	0.42
1:G:80:VAL:HB	1:G:158:LEU:HD23	2.01	0.42
1:G:314:ASN:HD22	1:G:331:MET:HE1	1.84	0.42
1:I:418:PHE:HB3	1:I:420:TRP:HE3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:243:GLN:HG3	1:L:273:ARG:HG3	2.00	0.42
1:U:314:ASN:HD22	1:U:331:MET:HE1	1.84	0.42
1:b:314:ASN:HD22	1:b:331:MET:HE1	1.84	0.42
1:A:418:PHE:HB3	1:A:420:TRP:HE3	1.83	0.42
1:B:314:ASN:HD22	1:B:331:MET:HE1	1.84	0.42
1:H:80:VAL:HB	1:H:158:LEU:HD23	2.01	0.42
1:M:418:PHE:HB3	1:M:420:TRP:HE3	1.83	0.42
1:O:367:ILE:HG21	1:O:396:LEU:HD11	2.02	0.42
1:Q:80:VAL:HB	1:Q:158:LEU:HD23	2.01	0.42
1:S:80:VAL:HB	1:S:158:LEU:HD23	2.01	0.42
1:S:246:CYS:SG	1:S:270:SER:OG	2.67	0.42
1:b:367:ILE:HG21	1:b:396:LEU:HD11	2.02	0.42
1:c:314:ASN:HD22	1:c:331:MET:HE1	1.84	0.42
1:d:314:ASN:HD22	1:d:331:MET:HE1	1.84	0.42
1:f:80:VAL:HB	1:f:158:LEU:HD23	2.01	0.42
1:f:246:CYS:SG	1:f:270:SER:OG	2.67	0.42
1:A:367:ILE:HG21	1:A:396:LEU:HD11	2.02	0.42
1:D:80:VAL:HB	1:D:158:LEU:HD23	2.01	0.42
1:I:367:ILE:HG21	1:I:396:LEU:HD11	2.02	0.42
1:K:418:PHE:HB3	1:K:420:TRP:HE3	1.83	0.42
1:M:80:VAL:HB	1:M:158:LEU:HD23	2.01	0.42
1:M:367:ILE:HG21	1:M:396:LEU:HD11	2.02	0.42
1:S:367:ILE:HG21	1:S:396:LEU:HD11	2.02	0.42
1:U:80:VAL:HB	1:U:158:LEU:HD23	2.01	0.42
1:U:418:PHE:HB3	1:U:420:TRP:HE3	1.83	0.42
1:a:367:ILE:HG21	1:a:396:LEU:HD11	2.02	0.42
1:b:386:VAL:HA	1:b:392:TYR:HE2	1.83	0.42
1:d:418:PHE:HB3	1:d:420:TRP:HE3	1.83	0.42
1:e:367:ILE:HG21	1:e:396:LEU:HD11	2.02	0.42
1:f:367:ILE:HG21	1:f:396:LEU:HD11	2.02	0.42
1:g:367:ILE:HG21	1:g:396:LEU:HD11	2.02	0.42
1:h:80:VAL:HB	1:h:158:LEU:HD23	2.01	0.42
1:A:46:LEU:HD23	1:A:70:CYS:HB3	2.02	0.42
1:A:314:ASN:HD22	1:A:331:MET:HE1	1.84	0.42
1:G:367:ILE:HG21	1:G:396:LEU:HD11	2.02	0.42
1:L:92:GLU:OE1	1:L:94:TRP:NE1	2.38	0.42
1:O:314:ASN:HD22	1:O:331:MET:HE1	1.84	0.42
1:R:246:CYS:SG	1:R:270:SER:OG	2.67	0.42
1:b:243:GLN:HG3	1:b:273:ARG:HG3	2.00	0.42
1:d:80:VAL:HB	1:d:158:LEU:HD23	2.01	0.42
1:F:367:ILE:HG21	1:F:396:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:46:LEU:HD23	1:J:70:CYS:HB3	2.02	0.42
1:J:314:ASN:HD22	1:J:331:MET:HE1	1.84	0.42
1:L:367:ILE:HG21	1:L:396:LEU:HD11	2.02	0.42
1:N:80:VAL:HB	1:N:158:LEU:HD23	2.01	0.42
1:N:314:ASN:HD22	1:N:331:MET:HE1	1.84	0.42
1:T:80:VAL:HB	1:T:158:LEU:HD23	2.01	0.42
1:a:80:VAL:HB	1:a:158:LEU:HD23	2.01	0.42
1:g:80:VAL:HB	1:g:158:LEU:HD23	2.01	0.42
1:h:367:ILE:HG21	1:h:396:LEU:HD11	2.02	0.42
1:C:80:VAL:HB	1:C:158:LEU:HD23	2.01	0.42
1:G:46:LEU:HD23	1:G:70:CYS:HB3	2.02	0.42
1:K:314:ASN:HD22	1:K:331:MET:HE1	1.84	0.42
1:Q:367:ILE:HG21	1:Q:396:LEU:HD11	2.02	0.42
1:R:367:ILE:HG21	1:R:396:LEU:HD11	2.02	0.42
1:U:367:ILE:HG21	1:U:396:LEU:HD11	2.02	0.42
1:d:367:ILE:HG21	1:d:396:LEU:HD11	2.02	0.42
1:e:46:LEU:HD23	1:e:70:CYS:HB3	2.02	0.42
1:C:47:ARG:O	1:C:103:TYR:OH	2.32	0.42
1:C:367:ILE:HG21	1:C:396:LEU:HD11	2.02	0.42
1:N:92:GLU:OE1	1:N:94:TRP:NE1	2.38	0.42
1:O:80:VAL:HB	1:O:158:LEU:HD23	2.02	0.42
1:R:314:ASN:HD22	1:R:331:MET:HE1	1.84	0.42
1:g:314:ASN:HD22	1:g:331:MET:HE1	1.84	0.42
1:D:46:LEU:HD23	1:D:70:CYS:HB3	2.02	0.42
1:F:46:LEU:HD23	1:F:70:CYS:HB3	2.02	0.42
1:I:80:VAL:HB	1:I:158:LEU:HD23	2.01	0.42
1:P:46:LEU:HD23	1:P:70:CYS:HB3	2.01	0.42
1:S:314:ASN:HD22	1:S:331:MET:HE1	1.84	0.42
1:f:314:ASN:HD22	1:f:331:MET:HE1	1.84	0.42
1:g:77:LYS:NZ	1:g:106:GLU:OE1	2.39	0.42
1:B:46:LEU:HD23	1:B:70:CYS:HB3	2.01	0.41
1:C:314:ASN:HD22	1:C:331:MET:HE1	1.84	0.41
1:K:367:ILE:HG21	1:K:396:LEU:HD11	2.02	0.41
1:D:367:ILE:HG21	1:D:396:LEU:HD11	2.02	0.41
1:H:46:LEU:HD23	1:H:70:CYS:HB3	2.02	0.41
1:S:92:GLU:OE1	1:S:94:TRP:NE1	2.38	0.41
1:U:46:LEU:HD23	1:U:70:CYS:HB3	2.02	0.41
1:d:46:LEU:HD23	1:d:70:CYS:HB3	2.02	0.41
1:O:46:LEU:HD23	1:O:70:CYS:HB3	2.02	0.41
1:c:367:ILE:HG21	1:c:396:LEU:HD11	2.02	0.41
1:N:46:LEU:HD23	1:N:70:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:441:THR:HG22	1:P:443:LYS:HG3	2.02	0.41
1:E:367:ILE:HG21	1:E:396:LEU:HD11	2.02	0.41
1:G:441:THR:HG22	1:G:443:LYS:HG3	2.02	0.41
1:I:46:LEU:HD23	1:I:70:CYS:HB3	2.02	0.41
1:J:367:ILE:HG21	1:J:396:LEU:HD11	2.02	0.41
1:K:46:LEU:HD23	1:K:70:CYS:HB3	2.02	0.41
1:N:77:LYS:NZ	1:N:106:GLU:OE1	2.39	0.41
1:R:243:GLN:HA	1:R:244:PRO:HD3	1.94	0.41
1:S:46:LEU:HD23	1:S:70:CYS:HB3	2.02	0.41
1:a:46:LEU:HD23	1:a:70:CYS:HB3	2.02	0.41
1:b:47:ARG:O	1:b:103:TYR:OH	2.32	0.41
1:c:46:LEU:HD23	1:c:70:CYS:HB3	2.02	0.41
1:e:243:GLN:HA	1:e:244:PRO:HD3	1.93	0.41
1:h:46:LEU:HD23	1:h:70:CYS:HB3	2.02	0.41
1:A:441:THR:HG22	1:A:443:LYS:HG3	2.02	0.41
1:Q:46:LEU:HD23	1:Q:70:CYS:HB3	2.02	0.41
1:e:441:THR:HG22	1:e:443:LYS:HG3	2.02	0.41
1:f:46:LEU:HD23	1:f:70:CYS:HB3	2.02	0.41
1:g:46:LEU:HD23	1:g:70:CYS:HB3	2.01	0.41
1:E:46:LEU:HD23	1:E:70:CYS:HB3	2.02	0.41
1:h:47:ARG:O	1:h:103:TYR:OH	2.32	0.41
1:i:367:ILE:HG21	1:i:396:LEU:HD11	2.02	0.41
1:B:367:ILE:HG21	1:B:396:LEU:HD11	2.02	0.41
1:F:441:THR:HG22	1:F:443:LYS:HG3	2.02	0.41
1:H:367:ILE:HG21	1:H:396:LEU:HD11	2.02	0.41
1:J:441:THR:HG22	1:J:443:LYS:HG3	2.02	0.41
1:M:46:LEU:HD23	1:M:70:CYS:HB3	2.01	0.41
1:M:441:THR:HG22	1:M:443:LYS:HG3	2.03	0.41
1:N:367:ILE:HG21	1:N:396:LEU:HD11	2.02	0.41
1:P:367:ILE:HG21	1:P:396:LEU:HD11	2.02	0.41
1:T:46:LEU:HD23	1:T:70:CYS:HB3	2.02	0.41
1:b:441:THR:HG22	1:b:443:LYS:HG3	2.03	0.41
1:h:441:THR:HG22	1:h:443:LYS:HG3	2.02	0.41
1:I:290:LYS:HD3	1:I:440:GLU:HG3	2.03	0.41
1:M:290:LYS:HD3	1:M:440:GLU:HG3	2.03	0.41
1:N:290:LYS:HD3	1:N:440:GLU:HG3	2.03	0.41
1:P:290:LYS:HD3	1:P:440:GLU:HG3	2.03	0.41
1:Q:441:THR:HG22	1:Q:443:LYS:HG3	2.02	0.41
1:R:46:LEU:HD23	1:R:70:CYS:HB3	2.02	0.41
1:T:243:GLN:HA	1:T:244:PRO:HD3	1.94	0.41
1:T:290:LYS:HD3	1:T:440:GLU:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:367:ILE:HG21	1:T:396:LEU:HD11	2.02	0.41
1:b:46:LEU:HD23	1:b:70:CYS:HB3	2.02	0.41
1:c:40:ILE:H	1:c:40:ILE:HG13	1.77	0.41
1:f:92:GLU:OE1	1:f:94:TRP:NE1	2.38	0.41
1:f:441:THR:HG22	1:f:443:LYS:HG3	2.02	0.41
1:i:46:LEU:HD23	1:i:70:CYS:HB3	2.02	0.41
1:C:46:LEU:HD23	1:C:70:CYS:HB3	2.02	0.41
1:H:441:THR:HG22	1:H:443:LYS:HG3	2.02	0.41
1:J:290:LYS:HD3	1:J:440:GLU:HG3	2.03	0.41
1:K:92:GLU:OE1	1:K:94:TRP:NE1	2.38	0.41
1:K:453:MET:HG2	1:d:425:SER:HB2	2.03	0.41
1:N:441:THR:HG22	1:N:443:LYS:HG3	2.02	0.41
1:R:92:GLU:OE1	1:R:94:TRP:NE1	2.38	0.41
1:S:290:LYS:HD3	1:S:440:GLU:HG3	2.03	0.41
1:S:441:THR:HG22	1:S:443:LYS:HG3	2.02	0.41
1:f:290:LYS:HD3	1:f:440:GLU:HG3	2.03	0.41
1:g:290:LYS:HD3	1:g:440:GLU:HG3	2.03	0.41
1:C:290:LYS:HD3	1:C:440:GLU:HG3	2.03	0.40
1:K:441:THR:HG22	1:K:443:LYS:HG3	2.02	0.40
1:L:46:LEU:HD23	1:L:70:CYS:HB3	2.02	0.40
1:O:290:LYS:HD3	1:O:440:GLU:HG3	2.03	0.40
1:g:193:GLU:OE2	1:g:228:LYS:NZ	2.45	0.40
1:D:290:LYS:HD3	1:D:440:GLU:HG3	2.03	0.40
1:D:441:THR:HG22	1:D:443:LYS:HG3	2.02	0.40
1:G:290:LYS:HD3	1:G:440:GLU:HG3	2.03	0.40
1:H:290:LYS:HD3	1:H:440:GLU:HG3	2.03	0.40
1:J:92:GLU:OE1	1:J:94:TRP:NE1	2.38	0.40
1:L:441:THR:HG22	1:L:443:LYS:HG3	2.02	0.40
1:U:441:THR:HG22	1:U:443:LYS:HG3	2.02	0.40
1:i:441:THR:HG22	1:i:443:LYS:HG3	2.03	0.40
1:B:40:ILE:H	1:B:40:ILE:HG13	1.77	0.40
1:H:224:ILE:HG21	1:i:418:PHE:HE2	1.87	0.40
1:b:290:LYS:HD3	1:b:440:GLU:HG3	2.03	0.40
1:d:441:THR:HG22	1:d:443:LYS:HG3	2.03	0.40
1:e:290:LYS:HD3	1:e:440:GLU:HG3	2.03	0.40
1:i:246:CYS:SG	1:i:270:SER:OG	2.67	0.40
1:O:441:THR:HG22	1:O:443:LYS:HG3	2.02	0.40
1:T:441:THR:HG22	1:T:443:LYS:HG3	2.03	0.40
1:U:290:LYS:HD3	1:U:440:GLU:HG3	2.03	0.40
1:a:290:LYS:HD3	1:a:440:GLU:HG3	2.03	0.40
1:d:290:LYS:HD3	1:d:440:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:441:THR:HG22	1:g:443:LYS:HG3	2.03	0.40
1:h:290:LYS:HD3	1:h:440:GLU:HG3	2.03	0.40
1:A:290:LYS:HD3	1:A:440:GLU:HG3	2.03	0.40
1:B:441:THR:HG22	1:B:443:LYS:HG3	2.03	0.40
1:R:441:THR:HG22	1:R:443:LYS:HG3	2.02	0.40
1:c:441:THR:HG22	1:c:443:LYS:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	413/478 (86%)	378 (92%)	35 (8%)	0	100	100
1	B	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	C	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	D	413/478 (86%)	377 (91%)	36 (9%)	0	100	100
1	E	413/478 (86%)	380 (92%)	33 (8%)	0	100	100
1	F	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	G	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	H	413/478 (86%)	377 (91%)	36 (9%)	0	100	100
1	I	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	J	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	K	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	L	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	M	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	N	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	O	413/478 (86%)	379 (92%)	34 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	Q	413/478 (86%)	378 (92%)	35 (8%)	0	100	100
1	R	413/478 (86%)	378 (92%)	35 (8%)	0	100	100
1	S	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	T	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	U	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	a	413/478 (86%)	380 (92%)	33 (8%)	0	100	100
1	b	413/478 (86%)	378 (92%)	35 (8%)	0	100	100
1	c	413/478 (86%)	378 (92%)	35 (8%)	0	100	100
1	d	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	e	413/478 (86%)	380 (92%)	33 (8%)	0	100	100
1	f	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	g	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	h	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
1	i	413/478 (86%)	379 (92%)	34 (8%)	0	100	100
All	All	12390/14340 (86%)	11364 (92%)	1026 (8%)	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 PDB entries followed by that with respect to all EM entries.

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	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	B	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	C	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	D	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	E	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	F	365/413 (88%)	364 (100%)	1 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	H	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	I	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	J	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	K	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	L	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	M	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	N	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	O	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	P	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	Q	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	R	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	S	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	T	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	U	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	a	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	b	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	c	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	d	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	e	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	f	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	g	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	h	365/413 (88%)	364 (100%)	1 (0%)	86	84
1	i	365/413 (88%)	364 (100%)	1 (0%)	86	84
All	All	10950/12390 (88%)	10920 (100%)	30 (0%)	84	84

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ILE
1	B	40	ILE
1	C	40	ILE
1	D	40	ILE
1	E	40	ILE

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Mol	Chain	Res	Type
1	F	40	ILE
1	G	40	ILE
1	H	40	ILE
1	I	40	ILE
1	J	40	ILE
1	K	40	ILE
1	L	40	ILE
1	M	40	ILE
1	N	40	ILE
1	O	40	ILE
1	P	40	ILE
1	Q	40	ILE
1	R	40	ILE
1	S	40	ILE
1	T	40	ILE
1	U	40	ILE
1	a	40	ILE
1	b	40	ILE
1	c	40	ILE
1	d	40	ILE
1	e	40	ILE
1	f	40	ILE
1	g	40	ILE
1	h	40	ILE
1	i	40	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (232) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	123	HIS
1	A	166	HIS
1	A	191	ASN
1	A	232	HIS
1	A	265	GLN
1	A	276	HIS
1	A	314	ASN
1	A	338	GLN
1	B	166	HIS
1	B	191	ASN
1	B	265	GLN
1	B	276	HIS

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Mol	Chain	Res	Type
1	B	314	ASN
1	B	338	GLN
1	B	378	ASN
1	B	442	GLN
1	C	83	HIS
1	C	157	HIS
1	C	166	HIS
1	C	232	HIS
1	C	265	GLN
1	C	276	HIS
1	C	314	ASN
1	C	338	GLN
1	C	378	ASN
1	C	442	GLN
1	D	83	HIS
1	D	166	HIS
1	D	191	ASN
1	D	232	HIS
1	D	265	GLN
1	D	276	HIS
1	D	314	ASN
1	D	338	GLN
1	D	378	ASN
1	E	83	HIS
1	E	123	HIS
1	E	166	HIS
1	E	191	ASN
1	E	265	GLN
1	E	276	HIS
1	E	314	ASN
1	E	338	GLN
1	F	123	HIS
1	F	166	HIS
1	F	191	ASN
1	F	232	HIS
1	F	276	HIS
1	F	314	ASN
1	F	338	GLN
1	F	378	ASN
1	F	442	GLN
1	G	123	HIS
1	G	191	ASN

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Mol	Chain	Res	Type
1	G	265	GLN
1	G	276	HIS
1	G	314	ASN
1	G	338	GLN
1	G	378	ASN
1	H	123	HIS
1	H	166	HIS
1	H	191	ASN
1	H	276	HIS
1	H	314	ASN
1	H	338	GLN
1	H	378	ASN
1	I	83	HIS
1	I	123	HIS
1	I	191	ASN
1	I	265	GLN
1	I	276	HIS
1	I	314	ASN
1	I	338	GLN
1	I	378	ASN
1	J	83	HIS
1	J	191	ASN
1	J	265	GLN
1	J	276	HIS
1	J	314	ASN
1	J	338	GLN
1	K	83	HIS
1	K	166	HIS
1	K	191	ASN
1	K	265	GLN
1	K	276	HIS
1	K	314	ASN
1	K	338	GLN
1	K	378	ASN
1	L	83	HIS
1	L	166	HIS
1	L	191	ASN
1	L	232	HIS
1	L	276	HIS
1	L	314	ASN
1	L	338	GLN
1	L	378	ASN

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Mol	Chain	Res	Type
1	L	442	GLN
1	M	191	ASN
1	M	265	GLN
1	M	276	HIS
1	M	314	ASN
1	M	338	GLN
1	N	83	HIS
1	N	150	ASN
1	N	166	HIS
1	N	191	ASN
1	N	265	GLN
1	N	276	HIS
1	N	314	ASN
1	N	338	GLN
1	O	191	ASN
1	O	265	GLN
1	O	276	HIS
1	O	314	ASN
1	O	338	GLN
1	P	83	HIS
1	P	150	ASN
1	P	166	HIS
1	P	191	ASN
1	P	232	HIS
1	P	265	GLN
1	P	276	HIS
1	P	314	ASN
1	P	338	GLN
1	Q	83	HIS
1	Q	166	HIS
1	Q	232	HIS
1	Q	276	HIS
1	Q	314	ASN
1	Q	338	GLN
1	Q	378	ASN
1	R	150	ASN
1	R	166	HIS
1	R	191	ASN
1	R	232	HIS
1	R	265	GLN
1	R	276	HIS
1	R	314	ASN

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Mol	Chain	Res	Type
1	R	338	GLN
1	R	378	ASN
1	S	83	HIS
1	S	213	HIS
1	S	276	HIS
1	S	314	ASN
1	S	338	GLN
1	S	378	ASN
1	T	74	HIS
1	T	150	ASN
1	T	191	ASN
1	T	232	HIS
1	T	276	HIS
1	T	314	ASN
1	T	338	GLN
1	T	378	ASN
1	U	166	HIS
1	U	265	GLN
1	U	276	HIS
1	U	314	ASN
1	U	338	GLN
1	U	442	GLN
1	a	123	HIS
1	a	166	HIS
1	a	191	ASN
1	a	232	HIS
1	a	265	GLN
1	a	276	HIS
1	a	314	ASN
1	a	338	GLN
1	b	123	HIS
1	b	150	ASN
1	b	166	HIS
1	b	191	ASN
1	b	276	HIS
1	b	314	ASN
1	b	338	GLN
1	b	378	ASN
1	b	442	GLN
1	c	123	HIS
1	c	166	HIS
1	c	191	ASN

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Mol	Chain	Res	Type
1	c	232	HIS
1	c	265	GLN
1	c	276	HIS
1	c	314	ASN
1	c	338	GLN
1	c	378	ASN
1	d	74	HIS
1	d	150	ASN
1	d	166	HIS
1	d	265	GLN
1	d	276	HIS
1	d	314	ASN
1	d	338	GLN
1	d	378	ASN
1	e	83	HIS
1	e	123	HIS
1	e	166	HIS
1	e	265	GLN
1	e	276	HIS
1	e	314	ASN
1	e	338	GLN
1	f	123	HIS
1	f	150	ASN
1	f	191	ASN
1	f	276	HIS
1	f	314	ASN
1	f	338	GLN
1	f	378	ASN
1	g	123	HIS
1	g	276	HIS
1	g	314	ASN
1	g	338	GLN
1	g	378	ASN
1	h	83	HIS
1	h	123	HIS
1	h	150	ASN
1	h	166	HIS
1	h	191	ASN
1	h	276	HIS
1	h	314	ASN
1	h	338	GLN
1	h	378	ASN

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Mol	Chain	Res	Type
1	i	83	HIS
1	i	123	HIS
1	i	166	HIS
1	i	232	HIS
1	i	276	HIS
1	i	314	ASN
1	i	338	GLN
1	i	378	ASN
1	i	442	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20673. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit ⓘ

This section was not generated.