



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Apr 9, 2019 – 01:28 PM EDT

PDB ID : 6J5T
EMDB ID: : EMD-0680
Title : Reconstitution and structure of a plant NLR resistosome conferring immunity
Authors : Wang, J.Z.; Wang, J.; Hu, M.J.; Wang, H.W.; Zhou, J.M.; Chai, J.J.
Deposited on : 2019-01-12
Resolution : 3.40 Å(reported)
Based on PDB ID : 3TL8

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

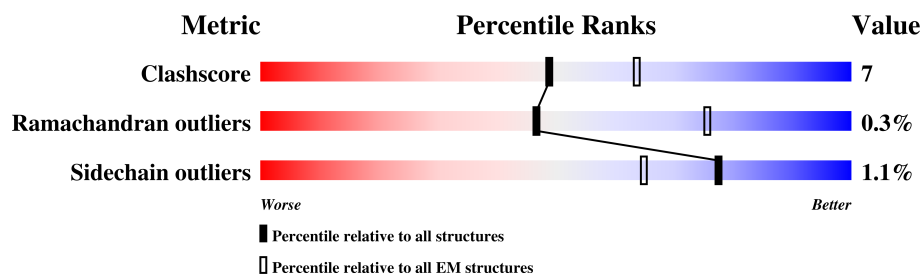
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	426	39% 6% 55%
1	D	426	38% 7% 55%
1	I	426	38% 7% 55%
1	J	426	38% 8% 55%
1	M	426	38% 8% 55%
2	B	351	67% 25% 7%
2	E	351	69% 24% 7%
2	H	351	70% 23% 7%
2	K	351	69% 24% 7%

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Mol	Chain	Length	Quality of chain
2	N	351	<div><div></div><div>69%24%7%</div></div>
3	C	852	<div><div></div><div>78%16%5%</div></div>
3	F	852	<div><div></div><div>78%16%5%</div></div>
3	G	852	<div><div></div><div>77%17%5%</div></div>
3	L	852	<div><div></div><div>78%16%5%</div></div>
3	O	852	<div><div></div><div>78%16%5%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 53488 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 Probable serine/threonine-protein kinase PBL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	193	Total	C	N	O	S	0	0
			1510	976	259	269	6		
1	A	193	Total	C	N	O	S	0	0
			1510	976	259	269	6		
1	D	193	Total	C	N	O	S	0	0
			1510	976	259	269	6		
1	J	193	Total	C	N	O	S	0	0
			1510	976	259	269	6		
1	M	193	Total	C	N	O	S	0	0
			1510	976	259	269	6		

- Molecule 2 is a protein called Protein kinase superfamily protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	327	Total	C	N	O	S	0	0
			2629	1686	447	479	17		
2	B	327	Total	C	N	O	S	0	0
			2629	1686	447	479	17		
2	E	327	Total	C	N	O	S	0	0
			2629	1686	447	479	17		
2	K	327	Total	C	N	O	S	0	0
			2629	1686	447	479	17		
2	N	327	Total	C	N	O	S	0	0
			2629	1686	447	479	17		

- Molecule 3 is a protein called Disease resistance RPP13-like protein 4.

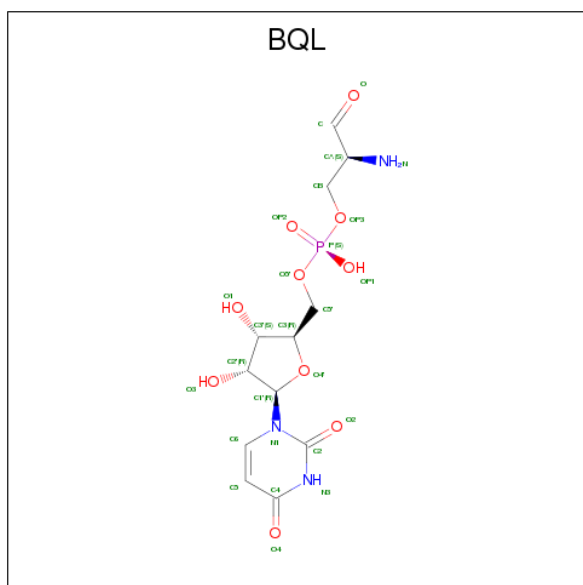
Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	808	Total	C	N	O	S	0	0
			6476	4097	1112	1228	39		
3	C	808	Total	C	N	O	S	0	0
			6476	4097	1112	1228	39		
3	F	808	Total	C	N	O	S	0	0
			6476	4097	1112	1228	39		

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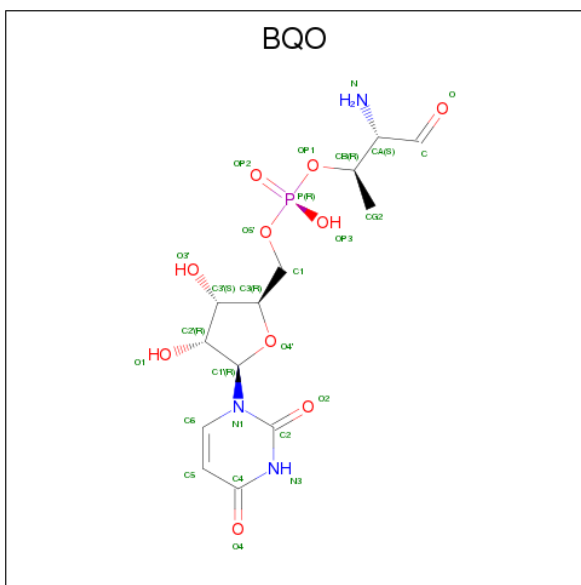
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	808	Total	C	N	O	S	0	0
			6476	4097	1112	1228	39		
3	O	808	Total	C	N	O	S	0	0
			6476	4097	1112	1228	39		

- Molecule 4 is [(2 {S})-2-azanyl-3-oxidanylidene-propyl] [(2 {R},3 {S},4 {R},5 {R})-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (three-letter code: BQL) (formula: C₁₂H₁₈N₃O₁₀P).



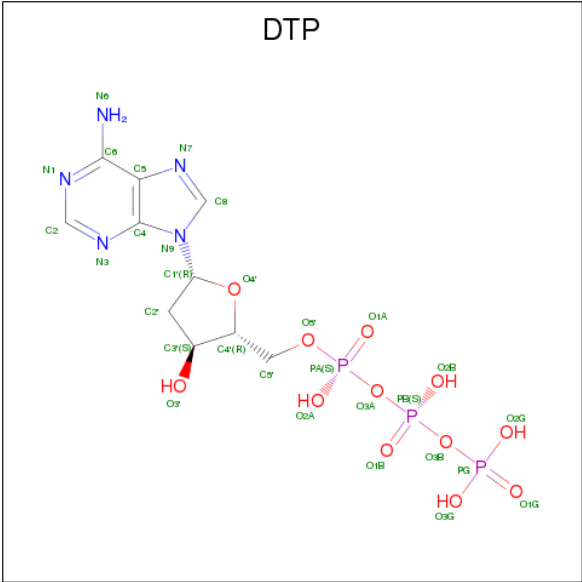
Mol	Chain	Residues	Atoms					AltConf
4	I	1	Total	C	N	O	P	0
			26	12	3	10	1	
4	A	1	Total	C	N	O	P	0
			26	12	3	10	1	
4	D	1	Total	C	N	O	P	0
			26	12	3	10	1	
4	J	1	Total	C	N	O	P	0
			26	12	3	10	1	
4	M	1	Total	C	N	O	P	0
			26	12	3	10	1	

- Molecule 5 is [(2 {R},3 {S})-3-azanyl-4-oxidanylidene-butan-2-yl] [(2 {R},3 {S},4 {R},5 {R})-5-[2,4-bis(oxidanylidene)pyrimidin-1-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (three-letter code: BQO) (formula: C₁₃H₂₀N₃O₁₀P).



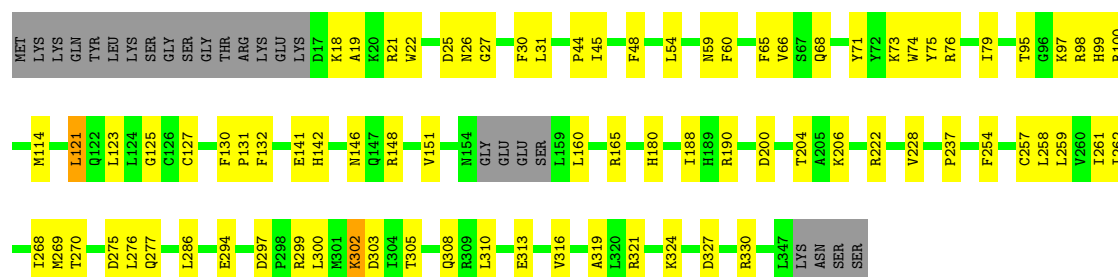
Mol	Chain	Residues	Atoms					AltConf
5	I	1	Total 25	C 13	N 3	O 8	P 1	0
5	A	1	Total 27	C 13	N 3	O 10	P 1	0
5	D	1	Total 27	C 13	N 3	O 10	P 1	0
5	J	1	Total 27	C 13	N 3	O 10	P 1	0
5	M	1	Total 27	C 13	N 3	O 10	P 1	0

- Molecule 6 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).

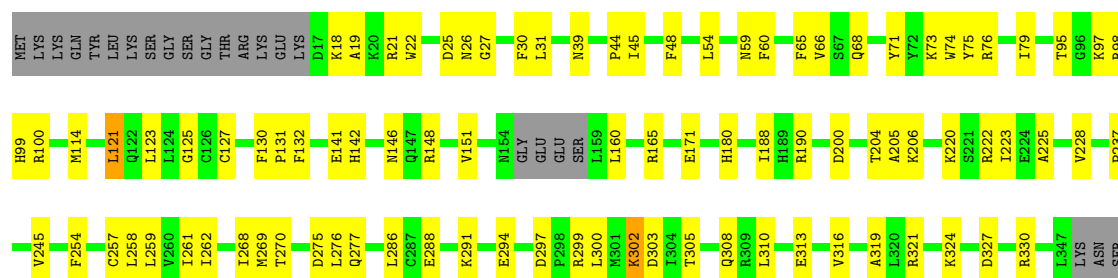


ARG

- Molecule 2: Protein kinase superfamily protein

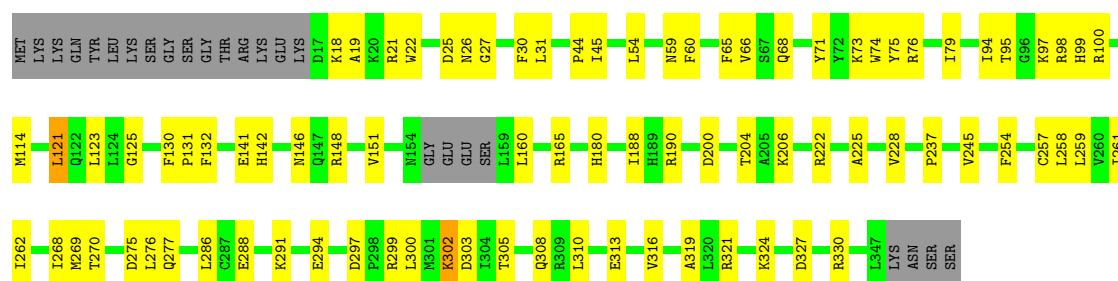
Chain H:  70% 23% 7%

- Molecule 2: Protein kinase superfamily protein

Chain B:  67% 25% 7%

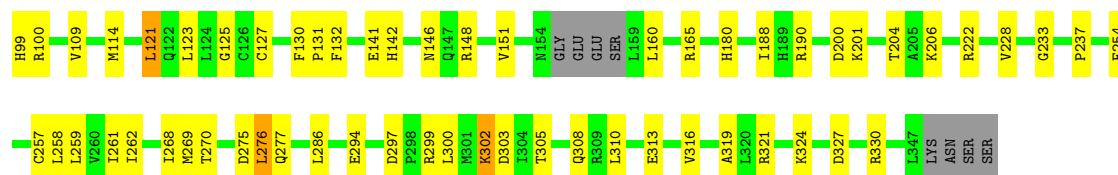
SER

- Molecule 2: Protein kinase superfamily protein

Chain E:  69% 24% 7%

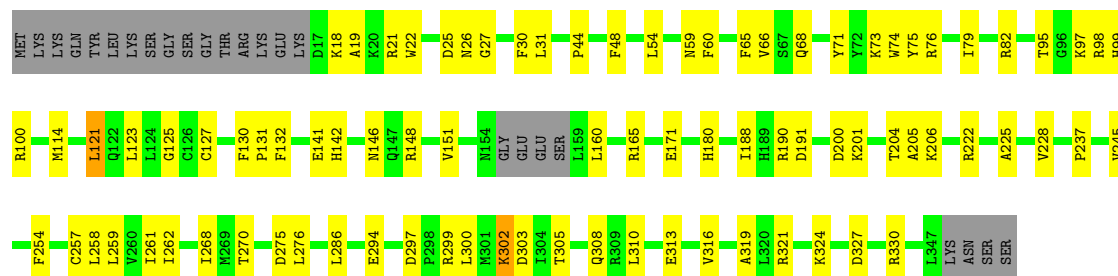
- Molecule 2: Protein kinase superfamily protein

Chain K:  69% 24% 7%



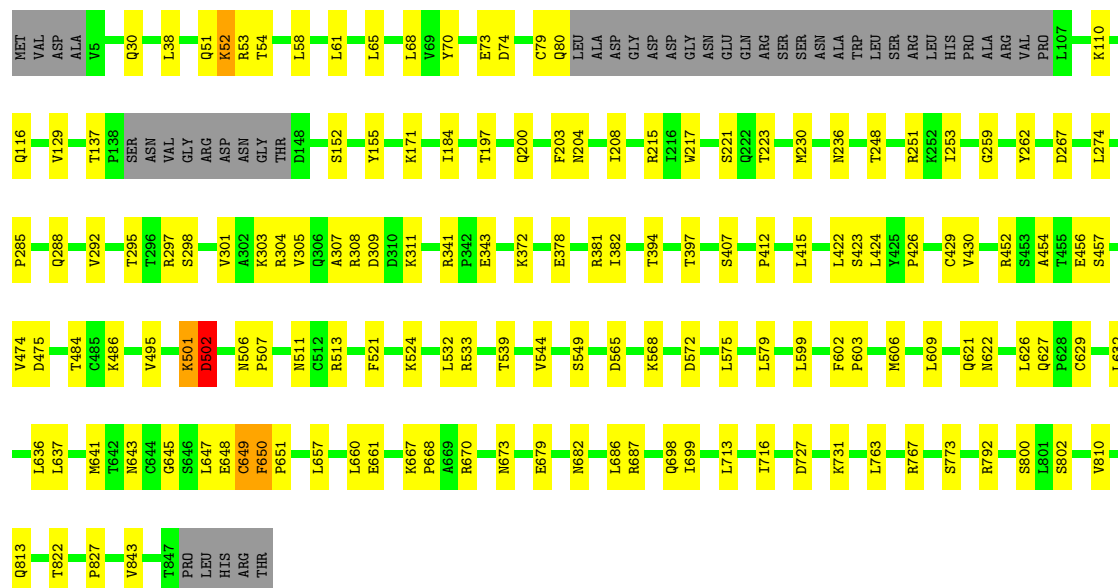
• Molecule 2: Protein kinase superfamily protein

Chain N: 69% 24% 7%



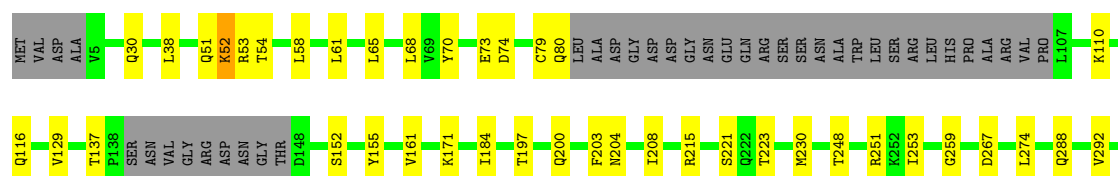
• Molecule 3: Disease resistance RPP13-like protein 4

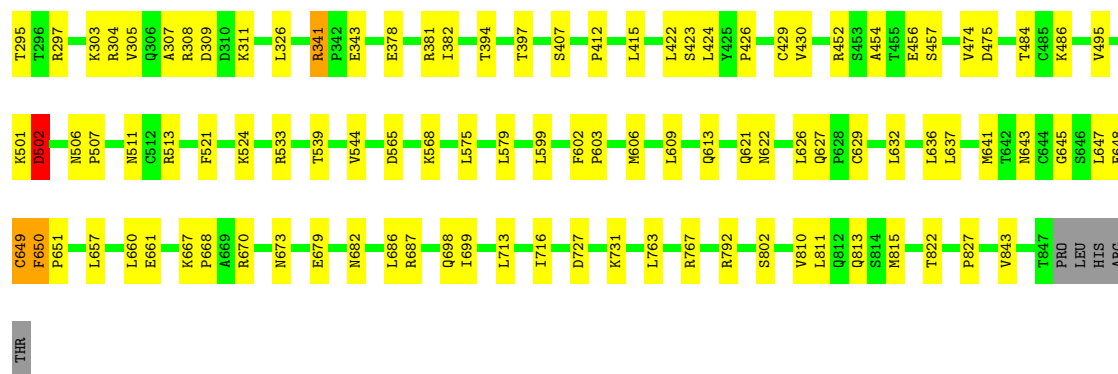
Chain G: 77% 17% 5%



• Molecule 3: Disease resistance RPP13-like protein 4

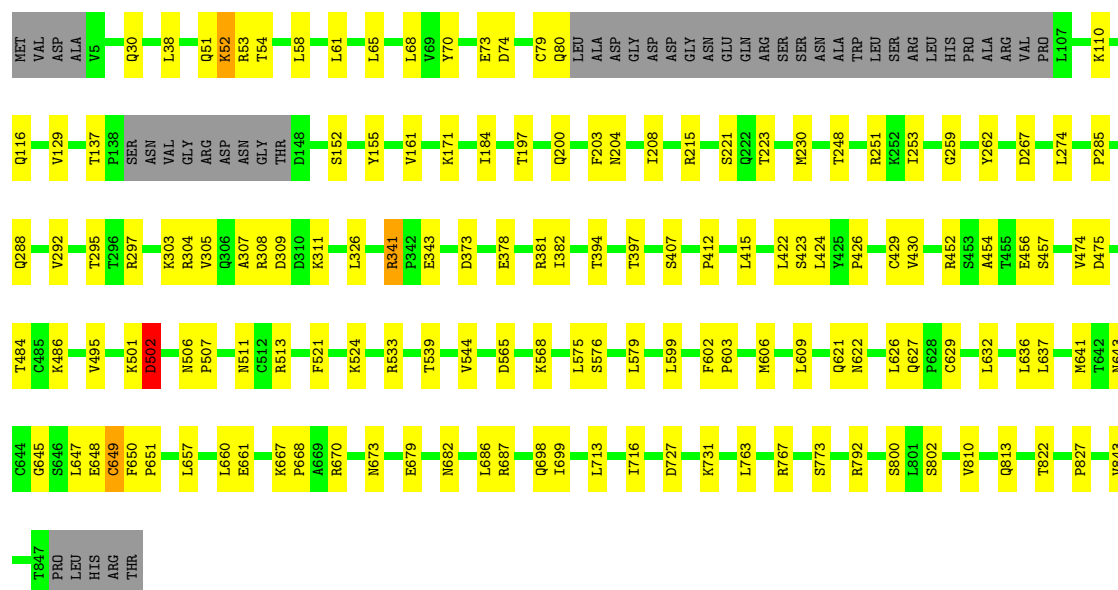
Chain C: 78% 16% 5%





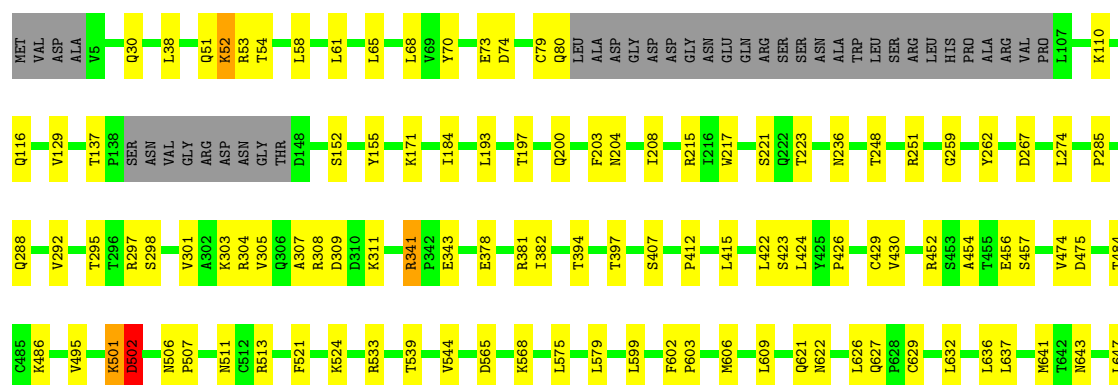
• Molecule 3: Disease resistance RPP13-like protein 4

Chain F: 78% 16% 5%



• Molecule 3: Disease resistance RPP13-like protein 4

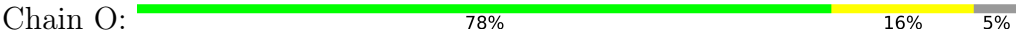
Chain L: 78% 16% 5%





HIS
ARG
THR

● Molecule 3: Disease resistance RPP13-like protein 4



PRO
LEU
HIS
ARG
THR

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	196707	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BQO, BQL, DTP

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 >2	RMSZ	# Z >2
1	A	0.31	0/1539	0.61	0/2078
1	D	0.31	0/1539	0.61	0/2078
1	I	0.31	0/1539	0.61	0/2078
1	J	0.31	0/1539	0.61	0/2078
1	M	0.31	0/1539	0.61	0/2078
2	B	0.41	0/2683	0.70	5/3621 (0.1%)
2	E	0.41	0/2683	0.70	5/3621 (0.1%)
2	H	0.41	0/2683	0.70	5/3621 (0.1%)
2	K	0.41	0/2683	0.70	5/3621 (0.1%)
2	N	0.41	0/2683	0.70	5/3621 (0.1%)
3	C	0.48	0/6596	0.66	3/8908 (0.0%)
3	F	0.48	0/6596	0.66	3/8908 (0.0%)
3	G	0.48	0/6596	0.66	3/8908 (0.0%)
3	L	0.48	0/6596	0.66	3/8908 (0.0%)
3	O	0.48	0/6596	0.66	3/8908 (0.0%)
All	All	0.45	0/54090	0.67	40/73035 (0.1%)

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	A	0	3
1	D	0	3
1	I	0	3
1	J	0	3
1	M	0	3
2	B	0	3
2	E	0	3
2	H	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	K	0	3
2	N	0	3
3	C	0	4
3	F	0	4
3	G	0	4
3	L	0	4
3	O	0	4
All	All	0	50

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	297	ASP	CB-CG-OD1	6.74	124.36	118.30
2	H	297	ASP	CB-CG-OD1	6.72	124.35	118.30
2	K	297	ASP	CB-CG-OD1	6.71	124.34	118.30
2	B	297	ASP	CB-CG-OD1	6.70	124.33	118.30
2	N	297	ASP	CB-CG-OD1	6.69	124.32	118.30
2	K	276	LEU	CA-CB-CG	6.57	130.40	115.30
2	H	276	LEU	CA-CB-CG	6.56	130.40	115.30
2	B	276	LEU	CA-CB-CG	6.56	130.39	115.30
2	N	276	LEU	CA-CB-CG	6.54	130.34	115.30
2	E	276	LEU	CA-CB-CG	6.54	130.33	115.30
2	B	310	LEU	CA-CB-CG	6.21	129.59	115.30
2	K	310	LEU	CA-CB-CG	6.21	129.59	115.30
2	E	310	LEU	CA-CB-CG	6.21	129.59	115.30
2	H	310	LEU	CA-CB-CG	6.19	129.54	115.30
2	N	310	LEU	CA-CB-CG	6.19	129.54	115.30
2	E	121	LEU	CA-CB-CG	6.08	129.29	115.30
2	B	121	LEU	CA-CB-CG	6.07	129.26	115.30
2	K	121	LEU	CA-CB-CG	6.07	129.26	115.30
2	N	121	LEU	CA-CB-CG	6.06	129.25	115.30
2	H	121	LEU	CA-CB-CG	6.06	129.23	115.30
3	C	424	LEU	CA-CB-CG	5.83	128.70	115.30
3	G	424	LEU	CA-CB-CG	5.81	128.66	115.30
3	O	424	LEU	CA-CB-CG	5.80	128.64	115.30
3	F	424	LEU	CA-CB-CG	5.79	128.62	115.30
3	L	424	LEU	CA-CB-CG	5.79	128.62	115.30
3	O	636	LEU	CA-CB-CG	5.55	128.06	115.30
3	C	636	LEU	CA-CB-CG	5.54	128.03	115.30
3	L	636	LEU	CA-CB-CG	5.53	128.02	115.30
3	G	636	LEU	CA-CB-CG	5.53	128.01	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	636	LEU	CA-CB-CG	5.53	128.01	115.30
3	C	422	LEU	CA-CB-CG	5.16	127.16	115.30
3	F	422	LEU	CA-CB-CG	5.15	127.14	115.30
3	O	422	LEU	CA-CB-CG	5.15	127.15	115.30
3	G	422	LEU	CA-CB-CG	5.14	127.12	115.30
3	L	422	LEU	CA-CB-CG	5.13	127.11	115.30
2	N	79	ILE	CG1-CB-CG2	-5.10	100.19	111.40
2	B	79	ILE	CG1-CB-CG2	-5.08	100.22	111.40
2	H	79	ILE	CG1-CB-CG2	-5.08	100.22	111.40
2	E	79	ILE	CG1-CB-CG2	-5.08	100.23	111.40
2	K	79	ILE	CG1-CB-CG2	-5.08	100.23	111.40

There are no chirality outliers.

All (50) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ALA	Peptide
1	A	169	TYR	Peptide
1	A	273	LEU	Peptide
2	B	130	PHE	Peptide
2	B	131	PRO	Peptide
2	B	132	PHE	Peptide
3	C	502	ASP	Peptide
3	C	506	ASN	Peptide
3	C	648	GLU	Peptide
3	C	649	CYS	Peptide
1	D	160	ALA	Peptide
1	D	169	TYR	Peptide
1	D	273	LEU	Peptide
2	E	130	PHE	Peptide
2	E	131	PRO	Peptide
2	E	132	PHE	Peptide
3	F	502	ASP	Peptide
3	F	506	ASN	Peptide
3	F	648	GLU	Peptide
3	F	649	CYS	Peptide
3	G	502	ASP	Peptide
3	G	506	ASN	Peptide
3	G	648	GLU	Peptide
3	G	649	CYS	Peptide
2	H	130	PHE	Peptide
2	H	131	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	H	132	PHE	Peptide
1	I	160	ALA	Peptide
1	I	169	TYR	Peptide
1	I	273	LEU	Peptide
1	J	160	ALA	Peptide
1	J	169	TYR	Peptide
1	J	273	LEU	Peptide
2	K	130	PHE	Peptide
2	K	131	PRO	Peptide
2	K	132	PHE	Peptide
3	L	502	ASP	Peptide
3	L	506	ASN	Peptide
3	L	648	GLU	Peptide
3	L	649	CYS	Peptide
1	M	160	ALA	Peptide
1	M	169	TYR	Peptide
1	M	273	LEU	Peptide
2	N	130	PHE	Peptide
2	N	131	PRO	Peptide
2	N	132	PHE	Peptide
3	O	502	ASP	Peptide
3	O	506	ASN	Peptide
3	O	648	GLU	Peptide
3	O	649	CYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1510	0	1539	17	0
1	D	1510	0	1539	18	0
1	I	1510	0	1539	17	0
1	J	1510	0	1539	20	0
1	M	1510	0	1539	18	0
2	B	2629	0	2654	54	0
2	E	2629	0	2654	52	0
2	H	2629	0	2654	49	0
2	K	2629	0	2654	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	2629	0	2654	54	0
3	C	6476	0	6506	80	0
3	F	6476	0	6506	81	0
3	G	6476	0	6506	83	0
3	L	6476	0	6506	81	0
3	O	6476	0	6506	82	0
4	A	26	0	0	0	0
4	D	26	0	0	0	0
4	I	26	0	0	0	0
4	J	26	0	0	0	0
4	M	26	0	0	0	0
5	A	27	0	0	1	0
5	D	27	0	0	1	0
5	I	25	0	0	0	0
5	J	27	0	0	1	0
5	M	27	0	0	1	0
6	C	30	0	12	1	0
6	F	30	0	12	1	0
6	G	30	0	12	1	0
6	L	30	0	12	2	0
6	O	30	0	12	1	0
All	All	53488	0	53555	713	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 7.

All (713) 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)
3:L:452:ARG:HD3	3:L:456:GLU:HG3	1.72	0.72
3:O:452:ARG:HD3	3:O:456:GLU:HG3	1.72	0.72
3:F:452:ARG:HD3	3:F:456:GLU:HG3	1.72	0.72
3:C:452:ARG:HD3	3:C:456:GLU:HG3	1.72	0.70
3:G:452:ARG:HD3	3:G:456:GLU:HG3	1.72	0.70
2:B:305:THR:HA	2:B:308:GLN:HB2	1.74	0.70
2:E:305:THR:HA	2:E:308:GLN:HB2	1.74	0.70
2:K:305:THR:HA	2:K:308:GLN:HB2	1.74	0.70
2:N:305:THR:HA	2:N:308:GLN:HB2	1.74	0.69
2:H:305:THR:HA	2:H:308:GLN:HB2	1.74	0.69
3:F:423:SER:HB3	3:F:495:VAL:HG12	1.75	0.68
3:L:423:SER:HB3	3:L:495:VAL:HG12	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:19:ALA:HA	2:K:22:TRP:HD1	1.59	0.68
2:E:19:ALA:HA	2:E:22:TRP:HD1	1.59	0.68
3:G:423:SER:HB3	3:G:495:VAL:HG12	1.75	0.68
3:O:423:SER:HB3	3:O:495:VAL:HG12	1.75	0.68
3:F:308:ARG:HH21	3:F:311:LYS:HE3	1.59	0.68
3:C:423:SER:HB3	3:C:495:VAL:HG12	1.75	0.67
2:H:19:ALA:HA	2:H:22:TRP:HD1	1.59	0.67
2:B:19:ALA:HA	2:B:22:TRP:HD1	1.59	0.67
3:C:308:ARG:HH21	3:C:311:LYS:HE3	1.59	0.67
3:G:670:ARG:HB2	3:G:673:ASN:HD22	1.61	0.66
2:N:19:ALA:HA	2:N:22:TRP:HD1	1.59	0.66
3:O:647:LEU:HD23	3:O:649:CYS:H	1.60	0.66
3:L:647:LEU:HD23	3:L:649:CYS:H	1.60	0.66
3:G:308:ARG:HH21	3:G:311:LYS:HE3	1.59	0.65
3:L:308:ARG:HH21	3:L:311:LYS:HE3	1.59	0.65
3:O:308:ARG:HH21	3:O:311:LYS:HE3	1.59	0.65
3:O:670:ARG:HB2	3:O:673:ASN:HD22	1.61	0.65
3:C:647:LEU:HD23	3:C:649:CYS:H	1.60	0.65
3:C:670:ARG:HB2	3:C:673:ASN:HD22	1.61	0.65
3:F:647:LEU:HD23	3:F:649:CYS:H	1.60	0.64
3:F:670:ARG:HB2	3:F:673:ASN:HD22	1.61	0.64
3:L:670:ARG:HB2	3:L:673:ASN:HD22	1.61	0.64
3:G:647:LEU:HD23	3:G:649:CYS:H	1.60	0.64
3:G:79:CYS:SG	3:G:80:GLN:N	2.73	0.62
3:C:79:CYS:SG	3:C:80:GLN:N	2.73	0.62
3:F:79:CYS:SG	3:F:80:GLN:N	2.73	0.61
3:L:79:CYS:SG	3:L:80:GLN:N	2.73	0.61
3:O:79:CYS:SG	3:O:80:GLN:N	2.73	0.61
2:B:321:ARG:HA	2:B:324:LYS:HE2	1.83	0.61
2:H:321:ARG:HA	2:H:324:LYS:HE2	1.83	0.60
3:O:203:PHE:O	3:O:215:ARG:NH1	2.34	0.60
3:G:203:PHE:O	3:G:215:ARG:NH1	2.34	0.60
3:F:203:PHE:O	3:F:215:ARG:NH1	2.34	0.60
2:E:321:ARG:HA	2:E:324:LYS:HE2	1.83	0.60
3:L:203:PHE:O	3:L:215:ARG:NH1	2.34	0.60
3:C:203:PHE:O	3:C:215:ARG:NH1	2.34	0.59
3:C:184:ILE:HG22	3:C:292:VAL:HB	1.85	0.59
3:G:713:LEU:HD21	3:G:716:ILE:HD11	1.84	0.59
2:N:321:ARG:HA	2:N:324:LYS:HE2	1.83	0.59
3:G:184:ILE:HG22	3:G:292:VAL:HB	1.85	0.59
3:C:713:LEU:HD21	3:C:716:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:184:ILE:HG22	3:F:292:VAL:HB	1.85	0.59
3:F:606:MET:HG3	3:F:609:LEU:HD12	1.85	0.59
3:F:713:LEU:HD21	3:F:716:ILE:HD11	1.84	0.59
2:K:321:ARG:HA	2:K:324:LYS:HE2	1.83	0.59
3:L:184:ILE:HG22	3:L:292:VAL:HB	1.85	0.59
3:L:713:LEU:HD21	3:L:716:ILE:HD11	1.84	0.58
1:M:202:ALA:HA	1:M:205:LEU:HD12	1.86	0.58
3:C:606:MET:HG3	3:C:609:LEU:HD12	1.85	0.58
2:H:160:LEU:HB2	2:H:165:ARG:HE	1.69	0.58
3:O:184:ILE:HG22	3:O:292:VAL:HB	1.85	0.58
3:O:713:LEU:HD21	3:O:716:ILE:HD11	1.84	0.58
3:L:606:MET:HG3	3:L:609:LEU:HD12	1.85	0.58
3:O:606:MET:HG3	3:O:609:LEU:HD12	1.85	0.58
2:H:142:HIS:ND1	2:H:200:ASP:O	2.37	0.58
2:N:160:LEU:HB2	2:N:165:ARG:HE	1.69	0.58
1:A:202:ALA:HA	1:A:205:LEU:HD12	1.86	0.57
2:H:299:ARG:O	2:H:302:LYS:NZ	2.38	0.57
5:A:502:BQO:OP3	2:B:100:ARG:NH1	2.37	0.57
3:C:565:ASP:OD1	3:C:565:ASP:N	2.37	0.57
2:K:142:HIS:ND1	2:K:200:ASP:O	2.37	0.57
2:K:160:LEU:HB2	2:K:165:ARG:HE	1.68	0.57
2:N:299:ARG:O	2:N:302:LYS:NZ	2.38	0.57
2:B:160:LEU:HB2	2:B:165:ARG:HE	1.69	0.57
2:E:142:HIS:ND1	2:E:200:ASP:O	2.37	0.57
3:F:565:ASP:N	3:F:565:ASP:OD1	2.37	0.57
3:G:606:MET:HG3	3:G:609:LEU:HD12	1.85	0.57
1:I:219:ASP:O	1:I:224:ASN:ND2	2.37	0.57
1:J:202:ALA:HA	1:J:205:LEU:HD12	1.87	0.57
2:K:299:ARG:O	2:K:302:LYS:NZ	2.38	0.57
2:N:142:HIS:ND1	2:N:200:ASP:O	2.37	0.57
2:B:299:ARG:O	2:B:302:LYS:NZ	2.38	0.57
2:B:142:HIS:ND1	2:B:200:ASP:O	2.37	0.57
2:E:160:LEU:HB2	2:E:165:ARG:HE	1.69	0.57
1:D:202:ALA:HA	1:D:205:LEU:HD12	1.87	0.57
5:M:502:BQO:OP3	2:N:100:ARG:NH1	2.37	0.57
1:I:202:ALA:HA	1:I:205:LEU:HD12	1.86	0.56
3:G:475:ASP:OD1	3:G:484:THR:OG1	2.23	0.56
3:L:629:CYS:HA	3:L:632:LEU:HD23	1.88	0.56
1:M:219:ASP:O	1:M:224:ASN:ND2	2.38	0.56
3:C:197:THR:HG21	6:C:901:DTP:H2'2	1.87	0.56
3:O:197:THR:HG21	6:O:901:DTP:H2'2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:475:ASP:OD1	3:C:484:THR:OG1	2.23	0.56
5:J:502:BQO:OP3	2:K:100:ARG:NH1	2.38	0.56
3:F:629:CYS:HA	3:F:632:LEU:HD23	1.88	0.56
3:L:475:ASP:OD1	3:L:484:THR:OG1	2.23	0.56
2:H:95:THR:O	2:H:98:ARG:NH1	2.39	0.56
3:L:513:ARG:O	3:L:533:ARG:N	2.37	0.56
2:N:95:THR:O	2:N:98:ARG:NH1	2.39	0.56
3:O:475:ASP:OD1	3:O:484:THR:OG1	2.23	0.56
3:O:629:CYS:HA	3:O:632:LEU:HD23	1.87	0.56
2:E:44:PRO:HG3	3:F:643:ASN:HD22	1.71	0.56
3:F:475:ASP:OD1	3:F:484:THR:OG1	2.23	0.55
2:E:299:ARG:O	2:E:302:LYS:NZ	2.38	0.55
3:F:452:ARG:HG3	3:L:381:ARG:HH11	1.71	0.55
3:L:565:ASP:OD1	3:L:565:ASP:N	2.37	0.55
2:B:95:THR:O	2:B:98:ARG:NH1	2.39	0.55
2:E:54:LEU:HD12	2:E:59:ASN:HD22	1.72	0.55
2:K:44:PRO:HG3	3:L:643:ASN:HD22	1.72	0.55
2:B:258:LEU:O	2:B:261:ILE:HB	2.07	0.55
2:B:54:LEU:HD12	2:B:59:ASN:HD22	1.72	0.55
2:B:44:PRO:HG3	3:C:643:ASN:HD22	1.72	0.55
5:D:502:BQO:OP3	2:E:100:ARG:NH1	2.39	0.55
3:C:513:ARG:O	3:C:533:ARG:N	2.38	0.55
2:H:258:LEU:HD23	2:H:319:ALA:HB2	1.89	0.55
3:C:452:ARG:O	3:C:457:SER:OG	2.25	0.55
2:N:54:LEU:HD12	2:N:59:ASN:HD22	1.72	0.55
3:C:629:CYS:HA	3:C:632:LEU:HD23	1.87	0.55
2:E:258:LEU:O	2:E:261:ILE:HB	2.07	0.55
2:K:95:THR:O	2:K:98:ARG:NH1	2.39	0.55
1:A:219:ASP:O	1:A:224:ASN:ND2	2.40	0.55
3:G:452:ARG:O	3:G:457:SER:OG	2.25	0.55
3:G:629:CYS:HA	3:G:632:LEU:HD23	1.88	0.55
2:B:258:LEU:HD23	2:B:319:ALA:HB2	1.89	0.54
2:E:95:THR:O	2:E:98:ARG:NH1	2.39	0.54
3:G:171:LYS:HG2	3:G:208:ILE:HD11	1.89	0.54
3:G:565:ASP:OD1	3:G:565:ASP:N	2.37	0.54
2:H:258:LEU:O	2:H:261:ILE:HB	2.07	0.54
2:H:54:LEU:HD12	2:H:59:ASN:HD22	1.72	0.54
2:H:97:LYS:O	2:H:99:HIS:ND1	2.40	0.54
2:K:54:LEU:HD12	2:K:59:ASN:HD22	1.72	0.54
3:G:197:THR:HG21	6:G:901:DTP:H2'2	1.88	0.54
3:F:452:ARG:O	3:F:457:SER:OG	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:565:ASP:N	3:O:565:ASP:OD1	2.37	0.54
3:O:513:ARG:O	3:O:533:ARG:N	2.38	0.54
1:J:219:ASP:O	1:J:224:ASN:ND2	2.40	0.54
2:K:258:LEU:O	2:K:261:ILE:HB	2.07	0.54
2:N:97:LYS:HD3	2:N:100:ARG:HB2	1.90	0.54
2:B:327:ASP:N	2:B:327:ASP:OD1	2.41	0.54
3:F:297:ARG:HH11	3:F:407:SER:HB2	1.73	0.54
2:K:97:LYS:HD3	2:K:100:ARG:HB2	1.90	0.54
3:O:171:LYS:HG2	3:O:208:ILE:HD11	1.89	0.54
2:H:44:PRO:HG3	3:G:643:ASN:HD22	1.72	0.54
2:E:97:LYS:O	2:E:99:HIS:ND1	2.40	0.54
3:G:297:ARG:HH11	3:G:407:SER:HB2	1.73	0.54
2:K:258:LEU:HD23	2:K:319:ALA:HB2	1.89	0.54
2:K:97:LYS:O	2:K:99:HIS:ND1	2.40	0.54
3:O:452:ARG:O	3:O:457:SER:OG	2.25	0.54
2:N:258:LEU:O	2:N:261:ILE:HB	2.07	0.54
1:M:255:LYS:HB2	2:N:228:VAL:HG13	1.90	0.53
3:C:171:LYS:HG2	3:C:208:ILE:HD11	1.89	0.53
1:D:219:ASP:O	1:D:224:ASN:ND2	2.42	0.53
3:F:171:LYS:HG2	3:F:208:ILE:HD11	1.89	0.53
2:B:165:ARG:HB3	2:B:261:ILE:HG23	1.91	0.53
2:E:258:LEU:HD23	2:E:319:ALA:HB2	1.89	0.53
2:E:165:ARG:HB3	2:E:261:ILE:HG23	1.91	0.53
3:L:452:ARG:O	3:L:457:SER:OG	2.25	0.53
2:N:97:LYS:O	2:N:99:HIS:ND1	2.40	0.53
3:F:513:ARG:O	3:F:533:ARG:N	2.37	0.53
3:L:197:THR:HG21	6:L:901:DTP:H2'2	1.90	0.53
1:I:268:VAL:HG11	2:H:237:PRO:HB3	1.91	0.53
3:L:171:LYS:HG2	3:L:208:ILE:HD11	1.89	0.53
2:N:258:LEU:HD23	2:N:319:ALA:HB2	1.89	0.53
3:O:297:ARG:HH11	3:O:407:SER:HB2	1.73	0.53
3:F:197:THR:HG21	6:F:901:DTP:H2'2	1.90	0.53
2:E:327:ASP:OD1	2:E:327:ASP:N	2.41	0.53
3:C:452:ARG:HG3	3:F:381:ARG:HH11	1.73	0.53
2:H:286:LEU:HD13	2:H:294:GLU:HB2	1.91	0.53
2:E:286:LEU:HD13	2:E:294:GLU:HB2	1.91	0.53
2:N:286:LEU:HD13	2:N:294:GLU:HB2	1.91	0.52
3:C:297:ARG:HH11	3:C:407:SER:HB2	1.73	0.52
3:F:155:TYR:HE1	3:F:204:ASN:HD22	1.58	0.52
2:K:286:LEU:HD13	2:K:294:GLU:HB2	1.91	0.52
2:E:97:LYS:HD3	2:E:100:ARG:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:165:ARG:HB3	2:H:261:ILE:HG23	1.91	0.52
2:B:286:LEU:HD13	2:B:294:GLU:HB2	1.91	0.52
3:G:452:ARG:HG3	3:C:381:ARG:HH11	1.74	0.52
1:D:272:ARG:HH12	1:D:276:LYS:HD3	1.74	0.52
2:H:97:LYS:HD3	2:H:100:ARG:HB2	1.90	0.52
3:L:155:TYR:HE1	3:L:204:ASN:HD22	1.58	0.52
2:N:165:ARG:HB3	2:N:261:ILE:HG23	1.91	0.52
2:B:324:LYS:O	2:B:330:ARG:NE	2.37	0.52
3:C:155:TYR:HE1	3:C:204:ASN:HD22	1.58	0.52
3:L:297:ARG:HH11	3:L:407:SER:HB2	1.73	0.52
2:N:327:ASP:OD1	2:N:327:ASP:N	2.41	0.52
2:K:165:ARG:HB3	2:K:261:ILE:HG23	1.91	0.52
2:B:97:LYS:HD3	2:B:100:ARG:HB2	1.90	0.51
3:F:575:LEU:HD12	3:F:599:LEU:HB2	1.92	0.51
3:F:668:PRO:O	3:F:698:GLN:NE2	2.43	0.51
3:O:155:TYR:HE1	3:O:204:ASN:HD22	1.58	0.51
1:A:326:ASP:HB2	1:A:332:GLN:HE21	1.76	0.51
3:G:513:ARG:O	3:G:533:ARG:N	2.37	0.51
2:K:324:LYS:O	2:K:330:ARG:NE	2.37	0.51
3:G:343:GLU:OE1	3:O:792:ARG:NH1	2.44	0.51
3:F:248:THR:HG22	3:F:251:ARG:HH21	1.76	0.51
2:N:324:LYS:O	2:N:330:ARG:NE	2.37	0.51
2:B:121:LEU:HA	2:B:206:LYS:HD3	1.93	0.51
3:O:248:THR:HG22	3:O:251:ARG:HH21	1.76	0.51
3:C:248:THR:HG22	3:C:251:ARG:HH21	1.76	0.51
3:C:575:LEU:HD12	3:C:599:LEU:HB2	1.92	0.51
2:E:324:LYS:O	2:E:330:ARG:NE	2.37	0.51
1:I:255:LYS:HB2	2:H:228:VAL:HG13	1.93	0.51
2:K:327:ASP:OD1	2:K:327:ASP:N	2.41	0.51
3:O:668:PRO:O	3:O:698:GLN:NE2	2.44	0.51
2:K:121:LEU:HA	2:K:206:LYS:HD3	1.93	0.51
3:G:184:ILE:HD12	3:G:305:VAL:HG12	1.93	0.51
3:L:452:ARG:HG3	3:O:381:ARG:HH11	1.74	0.51
3:L:668:PRO:O	3:L:698:GLN:NE2	2.43	0.51
3:G:381:ARG:HH11	3:O:452:ARG:HG3	1.76	0.51
3:F:70:TYR:O	3:F:74:ASP:HB2	2.11	0.51
3:L:575:LEU:HD12	3:L:599:LEU:HB2	1.92	0.51
3:O:184:ILE:HD12	3:O:305:VAL:HG12	1.93	0.51
2:B:97:LYS:O	2:B:99:HIS:ND1	2.40	0.51
2:E:121:LEU:HA	2:E:206:LYS:HD3	1.93	0.50
3:G:155:TYR:HE1	3:G:204:ASN:HD22	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:668:PRO:O	3:C:698:GLN:NE2	2.43	0.50
2:E:68:GLN:HG3	2:E:73:LYS:HG2	1.94	0.50
3:L:184:ILE:HD12	3:L:305:VAL:HG12	1.93	0.50
3:L:70:TYR:O	3:L:74:ASP:HB2	2.11	0.50
1:M:326:ASP:HB2	1:M:332:GLN:HE21	1.76	0.50
3:O:575:LEU:HD12	3:O:599:LEU:HB2	1.92	0.50
3:G:70:TYR:O	3:G:74:ASP:HB2	2.11	0.50
2:H:121:LEU:HA	2:H:206:LYS:HD3	1.93	0.50
2:N:270:THR:HB	2:N:275:ASP:HA	1.93	0.50
3:O:70:TYR:O	3:O:74:ASP:HB2	2.11	0.50
3:G:575:LEU:HD12	3:G:599:LEU:HB2	1.92	0.50
1:I:204:GLY:HA2	1:I:207:PHE:HD2	1.77	0.50
3:L:248:THR:HG22	3:L:251:ARG:HH21	1.76	0.50
3:C:792:ARG:NH1	3:F:343:GLU:OE1	2.45	0.50
3:G:668:PRO:O	3:G:698:GLN:NE2	2.44	0.50
1:I:326:ASP:HB2	1:I:332:GLN:HE21	1.77	0.50
1:A:268:VAL:HG11	2:B:237:PRO:HB3	1.93	0.50
3:C:184:ILE:HD12	3:C:305:VAL:HG12	1.93	0.50
3:C:70:TYR:O	3:C:74:ASP:HB2	2.11	0.50
3:G:699:ILE:HG13	3:G:731:LYS:HE3	1.94	0.50
2:K:68:GLN:HG3	2:K:73:LYS:HG2	1.94	0.50
3:O:626:LEU:HB3	3:O:651:PRO:HD3	1.94	0.50
1:D:326:ASP:HB2	1:D:332:GLN:HE21	1.76	0.50
3:F:184:ILE:HD12	3:F:305:VAL:HG12	1.93	0.50
3:O:687:ARG:HA	3:O:713:LEU:HA	1.94	0.50
3:O:699:ILE:HG13	3:O:731:LYS:HE3	1.94	0.50
2:H:66:VAL:N	2:H:74:TRP:O	2.42	0.50
3:L:626:LEU:HB3	3:L:651:PRO:HD3	1.94	0.50
2:B:68:GLN:HG3	2:B:73:LYS:HG2	1.94	0.49
3:F:579:LEU:HB2	3:F:603:PRO:HG2	1.94	0.49
3:C:622:ASN:OD1	3:C:622:ASN:N	2.45	0.49
2:E:270:THR:HB	2:E:275:ASP:HA	1.93	0.49
3:F:622:ASN:OD1	3:F:622:ASN:N	2.45	0.49
3:G:579:LEU:HB2	3:G:603:PRO:HG2	1.94	0.49
2:K:270:THR:HB	2:K:275:ASP:HA	1.94	0.49
3:F:51:GLN:NE2	3:L:137:THR:O	2.46	0.49
3:F:626:LEU:HB3	3:F:651:PRO:HD3	1.94	0.49
3:G:248:THR:HG22	3:G:251:ARG:HH21	1.76	0.49
1:J:204:GLY:HA2	1:J:207:PHE:HD2	1.77	0.49
2:N:121:LEU:HA	2:N:206:LYS:HD3	1.93	0.49
1:A:204:GLY:HA2	1:A:207:PHE:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:687:ARG:HA	3:L:713:LEU:HA	1.94	0.49
1:M:204:GLY:HA2	1:M:207:PHE:HD2	1.77	0.49
3:L:699:ILE:HG13	3:L:731:LYS:HE3	1.94	0.49
3:C:699:ILE:HG13	3:C:731:LYS:HE3	1.94	0.49
3:G:137:THR:O	3:O:51:GLN:NE2	2.45	0.49
2:B:160:LEU:H	2:B:165:ARG:HH21	1.60	0.49
2:B:270:THR:HB	2:B:275:ASP:HA	1.94	0.49
3:F:699:ILE:HG13	3:F:731:LYS:HE3	1.94	0.49
3:O:773:SER:HG	3:O:800:SER:HG	1.56	0.49
3:C:687:ARG:HA	3:C:713:LEU:HA	1.94	0.49
3:L:792:ARG:NH1	3:O:343:GLU:OE1	2.46	0.49
3:F:687:ARG:HA	3:F:713:LEU:HA	1.94	0.49
2:H:270:THR:HB	2:H:275:ASP:HA	1.94	0.49
2:H:327:ASP:OD1	2:H:327:ASP:N	2.41	0.49
1:A:353:ALA:HA	1:A:356:ARG:HD2	1.95	0.49
3:G:626:LEU:HB3	3:G:651:PRO:HD3	1.94	0.49
3:L:802:SER:HA	3:L:827:PRO:HD2	1.95	0.49
2:N:68:GLN:HG3	2:N:73:LYS:HG2	1.94	0.49
1:A:176:SER:H	1:A:179:ASN:HD22	1.60	0.48
2:B:65:PHE:HA	2:B:75:TYR:HA	1.95	0.48
1:J:326:ASP:HB2	1:J:332:GLN:HE21	1.77	0.48
2:K:121:LEU:HB2	2:K:206:LYS:HB3	1.95	0.48
3:L:579:LEU:HB2	3:L:603:PRO:HG2	1.94	0.48
2:N:27:GLY:O	2:N:31:LEU:N	2.46	0.48
2:N:65:PHE:HA	2:N:75:TYR:HA	1.95	0.48
3:C:579:LEU:HB2	3:C:603:PRO:HG2	1.94	0.48
3:G:687:ARG:HA	3:G:713:LEU:HA	1.94	0.48
3:G:802:SER:HA	3:G:827:PRO:HD2	1.95	0.48
3:L:502:ASP:N	3:L:502:ASP:OD1	2.47	0.48
1:M:268:VAL:HG11	2:N:237:PRO:HB3	1.95	0.48
2:B:146:ASN:HB2	2:B:151:VAL:HG22	1.96	0.48
2:B:60:PHE:HB2	2:B:75:TYR:HE2	1.78	0.48
2:H:121:LEU:HB2	2:H:206:LYS:HB3	1.95	0.48
2:H:68:GLN:HG3	2:H:73:LYS:HG2	1.94	0.48
1:J:268:VAL:HG11	2:K:237:PRO:HB3	1.95	0.48
3:O:802:SER:HA	3:O:827:PRO:HD2	1.95	0.48
3:F:454:ALA:HB2	3:F:637:LEU:HD13	1.95	0.48
2:H:60:PHE:HB2	2:H:75:TYR:HE2	1.78	0.48
3:L:622:ASN:N	3:L:622:ASN:OD1	2.45	0.48
2:N:160:LEU:H	2:N:165:ARG:HH21	1.60	0.48
3:O:579:LEU:HB2	3:O:603:PRO:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:792:ARG:NH1	3:C:343:GLU:OE1	2.46	0.48
3:C:637:LEU:HA	3:C:660:LEU:HA	1.96	0.48
1:D:255:LYS:HB2	2:E:228:VAL:HG13	1.94	0.48
1:D:350:ASN:HB2	1:D:356:ARG:HH22	1.79	0.48
3:F:394:THR:OG1	3:F:397:THR:OG1	2.29	0.48
1:I:353:ALA:HA	1:I:356:ARG:HD2	1.95	0.48
2:N:60:PHE:HB2	2:N:75:TYR:HE2	1.78	0.48
3:O:661:GLU:HA	3:O:686:LEU:HA	1.96	0.48
3:C:454:ALA:HB2	3:C:637:LEU:HD13	1.95	0.48
3:F:426:PRO:HG2	3:F:429:CYS:HB3	1.96	0.48
3:F:802:SER:HA	3:F:827:PRO:HD2	1.95	0.48
2:H:160:LEU:H	2:H:165:ARG:HH21	1.60	0.48
3:F:637:LEU:HA	3:F:660:LEU:HA	1.96	0.48
2:H:146:ASN:HB2	2:H:151:VAL:HG22	1.96	0.48
3:L:394:THR:OG1	3:L:397:THR:OG1	2.29	0.48
3:C:626:LEU:HB3	3:C:651:PRO:HD3	1.94	0.48
2:E:146:ASN:HB2	2:E:151:VAL:HG22	1.96	0.48
2:H:95:THR:HA	2:H:98:ARG:HH22	1.79	0.48
1:M:146:GLN:O	1:M:212:LYS:NZ	2.36	0.48
3:O:454:ALA:HB2	3:O:637:LEU:HD13	1.95	0.48
3:C:802:SER:HA	3:C:827:PRO:HD2	1.96	0.48
2:E:160:LEU:H	2:E:165:ARG:HH21	1.60	0.48
1:D:204:GLY:HA2	1:D:207:PHE:HD2	1.78	0.48
1:D:268:VAL:HG11	2:E:237:PRO:HB3	1.96	0.48
2:E:254:PHE:O	2:E:257:CYS:HB2	2.14	0.48
3:G:454:ALA:HB2	3:G:637:LEU:HD13	1.95	0.48
2:H:65:PHE:HA	2:H:75:TYR:HA	1.95	0.48
3:F:792:ARG:NH1	3:L:343:GLU:OE1	2.46	0.48
2:N:66:VAL:N	2:N:74:TRP:O	2.42	0.48
3:O:622:ASN:N	3:O:622:ASN:OD1	2.45	0.48
3:C:426:PRO:HG2	3:C:429:CYS:HB3	1.96	0.47
2:E:60:PHE:HB2	2:E:75:TYR:HE2	1.78	0.47
3:F:502:ASP:OD1	3:F:502:ASP:N	2.47	0.47
3:G:637:LEU:HA	3:G:660:LEU:HA	1.96	0.47
3:G:661:GLU:HA	3:G:686:LEU:HA	1.96	0.47
2:K:65:PHE:HA	2:K:75:TYR:HA	1.95	0.47
3:L:661:GLU:HA	3:L:686:LEU:HA	1.96	0.47
2:H:254:PHE:O	2:H:257:CYS:HB2	2.14	0.47
1:J:146:GLN:O	1:J:212:LYS:NZ	2.35	0.47
3:L:454:ALA:HB2	3:L:637:LEU:HD13	1.95	0.47
3:C:502:ASP:OD1	3:C:502:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLN:O	1:D:212:LYS:NZ	2.36	0.47
2:K:160:LEU:H	2:K:165:ARG:HH21	1.60	0.47
3:L:152:SER:O	3:L:200:GLN:NE2	2.47	0.47
3:L:637:LEU:HA	3:L:660:LEU:HA	1.96	0.47
3:L:426:PRO:HG2	3:L:429:CYS:HB3	1.96	0.47
1:M:350:ASN:HB2	1:M:356:ARG:HH22	1.79	0.47
2:N:121:LEU:HB2	2:N:206:LYS:HB3	1.96	0.47
3:O:502:ASP:OD1	3:O:502:ASP:N	2.47	0.47
3:F:773:SER:HG	3:F:800:SER:HG	1.59	0.47
3:G:152:SER:O	3:G:200:GLN:NE2	2.47	0.47
2:K:60:PHE:HB2	2:K:75:TYR:HE2	1.78	0.47
2:N:95:THR:HA	2:N:98:ARG:HH22	1.79	0.47
3:C:51:GLN:NE2	3:F:137:THR:O	2.48	0.47
3:L:51:GLN:NE2	3:O:137:THR:O	2.47	0.47
3:O:657:LEU:HD12	3:O:660:LEU:HD22	1.97	0.47
2:B:254:PHE:O	2:B:257:CYS:HB2	2.14	0.47
3:C:661:GLU:HA	3:C:686:LEU:HA	1.96	0.47
3:F:152:SER:O	3:F:200:GLN:NE2	2.48	0.47
2:K:27:GLY:O	2:K:31:LEU:N	2.46	0.47
3:O:152:SER:O	3:O:200:GLN:NE2	2.47	0.47
2:N:44:PRO:HG3	3:O:643:ASN:HD22	1.78	0.47
3:O:637:LEU:HA	3:O:660:LEU:HA	1.96	0.47
1:A:255:LYS:HB2	2:B:228:VAL:HG13	1.95	0.47
2:E:27:GLY:O	2:E:31:LEU:N	2.46	0.47
2:E:65:PHE:HA	2:E:75:TYR:HA	1.95	0.47
3:G:502:ASP:N	3:G:502:ASP:OD1	2.47	0.47
2:E:121:LEU:HB2	2:E:206:LYS:HB3	1.95	0.47
3:G:426:PRO:HG2	3:G:429:CYS:HB3	1.96	0.47
2:K:254:PHE:O	2:K:257:CYS:HB2	2.14	0.47
3:L:221:SER:OG	3:L:223:THR:O	2.33	0.47
2:N:146:ASN:HB2	2:N:151:VAL:HG22	1.96	0.47
3:O:426:PRO:HG2	3:O:429:CYS:HB3	1.96	0.47
1:I:350:ASN:HB2	1:I:356:ARG:HH22	1.79	0.47
1:J:350:ASN:HB2	1:J:356:ARG:HH22	1.79	0.47
1:M:353:ALA:HA	1:M:356:ARG:HD2	1.96	0.47
3:F:221:SER:OG	3:F:223:THR:O	2.33	0.47
2:K:146:ASN:HB2	2:K:151:VAL:HG22	1.96	0.47
1:A:350:ASN:HB2	1:A:356:ARG:HH22	1.79	0.46
2:B:121:LEU:HB2	2:B:206:LYS:HB3	1.95	0.46
3:L:521:PHE:HD1	3:L:524:LYS:HB3	1.80	0.46
3:O:521:PHE:HD1	3:O:524:LYS:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:THR:HB	3:C:58:LEU:HD23	1.97	0.46
1:D:176:SER:H	1:D:179:ASN:HD22	1.63	0.46
1:D:353:ALA:HA	1:D:356:ARG:HD2	1.98	0.46
2:E:200:ASP:OD2	2:E:204:THR:OG1	2.34	0.46
3:F:521:PHE:HD1	3:F:524:LYS:HB3	1.81	0.46
1:J:361:GLU:O	1:J:365:THR:OG1	2.28	0.46
2:K:66:VAL:N	2:K:74:TRP:O	2.42	0.46
3:C:38:LEU:HD11	3:C:73:GLU:HB3	1.97	0.46
3:F:661:GLU:HA	3:F:686:LEU:HA	1.96	0.46
2:K:95:THR:HA	2:K:98:ARG:HH22	1.79	0.46
2:N:300:LEU:HG	2:N:303:ASP:HB2	1.98	0.46
3:O:221:SER:OG	3:O:223:THR:O	2.33	0.46
2:E:95:THR:HA	2:E:98:ARG:HH22	1.79	0.46
3:G:521:PHE:HD1	3:G:524:LYS:HB3	1.81	0.46
3:L:412:PRO:HD2	3:L:415:LEU:HD12	1.98	0.46
1:M:174:LYS:O	1:M:180:HIS:NE2	2.47	0.46
3:O:38:LEU:HD11	3:O:73:GLU:HB3	1.97	0.46
3:O:602:PHE:HZ	3:O:627:GLN:H	1.63	0.46
3:C:412:PRO:HD2	3:C:415:LEU:HD12	1.98	0.46
3:F:30:GLN:HE22	3:F:116:GLN:HG2	1.81	0.46
3:G:38:LEU:HD11	3:G:73:GLU:HB3	1.97	0.46
3:G:412:PRO:HD2	3:G:415:LEU:HD12	1.98	0.46
3:G:51:GLN:NE2	3:C:137:THR:O	2.48	0.46
3:G:657:LEU:HD12	3:G:660:LEU:HD22	1.97	0.46
1:J:353:ALA:HA	1:J:356:ARG:HD2	1.97	0.46
2:N:254:PHE:O	2:N:257:CYS:HB2	2.14	0.46
3:L:602:PHE:HZ	3:L:627:GLN:H	1.63	0.46
2:B:200:ASP:OD2	2:B:204:THR:OG1	2.34	0.46
2:B:27:GLY:O	2:B:31:LEU:N	2.46	0.46
2:B:95:THR:HA	2:B:98:ARG:HH22	1.79	0.46
3:C:267:ASP:OD1	3:C:295:THR:OG1	2.34	0.46
1:D:208:LEU:HD12	1:D:217:TYR:CZ	2.51	0.46
3:F:412:PRO:HD2	3:F:415:LEU:HD12	1.98	0.46
1:J:255:LYS:HB2	2:K:228:VAL:HG13	1.97	0.46
1:I:270:THR:HG23	2:H:268:ILE:HG23	1.98	0.46
1:I:146:GLN:O	1:I:212:LYS:NZ	2.37	0.46
3:L:501:LYS:HB3	3:L:502:ASP:H	1.53	0.46
3:L:657:LEU:HD12	3:L:660:LEU:HD22	1.97	0.46
3:O:412:PRO:HD2	3:O:415:LEU:HD12	1.98	0.46
2:B:123:LEU:HD23	2:B:125:GLY:H	1.81	0.46
3:C:521:PHE:HD1	3:C:524:LYS:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:262:TYR:OH	3:F:285:PRO:O	2.27	0.46
2:H:200:ASP:OD2	2:H:204:THR:OG1	2.34	0.46
1:I:176:SER:H	1:I:179:ASN:HD22	1.63	0.46
2:K:123:LEU:HD23	2:K:125:GLY:H	1.81	0.46
3:C:30:GLN:HE22	3:C:116:GLN:HG2	1.81	0.45
3:G:54:THR:HB	3:G:58:LEU:HD23	1.98	0.45
2:K:200:ASP:OD2	2:K:204:THR:OG1	2.34	0.45
1:M:208:LEU:HD12	1:M:217:TYR:CZ	2.52	0.45
3:C:152:SER:O	3:C:200:GLN:NE2	2.47	0.45
3:C:221:SER:OG	3:C:223:THR:O	2.33	0.45
3:F:267:ASP:OD1	3:F:295:THR:OG1	2.34	0.45
1:I:174:LYS:O	1:I:180:HIS:NE2	2.49	0.45
2:N:200:ASP:OD2	2:N:204:THR:OG1	2.34	0.45
3:O:54:THR:HB	3:O:58:LEU:HD23	1.97	0.45
2:E:123:LEU:HD23	2:E:125:GLY:H	1.81	0.45
2:N:76:ARG:HH12	2:N:141:GLU:HA	1.82	0.45
3:F:475:ASP:OD1	3:F:475:ASP:N	2.50	0.45
3:O:430:VAL:HG13	3:O:474:VAL:HG21	1.98	0.45
3:F:54:THR:HB	3:F:58:LEU:HD23	1.97	0.45
3:F:602:PHE:HZ	3:F:627:GLN:H	1.63	0.45
1:J:208:LEU:HD12	1:J:217:TYR:CZ	2.51	0.45
3:L:30:GLN:HE22	3:L:116:GLN:HG2	1.81	0.45
2:E:76:ARG:HH12	2:E:141:GLU:HA	1.82	0.45
3:F:38:LEU:HD11	3:F:73:GLU:HB3	1.97	0.45
3:G:622:ASN:OD1	3:G:622:ASN:N	2.45	0.45
2:H:324:LYS:O	2:H:330:ARG:NE	2.37	0.45
1:I:208:LEU:HD12	1:I:217:TYR:CZ	2.52	0.45
1:J:176:SER:H	1:J:179:ASN:HD22	1.63	0.45
3:L:54:THR:HB	3:L:58:LEU:HD23	1.97	0.45
2:B:300:LEU:HG	2:B:303:ASP:HB2	1.98	0.45
2:B:66:VAL:N	2:B:74:TRP:O	2.42	0.45
3:C:602:PHE:HZ	3:C:627:GLN:H	1.63	0.45
1:D:174:LYS:O	1:D:180:HIS:NE2	2.50	0.45
3:G:430:VAL:HG13	3:G:474:VAL:HG21	1.98	0.45
3:G:602:PHE:HZ	3:G:627:GLN:H	1.63	0.45
2:H:123:LEU:HD23	2:H:125:GLY:H	1.81	0.45
2:K:19:ALA:HA	2:K:22:TRP:CD1	2.47	0.45
1:A:208:LEU:HD12	1:A:217:TYR:CZ	2.51	0.45
3:C:475:ASP:OD1	3:C:475:ASP:N	2.50	0.45
3:C:657:LEU:HD12	3:C:660:LEU:HD22	1.97	0.45
3:G:267:ASP:OD1	3:G:295:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:LYS:HB3	1:J:180:HIS:HE2	1.82	0.45
3:L:38:LEU:HD11	3:L:73:GLU:HB3	1.97	0.45
2:B:27:GLY:HA2	2:B:30:PHE:HB3	1.99	0.45
3:F:657:LEU:HD12	3:F:660:LEU:HD22	1.97	0.45
3:G:221:SER:OG	3:G:223:THR:O	2.33	0.45
3:G:394:THR:OG1	3:G:397:THR:OG1	2.29	0.45
1:J:174:LYS:O	1:J:180:HIS:NE2	2.48	0.45
3:L:475:ASP:N	3:L:475:ASP:OD1	2.50	0.45
1:M:176:SER:H	1:M:179:ASN:HD22	1.63	0.45
3:F:539:THR:HG21	3:F:568:LYS:HB2	1.99	0.45
2:K:76:ARG:HH12	2:K:141:GLU:HA	1.82	0.45
3:O:30:GLN:HE22	3:O:116:GLN:HG2	1.81	0.45
1:A:174:LYS:HB3	1:A:180:HIS:HE2	1.81	0.44
2:B:76:ARG:HH12	2:B:141:GLU:HA	1.82	0.44
2:E:300:LEU:HG	2:E:303:ASP:HB2	1.98	0.44
3:G:30:GLN:HE22	3:G:116:GLN:HG2	1.81	0.44
3:L:52:LYS:HD2	3:L:53:ARG:HB2	2.00	0.44
2:N:123:LEU:HD23	2:N:125:GLY:H	1.81	0.44
2:N:19:ALA:HA	2:N:22:TRP:CD1	2.47	0.44
3:O:184:ILE:HG13	3:O:307:ALA:HA	1.99	0.44
3:C:767:ARG:NH2	3:F:341:ARG:HH12	2.16	0.44
3:G:52:LYS:HD2	3:G:53:ARG:HB2	2.00	0.44
2:H:76:ARG:HH12	2:H:141:GLU:HA	1.82	0.44
2:H:27:GLY:HA2	2:H:30:PHE:HB3	1.99	0.44
2:E:45:ILE:N	3:F:621:GLN:OE1	2.50	0.44
3:F:430:VAL:HG13	3:F:474:VAL:HG21	1.98	0.44
3:G:773:SER:OG	3:G:800:SER:OG	2.30	0.44
2:H:27:GLY:O	2:H:31:LEU:N	2.46	0.44
2:K:300:LEU:HG	2:K:303:ASP:HB2	1.98	0.44
3:F:184:ILE:HG13	3:F:307:ALA:HA	1.99	0.44
2:K:71:TYR:OH	2:K:100:ARG:NH1	2.51	0.44
3:L:773:SER:OG	3:L:800:SER:OG	2.30	0.44
2:N:82:ARG:CZ	3:O:724:TYR:HB2	2.47	0.44
3:C:184:ILE:HG13	3:C:307:ALA:HA	1.99	0.44
3:C:52:LYS:HD2	3:C:53:ARG:HB2	1.99	0.44
3:G:262:TYR:OH	3:G:285:PRO:O	2.27	0.44
3:L:184:ILE:HG13	3:L:307:ALA:HA	1.99	0.44
3:L:430:VAL:HG13	3:L:474:VAL:HG21	1.98	0.44
3:C:430:VAL:HG13	3:C:474:VAL:HG21	1.98	0.44
2:E:19:ALA:O	2:E:22:TRP:HB2	2.18	0.44
2:E:71:TYR:OH	2:E:100:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:27:GLY:HA2	2:N:30:PHE:HB3	1.99	0.44
3:O:267:ASP:OD1	3:O:295:THR:OG1	2.34	0.44
2:H:300:LEU:HG	2:H:303:ASP:HB2	1.98	0.44
2:N:71:TYR:OH	2:N:100:ARG:NH1	2.51	0.44
2:B:19:ALA:O	2:B:22:TRP:HB2	2.18	0.44
3:F:61:LEU:HD22	3:F:129:VAL:HG11	2.00	0.44
3:G:184:ILE:HG13	3:G:307:ALA:HA	1.99	0.44
2:K:19:ALA:O	2:K:22:TRP:HB2	2.18	0.44
2:N:262:ILE:HD13	2:N:316:VAL:HG22	2.00	0.44
2:B:262:ILE:HD13	2:B:316:VAL:HG22	2.00	0.43
1:A:270:THR:HG23	2:B:268:ILE:HG23	2.00	0.43
2:E:27:GLY:HA2	2:E:30:PHE:HB3	1.99	0.43
3:F:52:LYS:HD2	3:F:53:ARG:HB2	2.00	0.43
3:G:65:LEU:HD23	3:G:68:LEU:HD12	2.00	0.43
3:G:539:THR:HG21	3:G:568:LYS:HB2	1.99	0.43
3:G:727:ASP:OD1	3:G:727:ASP:N	2.51	0.43
3:L:267:ASP:OD1	3:L:295:THR:OG1	2.34	0.43
3:C:539:THR:HG21	3:C:568:LYS:HB2	1.99	0.43
3:C:65:LEU:HD23	3:C:68:LEU:HD12	2.00	0.43
1:D:270:THR:HG23	2:E:268:ILE:HG23	2.00	0.43
3:G:810:VAL:HA	3:G:813:GLN:HG2	2.00	0.43
2:N:19:ALA:O	2:N:22:TRP:HB2	2.18	0.43
3:O:501:LYS:HB3	3:O:502:ASP:H	1.53	0.43
3:O:539:THR:HG21	3:O:568:LYS:HB2	1.99	0.43
3:C:727:ASP:OD1	3:C:727:ASP:N	2.51	0.43
3:C:810:VAL:HA	3:C:813:GLN:HG2	2.00	0.43
2:H:71:TYR:OH	2:H:100:ARG:NH1	2.51	0.43
3:C:61:LEU:HD22	3:C:129:VAL:HG11	2.00	0.43
3:F:381:ARG:HE	3:F:382:ILE:HG13	1.84	0.43
3:L:679:GLU:O	3:L:682:ASN:HB2	2.19	0.43
2:B:71:TYR:OH	2:B:100:ARG:NH1	2.51	0.43
3:F:679:GLU:O	3:F:682:ASN:HB2	2.19	0.43
2:K:25:ASP:OD1	2:K:26:ASN:N	2.52	0.43
3:L:539:THR:HG21	3:L:568:LYS:HB2	1.99	0.43
3:O:61:LEU:HD22	3:O:129:VAL:HG11	2.00	0.43
3:O:52:LYS:HD2	3:O:53:ARG:HB2	2.00	0.43
2:K:27:GLY:HA2	2:K:30:PHE:HB3	1.99	0.43
2:B:25:ASP:OD1	2:B:26:ASN:N	2.52	0.43
3:C:381:ARG:HE	3:C:382:ILE:HG13	1.84	0.43
3:C:679:GLU:O	3:C:682:ASN:HB2	2.19	0.43
2:E:25:ASP:OD1	2:E:26:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:475:ASP:OD1	3:G:475:ASP:N	2.50	0.43
2:H:19:ALA:O	2:H:22:TRP:HB2	2.18	0.43
2:H:262:ILE:HD13	2:H:316:VAL:HG22	2.00	0.43
2:K:262:ILE:HD13	2:K:316:VAL:HG22	2.00	0.43
3:L:262:TYR:OH	3:L:285:PRO:O	2.27	0.43
3:L:65:LEU:HD23	3:L:68:LEU:HD12	2.00	0.43
2:N:259:LEU:HD23	2:N:262:ILE:HD12	2.01	0.43
3:O:475:ASP:OD1	3:O:475:ASP:N	2.50	0.43
3:O:679:GLU:O	3:O:682:ASN:HB2	2.19	0.43
1:A:174:LYS:O	1:A:180:HIS:NE2	2.52	0.43
3:C:650:PHE:HD1	3:C:650:PHE:HA	1.72	0.43
2:E:66:VAL:N	2:E:74:TRP:O	2.42	0.43
3:G:381:ARG:HE	3:G:382:ILE:HG13	1.84	0.43
3:L:727:ASP:N	3:L:727:ASP:OD1	2.51	0.43
3:O:727:ASP:N	3:O:727:ASP:OD1	2.51	0.43
3:O:810:VAL:HA	3:O:813:GLN:HG2	2.00	0.43
2:B:180:HIS:HE1	2:B:188:ILE:HG23	1.84	0.42
2:B:27:GLY:O	2:B:30:PHE:HB3	2.19	0.42
2:B:288:GLU:O	2:B:291:LYS:NZ	2.48	0.42
3:F:810:VAL:HA	3:F:813:GLN:HG2	2.00	0.42
3:G:61:LEU:HD22	3:G:129:VAL:HG11	2.00	0.42
3:L:381:ARG:HE	3:L:382:ILE:HG13	1.84	0.42
3:O:237:LEU:HA	3:O:237:LEU:HD23	1.90	0.42
2:N:25:ASP:OD1	2:N:26:ASN:N	2.52	0.42
1:D:174:LYS:HB3	1:D:180:HIS:HE2	1.84	0.42
2:E:259:LEU:HD23	2:E:262:ILE:HD12	2.01	0.42
2:H:180:HIS:HE1	2:H:188:ILE:HG23	1.84	0.42
2:H:27:GLY:O	2:H:30:PHE:HB3	2.19	0.42
2:K:180:HIS:HE1	2:K:188:ILE:HG23	1.84	0.42
3:L:810:VAL:HA	3:L:813:GLN:HG2	2.00	0.42
1:M:274:THR:HG1	1:M:277:SER:H	1.65	0.42
3:O:381:ARG:HE	3:O:382:ILE:HG13	1.84	0.42
2:B:18:LYS:O	2:B:21:ARG:HB2	2.20	0.42
3:C:394:THR:OG1	3:C:397:THR:OG1	2.29	0.42
2:H:45:ILE:N	3:G:621:GLN:OE1	2.53	0.42
2:K:27:GLY:O	2:K:30:PHE:HB3	2.19	0.42
3:L:61:LEU:HD22	3:L:129:VAL:HG11	2.00	0.42
3:O:65:LEU:HD23	3:O:68:LEU:HD12	2.00	0.42
1:A:361:GLU:O	1:A:365:THR:OG1	2.27	0.42
3:C:230:MET:HE3	3:C:253:ILE:HD12	2.00	0.42
3:F:65:LEU:HD23	3:F:68:LEU:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:767:ARG:NH2	3:C:341:ARG:HH12	2.17	0.42
2:K:45:ILE:N	3:L:621:GLN:OE1	2.53	0.42
2:N:27:GLY:O	2:N:30:PHE:HB3	2.19	0.42
2:H:25:ASP:OD1	2:H:26:ASN:N	2.52	0.42
2:N:18:LYS:O	2:N:21:ARG:HB2	2.20	0.42
2:B:259:LEU:HD23	2:B:262:ILE:HD12	2.01	0.42
3:C:544:VAL:HA	3:C:568:LYS:HB3	2.02	0.42
2:E:27:GLY:O	2:E:30:PHE:HB3	2.19	0.42
3:G:274:LEU:HD23	3:G:304:ARG:HG2	2.02	0.42
3:G:544:VAL:HA	3:G:568:LYS:HB3	2.02	0.42
3:L:303:LYS:NZ	3:L:309:ASP:OD1	2.53	0.42
2:E:288:GLU:O	2:E:291:LYS:NZ	2.48	0.42
2:E:262:ILE:HD13	2:E:316:VAL:HG22	2.00	0.42
3:F:303:LYS:NZ	3:F:309:ASP:OD1	2.53	0.42
3:F:727:ASP:N	3:F:727:ASP:OD1	2.51	0.42
3:G:679:GLU:O	3:G:682:ASN:HB2	2.19	0.42
2:K:259:LEU:HD23	2:K:262:ILE:HD12	2.01	0.42
1:M:361:GLU:HA	1:M:364:VAL:HG22	2.02	0.42
2:N:31:LEU:HD12	2:N:31:LEU:HA	1.93	0.42
3:O:262:TYR:OH	3:O:285:PRO:O	2.27	0.42
2:B:269:MET:HB3	2:B:277:GLN:HB2	2.02	0.41
2:E:180:HIS:HE1	2:E:188:ILE:HG23	1.84	0.41
3:F:822:THR:HG22	3:F:843:VAL:HG12	2.02	0.41
3:G:501:LYS:HB3	3:G:502:ASP:H	1.53	0.41
1:J:250:THR:OG1	1:J:251:HIS:N	2.53	0.41
1:J:272:ARG:HD3	2:K:276:LEU:HB3	2.01	0.41
2:K:48:PHE:HB2	2:K:127:CYS:HB2	2.02	0.41
3:L:767:ARG:NH2	3:O:341:ARG:HH12	2.18	0.41
3:C:822:THR:HG22	3:C:843:VAL:HG12	2.02	0.41
1:D:350:ASN:O	1:D:356:ARG:NH2	2.52	0.41
3:F:274:LEU:HD23	3:F:304:ARG:HG2	2.02	0.41
3:G:303:LYS:NZ	3:G:309:ASP:OD1	2.53	0.41
2:N:48:PHE:HB2	2:N:127:CYS:HB2	2.02	0.41
3:O:274:LEU:HD23	3:O:304:ARG:HG2	2.02	0.41
3:G:822:THR:HG22	3:G:843:VAL:HG12	2.02	0.41
1:I:174:LYS:HB3	1:I:180:HIS:HE2	1.85	0.41
1:I:361:GLU:HA	1:I:364:VAL:HG22	2.02	0.41
1:J:361:GLU:HA	1:J:364:VAL:HG22	2.02	0.41
3:L:274:LEU:HD23	3:L:304:ARG:HG2	2.02	0.41
3:L:298:SER:HB2	3:L:301:VAL:HG22	2.03	0.41
3:F:767:ARG:NH2	3:L:341:ARG:HH12	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:250:THR:OG1	1:M:251:HIS:N	2.52	0.41
2:N:180:HIS:HE1	2:N:188:ILE:HG23	1.85	0.41
2:E:19:ALA:HA	2:E:22:TRP:CD1	2.47	0.41
2:H:18:LYS:O	2:H:21:ARG:HB2	2.20	0.41
2:H:259:LEU:HD23	2:H:262:ILE:HD12	2.01	0.41
3:L:193:LEU:N	6:L:901:DTP:O2B	2.50	0.41
1:M:270:THR:HG23	2:N:268:ILE:HG23	2.02	0.41
2:B:45:ILE:N	3:C:621:GLN:OE1	2.53	0.41
3:C:274:LEU:HD23	3:C:304:ARG:HG2	2.02	0.41
2:E:18:LYS:O	2:E:21:ARG:HB2	2.20	0.41
2:E:269:MET:HB3	2:E:277:GLN:HB2	2.02	0.41
3:O:303:LYS:NZ	3:O:309:ASP:OD1	2.53	0.41
3:O:378:GLU:HB2	3:O:381:ARG:NH2	2.36	0.41
3:F:230:MET:HE3	3:F:253:ILE:HD12	2.01	0.41
3:G:532:LEU:HD13	3:G:532:LEU:HA	1.90	0.41
3:G:650:PHE:HD1	3:G:650:PHE:HA	1.72	0.41
3:L:544:VAL:HA	3:L:568:LYS:HB3	2.02	0.41
3:F:378:GLU:HB2	3:F:381:ARG:NH2	2.36	0.41
3:G:259:GLY:H	3:G:288:GLN:NE2	2.19	0.41
2:H:269:MET:HB3	2:H:277:GLN:HB2	2.02	0.41
3:L:378:GLU:HB2	3:L:381:ARG:NH2	2.36	0.41
3:O:259:GLY:H	3:O:288:GLN:NE2	2.19	0.41
2:B:225:ALA:HB2	2:B:245:VAL:HG23	2.03	0.41
3:C:259:GLY:H	3:C:288:GLN:NE2	2.19	0.41
3:C:303:LYS:NZ	3:C:309:ASP:OD1	2.53	0.41
3:C:378:GLU:HB2	3:C:381:ARG:NH2	2.36	0.41
3:F:645:GLY:O	3:F:667:LYS:NZ	2.54	0.41
3:G:645:GLY:O	3:G:667:LYS:NZ	2.54	0.41
3:L:822:THR:HG22	3:L:843:VAL:HG12	2.02	0.41
2:N:191:ASP:OD1	2:N:191:ASP:N	2.40	0.41
3:O:532:LEU:HA	3:O:532:LEU:HD13	1.90	0.41
3:C:161:VAL:HG21	3:C:326:LEU:HB2	2.03	0.41
3:C:811:LEU:O	3:C:815:MET:N	2.54	0.41
1:D:250:THR:OG1	1:D:251:HIS:N	2.51	0.41
2:E:225:ALA:HB2	2:E:245:VAL:HG23	2.03	0.41
3:F:161:VAL:HG21	3:F:326:LEU:HB2	2.03	0.41
3:F:544:VAL:HA	3:F:568:LYS:HB3	2.02	0.41
3:G:230:MET:HE3	3:G:253:ILE:HD12	2.03	0.41
2:K:269:MET:HB3	2:K:277:GLN:HB2	2.02	0.41
3:O:544:VAL:HA	3:O:568:LYS:HB3	2.02	0.41
3:G:372:LYS:HA	3:G:372:LYS:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:298:SER:HB2	3:O:301:VAL:HG22	2.03	0.41
3:O:645:GLY:O	3:O:667:LYS:NZ	2.54	0.41
1:A:361:GLU:HA	1:A:364:VAL:HG22	2.02	0.41
2:B:48:PHE:HB2	2:B:127:CYS:HB2	2.02	0.41
3:C:645:GLY:O	3:C:667:LYS:NZ	2.54	0.41
2:E:94:ILE:HG23	2:E:94:ILE:HD12	1.89	0.41
3:F:373:ASP:N	3:F:373:ASP:OD1	2.48	0.41
2:K:18:LYS:O	2:K:21:ARG:HB2	2.20	0.41
3:O:502:ASP:O	3:O:504:PHE:N	2.54	0.41
3:O:846:LYS:HB2	3:O:846:LYS:HE2	1.95	0.41
3:O:822:THR:HG22	3:O:843:VAL:HG12	2.02	0.40
2:B:39:ASN:OD1	3:C:568:LYS:NZ	2.40	0.40
3:G:298:SER:HB2	3:G:301:VAL:HG22	2.03	0.40
3:G:549:SER:HB2	3:G:572:ASP:HB2	2.04	0.40
2:H:48:PHE:HB2	2:H:127:CYS:HB2	2.02	0.40
1:I:159:CYS:HB2	1:I:161:GLU:HG3	2.03	0.40
3:L:259:GLY:H	3:L:288:GLN:NE2	2.19	0.40
2:N:201:LYS:HE2	2:N:201:LYS:HB2	1.95	0.40
3:G:217:TRP:O	3:G:236:ASN:ND2	2.55	0.40
3:G:378:GLU:HB2	3:G:381:ARG:NH2	2.36	0.40
1:J:350:ASN:O	1:J:356:ARG:NH2	2.54	0.40
1:J:270:THR:HG23	2:K:268:ILE:HG23	2.02	0.40
2:K:33:GLU:HG2	2:K:109:VAL:HG21	2.04	0.40
3:L:217:TRP:O	3:L:236:ASN:ND2	2.55	0.40
2:N:225:ALA:HB2	2:N:245:VAL:HG23	2.03	0.40
3:O:811:LEU:O	3:O:815:MET:N	2.54	0.40
3:F:259:GLY:H	3:F:288:GLN:NE2	2.19	0.40
3:F:513:ARG:HD3	3:F:513:ARG:HA	1.86	0.40
3:F:576:SER:HA	3:F:603:PRO:HG3	2.04	0.40
1:I:149:HIS:HB2	1:I:152:LEU:HD12	2.03	0.40
3:L:513:ARG:HA	3:L:513:ARG:HD3	1.86	0.40
1:A:355:LEU:H	1:A:356:ARG:NH1	2.20	0.40
1:A:350:ASN:O	1:A:356:ARG:NH2	2.55	0.40
2:B:171:GLU:HG3	2:B:205:ALA:HB3	2.04	0.40
2:B:220:LYS:HD2	2:B:223:ILE:HD11	2.03	0.40
3:C:613:GLN:O	3:C:637:LEU:N	2.52	0.40
1:D:272:ARG:CZ	1:D:274:THR:HG21	2.52	0.40
2:H:31:LEU:HD12	2:H:31:LEU:HA	1.92	0.40
1:J:269:ALA:HA	2:K:233:GLY:HA2	2.02	0.40
2:K:201:LYS:HB2	2:K:201:LYS:HE2	1.95	0.40
3:L:846:LYS:HB2	3:L:846:LYS:HE2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:149:HIS:HB2	1:M:152:LEU:HD12	2.04	0.40
1:M:174:LYS:HB3	1:M:180:HIS:HE2	1.86	0.40
2:N:171:GLU:HG3	2:N:205:ALA:HB3	2.04	0.40
3:O:372:LYS:HA	3:O:372:LYS:HD3	1.92	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	185/426 (43%)	155 (84%)	30 (16%)	0	100	100
1	D	185/426 (43%)	154 (83%)	31 (17%)	0	100	100
1	I	185/426 (43%)	155 (84%)	30 (16%)	0	100	100
1	J	185/426 (43%)	155 (84%)	30 (16%)	0	100	100
1	M	185/426 (43%)	156 (84%)	29 (16%)	0	100	100
2	B	323/351 (92%)	293 (91%)	30 (9%)	0	100	100
2	E	323/351 (92%)	293 (91%)	30 (9%)	0	100	100
2	H	323/351 (92%)	293 (91%)	30 (9%)	0	100	100
2	K	323/351 (92%)	293 (91%)	30 (9%)	0	100	100
2	N	323/351 (92%)	293 (91%)	30 (9%)	0	100	100
3	C	802/852 (94%)	709 (88%)	89 (11%)	4 (0%)	31	69
3	F	802/852 (94%)	711 (89%)	87 (11%)	4 (0%)	31	69
3	G	802/852 (94%)	709 (88%)	89 (11%)	4 (0%)	31	69
3	L	802/852 (94%)	709 (88%)	89 (11%)	4 (0%)	31	69
3	O	802/852 (94%)	709 (88%)	89 (11%)	4 (0%)	31	69
All	All	6550/8145 (80%)	5787 (88%)	743 (11%)	20 (0%)	47	77

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	501	LYS
3	G	507	PRO
3	G	650	PHE
3	C	501	LYS
3	C	507	PRO
3	C	650	PHE
3	F	501	LYS
3	F	507	PRO
3	F	650	PHE
3	L	501	LYS
3	L	507	PRO
3	L	650	PHE
3	O	501	LYS
3	O	507	PRO
3	O	650	PHE
3	G	502	ASP
3	C	502	ASP
3	F	502	ASP
3	L	502	ASP
3	O	502	ASP

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	158/355 (44%)	158 (100%)	0	100	100
1	D	158/355 (44%)	158 (100%)	0	100	100
1	I	158/355 (44%)	158 (100%)	0	100	100
1	J	158/355 (44%)	158 (100%)	0	100	100
1	M	158/355 (44%)	158 (100%)	0	100	100
2	B	293/314 (93%)	287 (98%)	6 (2%)	58	82
2	E	293/314 (93%)	287 (98%)	6 (2%)	58	82
2	H	293/314 (93%)	287 (98%)	6 (2%)	58	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	293/314 (93%)	287 (98%)	6 (2%)	58	82
2	N	293/314 (93%)	287 (98%)	6 (2%)	58	82
3	C	736/772 (95%)	729 (99%)	7 (1%)	78	89
3	F	736/772 (95%)	729 (99%)	7 (1%)	78	89
3	G	736/772 (95%)	729 (99%)	7 (1%)	78	89
3	L	736/772 (95%)	729 (99%)	7 (1%)	78	89
3	O	736/772 (95%)	729 (99%)	7 (1%)	78	89
All	All	5935/7205 (82%)	5870 (99%)	65 (1%)	77	89

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	114	MET
2	H	148	ARG
2	H	190	ARG
2	H	222	ARG
2	H	302	LYS
2	H	313	GLU
3	G	52	LYS
3	G	110	LYS
3	G	341	ARG
3	G	486	LYS
3	G	511	ASN
3	G	641	MET
3	G	763	LEU
2	B	114	MET
2	B	148	ARG
2	B	190	ARG
2	B	222	ARG
2	B	302	LYS
2	B	313	GLU
3	C	52	LYS
3	C	110	LYS
3	C	341	ARG
3	C	486	LYS
3	C	511	ASN
3	C	641	MET
3	C	763	LEU
2	E	114	MET
2	E	148	ARG

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Mol	Chain	Res	Type
2	E	190	ARG
2	E	222	ARG
2	E	302	LYS
2	E	313	GLU
3	F	52	LYS
3	F	110	LYS
3	F	341	ARG
3	F	486	LYS
3	F	511	ASN
3	F	641	MET
3	F	763	LEU
2	K	114	MET
2	K	148	ARG
2	K	190	ARG
2	K	222	ARG
2	K	302	LYS
2	K	313	GLU
3	L	52	LYS
3	L	110	LYS
3	L	341	ARG
3	L	486	LYS
3	L	511	ASN
3	L	641	MET
3	L	763	LEU
2	N	114	MET
2	N	148	ARG
2	N	190	ARG
2	N	222	ARG
2	N	302	LYS
2	N	313	GLU
3	O	52	LYS
3	O	110	LYS
3	O	341	ARG
3	O	486	LYS
3	O	511	ASN
3	O	641	MET
3	O	763	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	179	ASN

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Mol	Chain	Res	Type
1	I	332	GLN
2	H	59	ASN
2	H	180	HIS
2	H	189	HIS
3	G	236	ASN
3	G	288	GLN
3	G	322	ASN
3	G	511	ASN
3	G	643	ASN
3	G	673	ASN
3	G	698	GLN
1	A	179	ASN
1	A	332	GLN
2	B	59	ASN
2	B	180	HIS
2	B	189	HIS
3	C	236	ASN
3	C	322	ASN
3	C	511	ASN
3	C	643	ASN
3	C	673	ASN
3	C	698	GLN
1	D	179	ASN
1	D	332	GLN
2	E	59	ASN
2	E	180	HIS
2	E	189	HIS
3	F	288	GLN
3	F	322	ASN
3	F	511	ASN
3	F	643	ASN
3	F	673	ASN
3	F	698	GLN
1	J	179	ASN
1	J	332	GLN
2	K	59	ASN
2	K	180	HIS
2	K	189	HIS
3	L	236	ASN
3	L	288	GLN
3	L	322	ASN
3	L	511	ASN

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Mol	Chain	Res	Type
3	L	643	ASN
3	L	673	ASN
3	L	698	GLN
1	M	179	ASN
1	M	332	GLN
2	N	59	ASN
2	N	180	HIS
2	N	189	HIS
3	O	236	ASN
3	O	288	GLN
3	O	322	ASN
3	O	511	ASN
3	O	643	ASN
3	O	673	ASN
3	O	698	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

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	BQL	A	501	1,5	22,27,27	0.83	1 (4%)	22,39,39	1.14	2 (9%)
5	BQO	A	502	1,4	22,28,28	1.71	5 (22%)	23,41,41	1.36	4 (17%)
6	DTP	C	901	-	26,32,32	0.75	0	29,50,50	0.86	2 (6%)
4	BQL	D	501	1,5	22,27,27	0.83	1 (4%)	22,39,39	1.18	2 (9%)
5	BQO	D	502	1,4	22,28,28	1.71	5 (22%)	23,41,41	1.36	3 (13%)
6	DTP	F	901	-	26,32,32	0.75	0	29,50,50	0.88	2 (6%)
6	DTP	G	901	-	26,32,32	0.75	0	29,50,50	0.87	1 (3%)
4	BQL	I	501	1,5	22,27,27	0.82	1 (4%)	22,39,39	1.07	2 (9%)
5	BQO	I	502	1,4	18,26,28	2.05	5 (27%)	16,36,41	1.48	3 (18%)
4	BQL	J	501	1,5	22,27,27	0.84	1 (4%)	22,39,39	1.15	2 (9%)
5	BQO	J	502	1,4	22,28,28	1.70	5 (22%)	23,41,41	1.35	4 (17%)
6	DTP	L	901	-	26,32,32	0.75	0	29,50,50	0.88	2 (6%)
4	BQL	M	501	1,5	22,27,27	0.81	1 (4%)	22,39,39	1.09	2 (9%)
5	BQO	M	502	1,4	22,28,28	1.73	5 (22%)	23,41,41	1.39	5 (21%)
6	DTP	O	901	-	26,32,32	0.75	0	29,50,50	0.87	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BQL	A	501	1,5	-	0/11/34/34	0/2/2/2
5	BQO	A	502	1,4	-	0/15/37/37	0/2/2/2
6	DTP	C	901	-	-	0/18/34/34	0/3/3/3
4	BQL	D	501	1,5	-	0/11/34/34	0/2/2/2
5	BQO	D	502	1,4	-	0/15/37/37	0/2/2/2
6	DTP	F	901	-	-	0/18/34/34	0/3/3/3
6	DTP	G	901	-	-	0/18/34/34	0/3/3/3
4	BQL	I	501	1,5	-	0/11/34/34	0/2/2/2
5	BQO	I	502	1,4	-	0/6/33/37	0/2/2/2
4	BQL	J	501	1,5	-	0/11/34/34	0/2/2/2
5	BQO	J	502	1,4	-	0/15/37/37	0/2/2/2
6	DTP	L	901	-	-	0/18/34/34	0/3/3/3
4	BQL	M	501	1,5	-	0/11/34/34	0/2/2/2
5	BQO	M	502	1,4	-	0/15/37/37	0/2/2/2
6	DTP	O	901	-	-	0/18/34/34	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	502	BQO	OP1-CB	-4.83	1.39	1.45
5	D	502	BQO	C3'-C2'	-2.55	1.46	1.53
5	A	502	BQO	C3'-C2'	-2.52	1.46	1.53
5	I	502	BQO	C3'-C2'	-2.51	1.46	1.53
5	J	502	BQO	C3'-C2'	-2.50	1.46	1.53
5	M	502	BQO	C6-N1	-2.48	1.32	1.35
5	I	502	BQO	C6-N1	-2.48	1.32	1.35
5	M	502	BQO	C3'-C2'	-2.45	1.47	1.53
5	A	502	BQO	C6-N1	-2.44	1.32	1.35
5	J	502	BQO	C6-N1	-2.42	1.32	1.35
5	D	502	BQO	C6-N1	-2.38	1.32	1.35
5	M	502	BQO	O4-C4	-2.34	1.18	1.24
5	A	502	BQO	O4-C4	-2.31	1.18	1.24
5	I	502	BQO	O4-C4	-2.31	1.18	1.24
5	J	502	BQO	O4-C4	-2.30	1.18	1.24
5	D	502	BQO	O4-C4	-2.30	1.18	1.24
4	J	501	BQL	C2-N3	-2.17	1.33	1.38
4	D	501	BQL	C2-N3	-2.08	1.34	1.38
4	A	501	BQL	C2-N3	-2.08	1.34	1.38
4	I	501	BQL	C2-N3	-2.08	1.34	1.38
4	M	501	BQL	C2-N3	-2.04	1.34	1.38
5	J	502	BQO	P-OP3	2.03	1.65	1.55
5	M	502	BQO	P-OP3	2.05	1.65	1.55
5	D	502	BQO	P-OP3	2.05	1.65	1.55
5	A	502	BQO	P-OP3	2.06	1.65	1.55
5	I	502	BQO	O4'-C1'	4.35	1.47	1.41
5	A	502	BQO	O4'-C1'	4.38	1.47	1.41
5	J	502	BQO	O4'-C1'	4.42	1.47	1.41
5	M	502	BQO	O4'-C1'	4.45	1.47	1.41
5	D	502	BQO	O4'-C1'	4.45	1.47	1.41

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	502	BQO	C3-O4'-C1'	-3.03	106.67	109.83
5	D	502	BQO	C3-O4'-C1'	-3.01	106.69	109.83
5	A	502	BQO	C3-O4'-C1'	-2.98	106.72	109.83
5	J	502	BQO	C3-O4'-C1'	-2.94	106.76	109.83
5	M	502	BQO	C3-O4'-C1'	-2.85	106.86	109.83
4	D	501	BQL	O-C-CA	-2.61	117.97	124.98
5	M	502	BQO	CG2-CB-CA	-2.54	108.10	113.10
5	A	502	BQO	CG2-CB-CA	-2.53	108.13	113.10
4	M	501	BQL	O-C-CA	-2.45	118.42	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	501	BQL	O-C-CA	-2.43	118.45	124.98
5	J	502	BQO	CG2-CB-CA	-2.36	108.45	113.10
4	I	501	BQL	O-C-CA	-2.36	118.65	124.98
4	A	501	BQL	O-C-CA	-2.35	118.69	124.98
5	M	502	BQO	P-O5'-C1	-2.30	108.19	121.68
5	D	502	BQO	P-O5'-C1	-2.28	108.33	121.68
5	J	502	BQO	P-O5'-C1	-2.17	108.97	121.68
5	A	502	BQO	P-O5'-C1	-2.11	109.29	121.68
6	L	901	DTP	PA-O3A-PB	-2.06	126.02	132.57
6	O	901	DTP	PA-O3A-PB	-2.03	126.13	132.57
5	I	502	BQO	CG2-CB-CA	-2.02	109.12	113.10
6	C	901	DTP	PA-O3A-PB	-2.02	126.15	132.57
6	F	901	DTP	PA-O3A-PB	-2.02	126.15	132.57
5	M	502	BQO	C1-C3-C3'	-2.01	107.65	115.21
6	F	901	DTP	C5-C6-N6	2.17	123.78	120.38
6	L	901	DTP	C5-C6-N6	2.18	123.81	120.38
6	O	901	DTP	C5-C6-N6	2.19	123.81	120.38
6	C	901	DTP	C5-C6-N6	2.20	123.84	120.38
6	G	901	DTP	C5-C6-N6	2.20	123.84	120.38
4	I	501	BQL	O4'-C1'-N1	2.25	112.44	108.06
4	M	501	BQL	O4'-C1'-N1	2.37	112.69	108.06
4	A	501	BQL	O4'-C1'-N1	2.38	112.72	108.06
4	J	501	BQL	O4'-C1'-N1	2.55	113.04	108.06
5	I	502	BQO	C2'-C3'-C3	2.66	107.69	102.60
5	M	502	BQO	C2'-C3'-C3	2.68	107.73	102.60
5	A	502	BQO	C2'-C3'-C3	2.70	107.77	102.60
4	D	501	BQL	O4'-C1'-N1	2.74	113.42	108.06
5	J	502	BQO	C2'-C3'-C3	2.80	107.95	102.60
5	D	502	BQO	C2'-C3'-C3	2.94	108.22	102.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	502	BQO	1	0
6	C	901	DTP	1	0
5	D	502	BQO	1	0
6	F	901	DTP	1	0
6	G	901	DTP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	502	BQO	1	0
6	L	901	DTP	2	0
5	M	502	BQO	1	0
6	O	901	DTP	1	0

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.