



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:14 PM UTC

PDB ID : 5KZP / pdb_00005kzp
Title : Structure of the HCV1-C1 Antibody-Antigen Complex
Authors : Piepenbrink, K.H.; Sundberg, E.J.
Deposited on : 2016-07-25
Resolution : 2.26 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

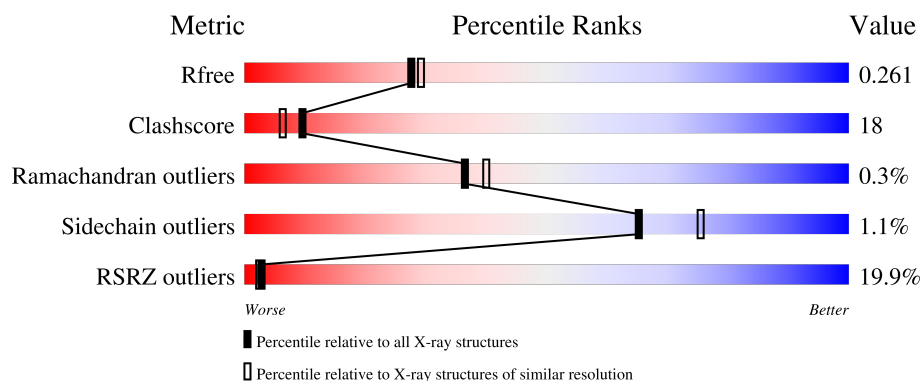
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	E	226	46% 61% 35% .
1	F	226	23% 83% 16%
1	G	226	19% 71% 27% .
1	H	226	8% 84% 15%
2	I	213	24% 70% 27% .

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Mol	Chain	Length	Quality of chain
2	J	213	
2	K	213	
2	L	213	
3	A	15	
3	B	15	
3	C	15	
3	D	15	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACT	E	301	-	-	X	-
4	ACT	F	301	-	-	X	-
4	ACT	G	301	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14615 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 HCV1-C1 Antibody Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	226	Total	C	N	O	S	0	2	0
			1742	1109	291	334	8			
1	E	226	Total	C	N	O	S	0	1	0
			1727	1100	286	333	8			
1	F	226	Total	C	N	O	S	0	1	0
			1734	1103	290	333	8			
1	G	226	Total	C	N	O	S	0	1	0
			1733	1100	292	333	8			

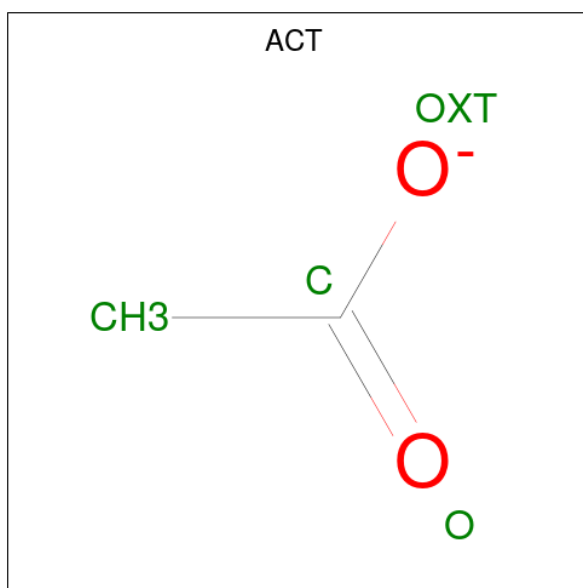
- Molecule 2 is a protein called HCV1-C1 Antibody Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	3	0
			1658	1035	285	334	4			
2	I	212	Total	C	N	O	S	0	4	0
			1661	1039	284	334	4			
2	J	212	Total	C	N	O	S	0	4	0
			1660	1036	284	336	4			
2	K	211	Total	C	N	O	S	0	1	0
			1625	1014	278	329	4			

- Molecule 3 is a protein called C1 Epitope.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	15	Total	C	N	O	S	0	0	0
			120	73	23	22	2			
3	B	15	Total	C	N	O	S	0	1	0
			125	76	24	23	2			
3	C	15	Total	C	N	O	S	0	1	0
			125	76	24	23	2			
3	D	15	Total	C	N	O	S	0	0	0
			120	73	23	22	2			

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total C O 4 2 2	0	0
4	E	1	Total C O 4 2 2	0	0
4	F	1	Total C O 4 2 2	0	0
4	G	1	Total C O 4 2 2	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	2	Total Ca 2 2	0	0
5	L	2	Total Ca 2 2	0	0
5	A	1	Total Ca 1 1	0	0
5	E	1	Total Ca 1 1	0	0
5	I	1	Total Ca 1 1	0	0
5	F	4	Total Ca 4 4	0	0
5	J	2	Total Ca 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	Ca 1	0	0
5	G	2	Total 2	Ca 2	0	0
5	K	5	Total 5	Ca 5	0	0

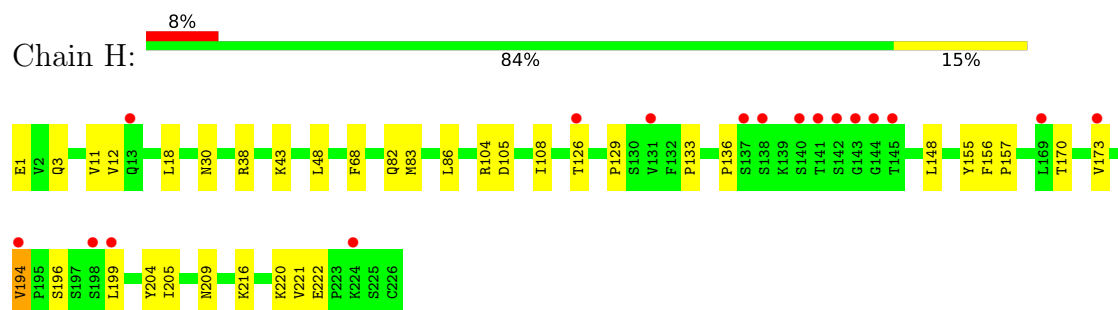
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	83	Total 83	O 83	0	0
6	L	85	Total 85	O 85	0	0
6	A	7	Total 7	O 7	0	0
6	E	48	Total 48	O 48	0	0
6	I	53	Total 53	O 53	0	0
6	B	10	Total 10	O 10	0	0
6	F	68	Total 68	O 68	0	0
6	J	76	Total 76	O 76	0	0
6	C	6	Total 6	O 6	0	0
6	G	60	Total 60	O 60	0	0
6	K	49	Total 49	O 49	0	0
6	D	3	Total 3	O 3	0	0

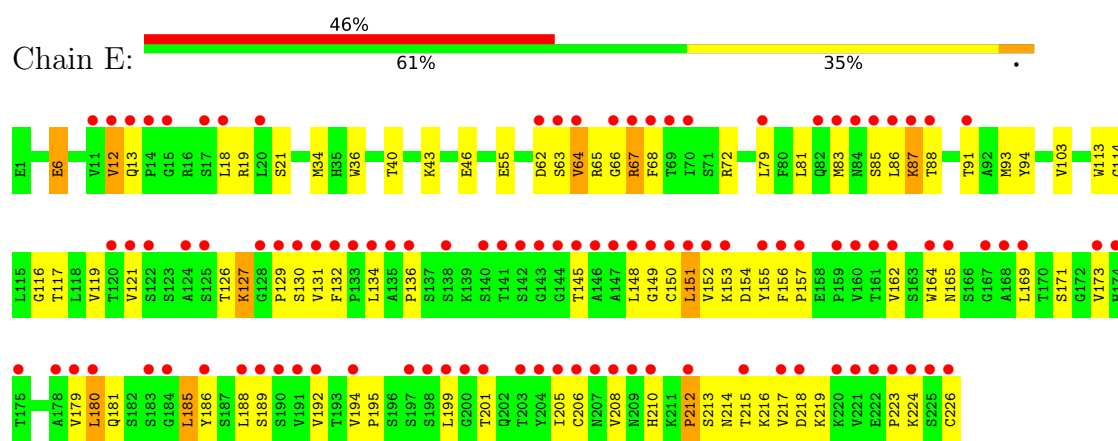
3 Residue-property plots [i](#)

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.

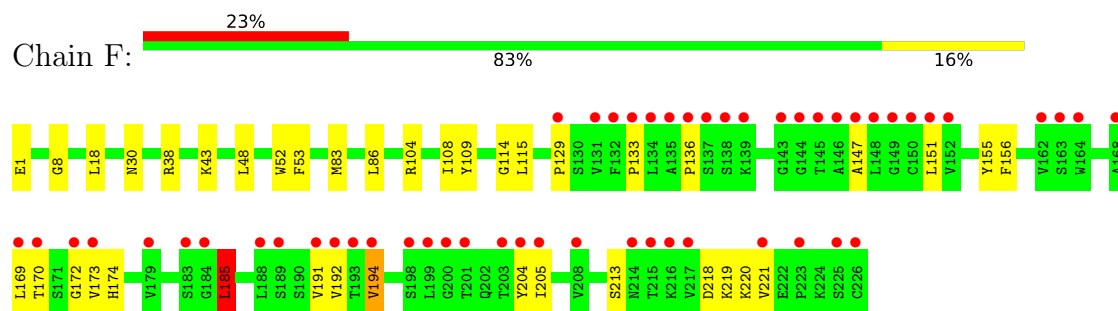
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



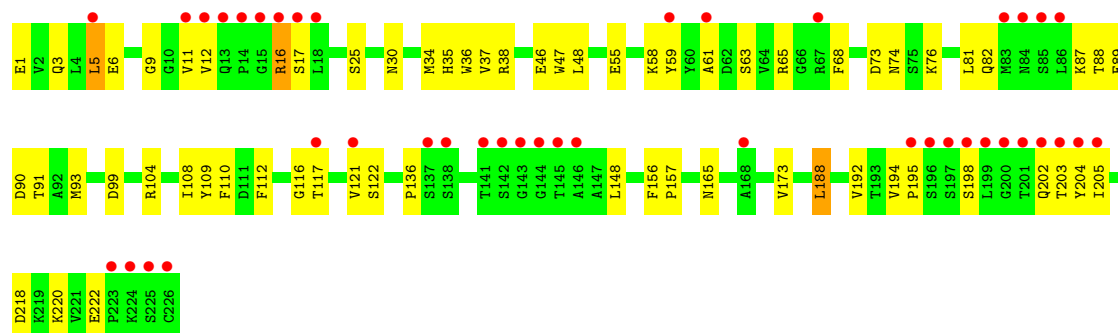
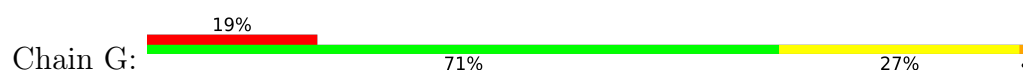
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



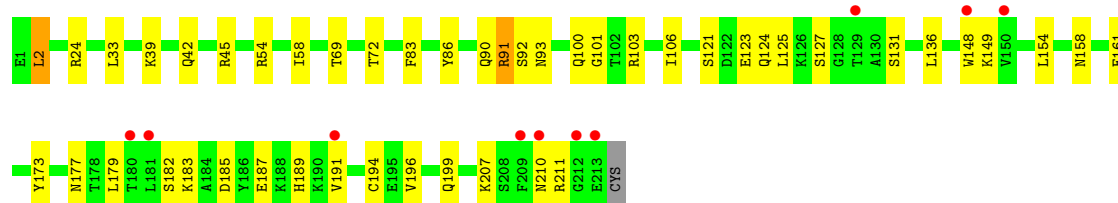
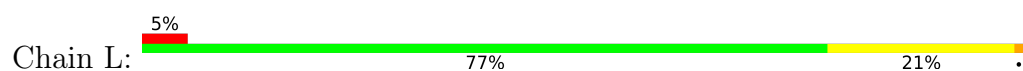
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



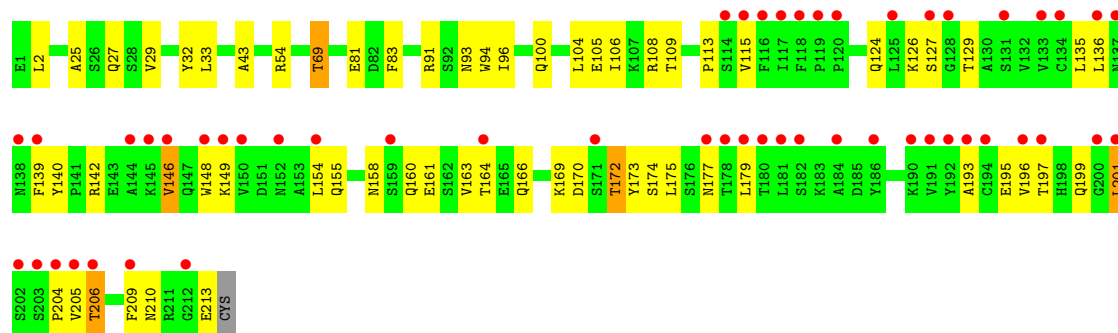
- Molecule 1: HCV1-C1 Antibody Fab Heavy Chain



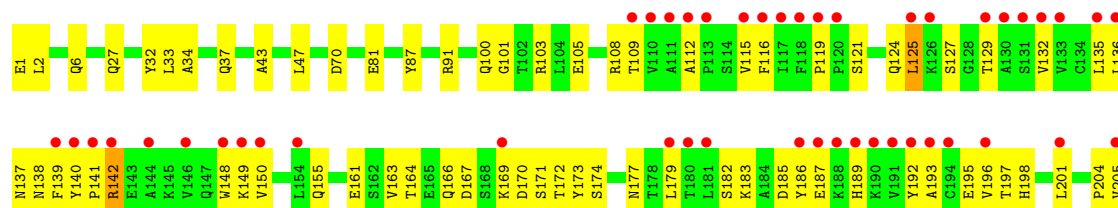
• Molecule 2: HCV1-C1 Antibody Fab Light Chain

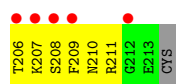


• Molecule 2: HCV1-C1 Antibody Fab Light Chain

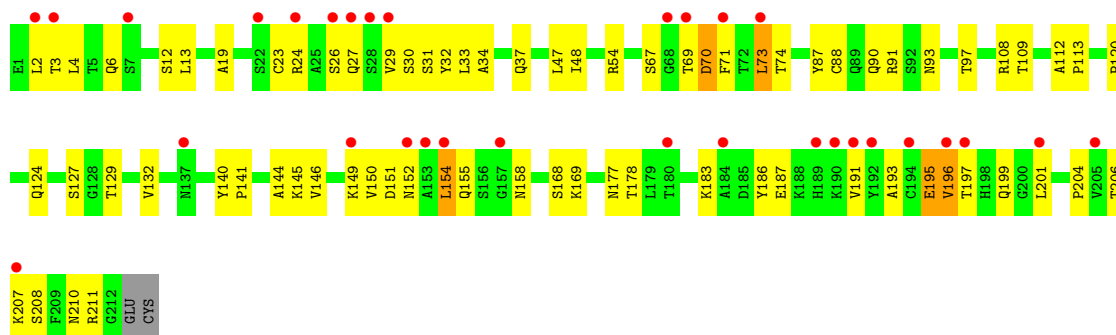


• Molecule 2: HCV1-C1 Antibody Fab Light Chain

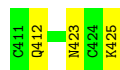
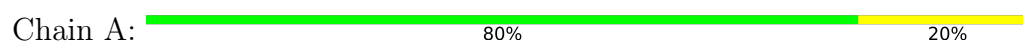




● Molecule 2: HCV1-C1 Antibody Fab Light Chain



● Molecule 3: C1 Epitope



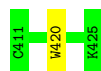
● Molecule 3: C1 Epitope



● Molecule 3: C1 Epitope



● Molecule 3: C1 Epitope



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	47.07Å 94.54Å 126.76Å 91.84° 94.95° 97.91°	Depositor
Resolution (Å)	29.49 – 2.26 29.49 – 2.26	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.49-2.26) 85.3 (29.49-2.26)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.26Å)	Xtriage
Refinement program	PHENIX 1.10pre_2124	Depositor
R, R_{free}	0.218 , 0.261 0.219 , 0.261	Depositor DCC
R_{free} test set	4685 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	35.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.1	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	0.93	EDS
Total number of atoms	14615	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	E	0.70	3/1774 (0.2%)	1.13	21/2416 (0.9%)
1	F	0.54	2/1780 (0.1%)	0.84	4/2422 (0.2%)
1	G	0.48	0/1779	0.81	4/2421 (0.2%)
1	H	0.63	4/1792 (0.2%)	0.79	4/2438 (0.2%)
2	I	0.53	0/1708	0.83	6/2320 (0.3%)
2	J	0.55	0/1707	0.82	3/2319 (0.1%)
2	K	0.49	0/1663	0.93	7/2263 (0.3%)
2	L	0.51	0/1702	0.76	2/2312 (0.1%)
3	A	0.55	0/122	0.71	0/163
3	B	0.55	0/130	0.69	0/174
3	C	0.41	0/130	0.68	0/174
3	D	0.45	0/122	0.59	0/163
All	All	0.56	9/14409 (0.1%)	0.86	51/19585 (0.3%)

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	E	0	1
2	J	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	194	VAL	C-O	13.31	1.33	1.24
1	E	6	GLU	CD-OE2	-11.20	1.04	1.25
1	H	222	GLU	CA-C	-10.26	1.42	1.52
1	F	194	VAL	C-O	9.64	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	222	GLU	C-O	9.04	1.33	1.24
1	H	194	VAL	C-O	-7.24	1.18	1.24
1	E	6	GLU	CD-OE1	-6.96	1.12	1.25
1	F	194	VAL	CA-C	-6.16	1.46	1.52
1	H	194	VAL	CA-C	5.42	1.58	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	73	LEU	CB-CG-CD2	-13.63	69.82	110.70
1	F	185	LEU	CD1-CG-CD2	-13.35	81.42	110.80
2	K	73	LEU	CB-CG-CD1	13.25	150.45	110.70
1	E	87	LYS	CB-CG-CD	12.49	140.03	111.30
1	H	222	GLU	O-C-N	-10.88	113.06	121.55
1	F	185	LEU	CB-CG-CD1	-10.52	79.15	110.70
1	F	185	LEU	CB-CG-CD2	10.49	142.18	110.70
2	K	73	LEU	CD1-CG-CD2	-10.38	87.97	110.80
1	E	67	ARG	CB-CG-CD	-10.22	87.80	111.30
1	E	185	LEU	CB-CG-CD2	-7.83	87.22	110.70
1	E	66	GLY	CA-C-N	-7.79	108.96	122.36
1	E	66	GLY	C-N-CA	-7.79	108.96	122.36
1	F	194	VAL	O-C-N	-7.67	116.35	121.72
2	I	195	GLU	CA-CB-CG	7.09	128.27	114.10
1	H	222	GLU	CA-C-N	6.99	126.95	120.03
1	H	222	GLU	C-N-CA	6.99	126.95	120.03
2	I	146	VAL	CG1-CB-CG2	6.90	125.97	110.80
1	E	173	VAL	CA-C-N	6.71	132.61	122.95
1	E	173	VAL	C-N-CA	6.71	132.61	122.95
1	E	151	LEU	CA-CB-CG	6.61	139.42	116.30
1	E	67	ARG	CG-CD-NE	6.47	126.25	112.00
1	E	12	VAL	CG1-CB-CG2	6.46	125.00	110.80
2	I	172	THR	OG1-CB-CG2	6.27	121.85	109.30
1	E	185	LEU	N-CA-C	6.09	119.12	109.50
1	E	113	TRP	CA-C-N	-6.02	116.31	122.27
1	E	113	TRP	C-N-CA	-6.02	116.31	122.27
2	I	172	THR	CA-CB-CG2	5.93	120.58	110.50
1	E	67	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	G	16	ARG	CA-C-N	5.74	130.92	123.00
1	G	16	ARG	C-N-CA	5.74	130.92	123.00
1	E	67	ARG	CD-NE-CZ	5.66	132.33	124.40
2	J	205	VAL	N-CA-C	5.65	115.99	107.80
2	L	2	LEU	CB-CG-CD1	-5.62	93.85	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	216	LYS	CD-CE-NZ	-5.61	93.94	111.90
2	I	201	LEU	CB-CG-CD2	-5.61	93.86	110.70
1	E	87	LYS	N-CA-C	5.57	118.66	109.85
2	I	206	THR	OG1-CB-CG2	5.57	120.44	109.30
1	G	5	LEU	CA-CB-CG	5.55	135.74	116.30
1	H	194	VAL	O-C-N	5.52	125.58	121.72
2	J	142	ARG	CA-C-N	-5.38	113.41	120.95
2	J	142	ARG	C-N-CA	-5.38	113.41	120.95
2	L	91	ARG	NE-CZ-NH1	-5.28	116.22	121.50
1	G	16	ARG	CA-CB-CG	5.24	124.59	114.10
2	K	196	VAL	CA-C-N	-5.21	115.65	122.99
2	K	196	VAL	C-N-CA	-5.21	115.65	122.99
2	K	195	GLU	N-CA-CB	5.20	118.73	110.57
2	K	73	LEU	CA-CB-CG	-5.15	98.28	116.30
1	E	150	CYS	CA-C-N	-5.09	115.70	122.72
1	E	150	CYS	C-N-CA	-5.09	115.70	122.72
1	E	87	LYS	CA-C-N	5.07	127.78	120.38
1	E	87	LYS	C-N-CA	5.07	127.78	120.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	67	ARG	Sidechain
2	J	125	LEU	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	E	1727	0	1681	96	0
1	F	1734	0	1705	48	0
1	G	1733	0	1696	78	0
1	H	1742	0	1709	27	0
2	I	1661	0	1626	66	0
2	J	1660	0	1617	80	0
2	K	1625	0	1567	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1658	0	1616	38	0
3	A	120	0	111	1	0
3	B	125	0	117	1	0
3	C	125	0	117	1	0
3	D	120	0	111	3	0
4	E	4	0	3	7	0
4	F	4	0	3	2	0
4	G	4	0	3	2	0
4	H	4	0	3	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	F	4	0	0	0	0
5	G	2	0	0	0	0
5	H	2	0	0	0	0
5	I	1	0	0	0	0
5	J	2	0	0	0	0
5	K	5	0	0	0	0
5	L	2	0	0	0	0
6	A	7	0	0	0	0
6	B	10	0	0	1	0
6	C	6	0	0	1	0
6	D	3	0	0	0	0
6	E	48	0	0	11	0
6	F	68	0	0	6	0
6	G	60	0	0	19	0
6	H	83	0	0	3	0
6	I	53	0	0	6	0
6	J	76	0	0	7	0
6	K	49	0	0	15	0
6	L	85	0	0	9	0
All	All	14615	0	13685	494	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 18.

All (494) 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)
2:I:170:ASP:OD2	2:I:172:THR:HG23	1.09	1.25
1:E:12:VAL:HG12	6:E:406:HOH:O	1.18	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:LEU:HD11	2:L:93:ASN:HB3	1.31	1.10
2:I:170:ASP:OD2	2:I:172:THR:CG2	1.99	1.08
1:F:205:ILE:HD12	1:F:220:LYS:HD2	1.33	1.07
2:K:195:GLU:HG3	2:K:206:THR:HG23	1.35	1.03
1:E:68:PHE:CD2	1:E:83:MET:HB2	1.93	1.02
2:J:195:GLU:OE1	2:J:206:THR:OG1	1.78	0.99
1:E:126:THR:O	1:E:127:LYS:HE2	1.61	0.99
1:F:205:ILE:HD11	1:F:218:ASP:HB3	1.41	0.98
1:E:145:THR:HA	1:E:195:PRO:HA	1.45	0.97
1:H:3:GLN:NE2	6:H:401:HOH:O	1.98	0.95
1:G:16:ARG:HD3	1:G:17:SER:H	1.27	0.95
2:K:191:VAL:O	6:K:401:HOH:O	1.85	0.95
2:I:155:GLN:HB3	2:I:158:ASN:HD21	1.32	0.95
2:K:191:VAL:HG12	2:K:210:ASN:HD22	1.32	0.94
2:J:149:LYS:HD3	2:J:193:ALA:HB3	1.50	0.94
1:G:46:GLU:OE2	6:G:401:HOH:O	1.86	0.94
2:K:186:TYR:O	2:K:211:ARG:NH2	2.01	0.94
2:K:145:LYS:HB3	2:K:197:THR:HG22	1.50	0.93
2:J:150:VAL:HG23	2:J:155:GLN:NE2	1.84	0.92
2:K:195:GLU:HG3	2:K:206:THR:CG2	2.00	0.91
2:I:149:LYS:HE3	2:I:193:ALA:HB3	1.53	0.90
2:I:169:LYS:NZ	6:I:401:HOH:O	2.04	0.89
2:L:2:LEU:HB3	6:L:468:HOH:O	1.75	0.87
1:G:16:ARG:CD	1:G:17:SER:H	1.87	0.87
1:G:36:TRP:O	6:G:402:HOH:O	1.93	0.86
1:E:180:LEU:O	2:I:160:GLN:NE2	2.07	0.86
2:K:195:GLU:CG	2:K:206:THR:HG23	2.04	0.85
1:G:198:SER:OG	6:G:403:HOH:O	1.94	0.85
2:K:24:ARG:NH2	2:K:70:ASP:OD1	2.09	0.85
1:G:90:ASP:OD1	6:G:404:HOH:O	1.95	0.85
1:E:165:ASN:HD21	1:E:169:LEU:HB3	1.40	0.85
2:L:2:LEU:CD1	2:L:93:ASN:HB3	2.07	0.84
2:J:150:VAL:CG2	2:J:155:GLN:NE2	2.40	0.84
1:E:64:VAL:HG13	1:E:68:PHE:CD1	2.13	0.84
3:C:411:CYS:N	6:C:601:HOH:O	2.10	0.84
1:E:6:GLU:OE1	1:E:114:GLY:HA3	1.78	0.84
2:K:32:TYR:HB3	2:K:91:ARG:HG3	1.60	0.84
1:F:205:ILE:HD12	1:F:220:LYS:CD	2.08	0.83
1:E:136:PRO:HB2	1:E:199:LEU:HD21	1.61	0.83
2:K:97:THR:O	6:K:403:HOH:O	1.96	0.82
2:J:142:ARG:HH21	2:J:163:VAL:HB	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:148:TRP:NE1	2:L:177:ASN:OD1	2.14	0.80
2:J:140:TYR:CD2	2:J:141:PRO:HA	2.16	0.80
1:E:205:ILE:HD11	1:E:218:ASP:HB3	1.63	0.80
2:J:148:TRP:NE1	2:J:177:ASN:OD1	2.14	0.80
2:K:6:GLN:HE22	2:K:87:TYR:HA	1.46	0.80
2:I:164:THR:HG22	2:I:174:SER:H	1.45	0.79
1:E:63:SER:O	1:E:64:VAL:HG23	1.82	0.79
2:J:150:VAL:HG23	2:J:155:GLN:HE21	1.46	0.78
2:K:129:THR:OG1	6:K:404:HOH:O	2.02	0.78
1:G:88:THR:HA	1:G:121:VAL:HG13	1.65	0.78
1:E:154:ASP:OD1	1:E:185:LEU:HD21	1.84	0.77
3:B:411:CYS:N	6:B:501:HOH:O	2.16	0.77
1:E:13:GLN:N	6:E:406:HOH:O	2.17	0.77
2:K:149:LYS:HZ3	2:K:193:ALA:HB3	1.50	0.77
1:E:64:VAL:CG1	1:E:68:PHE:CD1	2.67	0.76
2:K:191:VAL:HG12	2:K:210:ASN:ND2	2.01	0.76
1:G:3:GLN:O	6:G:405:HOH:O	2.04	0.76
2:K:168:SER:OG	6:K:405:HOH:O	2.04	0.75
1:H:1:GLU:N	6:H:402:HOH:O	2.19	0.75
2:I:108:ARG:NH1	2:I:109:THR:OG1	2.12	0.75
1:E:131:VAL:HG21	1:E:217:VAL:HG21	1.67	0.74
2:K:199:GLN:OE1	6:K:406:HOH:O	2.05	0.74
1:F:205:ILE:CD1	1:F:220:LYS:HD2	2.14	0.74
1:E:165:ASN:ND2	1:E:169:LEU:HB3	2.02	0.73
1:G:63:SER:O	6:G:406:HOH:O	2.05	0.73
2:I:106:ILE:H	2:I:166:GLN:HE22	1.34	0.73
2:L:161:GLU:HB3	2:L:177:ASN:HD22	1.54	0.72
2:I:2[B]:LEU:HD21	2:I:29:VAL:HG12	1.70	0.72
2:I:209:PHE:HZ	2:I:213:GLU:HB3	1.53	0.72
1:E:12:VAL:HG21	1:E:18:LEU:CD1	2.19	0.72
1:E:40:THR:HG23	1:E:43:LYS:H	1.55	0.72
2:J:140:TYR:HD2	2:J:141:PRO:CA	2.01	0.72
2:K:29:VAL:HG11	2:K:90:GLN:HG3	1.71	0.72
1:F:1:GLU:OE1	1:F:1:GLU:N	2.16	0.72
1:E:83:MET:HG3	1:E:86:LEU:HD21	1.72	0.71
1:G:194:VAL:HG12	1:G:195:PRO:HD2	1.72	0.71
2:K:90:GLN:NE2	2:K:93:ASN:H	1.87	0.71
1:G:16:ARG:HD3	1:G:17:SER:N	2.04	0.71
1:E:165:ASN:OD1	1:E:169:LEU:N	2.24	0.71
1:E:87:LYS:HG3	1:E:88:THR:H	1.54	0.70
1:G:16:ARG:NH2	6:G:408:HOH:O	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:116:GLY:O	6:E:402:HOH:O	2.08	0.70
1:F:156:PHE:HB2	1:F:185:LEU:HD11	1.73	0.70
2:J:108:ARG:HG3	2:J:140:TYR:CD1	2.25	0.70
1:G:87:LYS:NZ	1:G:89:GLU:OE1	2.24	0.70
1:E:91:THR:HG22	6:E:401:HOH:O	1.91	0.70
1:F:205:ILE:CD1	1:F:218:ASP:HB3	2.20	0.70
2:J:125:LEU:HD23	2:J:183:LYS:HG3	1.74	0.69
1:H:194:VAL:HG11	1:H:204:TYR:OH	1.92	0.69
2:K:149:LYS:NZ	2:K:193:ALA:HB3	2.07	0.69
1:F:213:SER:O	6:F:401:HOH:O	2.08	0.69
2:L:39:LYS:NZ	6:L:403:HOH:O	2.24	0.69
2:J:70[B]:ASP:OD1	6:J:401:HOH:O	2.10	0.69
1:F:133:PRO:HB3	1:F:219:LYS:HZ3	1.58	0.69
1:E:68:PHE:CG	1:E:83:MET:HB2	2.28	0.68
2:L:207:LYS:HE3	2:L:207:LYS:HA	1.75	0.68
1:E:224:LYS:NZ	6:E:404:HOH:O	2.14	0.68
1:F:205:ILE:HD11	1:F:218:ASP:CB	2.22	0.68
1:H:43:LYS:HA	1:H:43:LYS:HE2	1.76	0.68
2:L:207:LYS:O	6:L:401:HOH:O	2.11	0.67
1:G:63:SER:N	6:G:410:HOH:O	2.26	0.67
1:G:35:HIS:HD2	1:G:47:TRP:HE1	1.43	0.67
2:K:183:LYS:HA	2:K:186:TYR:HB3	1.76	0.67
2:I:149:LYS:CE	2:I:193:ALA:HB3	2.24	0.67
1:G:91:THR:O	6:G:407:HOH:O	2.12	0.67
1:G:9:GLY:H	1:G:117:THR:HG21	1.59	0.67
2:K:90:GLN:HE21	2:K:93:ASN:H	1.41	0.67
2:J:140:TYR:HD2	2:J:141:PRO:N	1.93	0.67
2:K:145:LYS:HB3	2:K:197:THR:CG2	2.25	0.67
2:K:150:VAL:HA	6:K:401:HOH:O	1.94	0.67
2:J:139:PHE:CE2	2:J:142:ARG:HA	2.30	0.66
1:E:86:LEU:HB3	1:E:121:VAL:HG21	1.78	0.66
2:I:209:PHE:CZ	2:I:213:GLU:HB3	2.30	0.66
2:K:91:ARG:NH1	6:K:402:HOH:O	1.91	0.66
2:K:195:GLU:CD	2:K:206:THR:HG23	2.20	0.66
1:H:133:PRO:HB3	1:H:221:VAL:HG12	1.78	0.66
2:K:144:ALA:O	6:K:407:HOH:O	2.14	0.65
1:F:104:ARG:H	4:F:301:ACT:H1	1.59	0.65
1:F:169:LEU:HD21	1:F:192:VAL:HG21	1.79	0.65
2:I:43:ALA:O	6:I:403:HOH:O	2.14	0.64
1:E:19:ARG:NH1	6:E:409:HOH:O	2.30	0.64
1:E:213:SER:O	1:E:215:THR:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2[A]:LEU:CD1	2:I:93:ASN:HB3	2.27	0.64
2:J:6:GLN:HE22	2:J:87:TYR:HA	1.63	0.63
1:G:104[A]:ARG:NH2	6:G:411:HOH:O	2.26	0.63
2:J:142:ARG:HH21	2:J:163:VAL:CB	2.09	0.63
2:K:27:GLN:O	6:K:408:HOH:O	2.15	0.63
2:K:108:ARG:NH1	2:K:109:THR:OG1	2.31	0.63
2:L:194:CYS:N	6:L:401:HOH:O	2.31	0.62
1:E:213:SER:O	1:E:213:SER:OG	2.16	0.62
2:J:149:LYS:H	2:J:149:LYS:HD2	1.64	0.62
2:I:161:GLU:HB3	2:I:177:ASN:HD22	1.65	0.62
2:J:108:ARG:NH1	2:J:109:THR:OG1	2.33	0.62
1:H:104:ARG:HE	4:E:301:ACT:H1	1.65	0.61
1:E:88:THR:O	1:E:91:THR:HG23	2.00	0.61
2:J:132:VAL:CG1	2:J:179:LEU:HB3	2.29	0.61
2:K:90:GLN:HB2	6:K:436:HOH:O	1.99	0.61
1:G:37:VAL:HG22	6:G:402:HOH:O	1.99	0.61
2:I:155:GLN:OE1	2:I:158:ASN:ND2	2.34	0.61
2:J:142:ARG:NH2	2:J:163:VAL:HB	2.13	0.61
2:I:136:LEU:HD13	2:I:175:LEU:HD22	1.81	0.61
2:J:140:TYR:CD2	2:J:141:PRO:CA	2.79	0.61
1:G:205:ILE:HD11	1:G:218:ASP:C	2.25	0.61
2:L:189:HIS:O	2:L:211:ARG:NH2	2.19	0.61
1:G:104[B]:ARG:H	4:G:301:ACT:H2	1.64	0.61
2:L:2:LEU:HD11	2:L:93:ASN:CB	2.21	0.61
2:J:163:VAL:HG13	2:J:174:SER:O	2.00	0.61
1:E:62:ASP:OD1	1:E:65:ARG:NH1	2.34	0.61
1:G:194:VAL:CG1	1:G:195:PRO:HD2	2.30	0.61
1:E:129:PRO:HB3	1:E:155:TYR:HB3	1.83	0.60
1:G:104[A]:ARG:H	4:G:301:ACT:H2	1.64	0.60
1:F:104:ARG:HG3	4:F:301:ACT:H3	1.82	0.60
1:F:174:HIS:HE1	2:J:138:ASN:OD1	1.83	0.60
2:I:2[B]:LEU:HD21	2:I:29:VAL:CG1	2.31	0.60
2:K:69:THR:HG22	6:K:408:HOH:O	2.01	0.60
2:K:4:LEU:HD12	6:K:403:HOH:O	2.02	0.59
1:G:202:GLN:OE1	1:G:203:THR:N	2.27	0.59
2:K:37:GLN:HB2	2:K:47:LEU:HD11	1.82	0.59
1:E:94:TYR:CD1	1:E:119:VAL:CG2	2.85	0.59
2:L:191:VAL:CG1	2:L:210:ASN:OD1	2.50	0.59
2:J:182:SER:OG	2:J:185:ASP:OD2	2.18	0.59
1:G:38:ARG:HD3	1:G:48:LEU:HD21	1.83	0.59
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:LYS:HD2	1:G:88:THR:N	2.19	0.58
1:H:196:SER:O	1:H:199:LEU:HD13	2.02	0.58
1:E:87:LYS:CG	1:E:88:THR:N	2.65	0.58
1:E:12:VAL:CG2	1:E:18:LEU:CD1	2.82	0.58
1:E:64:VAL:HG11	1:E:68:PHE:CD1	2.39	0.58
2:I:2[A]:LEU:HD11	2:I:93:ASN:HB3	1.84	0.58
2:J:132:VAL:HG12	2:J:179:LEU:HB3	1.86	0.58
1:G:87:LYS:HZ2	1:G:88:THR:HG22	1.68	0.58
1:E:87:LYS:HG3	1:E:88:THR:N	2.19	0.58
1:F:156:PHE:HB2	1:F:185:LEU:CD1	2.33	0.58
1:F:191:VAL:HG11	2:J:135:LEU:HD12	1.85	0.58
1:G:194:VAL:HG11	1:G:204:TYR:OH	2.04	0.58
2:J:149:LYS:HD2	2:J:149:LYS:N	2.19	0.57
2:I:105:GLU:HG2	2:I:106:ILE:N	2.19	0.57
2:I:139:PHE:C	2:I:172:THR:HG1	2.07	0.57
2:J:1:GLU:O	6:J:402:HOH:O	2.17	0.57
2:J:170:ASP:OD1	2:J:172:THR:HG22	2.04	0.57
1:G:12:VAL:O	1:G:121:VAL:HA	2.05	0.57
1:E:93:MET:HG2	6:E:403:HOH:O	2.04	0.56
2:I:100:GLN:O	6:I:404:HOH:O	2.17	0.56
1:G:112:PHE:HB3	6:G:435:HOH:O	2.03	0.56
2:K:120:PRO:HD3	2:K:132:VAL:HG22	1.87	0.56
2:I:155:GLN:HB3	2:I:158:ASN:ND2	2.14	0.56
1:H:108:ILE:HB	2:L:91:ARG:HD2	1.87	0.56
2:I:161:GLU:HB3	2:I:177:ASN:ND2	2.20	0.56
2:J:142:ARG:HD2	2:J:173:TYR:CE1	2.41	0.56
1:G:87:LYS:NZ	1:G:88:THR:HG22	2.20	0.56
1:F:43:LYS:NZ	6:F:406:HOH:O	2.35	0.56
2:K:177:ASN:HD22	2:K:178:THR:N	2.03	0.56
2:I:158:ASN:OD1	2:I:158:ASN:N	2.38	0.56
1:E:188:LEU:HD12	1:E:189:SER:N	2.21	0.56
1:G:198:SER:HB2	6:G:422:HOH:O	2.06	0.56
2:L:103:ARG:NH1	2:L:173:TYR:OH	2.36	0.55
1:E:132:PHE:CD1	2:I:124:GLN:HB2	2.41	0.55
2:I:113:PRO:HD2	2:I:201:LEU:CD1	2.35	0.55
2:J:150:VAL:HG21	2:J:155:GLN:NE2	2.20	0.55
2:L:199:GLN:HB2	6:L:466:HOH:O	2.06	0.55
1:E:103:VAL:H	4:E:301:ACT:CH3	2.19	0.55
1:E:156:PHE:CD1	1:E:157:PRO:HA	2.43	0.54
2:L:123:GLU:OE1	2:L:123:GLU:N	2.31	0.54
1:E:85:SER:O	1:E:85:SER:OG	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:TYR:N	1:E:185:LEU:HD11	2.23	0.54
2:K:183:LYS:HA	2:K:186:TYR:CB	2.37	0.54
1:E:12:VAL:O	1:E:121:VAL:HA	2.08	0.54
1:E:12:VAL:HG21	1:E:18:LEU:HD12	1.89	0.54
2:K:195:GLU:OE2	2:K:204:PRO:HB2	2.08	0.54
2:I:209:PHE:HZ	2:I:213:GLU:CB	2.18	0.54
1:F:170:THR:O	1:F:173:VAL:HG22	2.08	0.54
4:H:301:ACT:H2	4:E:301:ACT:OXT	2.08	0.54
1:E:87:LYS:CG	1:E:88:THR:H	2.21	0.54
2:L:90:GLN:OE1	2:L:92:SER:N	2.42	0.53
2:J:124:GLN:O	2:J:127:SER:N	2.36	0.53
1:F:129:PRO:HB3	1:F:155:TYR:HB3	1.91	0.53
1:G:35:HIS:HD2	1:G:47:TRP:NE1	2.05	0.53
1:G:194:VAL:HG12	6:G:422:HOH:O	2.07	0.53
2:K:3:THR:OG1	2:K:26:SER:HB3	2.08	0.53
2:I:113:PRO:HD2	2:I:201:LEU:HD12	1.91	0.53
2:K:73:LEU:HG	2:K:74:THR:N	2.23	0.53
2:I:164:THR:CG2	2:I:174:SER:H	2.20	0.53
2:J:139:PHE:HE2	2:J:142:ARG:HA	1.73	0.53
2:K:177:ASN:HD22	2:K:178:THR:H	1.53	0.53
1:F:83:MET:HE2	1:F:86:LEU:HD21	1.91	0.52
2:J:169:LYS:NZ	6:J:409:HOH:O	2.42	0.52
2:L:45[A]:ARG:NH1	6:L:403:HOH:O	2.41	0.52
1:E:121:VAL:N	6:E:401:HOH:O	2.00	0.52
2:I:196:VAL:HG12	2:I:205:VAL:O	2.09	0.52
1:E:179:VAL:O	1:E:186:TYR:HA	2.10	0.52
1:E:210:HIS:HD2	1:E:212:PRO:HD2	1.74	0.52
2:J:142:ARG:HH21	2:J:163:VAL:CG1	2.22	0.52
2:J:115:VAL:O	2:J:207:LYS:HG3	2.10	0.51
1:H:170:THR:O	1:H:173:VAL:HG22	2.09	0.51
1:E:134:LEU:HD21	1:E:151:LEU:HD22	1.91	0.51
1:H:11:VAL:HG21	1:H:157:PRO:HG3	1.93	0.51
1:F:205:ILE:CD1	1:F:220:LYS:CD	2.83	0.51
2:J:161:GLU:HB3	2:J:177:ASN:HD22	1.74	0.51
1:G:58:LYS:O	1:G:59:TYR:HD1	1.92	0.51
2:K:124:GLN:O	2:K:127:SER:OG	2.28	0.51
1:E:94:TYR:CE1	1:E:119:VAL:HG23	2.46	0.51
2:J:108:ARG:HG3	2:J:140:TYR:CE1	2.44	0.51
1:G:1:GLU:OE2	1:G:3:GLN:NE2	2.44	0.51
2:L:124:GLN:O	2:L:127:SER:OG	2.20	0.51
1:E:68:PHE:CE2	1:E:83:MET:HB2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:ARG:HB3	1:G:48:LEU:HD11	1.93	0.51
2:J:167[A]:ASP:OD2	2:J:169:LYS:HB2	2.10	0.51
2:L:131:SER:HA	2:L:179:LEU:O	2.11	0.51
1:F:83:MET:HB3	1:F:86:LEU:HD21	1.91	0.51
1:F:220:LYS:HD3	1:F:220:LYS:N	2.26	0.51
1:G:35:HIS:HE1	1:G:99:ASP:HB2	1.75	0.51
1:H:38:ARG:HD3	1:H:48:LEU:HD11	1.93	0.51
2:K:48:ILE:HD13	2:K:54:ARG:HA	1.93	0.51
1:E:94:TYR:CE1	1:E:119:VAL:CG2	2.93	0.50
2:I:108:ARG:NE	2:I:109:THR:O	2.41	0.50
1:G:87:LYS:HE3	1:G:89:GLU:HB2	1.92	0.50
2:L:149:LYS:HG2	2:L:154:LEU:HD23	1.92	0.50
1:F:219:LYS:NZ	1:F:221:VAL:HG22	2.26	0.50
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.91	0.50
1:G:25:SER:N	6:G:405:HOH:O	2.29	0.50
2:K:33:LEU:HD23	2:K:34:ALA:N	2.27	0.50
2:L:183:LYS:HE2	2:L:187:GLU:OE2	2.12	0.50
2:J:124:GLN:O	2:J:127:SER:HB2	2.12	0.50
2:K:4:LEU:HD13	2:K:88:CYS:SG	2.51	0.50
2:K:149:LYS:HZ3	2:K:193:ALA:CB	2.23	0.50
2:J:189:HIS:O	2:J:211:ARG:NH1	2.44	0.50
2:K:113:PRO:HD2	2:K:201:LEU:CD1	2.41	0.50
2:J:100:GLN:HG2	6:J:423:HOH:O	2.11	0.50
2:J:172:THR:HG23	6:J:413:HOH:O	2.11	0.50
2:I:115:VAL:HA	2:I:135:LEU:O	2.11	0.50
2:J:81:GLU:CD	2:J:81:GLU:H	2.20	0.50
1:F:147:ALA:HB3	2:J:116:PHE:HD2	1.78	0.49
1:F:205:ILE:HA	1:F:220:LYS:HA	1.94	0.49
1:G:87:LYS:HD2	1:G:87:LYS:C	2.37	0.49
1:F:205:ILE:HG13	1:F:219:LYS:C	2.38	0.49
1:G:173:VAL:HG22	1:G:192:VAL:CG1	2.42	0.49
2:L:42:GLN:OE1	6:L:402:HOH:O	2.20	0.49
2:L:182:SER:OG	2:L:185:ASP:OD1	2.29	0.49
2:J:2:LEU:HD23	2:J:2:LEU:N	2.26	0.49
1:G:108:ILE:HB	2:K:91:ARG:HD2	1.95	0.49
1:E:180:LEU:HD12	1:E:181:GLN:O	2.13	0.49
1:G:220:LYS:NZ	1:G:222:GLU:OE2	2.33	0.49
1:H:105:ASP:HB3	6:H:467:HOH:O	2.13	0.49
2:K:33:LEU:HD13	2:K:71:PHE:CG	2.48	0.49
1:E:162:VAL:HG22	1:E:208:VAL:HG22	1.94	0.49
2:J:119:PRO:HG3	2:J:209:PHE:CG	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:ASP:O	1:E:63:SER:OG	2.23	0.49
2:K:4:LEU:HD13	2:K:23:CYS:SG	2.53	0.48
1:E:68:PHE:HA	6:E:411:HOH:O	2.12	0.48
2:I:81:GLU:CD	2:I:81:GLU:H	2.21	0.48
2:J:6:GLN:NE2	2:J:101:GLY:H	2.10	0.48
1:E:6:GLU:HA	1:E:21:SER:O	2.14	0.48
1:E:46:GLU:OE1	6:E:407:HOH:O	2.20	0.48
1:E:103:VAL:H	4:E:301:ACT:H2	1.78	0.48
2:I:105:GLU:HG3	2:I:173:TYR:HH	1.77	0.48
1:G:59:TYR:HD2	3:D:420:TRP:HZ3	1.59	0.48
2:L:121:SER:HB2	2:L:123:GLU:OE1	2.14	0.48
1:E:55:GLU:OE2	1:E:72:ARG:O	2.32	0.48
1:E:208:VAL:HB	1:E:217:VAL:HG22	1.96	0.48
1:F:151:LEU:HD13	6:F:402:HOH:O	2.13	0.48
2:K:4:LEU:HD11	6:K:436:HOH:O	2.12	0.48
1:E:12:VAL:CG2	1:E:18:LEU:HD11	2.43	0.48
2:K:149:LYS:CD	2:K:193:ALA:HB3	2.43	0.48
2:K:193:ALA:HB2	2:K:208:SER:HB3	1.95	0.48
1:E:12:VAL:HG21	1:E:18:LEU:CG	2.44	0.48
1:G:61:ALA:HA	6:G:415:HOH:O	2.13	0.48
1:G:47:TRP:HA	6:G:402:HOH:O	2.13	0.47
1:F:133:PRO:HB3	1:F:219:LYS:NZ	2.26	0.47
1:F:133:PRO:HD2	2:J:121:SER:CB	2.44	0.47
2:J:2:LEU:HD22	2:J:27:GLN:HG2	1.95	0.47
1:H:133:PRO:HD2	2:L:121:SER:CB	2.44	0.47
1:F:8:GLY:O	1:F:18[B]:LEU:HD11	2.14	0.47
1:H:12:VAL:HG11	1:H:18:LEU:HG	1.96	0.47
3:A:423:ASN:OD1	3:A:425:LYS:NZ	2.47	0.47
1:G:87:LYS:HZ1	1:G:89:GLU:CD	2.21	0.47
1:E:93:MET:HE3	1:E:116:GLY:C	2.40	0.47
2:I:155:GLN:CB	2:I:158:ASN:HD21	2.17	0.47
1:G:109:TYR:CD1	2:K:34:ALA:HB2	2.50	0.47
2:I:148:TRP:NE1	2:I:177:ASN:OD1	2.35	0.47
1:G:30:ASN:ND2	1:G:74:ASN:HB3	2.29	0.47
2:I:146:VAL:HG21	2:I:177:ASN:ND2	2.30	0.47
2:I:193:ALA:HB1	2:I:206:THR:CG2	2.44	0.47
2:J:103[B]:ARG:HH12	2:J:166:GLN:HB2	1.79	0.47
1:G:194:VAL:HG12	1:G:195:PRO:CD	2.43	0.47
1:G:6:GLU:CD	1:G:116:GLY:H	2.22	0.47
1:G:68:PHE:HA	1:G:82:GLN:O	2.14	0.47
1:E:93:MET:HE3	1:E:117:THR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:PRO:HG3	1:E:148:LEU:HB3	1.97	0.47
2:K:149:LYS:CG	2:K:193:ALA:HB3	2.44	0.47
2:K:183:LYS:O	2:K:187:GLU:HG2	2.14	0.47
2:K:207:LYS:HD3	2:K:208:SER:H	1.80	0.46
1:F:194:VAL:HG11	1:F:204:TYR:CZ	2.49	0.46
2:J:108:ARG:CG	2:J:140:TYR:CD1	2.96	0.46
2:K:169:LYS:HG2	6:K:405:HOH:O	2.14	0.46
1:E:199:LEU:HG	1:E:223:PRO:HG3	1.98	0.46
1:H:204:TYR:O	1:H:205:ILE:HD13	2.15	0.46
1:E:36:TRP:CZ2	1:E:79:LEU:HD23	2.50	0.46
1:E:12:VAL:HG21	1:E:18:LEU:HG	1.98	0.46
1:F:115:LEU:HD12	1:F:115:LEU:H	1.81	0.46
1:E:64:VAL:HG11	1:E:68:PHE:HD1	1.79	0.46
2:I:25:ALA:O	2:I:69:THR:OG1	2.33	0.46
2:L:54:ARG:HD2	2:L:58:ILE:O	2.16	0.46
1:E:199:LEU:C	1:E:201:THR:H	2.23	0.46
2:I:2[A]:LEU:CD2	2:I:27:GLN:HG2	2.45	0.46
1:G:173:VAL:HG22	1:G:192:VAL:HG12	1.98	0.46
1:E:154:ASP:HA	1:E:185:LEU:HD11	1.98	0.46
1:F:219:LYS:HE3	1:F:219:LYS:HB3	1.75	0.46
2:J:135:LEU:CD2	2:J:137:ASN:HB2	2.45	0.46
1:F:52:TRP:CD1	1:F:53:PHE:H	2.34	0.45
2:K:154:LEU:HD12	2:K:154:LEU:H	1.80	0.45
2:I:83:PHE:CD1	2:I:104:LEU:HD22	2.51	0.45
2:J:197:THR:HG23	2:J:204:PRO:HG3	1.99	0.45
1:H:126:THR:HA	1:H:156:PHE:O	2.17	0.45
2:I:209:PHE:CD1	2:I:210:ASN:N	2.82	0.45
1:F:109:TYR:CD1	2:J:34:ALA:HB2	2.52	0.45
1:E:114:GLY:O	2:I:43:ALA:HB2	2.16	0.45
1:E:132:PHE:CE1	2:I:124:GLN:HB2	2.51	0.45
2:K:149:LYS:HE2	2:K:152:ASN:ND2	2.32	0.45
1:H:68:PHE:HA	1:H:82:GLN:O	2.17	0.45
1:H:104:ARG:HE	4:E:301:ACT:CH3	2.28	0.45
1:E:103:VAL:HG23	4:E:301:ACT:H3	1.99	0.45
2:I:136:LEU:HD22	2:I:175:LEU:HD13	1.98	0.45
2:J:124:GLN:HG2	2:J:129:THR:O	2.16	0.45
2:K:149:LYS:NZ	2:K:193:ALA:CB	2.77	0.45
2:L:123:GLU:H	2:L:123:GLU:CD	2.18	0.44
2:L:191:VAL:HG12	2:L:210:ASN:OD1	2.16	0.44
1:E:188:LEU:HD12	1:E:189:SER:H	1.81	0.44
1:F:108:ILE:HB	2:J:91:ARG:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:112:ALA:HB1	2:K:201:LEU:HD11	1.98	0.44
1:E:210:HIS:CD2	1:E:212:PRO:HD2	2.50	0.44
1:F:136:PRO:HD3	1:F:221:VAL:HG12	2.00	0.44
2:J:100:GLN:NE2	6:J:406:HOH:O	2.32	0.44
1:G:65:ARG:HA	6:G:442:HOH:O	2.16	0.44
1:G:165:ASN:OD1	1:G:205:ILE:HG22	2.18	0.44
1:E:13:GLN:O	6:E:406:HOH:O	2.21	0.44
2:J:32:TYR:HB3	2:J:91:ARG:HG3	2.00	0.44
2:J:33:LEU:HG	2:J:34:ALA:N	2.32	0.44
2:J:198:HIS:HB3	2:J:201:LEU:CD2	2.47	0.44
2:K:151:ASP:HA	2:K:191:VAL:HG23	1.99	0.44
2:I:94:TRP:C	2:I:96:ILE:HG13	2.41	0.44
1:F:38:ARG:HD3	1:F:48:LEU:HD11	1.99	0.44
1:G:47:TRP:CD1	6:G:402:HOH:O	2.71	0.44
2:K:29:VAL:O	2:K:31:SER:N	2.51	0.44
2:L:83:PHE:CZ	2:L:106:ILE:HD13	2.53	0.44
2:I:32:TYR:HB3	2:I:91:ARG:HG3	2.00	0.44
2:J:136:LEU:HD21	2:J:196:VAL:HG21	2.00	0.44
1:E:36:TRP:NE1	1:E:81:LEU:HB2	2.32	0.44
1:G:38:ARG:CD	1:G:48:LEU:HD21	2.47	0.44
1:G:205:ILE:HD11	1:G:218:ASP:HB3	1.99	0.44
2:I:113:PRO:HB3	2:I:139:PHE:HB3	2.00	0.43
1:H:136:PRO:HG3	1:H:148:LEU:HD22	2.00	0.43
2:L:72:THR:HG23	6:L:470:HOH:O	2.18	0.43
1:F:156:PHE:CB	1:F:185:LEU:HD11	2.46	0.43
1:F:219:LYS:HZ2	1:F:221:VAL:HG22	1.82	0.43
1:G:34:MET:HE3	1:G:34:MET:HB3	1.83	0.43
2:I:124:GLN:HG2	2:I:129:THR:O	2.18	0.43
2:K:4:LEU:HA	2:K:24:ARG:O	2.18	0.43
1:E:210:HIS:CE1	1:E:213:SER:HB3	2.53	0.43
2:I:124:GLN:O	2:I:127:SER:HB2	2.17	0.43
2:I:139:PHE:O	2:I:172:THR:OG1	2.18	0.43
2:I:149:LYS:N	6:I:407:HOH:O	2.40	0.43
1:G:35:HIS:CE1	1:G:99:ASP:HB2	2.53	0.43
1:G:61:ALA:O	1:G:65:ARG:HG2	2.18	0.43
2:K:140:TYR:CD1	2:K:141:PRO:HA	2.53	0.43
2:L:100[A]:GLN:HG2	6:L:442:HOH:O	2.17	0.43
2:I:126:LYS:HD2	2:I:126:LYS:O	2.18	0.43
2:I:172:THR:OG1	2:I:173:TYR:N	2.50	0.43
1:F:174:HIS:CE1	2:J:174:SER:OG	2.72	0.43
1:G:58:LYS:O	1:G:59:TYR:CD1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:GLY:N	6:F:407:HOH:O	2.35	0.43
2:J:149:LYS:HZ1	2:J:195:GLU:HB2	1.83	0.43
1:G:55:GLU:O	1:G:58:LYS:HE2	2.18	0.43
1:H:209:ASN:CG	1:H:216:LYS:HG2	2.44	0.43
2:I:197:THR:HG23	2:I:204:PRO:HG3	2.01	0.43
2:L:24:ARG:HA	2:L:69:THR:O	2.18	0.43
1:E:36:TRP:NE1	1:E:79:LEU:HD21	2.33	0.43
1:E:129:PRO:HA	1:E:154:ASP:O	2.19	0.43
2:J:193:ALA:HB1	2:J:206:THR:HG22	2.01	0.43
1:E:130:SER:N	1:E:153:LYS:O	2.52	0.43
1:E:226:CYS:SG	2:I:213:GLU:C	3.02	0.43
2:I:105:GLU:OE2	2:I:140:TYR:OH	2.27	0.43
1:G:11:VAL:HG21	1:G:157:PRO:HG3	2.00	0.43
2:J:167[A]:ASP:OD2	2:J:169:LYS:HE2	2.19	0.42
1:G:38:ARG:HE	1:G:46:GLU:HG2	1.83	0.42
1:G:59:TYR:HD2	3:D:420:TRP:CZ3	2.36	0.42
1:G:93:MET:HE3	1:G:116:GLY:C	2.44	0.42
1:H:148:LEU:HD13	1:H:221:VAL:HG21	2.01	0.42
2:I:113:PRO:HD2	2:I:201:LEU:HD11	2.02	0.42
2:L:136:LEU:HD11	2:L:196:VAL:HG11	2.01	0.42
1:H:129:PRO:HB3	1:H:155:TYR:HB3	2.00	0.42
1:F:1:GLU:N	6:F:413:HOH:O	2.53	0.42
1:H:133:PRO:HD2	2:L:121:SER:HB3	2.01	0.42
2:I:148:TRP:HB3	2:I:179:LEU:HD22	2.01	0.42
2:J:112:ALA:HB2	6:J:443:HOH:O	2.18	0.42
1:H:104:ARG:HH21	4:E:301:ACT:H1	1.85	0.42
2:L:86:TYR:O	2:L:101:GLY:HA2	2.20	0.42
2:I:142:ARG:HE	2:I:163:VAL:HG11	1.83	0.42
2:K:146:VAL:HG12	2:K:196:VAL:HG22	2.01	0.42
2:I:54:ARG:NH2	6:I:410:HOH:O	2.52	0.42
1:F:30:ASN:HB2	6:F:440:HOH:O	2.19	0.42
1:G:59:TYR:CD2	3:D:420:TRP:HZ3	2.36	0.42
1:G:136:PRO:HD3	1:G:148:LEU:HB3	2.01	0.42
2:K:149:LYS:HG3	2:K:193:ALA:HB3	2.00	0.42
1:G:35:HIS:CD2	1:G:110:PHE:HE2	2.38	0.42
2:J:125:LEU:HD21	2:J:186:TYR:CD2	2.55	0.42
1:F:173:VAL:HG12	1:F:192:VAL:HB	2.01	0.42
1:E:6:GLU:OE1	1:E:114:GLY:CA	2.60	0.41
1:E:126:THR:HG22	1:E:213:SER:HB2	2.02	0.41
1:G:36:TRP:NE1	1:G:81:LEU:HB2	2.35	0.41
2:J:115:VAL:O	2:J:116:PHE:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:SER:HB3	1:G:156:PHE:HZ	1.85	0.41
1:E:149:GLY:HA2	1:E:164:TRP:CH2	2.54	0.41
1:E:206:CYS:SG	1:E:219:LYS:HB3	2.61	0.41
2:I:193:ALA:HB1	2:I:206:THR:HG23	2.02	0.41
1:F:204:TYR:O	1:F:221:VAL:N	2.46	0.41
1:G:93:MET:HE3	1:G:117:THR:N	2.36	0.41
2:K:113:PRO:HD2	2:K:201:LEU:HD11	2.01	0.41
2:K:195:GLU:OE1	2:K:206:THR:HG23	2.20	0.41
2:L:158:ASN:OD1	2:L:158:ASN:N	2.53	0.41
1:E:154:ASP:C	1:E:185:LEU:HD11	2.45	0.41
2:J:142:ARG:HE	2:J:163:VAL:HG11	1.85	0.41
2:J:186:TYR:O	2:J:211:ARG:NH1	2.53	0.41
1:G:35:HIS:CD2	1:G:47:TRP:HE1	2.29	0.41
1:G:188:LEU:C	1:G:188:LEU:HD12	2.45	0.41
2:L:125:LEU:HA	2:L:125:LEU:HD23	1.77	0.41
1:E:34:MET:CB	1:E:79:LEU:HD13	2.51	0.41
1:E:152:VAL:N	1:E:188:LEU:O	2.41	0.41
1:E:215:THR:HG22	1:E:217:VAL:HG13	2.01	0.41
2:I:136:LEU:HB2	2:I:175:LEU:HB3	2.02	0.41
2:K:155:GLN:OE1	2:K:158:ASN:ND2	2.54	0.41
2:J:183:LYS:O	2:J:187:GLU:HG2	2.21	0.41
1:G:73:ASP:OD1	1:G:76:LYS:HG2	2.21	0.41
1:E:169:LEU:HD21	1:E:192:VAL:HG21	2.03	0.41
2:J:140:TYR:CD2	2:J:140:TYR:C	2.99	0.41
2:J:193:ALA:HB1	2:J:206:THR:CG2	2.51	0.41
2:K:197:THR:CG2	2:K:197:THR:O	2.69	0.41
2:J:142:ARG:HD2	2:J:173:TYR:CD1	2.56	0.41
2:J:193:ALA:HB2	2:J:208:SER:HB3	2.03	0.41
1:G:9:GLY:HA3	1:G:117:THR:HG22	2.03	0.41
2:K:19:ALA:O	2:K:74:THR:HA	2.20	0.41
2:K:207:LYS:HA	2:K:207:LYS:HE2	2.03	0.41
2:J:192:TYR:HB2	2:J:209:PHE:CZ	2.56	0.40
2:K:2:LEU:HD12	2:K:90:GLN:OE1	2.21	0.40
2:K:91:ARG:NH2	6:K:413:HOH:O	2.55	0.40
1:H:136:PRO:HG3	1:H:148:LEU:CD2	2.51	0.40
2:I:148:TRP:HE3	6:I:407:HOH:O	2.04	0.40
2:K:12:SER:O	2:K:13:LEU:HD23	2.21	0.40
1:F:114:GLY:O	2:J:43:ALA:HB2	2.21	0.40
1:E:129:PRO:CB	1:E:155:TYR:HB3	2.49	0.40
1:H:205:ILE:CD1	1:H:220:LYS:HG3	2.51	0.40

There are no symmetry-related clashes.

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	E	225/226 (100%)	212 (94%)	10 (4%)	3 (1%)	9	6
1	F	225/226 (100%)	216 (96%)	9 (4%)	0	100	100
1	G	225/226 (100%)	216 (96%)	9 (4%)	0	100	100
1	H	226/226 (100%)	217 (96%)	9 (4%)	0	100	100
2	I	214/213 (100%)	207 (97%)	7 (3%)	0	100	100
2	J	214/213 (100%)	205 (96%)	8 (4%)	1 (0%)	24	24
2	K	210/213 (99%)	199 (95%)	10 (5%)	1 (0%)	24	24
2	L	213/213 (100%)	208 (98%)	5 (2%)	0	100	100
3	A	13/15 (87%)	13 (100%)	0	0	100	100
3	B	14/15 (93%)	14 (100%)	0	0	100	100
3	C	14/15 (93%)	12 (86%)	2 (14%)	0	100	100
3	D	13/15 (87%)	13 (100%)	0	0	100	100
All	All	1806/1816 (99%)	1732 (96%)	69 (4%)	5 (0%)	36	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	64	VAL
1	E	214	ASN
2	K	30	SER
2	J	210	ASN
1	E	212	PRO

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	E	194/195 (100%)	191 (98%)	3 (2%)	57	68
1	F	196/195 (100%)	195 (100%)	1 (0%)	81	87
1	G	195/195 (100%)	193 (99%)	2 (1%)	68	77
1	H	197/195 (101%)	195 (99%)	2 (1%)	68	77
2	I	188/185 (102%)	184 (98%)	4 (2%)	47	58
2	J	188/185 (102%)	186 (99%)	2 (1%)	65	75
2	K	182/185 (98%)	179 (98%)	3 (2%)	55	66
2	L	187/185 (101%)	186 (100%)	1 (0%)	81	87
3	A	14/14 (100%)	13 (93%)	1 (7%)	13	12
3	B	15/14 (107%)	15 (100%)	0	100	100
3	C	15/14 (107%)	15 (100%)	0	100	100
3	D	14/14 (100%)	14 (100%)	0	100	100
All	All	1585/1576 (101%)	1566 (99%)	19 (1%)	65	74

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	30[A]	ASN
1	H	30[B]	ASN
2	L	33	LEU
3	A	412	GLN
1	E	127	LYS
1	E	171	SER
1	E	180	LEU
2	I	33	LEU
2	I	69	THR
2	I	154	LEU
2	I	199	GLN
1	F	185	LEU
2	J	105	GLU
2	J	164	THR
1	G	5	LEU
1	G	188	LEU
2	K	67	SER
2	K	70	ASP
2	K	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	37	GLN
2	L	147	GLN
3	A	412	GLN
1	E	39	GLN
1	E	181	GLN
1	E	210	HIS
2	I	38	GLN
2	I	166	GLN
1	F	39	GLN
1	F	174	HIS
1	F	209	ASN
2	J	6	GLN
2	J	38	GLN
2	J	100	GLN
2	J	124	GLN
2	J	137	ASN
2	J	155	GLN
1	G	35	HIS
1	G	39	GLN
1	G	84	ASN
2	K	38	GLN
2	K	90	GLN
2	K	152	ASN
2	K	177	ASN
2	K	199	GLN
2	K	210	ASN
3	D	417	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 25 ligands modelled in this entry, 21 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACT	F	301	-	3,3,3	0.60	0	3,3,3	1.57	1 (33%)
4	ACT	G	301	-	3,3,3	1.13	0	3,3,3	1.48	1 (33%)
4	ACT	H	301	-	3,3,3	0.71	0	3,3,3	1.04	0
4	ACT	E	301	-	3,3,3	0.99	0	3,3,3	1.21	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	G	301	ACT	OXT-C-O	-2.09	114.26	122.03
4	F	301	ACT	OXT-C-CH3	2.02	123.54	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	301	ACT	2	0
4	G	301	ACT	2	0
4	H	301	ACT	1	0
4	E	301	ACT	7	0

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	E	226/226 (100%)	1.87	105 (46%) 0 0	26, 116, 200, 238	1 (0%)
1	F	226/226 (100%)	0.86	53 (23%) 2 1	24, 58, 179, 230	1 (0%)
1	G	226/226 (100%)	1.07	42 (18%) 3 3	37, 68, 138, 213	1 (0%)
1	H	226/226 (100%)	0.27	17 (7%) 20 18	21, 49, 128, 170	2 (0%)
2	I	212/213 (99%)	1.01	52 (24%) 2 1	28, 75, 191, 220	4 (1%)
2	J	212/213 (99%)	0.93	51 (24%) 2 1	21, 62, 151, 171	4 (1%)
2	K	211/213 (99%)	1.05	31 (14%) 6 5	40, 73, 122, 152	1 (0%)
2	L	212/213 (99%)	0.25	10 (4%) 36 35	16, 48, 120, 138	3 (1%)
3	A	15/15 (100%)	-0.37	0 100 100	30, 38, 45, 52	0
3	B	15/15 (100%)	-0.08	0 100 100	23, 43, 53, 58	1 (6%)
3	C	15/15 (100%)	0.06	0 100 100	28, 41, 59, 72	1 (6%)
3	D	15/15 (100%)	0.32	0 100 100	50, 63, 71, 71	0
All	All	1811/1816 (99%)	0.89	361 (19%) 3 2	16, 66, 171, 238	19 (1%)

All (361) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	168	ALA	5.9
1	G	11	VAL	5.7
1	E	152	VAL	5.4
1	F	172	GLY	5.3
1	G	199	LEU	5.3
1	E	160	VAL	5.2
2	J	186	TYR	5.1
1	E	134	LEU	5.0
1	E	205	ILE	4.9
1	E	133	PRO	4.7
1	E	150	CYS	4.7

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Mol	Chain	Res	Type	RSRZ
2	I	184	ALA	4.6
2	I	192	TYR	4.6
2	I	178	THR	4.5
1	E	169	LEU	4.4
2	I	180	THR	4.4
1	E	162	VAL	4.3
1	F	137	SER	4.3
1	E	212	PRO	4.3
1	E	68	PHE	4.2
1	F	208	VAL	4.2
2	I	181	LEU	4.2
1	E	146	ALA	4.1
2	J	132	VAL	4.1
1	E	135	ALA	4.1
1	G	15	GLY	4.1
2	I	133	VAL	4.1
1	F	147	ALA	4.1
2	K	154	LEU	4.1
1	E	204	TYR	4.1
1	F	204	TYR	4.0
1	E	151	LEU	4.0
2	I	119	PRO	4.0
2	J	142	ARG	4.0
1	F	191	VAL	3.9
1	E	199	LEU	3.9
1	F	199	LEU	3.9
2	I	116	PHE	3.9
2	J	135	LEU	3.9
2	I	118	PHE	3.8
1	F	194	VAL	3.8
2	I	154	LEU	3.8
2	J	181	LEU	3.8
2	K	73	LEU	3.8
1	F	193	THR	3.8
1	E	226	CYS	3.8
2	J	116	PHE	3.8
1	G	224	LYS	3.8
1	E	64	VAL	3.8
2	J	117	ILE	3.8
1	E	208	VAL	3.7
1	E	15	GLY	3.7
2	J	150	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	J	144	ALA	3.7
2	J	115	VAL	3.6
2	J	209	PHE	3.6
1	E	143	GLY	3.6
1	F	217	VAL	3.6
2	I	136	LEU	3.6
2	I	114[A]	SER	3.6
1	E	18	LEU	3.6
1	F	150	CYS	3.6
1	E	186	TYR	3.5
1	G	143	GLY	3.5
1	E	192	VAL	3.5
2	K	27	GLN	3.5
1	H	143	GLY	3.5
1	F	169	LEU	3.5
2	I	194	CYS	3.5
2	J	205	VAL	3.4
1	G	226	CYS	3.4
1	F	192	VAL	3.4
1	E	157	PRO	3.4
2	J	196	VAL	3.4
1	E	178	ALA	3.4
1	F	205	ILE	3.3
1	E	209	ASN	3.3
1	E	148	LEU	3.3
1	G	201	THR	3.3
1	E	132	PHE	3.3
1	E	175	THR	3.3
2	I	186	TYR	3.3
1	H	138	SER	3.3
1	F	226	CYS	3.3
1	G	142	SER	3.3
2	I	148	TRP	3.3
2	J	148	TRP	3.3
2	J	140	TYR	3.2
1	E	215	THR	3.2
1	F	145	THR	3.2
2	J	118	PHE	3.2
1	E	121	VAL	3.2
2	L	181	LEU	3.2
1	G	195	PRO	3.2
1	E	141	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	G	197	SER	3.2
1	E	147	ALA	3.2
1	E	191	VAL	3.2
2	J	212	GLY	3.2
1	G	17	SER	3.1
1	H	169	LEU	3.1
1	F	188	LEU	3.1
2	K	2	LEU	3.1
2	K	28	SER	3.1
1	E	149	GLY	3.1
1	E	11	VAL	3.1
2	J	133	VAL	3.1
1	G	145	THR	3.1
2	J	139	PHE	3.1
1	E	173	VAL	3.1
2	K	191	VAL	3.1
2	K	201	LEU	3.1
1	E	140	SER	3.1
2	I	212	GLY	3.1
2	I	182	SER	3.0
1	E	206	CYS	3.0
2	K	24	ARG	3.0
1	F	135	ALA	3.0
1	F	146	ALA	3.0
1	E	164	TRP	3.0
1	G	200	GLY	3.0
1	G	146	ALA	3.0
2	I	120	PRO	3.0
1	E	188	LEU	3.0
2	J	109	THR	3.0
1	G	198	SER	3.0
1	F	149	GLY	3.0
2	L	213	GLU	3.0
1	E	86	LEU	3.0
1	F	134	LEU	3.0
1	F	151	LEU	3.0
2	I	205	VAL	3.0
1	F	201	THR	3.0
2	K	205	VAL	2.9
2	I	197	THR	2.9
2	L	212	GLY	2.9
1	G	18	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	I	196	VAL	2.9
1	H	137	SER	2.9
1	H	140	SER	2.9
2	K	68	GLY	2.9
2	K	196	VAL	2.9
2	K	197	THR	2.9
1	E	142	SER	2.9
1	E	165	ASN	2.9
2	K	192	TYR	2.9
1	F	173	VAL	2.9
1	E	194	VAL	2.8
2	I	115	VAL	2.8
2	I	146	VAL	2.8
2	I	191	VAL	2.8
1	E	174	HIS	2.8
1	F	129	PRO	2.8
1	E	79	LEU	2.8
2	I	150	VAL	2.8
1	E	130	SER	2.8
1	G	14	PRO	2.8
1	E	155	TYR	2.8
1	E	83	MET	2.8
2	J	149	LYS	2.8
1	E	12	VAL	2.8
1	F	170	THR	2.8
1	E	167	GLY	2.8
1	F	136	PRO	2.8
2	J	141	PRO	2.8
1	E	180	LEU	2.8
1	E	161	THR	2.7
1	E	223	PRO	2.7
2	J	110	VAL	2.7
2	I	206	THR	2.7
1	G	144	GLY	2.7
1	H	224	LYS	2.7
2	J	154	LEU	2.7
2	K	153	ALA	2.7
1	G	117	THR	2.7
1	E	17	SER	2.7
1	E	183	SER	2.7
1	E	197	SER	2.7
1	E	131	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	K	149	LYS	2.7
2	I	127	SER	2.7
2	I	159	SER	2.7
2	I	179	LEU	2.7
2	J	189	HIS	2.6
1	E	156	PHE	2.6
1	F	216	LYS	2.6
2	J	192	TYR	2.6
2	L	191	VAL	2.6
1	E	128	GLY	2.6
1	G	13	GLN	2.6
2	J	111	ALA	2.6
1	E	210	HIS	2.6
1	H	13	GLN	2.6
1	E	220	LYS	2.6
1	E	67	ARG	2.6
1	E	179	VAL	2.6
1	E	224	LYS	2.6
2	I	144	ALA	2.6
1	F	143	GLY	2.6
2	I	145	LYS	2.6
2	L	210	ASN	2.5
1	E	66	GLY	2.5
1	E	217	VAL	2.5
1	F	131	VAL	2.5
2	J	131	SER	2.5
1	E	124	ALA	2.5
2	K	184	ALA	2.5
1	E	200	GLY	2.5
1	F	164	TRP	2.5
1	G	86	LEU	2.5
1	E	218	ASP	2.5
2	I	177	ASN	2.5
1	E	91	THR	2.5
1	E	201	THR	2.5
1	F	138	SER	2.5
1	G	16	ARG	2.5
1	F	148	LEU	2.5
2	J	207	LYS	2.5
2	J	120	PRO	2.5
1	E	88	THR	2.4
1	H	198	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	85	SER	2.4
1	G	12	VAL	2.4
1	G	59	TYR	2.4
1	G	61	ALA	2.4
1	G	168	ALA	2.4
2	K	180	THR	2.4
1	E	189	SER	2.4
2	L	150	VAL	2.4
2	I	125	LEU	2.4
2	J	136	LEU	2.4
2	L	129	THR	2.4
1	F	183	SER	2.4
1	E	87	LYS	2.4
1	E	136	PRO	2.4
1	F	200	GLY	2.4
2	I	128	GLY	2.4
1	F	203	THR	2.4
1	E	20	LEU	2.4
2	J	179	LEU	2.4
1	G	204	TYR	2.3
2	I	164	THR	2.3
2	J	206	THR	2.3
1	F	225	SER	2.3
2	I	131	SER	2.3
2	K	29	VAL	2.3
1	H	199	LEU	2.3
1	G	5	LEU	2.3
2	I	204	PRO	2.3
2	K	207	LYS	2.3
2	I	200	GLY	2.3
2	J	130	ALA	2.3
1	E	145	THR	2.3
2	K	3	THR	2.3
1	E	63	SER	2.3
2	J	191	VAL	2.3
2	I	152	ASN	2.3
2	K	137	ASN	2.3
1	E	69	THR	2.3
2	J	129	THR	2.3
1	G	205	ILE	2.3
2	I	209	PHE	2.3
2	J	188	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	193	ALA	2.3
1	G	141	THR	2.3
1	E	190	SER	2.3
2	I	171	SER	2.3
2	K	26	SER	2.3
1	E	222	GLU	2.3
2	K	190	LYS	2.3
1	F	132	PHE	2.2
2	I	139	PHE	2.2
2	J	201	LEU	2.2
2	I	134	CYS	2.2
2	J	194	CYS	2.2
1	E	14	PRO	2.2
1	E	120	THR	2.2
1	H	142	SER	2.2
1	E	138	SER	2.2
1	G	196	SER	2.2
1	G	202	GLN	2.2
1	E	153	LYS	2.2
1	G	121	VAL	2.2
2	J	146	VAL	2.2
1	E	129	PRO	2.2
1	G	223	PRO	2.2
2	J	187	GLU	2.2
1	E	13	GLN	2.2
2	I	149	LYS	2.2
1	H	126	THR	2.2
1	E	198	SER	2.2
1	G	138	SER	2.2
2	I	201	LEU	2.2
1	H	194	VAL	2.2
1	E	207	ASN	2.2
1	F	214	ASN	2.2
1	G	67	ARG	2.2
1	E	184	GLY	2.2
1	E	203	THR	2.2
2	I	193	ALA	2.2
1	E	225	SER	2.2
1	G	85	SER	2.2
1	G	225	SER	2.2
1	F	152	VAL	2.2
2	I	137	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	71	PHE	2.2
1	F	133	PRO	2.2
2	I	190	LYS	2.2
1	E	82	GLN	2.2
1	E	144	GLY	2.2
1	G	203	THR	2.2
2	I	203	SER	2.2
2	K	69	THR	2.2
1	E	70	ILE	2.1
2	I	117	ILE	2.1
1	E	221	VAL	2.1
2	L	209	PHE	2.1
2	J	190	LYS	2.1
2	J	113	PRO	2.1
2	J	119	PRO	2.1
1	F	184	GLY	2.1
2	K	194	CYS	2.1
1	H	141	THR	2.1
1	H	145	THR	2.1
1	E	125	SER	2.1
1	F	189	SER	2.1
1	F	139	LYS	2.1
2	J	169	LYS	2.1
2	K	152	ASN	2.1
1	E	159	PRO	2.1
1	F	144	GLY	2.1
2	L	180	THR	2.1
2	J	180	THR	2.1
1	G	83	MET	2.1
1	E	62	ASP	2.1
1	G	84	ASN	2.1
1	H	173	VAL	2.1
1	F	162	VAL	2.1
1	F	179	VAL	2.1
1	F	163	SER	2.1
1	F	215	THR	2.1
1	G	137	SER	2.1
2	K	7	SER	2.1
2	K	22	SER	2.1
2	J	112	ALA	2.1
2	J	126	LYS	2.1
2	J	125	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	144	GLY	2.1
2	K	157	GLY	2.1
1	F	198	SER	2.0
2	I	202	SER	2.0
2	J	208	SER	2.0
1	F	168	ALA	2.0
1	E	84	ASN	2.0
2	I	138	ASN	2.0
1	F	223	PRO	2.0
1	H	131	VAL	2.0
1	F	221	VAL	2.0
2	L	148	TRP	2.0
1	E	122	SER	2.0
2	K	189	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CA	G	303	1/1	0.57	0.18	120,120,120,120	0
5	CA	K	304	1/1	0.65	0.23	110,110,110,110	0
5	CA	J	302	1/1	0.78	0.19	142,142,142,142	0
5	CA	K	303	1/1	0.84	0.16	114,114,114,114	0
4	ACT	E	301	4/4	0.84	0.12	39,46,48,57	0
5	CA	K	305	1/1	0.84	0.21	98,98,98,98	0
5	CA	C	501	1/1	0.87	0.21	103,103,103,103	0
5	CA	A	501	1/1	0.88	0.19	117,117,117,117	0
5	CA	K	302	1/1	0.90	0.10	96,96,96,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	L	301	1/1	0.90	0.13	89,89,89,89	0
4	ACT	G	301	4/4	0.91	0.09	36,44,47,54	0
4	ACT	H	301	4/4	0.91	0.12	44,44,47,48	0
5	CA	J	301	1/1	0.92	0.07	76,76,76,76	0
5	CA	H	302	1/1	0.92	0.07	75,75,75,75	0
4	ACT	F	301	4/4	0.93	0.10	36,42,45,48	0
5	CA	F	303	1/1	0.94	0.08	97,97,97,97	0
5	CA	G	302	1/1	0.94	0.07	86,86,86,86	0
5	CA	F	305	1/1	0.94	0.13	80,80,80,80	0
5	CA	K	301	1/1	0.94	0.11	101,101,101,101	0
5	CA	F	304	1/1	0.96	0.06	74,74,74,74	0
5	CA	E	302	1/1	0.96	0.07	75,75,75,75	0
5	CA	F	302	1/1	0.96	0.08	81,81,81,81	0
5	CA	H	303	1/1	0.96	0.07	65,65,65,65	0
5	CA	L	302	1/1	0.99	0.05	60,60,60,60	0
5	CA	I	301	1/1	0.99	0.04	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.