Full wwPDB EM Validation Report ⓘ

Dec 19, 2024 – 02:07 PM JST

PDB ID	:	8ZPV
EMDB ID	:	EMD-60355
Title	:	Nipah virus polymerase complex
Authors	:	Wang, Y.R.; Zhang, H.Q.
Deposited on	:	2024-05-31
Resolution	:	2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

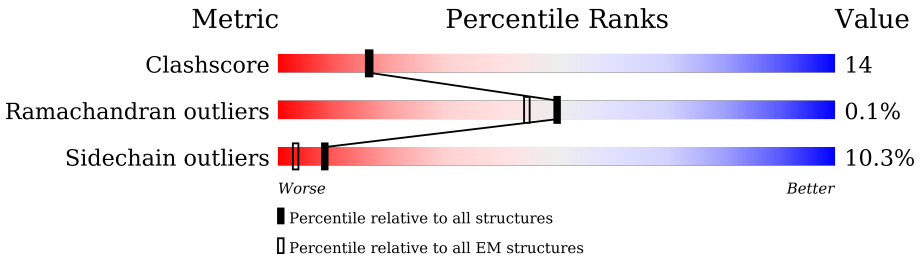
EMDB validation analysis	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	2244	42% 13% · 43%
2	B	709	· · · 93%
2	C	709	· · · 92%
2	D	709	8% 7% · 83%
2	E	709	· · · 92%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12440 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1275	Total	C	N	O	S	0	0
			10260	6533	1758	1903	66		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	581	THR	GLU	conflict	UNP Q997F0

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	51	Total	C	N	O	S	0	0
			400	252	70	77	1		
2	C	54	Total	C	N	O	S	0	0
			425	269	75	80	1		
2	D	117	Total	C	N	O	S	0	0
			922	573	161	183	5		
2	E	55	Total	C	N	O	S	0	0
			431	272	76	82	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

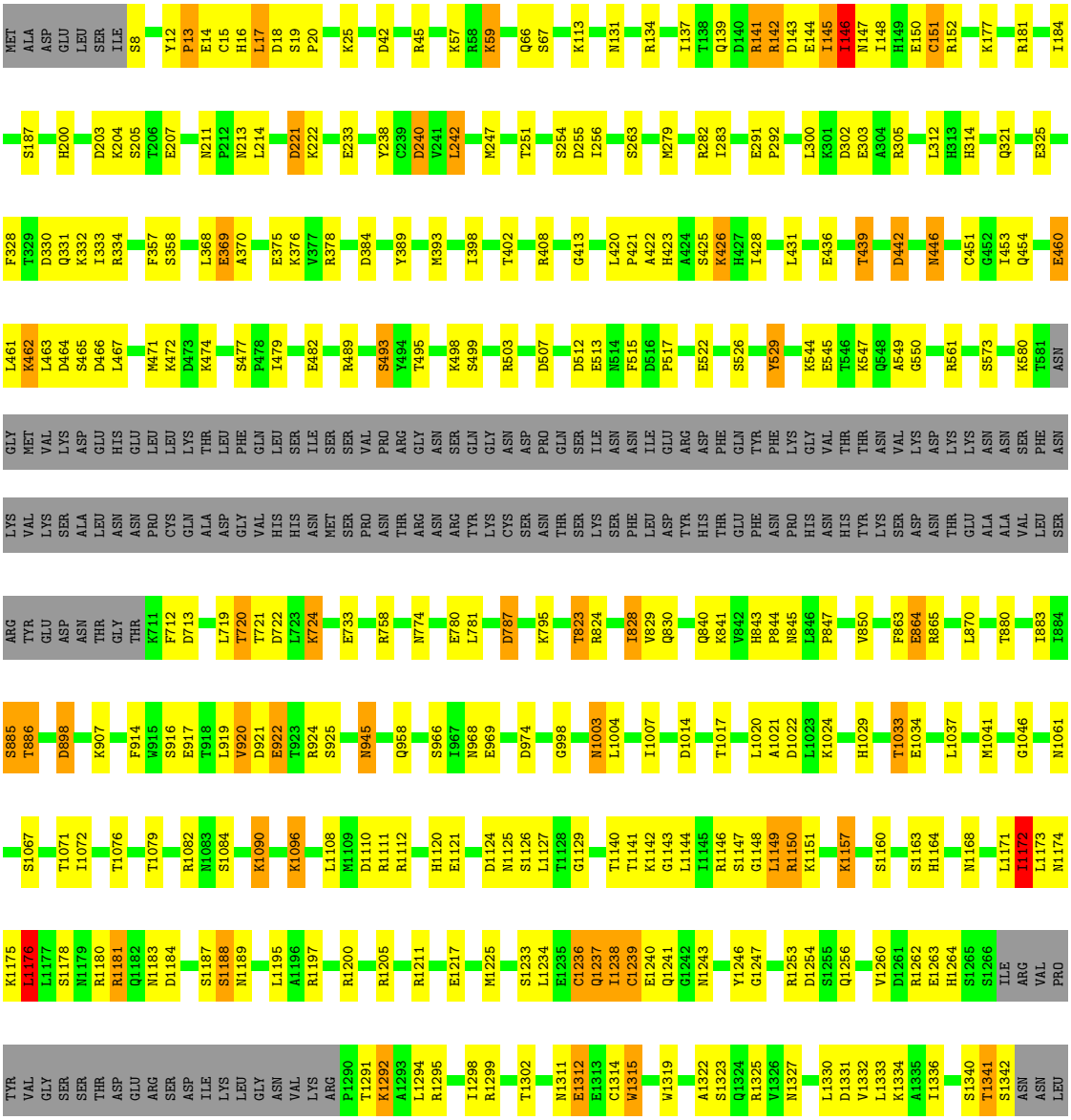
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

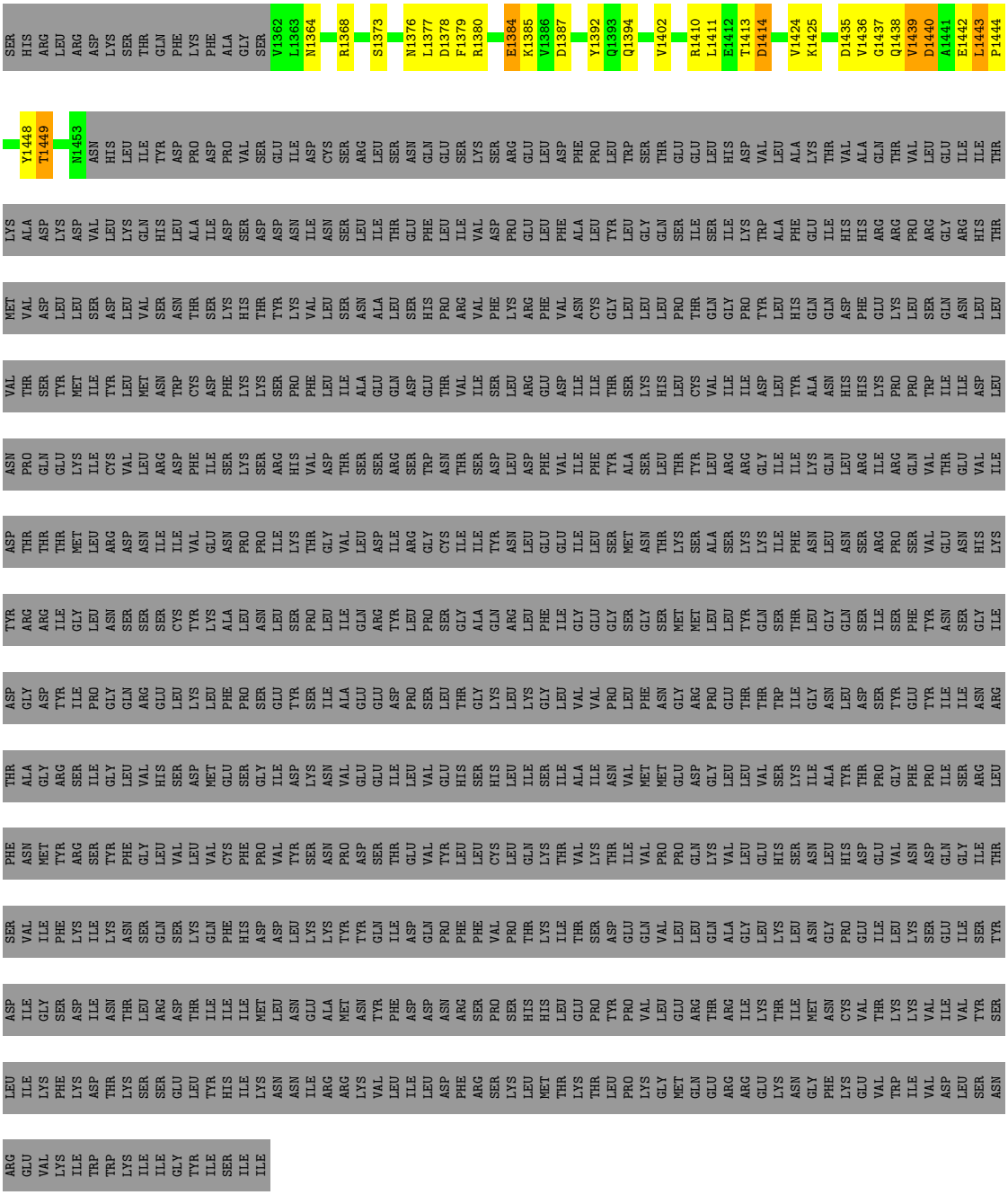
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RNA-directed RNA polymerase L

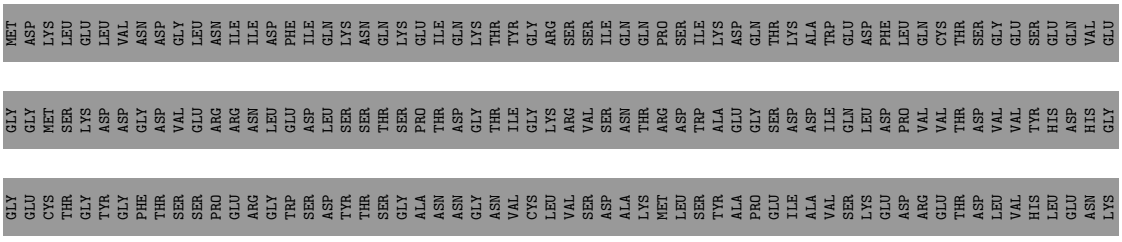
Chain A:

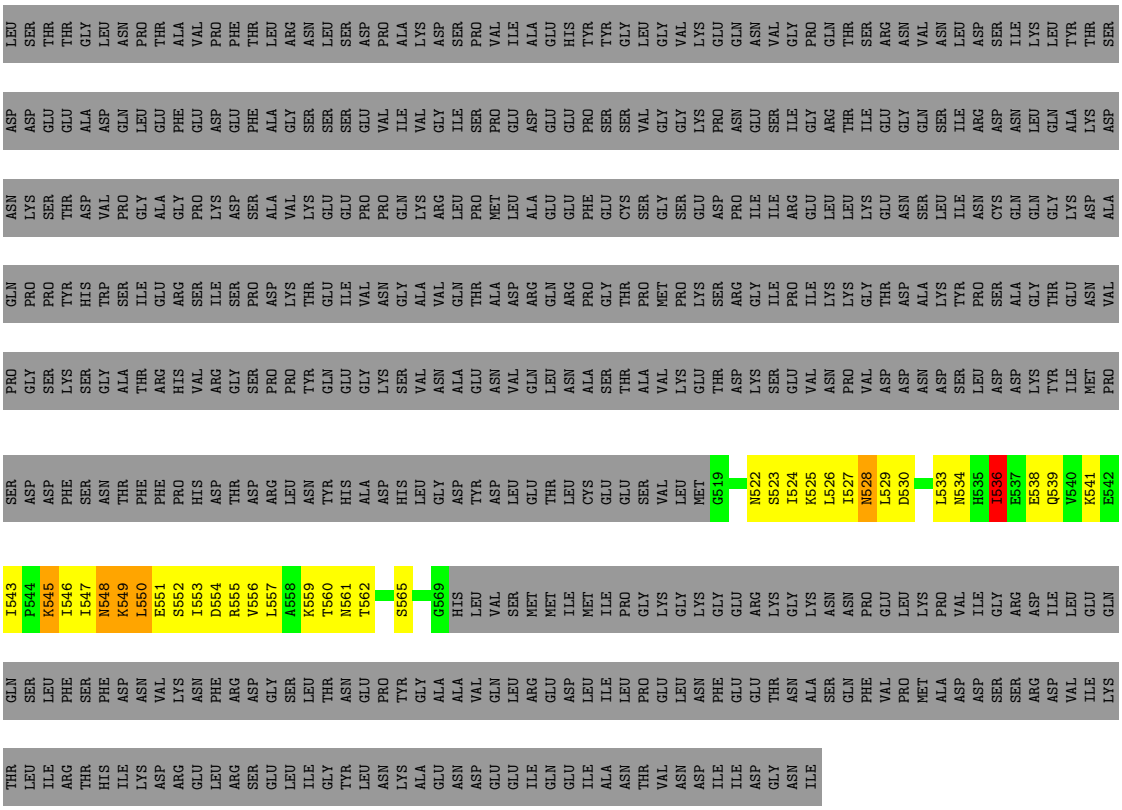




• Molecule 2: Phosphoprotein

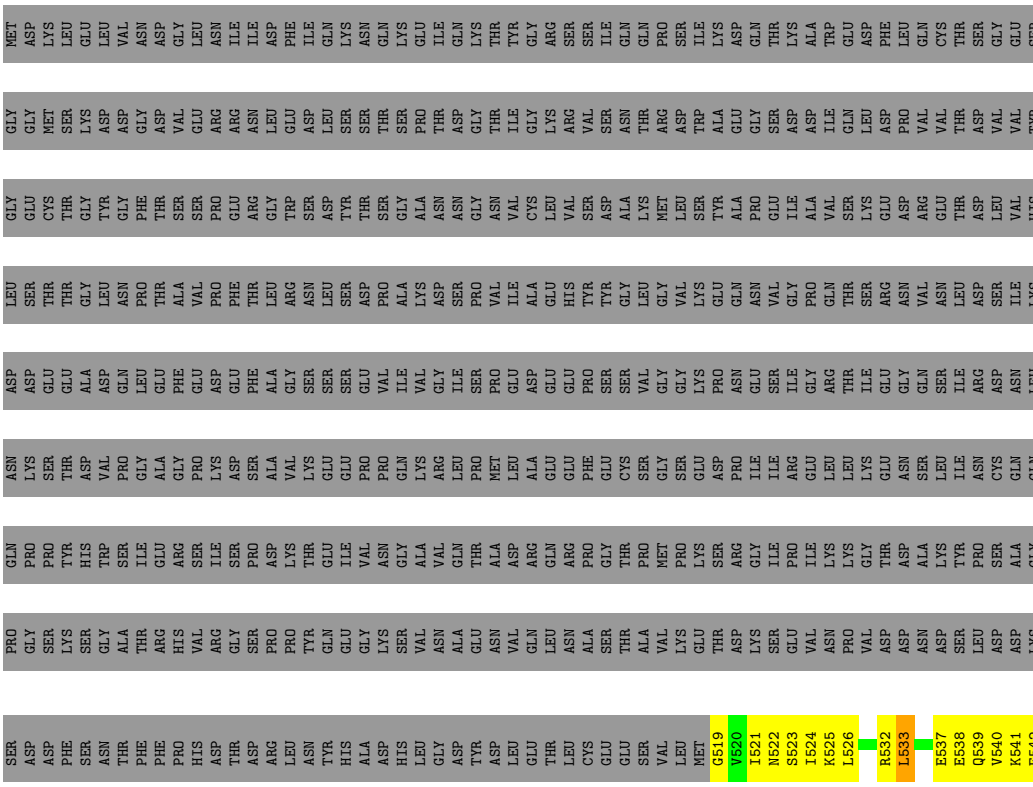
Chain B: 93%

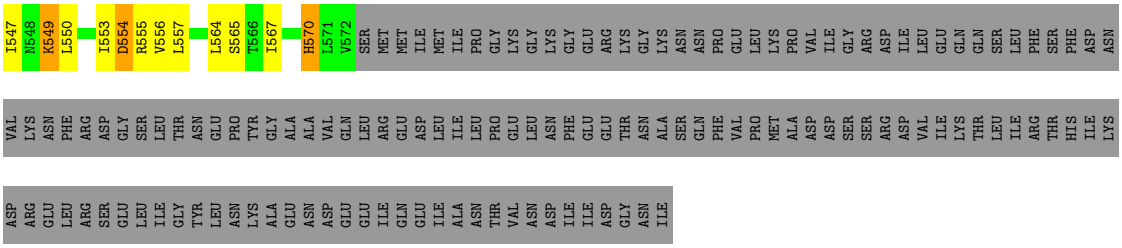




• Molecule 2: Phosphoprotein

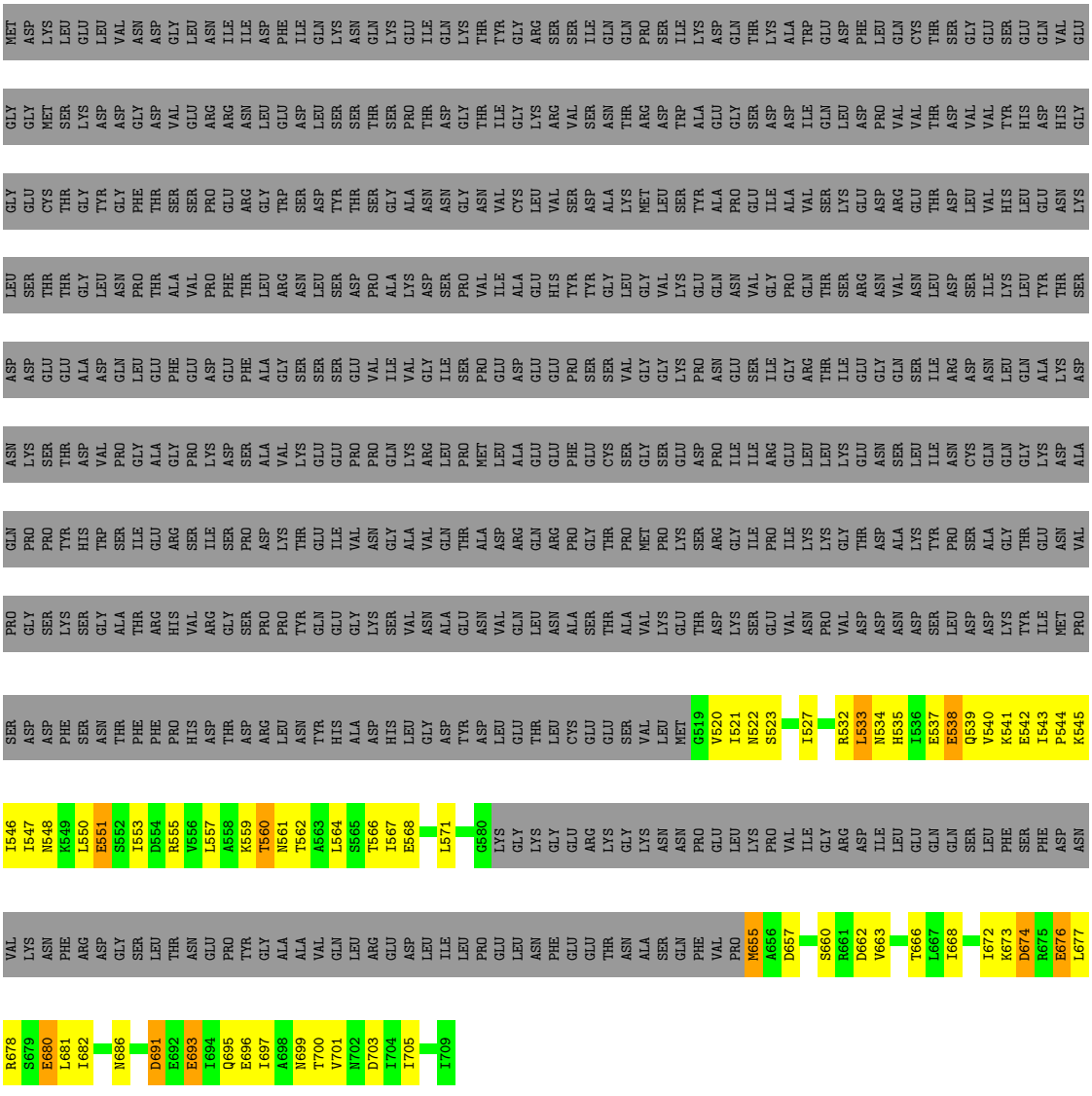
Chain C: 92%





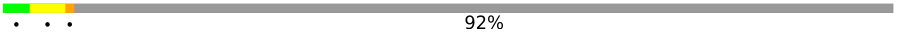
• Molecule 2: Phosphoprotein

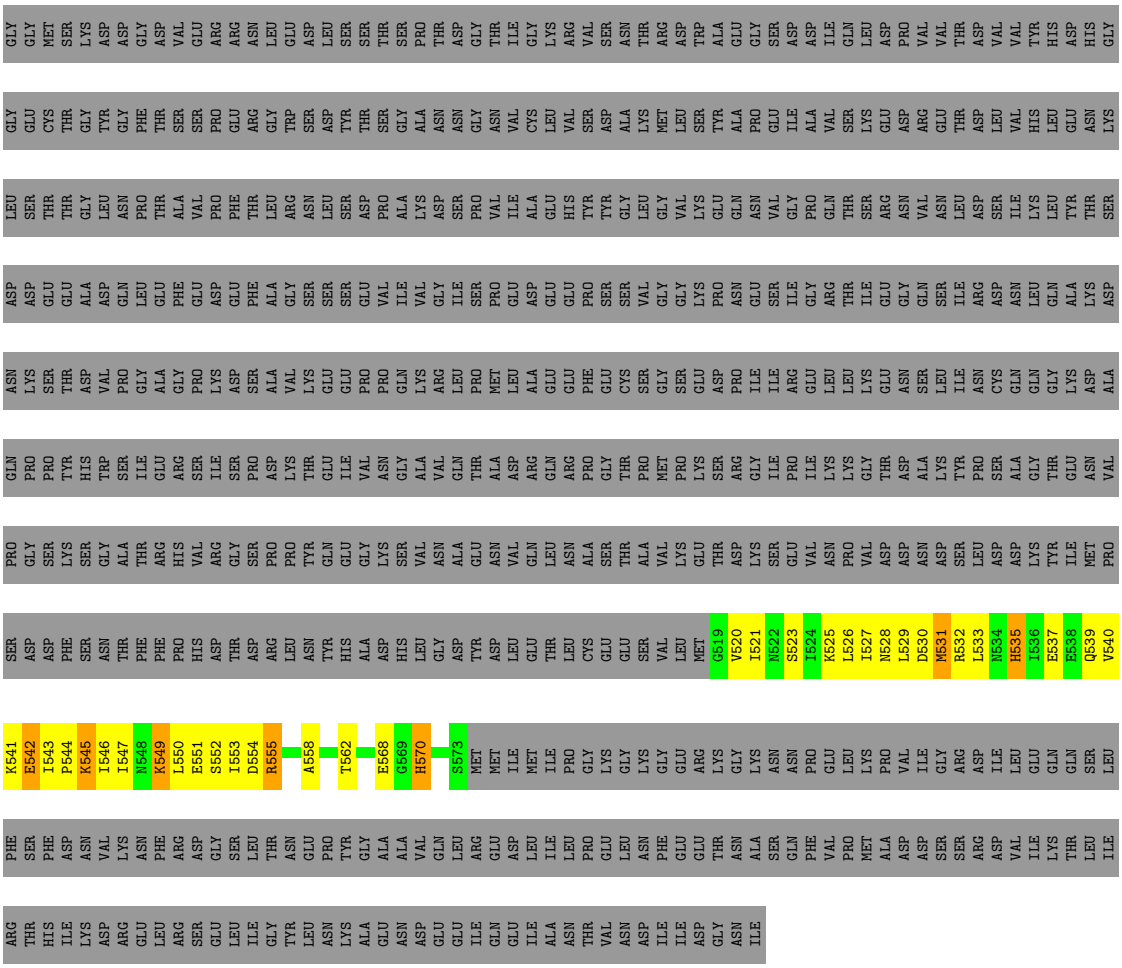
Chain D:



• Molecule 2: Phosphoprotein

Chain E:




GLY GLY MET SER LYS ASP ASP GLY ASP VAL GLU ARG ARG ASN LEU GLU ASP LEU SER SER THR SER PRO THR ASP GLY THR ILE GLY LYS ARG VAL SER ASN THR ARG ASP TRP ALA GLU GLY SER ASP ASP ILE GLN LEU ASP PRO VAL VAL THR ASP VAL VAL TYR HIS ASP HIS GLY
GLY GLU CYS THR GLY TYR GLY PHE THR SER SER PRO GLU ARG GLY TRP SER ASP TYR THR SER GLY ALA ALA ASN ASN GLY ASN VAL CYS LEU VAL SER ASP ALA LYS MET LEU SER TYR ALA PRO GLU ILE ALA VAL SER LYS GLU ASP ARG GLU THR ASP LEU VAL HIS LEU GLU ASN LYS
LEU SER THR THR GLY LEU ASN PRO THR ALA VAL PRO PHE THR LEU ARG ASN LEU SER ASP PRO ALA LYS ASP SER PRO VAL ILE ALA GLU HIS TYR TYR GLY LEU VAL PRO GLN THR SER ARG ASN VAL SER LEU ASP SER ILE LYS LEU GLU ASN SER
ASP ASP GLU GLU ALA ASP GLN LEU GLU PHE GLU ASP GLU PHE ALA GLY SER SER SER GLU VAL ILE VAL GLY ILE SER PRO GLU ASP GLU GLU PRO SER SER VAL GLY GLY LYS PRO ASN GLU SER ILE GLY ARG THR ILE GLU GLY GLN LEU ASN GLU GLN ASP ASP SER ILE LYS GLN ALA LYS ASP
ASN LYS SER THR ASP VAL PRO GLY ALA GLY PRO PRO LYS ASP SER ALA VAL LYS GLU GLU PRO PRO GLN LYS ARG LEU PRO MET LEU ALA GLU GLU PHE GLU GLU ASP SER GLU ASP PRO ILE ILE ARG GLU LEU LEU LYS GLU GLN ASN SER LEU ILE ASN CYS GLN GLN GLY LYS ASP ALA
GLN PRO PRO TYR HIS TRP SER ILE GLU ARG SER ILE SER PRO ASP LYS THR GLU ILE VAL ASN GLY ALA VAL GLN THR ALA ASP ARG GLN ARG PRO GLY THR PRO MET PRO LYS SER ARG GLY ILE PRO ILE LYS LYS GLY THR GLY GLU ASP ASN SER LEU ILE ASP ALA LYS TYR PRO SER GLY THR GLU ASN VAL
PRO GLY SER LYS SER GLY ALA THR ARG HIS VAL ARG GLY SER PRO PRO TYR GLN GLU GLY SER VAL ASN ALA GLU ASN VAL GLN LEU ASN ALA SER THR ALA VAL LYS GLU THR ASP LYS SER GLU VAL ASN PRO VAL ASP ASP ASN SER LEU ASP LYS TYR ILE MET PRO
SER ASP ASP PHE SER ASN THR PHE PHE PRO HIS ASP THR ASP ASN TYR HIS ALA ASP HIS LEU GLY ASP TYR ASP LEU GLU THR LEU CYS GLU GLU SER VAL LEU MET G519 V520 I521 N522 S523 I524 K525 L526 I527 N528 L529 D530 M531 R532 L533 N534 H535 I536 E537 E538 Q539 V540
K541 E542 I543 P544 K545 I546 I547 N548 K549 L550 E551 S552 I553 D554 R555 A558 T562 E568 G569 H570 S573 MET MET ILE MET ILE PRO GLY LYS GLY LYS GLY GLU ARG LYS GLY LYS ASN ASN PRO GLU LEU LYS PRO VAL ILE GLY ARG ASP ILE LEU GLU GLN SER LEU
PHE SER PHE ASP ASN VAL LYS ASN PHE ARG ASP GLY SER LEU THR ASN GLU PRO TYR GLY ALA ALA VAL GLN LEU ARG GLU ASP LEU ILE LEU PRO GLU LEU LEU ASN PHE GLU GLU GLU THR ASN ALA SER GLN PHE VAL PRO MET ALA ASP ASP SER SER ARG ASP VAL ILE LYS THR LEU ILE
ARG THR HIS ILE LYS ASP ARG GLU LEU ARG SER GLU LEU ILE GLY TYR LEU ASN LYS ALA GLU ASN ASP GLU GLU ILE GLN GLU ILE ALA ASN THR VAL ASN ASP ILE ILE ASP GLY ASN ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	523611	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.42	10/10470 (0.1%)	0.50	6/14152 (0.0%)
2	B	0.27	0/401	0.53	0/539
2	C	0.27	0/427	0.58	0/575
2	D	0.25	0/926	0.47	0/1245
2	E	0.24	0/433	0.57	0/583
All	All	0.40	10/12657 (0.1%)	0.50	6/17094 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
2	B	0	1
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	PRO	N-CA	12.55	1.68	1.47
1	A	1175	LYS	C-O	-9.45	1.05	1.23
1	A	1176	LEU	C-O	-9.13	1.05	1.23
1	A	1172	ILE	C-O	-7.01	1.10	1.23
1	A	1178	SER	CA-CB	-6.97	1.42	1.52
1	A	1173	LEU	C-O	-5.95	1.12	1.23
1	A	1171	LEU	C-O	-5.92	1.12	1.23
1	A	1174	ASN	C-O	-5.85	1.12	1.23
1	A	12	TYR	C-N	5.80	1.45	1.34
1	A	1178	SER	C-O	-5.55	1.12	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	13	PRO	CA-N-CD	-7.11	101.55	111.50
1	A	13	PRO	N-CA-C	-6.28	95.78	112.10
1	A	1174	ASN	CB-CA-C	-6.08	98.25	110.40
1	A	1180	ARG	CB-CA-C	-5.61	99.19	110.40
1	A	1180	ARG	CB-CG-CD	-5.35	97.70	111.60
1	A	1181	ARG	CB-CG-CD	5.07	124.77	111.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1172	ILE	Mainchain
1	A	1237	GLN	Peptide
1	A	1238	ILE	Peptide
1	A	145	ILE	Peptide
1	A	828	ILE	Peptide
2	B	536	ILE	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	10260	0	10301	223	0
2	B	400	0	433	40	0
2	C	425	0	460	35	0
2	D	922	0	959	55	0
2	E	431	0	465	38	0
3	A	2	0	0	0	0
All	All	12440	0	12618	351	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 14.

All (351) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PRO:N	1:A:13:PRO:CA	1.68	1.47
1:A:1236:CYS:HB3	1:A:1239:CYS:HA	1.49	0.93
1:A:426:LYS:H	1:A:426:LYS:CE	1.90	0.85
2:C:532:ARG:HG3	2:D:533:LEU:HD23	1.57	0.85
2:C:543:ILE:HG13	2:C:544:PRO:HD3	1.58	0.85
1:A:145:ILE:O	1:A:147:ASN:N	2.09	0.85
1:A:291:GLU:HG2	1:A:292:PRO:HD3	1.62	0.81
1:A:14:GLU:N	1:A:14:GLU:OE2	2.16	0.78
2:B:527:ILE:HG13	2:E:525:LYS:HE3	1.67	0.77
2:B:557:LEU:O	2:B:561:ASN:HB2	1.83	0.77
2:B:556:VAL:O	2:B:560:THR:OG1	2.03	0.76
1:A:421:PRO:HB3	2:B:559:LYS:HE3	1.68	0.76
1:A:13:PRO:N	1:A:13:PRO:C	2.38	0.76
1:A:426:LYS:H	1:A:426:LYS:HE2	1.52	0.75
1:A:1378:ASP:H	1:A:1380:ARG:HG3	1.51	0.75
2:B:530:ASP:O	2:E:532:ARG:NH2	2.20	0.74
1:A:1238:ILE:H	1:A:1240:GLU:H	1.34	0.74
2:D:532:ARG:NH2	2:E:537:GLU:OE2	2.21	0.73
1:A:545:GLU:HG3	1:A:550:GLY:HA2	1.69	0.73
1:A:16:HIS:CE1	1:A:916:SER:HB3	2.25	0.72
2:D:691:ASP:OD1	2:D:691:ASP:N	2.20	0.72
2:C:553:ILE:HA	2:C:556:VAL:HG12	1.72	0.72
2:E:547:ILE:HA	2:E:550:LEU:HD12	1.70	0.71
2:D:532:ARG:NH1	2:E:533:LEU:O	2.20	0.71
1:A:141:ARG:NH1	1:A:144:GLU:O	2.24	0.71
2:D:701:VAL:O	2:D:705:ILE:HG12	1.91	0.71
1:A:255:ASP:OD1	1:A:256:ILE:N	2.25	0.70
1:A:463:LEU:HD13	1:A:517:PRO:HB2	1.73	0.69
1:A:1176:LEU:HD23	1:A:1176:LEU:O	1.92	0.69
1:A:145:ILE:HD12	1:A:145:ILE:H	1.60	0.67
1:A:17:LEU:C	1:A:17:LEU:HD22	2.14	0.67
1:A:422:ALA:H	2:B:559:LYS:HZ1	1.41	0.66
2:D:547:ILE:HD13	2:D:550:LEU:HD21	1.76	0.66
2:B:551:GLU:O	2:B:555:ARG:CB	2.43	0.66
1:A:375:GLU:OE2	1:A:378:ARG:NH1	2.29	0.66
1:A:924:ARG:NH2	1:A:998:GLY:O	2.29	0.66
1:A:312:LEU:HD23	2:D:663:VAL:HG23	1.79	0.65
1:A:1238:ILE:HB	1:A:1241:GLN:H	1.60	0.65
2:B:551:GLU:O	2:B:555:ARG:HB2	1.96	0.65
2:D:672:ILE:O	2:D:678:ARG:NH1	2.30	0.65
2:D:548:ASN:HA	2:D:551:GLU:HG3	1.79	0.65
2:C:547:ILE:HA	2:C:550:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HD13	1:A:17:LEU:O	1.97	0.64
2:D:655:MET:SD	2:D:655:MET:N	2.71	0.64
1:A:921:ASP:OD2	1:A:968:ASN:ND2	2.31	0.64
1:A:1112:ARG:HH22	1:A:1437:GLY:HA3	1.62	0.64
1:A:442:ASP:O	1:A:446:ASN:ND2	2.31	0.64
2:D:532:ARG:HE	2:D:535:HIS:HE1	1.44	0.64
1:A:1291:THR:HA	1:A:1295:ARG:HE	1.63	0.63
1:A:1334:LYS:NZ	1:A:1336:ILE:O	2.24	0.63
1:A:8:SER:HB2	1:A:1150:ARG:HH11	1.63	0.63
1:A:795:LYS:NZ	2:C:570:HIS:O	2.24	0.62
2:D:566:THR:HG23	2:D:567:ILE:HG12	1.81	0.62
1:A:1410:ARG:NH1	1:A:1414:ASP:OD1	2.33	0.62
1:A:462:LYS:H	1:A:462:LYS:HD2	1.64	0.61
1:A:1126:SER:OG	1:A:1127:LEU:N	2.32	0.61
2:C:555:ARG:NE	2:C:555:ARG:HA	2.15	0.61
1:A:279:MET:HE2	1:A:283:ILE:HA	1.81	0.60
1:A:1168:ASN:O	1:A:1172:ILE:HG13	2.00	0.60
2:B:536:ILE:HG23	2:C:540:VAL:HG21	1.82	0.60
1:A:8:SER:HB3	1:A:1149:LEU:HD21	1.84	0.60
1:A:240:ASP:N	1:A:240:ASP:OD1	2.35	0.60
1:A:1046:GLY:O	1:A:1061:ASN:ND2	2.35	0.60
1:A:137:ILE:HG21	1:A:1402:VAL:HG21	1.83	0.59
2:C:522:ASN:O	2:C:526:LEU:HG	2.02	0.59
2:E:544:PRO:HA	2:E:547:ILE:HD11	1.85	0.59
1:A:823:THR:OG1	1:A:824:ARG:N	2.36	0.59
1:A:42:ASP:OD1	1:A:42:ASP:N	2.35	0.58
2:D:544:PRO:HA	2:D:547:ILE:HB	1.86	0.58
1:A:358:SER:HB3	1:A:907:LYS:HB2	1.86	0.58
1:A:1084:SER:O	1:A:1090:LYS:NZ	2.37	0.57
1:A:19:SER:HB2	1:A:20:PRO:HD2	1.87	0.57
1:A:828:ILE:HG22	1:A:829:VAL:H	1.70	0.56
1:A:145:ILE:HG22	1:A:146:ILE:H	1.69	0.56
1:A:376:LYS:HD3	1:A:549:ALA:HB1	1.86	0.56
2:D:539:GLN:NE2	2:E:540:VAL:O	2.36	0.56
1:A:147:ASN:O	1:A:150:GLU:N	2.39	0.56
1:A:898:ASP:O	1:A:1368:ARG:NH1	2.38	0.56
2:D:546:ILE:HG12	2:E:547:ILE:HD13	1.88	0.56
1:A:1111:ARG:HD3	1:A:1440:ASP:O	2.05	0.56
2:B:525:LYS:HZ1	2:C:526:LEU:HD13	1.71	0.55
1:A:330:ASP:OD2	1:A:333:ILE:N	2.33	0.55
1:A:1037:LEU:HD22	1:A:1187:SER:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1364:ASN:N	1:A:1364:ASN:OD1	2.39	0.55
2:D:678:ARG:O	2:D:682:ILE:HD12	2.06	0.55
1:A:16:HIS:HE1	1:A:916:SER:HB3	1.72	0.55
1:A:302:ASP:OD1	1:A:303:GLU:N	2.36	0.55
2:D:660:SER:HA	2:D:663:VAL:HG12	1.89	0.55
1:A:16:HIS:ND1	1:A:916:SER:HA	2.22	0.55
2:C:546:ILE:O	2:C:549:LYS:HG3	2.06	0.55
2:C:544:PRO:HA	2:C:547:ILE:HG13	1.89	0.55
2:B:525:LYS:O	2:B:529:LEU:HG	2.07	0.55
1:A:184:ILE:O	1:A:187:SER:OG	2.25	0.54
1:A:439:THR:OG1	1:A:442:ASP:OD1	2.21	0.54
2:C:533:LEU:HD23	2:C:533:LEU:H	1.71	0.54
2:E:528:ASN:O	2:E:532:ARG:HD3	2.07	0.54
1:A:131:ASN:HD22	1:A:1029:HIS:HE1	1.56	0.54
1:A:513:GLU:N	1:A:513:GLU:OE1	2.40	0.54
2:D:543:ILE:O	2:D:546:ILE:HG13	2.08	0.54
2:B:546:ILE:HG12	2:C:547:ILE:HD13	1.89	0.54
1:A:442:ASP:OD1	1:A:442:ASP:N	2.38	0.54
1:A:378:ARG:NH2	1:A:787:ASP:O	2.40	0.54
1:A:460:GLU:OE1	1:A:462:LYS:NZ	2.35	0.54
2:B:539:GLN:HG3	2:C:541:LYS:HZ2	1.72	0.53
1:A:431:LEU:HD11	1:A:436:GLU:HB2	1.89	0.53
1:A:1148:GLY:HA2	1:A:1151:LYS:HG2	1.91	0.53
2:D:559:LYS:HA	2:D:562:THR:HG22	1.90	0.53
1:A:1121:GLU:OE1	1:A:1299:ARG:NH1	2.36	0.53
1:A:369:GLU:OE1	1:A:370:ALA:N	2.41	0.53
2:E:551:GLU:N	2:E:551:GLU:OE1	2.39	0.53
1:A:8:SER:HB2	1:A:1150:ARG:NH1	2.24	0.53
1:A:780:GLU:OE1	1:A:780:GLU:N	2.39	0.53
2:B:539:GLN:HG3	2:C:541:LYS:NZ	2.23	0.53
2:E:526:LEU:HA	2:E:529:LEU:HG	1.90	0.53
2:B:536:ILE:HD11	2:C:537:GLU:HA	1.91	0.52
2:B:546:ILE:HD12	2:B:549:LYS:HG2	1.91	0.52
1:A:150:GLU:OE2	1:A:945:ASN:ND2	2.43	0.52
1:A:503:ARG:NH1	1:A:507:ASP:OD1	2.41	0.52
1:A:580:LYS:HA	1:A:830:GLN:HG2	1.90	0.52
1:A:1110:ASP:OD1	1:A:1211:ARG:NH1	2.34	0.52
1:A:840:GLN:NE2	1:A:841:LYS:O	2.43	0.52
1:A:1387:ASP:N	1:A:1387:ASP:OD1	2.43	0.52
2:B:523:SER:O	2:B:527:ILE:HD12	2.10	0.52
1:A:423:HIS:CE1	2:B:555:ARG:HA	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LYS:HZ1	1:A:561:ARG:HD2	1.75	0.52
2:D:695:GLN:O	2:D:699:ASN:ND2	2.43	0.52
1:A:247:MET:O	1:A:251:THR:HG22	2.10	0.51
1:A:919:LEU:O	1:A:921:ASP:N	2.43	0.51
1:A:1188:SER:OG	1:A:1189:ASN:N	2.43	0.51
2:C:550:LEU:HD21	2:D:550:LEU:HD13	1.91	0.51
1:A:203:ASP:OD1	1:A:204:LYS:N	2.41	0.51
1:A:465:SER:O	1:A:465:SER:OG	2.26	0.51
2:C:546:ILE:HD12	2:C:547:ILE:N	2.26	0.51
1:A:466:ASP:OD1	1:A:467:LEU:N	2.43	0.51
1:A:1341:THR:OG1	1:A:1342:SER:N	2.40	0.51
1:A:1380:ARG:HA	1:A:1385:LYS:HA	1.92	0.51
1:A:885:SER:OG	1:A:886:THR:N	2.44	0.51
2:E:552:SER:HA	2:E:555:ARG:NH2	2.26	0.51
1:A:512:ASP:OD1	1:A:515:PHE:N	2.44	0.51
2:B:553:ILE:HD12	2:E:553:ILE:HD11	1.93	0.51
2:C:553:ILE:HD12	2:D:553:ILE:HB	1.93	0.51
1:A:886:THR:O	1:A:886:THR:OG1	2.29	0.51
2:D:546:ILE:HD13	2:E:547:ILE:HB	1.92	0.50
2:B:557:LEU:HD21	2:C:557:LEU:HD13	1.93	0.50
1:A:1254:ASP:H	1:A:1413:THR:HG1	1.56	0.50
1:A:1323:SER:O	1:A:1448:TYR:OH	2.29	0.50
1:A:529:TYR:O	1:A:758:ARG:NH1	2.43	0.50
1:A:733:GLU:OE2	1:A:733:GLU:N	2.44	0.50
1:A:479:ILE:HG12	1:A:482:GLU:HG2	1.94	0.50
1:A:1436:VAL:O	1:A:1438:GLN:HG2	2.10	0.50
1:A:1376:ASN:OD1	1:A:1377:LEU:N	2.44	0.49
1:A:1436:VAL:HG22	1:A:1437:GLY:H	1.77	0.49
1:A:142:ARG:H	1:A:142:ARG:HD3	1.78	0.49
1:A:522:GLU:O	1:A:526:SER:OG	2.18	0.49
1:A:787:ASP:OD1	1:A:787:ASP:N	2.38	0.49
1:A:1311:ASN:OD1	1:A:1312:GLU:N	2.45	0.49
1:A:57:LYS:O	1:A:59:LYS:NZ	2.33	0.49
1:A:493:SER:O	1:A:493:SER:OG	2.28	0.49
2:D:697:ILE:HA	2:D:700:THR:HG22	1.94	0.49
2:C:519:GLY:O	2:C:523:SER:OG	2.25	0.49
1:A:15:CYS:HB2	1:A:177:LYS:HE3	1.95	0.49
1:A:1096:LYS:H	1:A:1096:LYS:HD3	1.77	0.49
2:E:542:GLU:HA	2:E:545:LYS:NZ	2.28	0.49
1:A:1238:ILE:O	1:A:1239:CYS:HB2	2.13	0.48
2:B:543:ILE:O	2:B:547:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:668:ILE:O	2:D:672:ILE:HG13	2.13	0.48
1:A:1124:ASP:O	1:A:1129:GLY:HA3	2.13	0.48
2:B:539:GLN:HE21	2:C:541:LYS:HD2	1.78	0.48
1:A:1238:ILE:HD12	1:A:1241:GLN:HA	1.95	0.48
1:A:200:HIS:NE2	1:A:207:GLU:OE2	2.41	0.48
1:A:1033:THR:OG1	1:A:1034:GLU:N	2.46	0.48
2:D:542:GLU:OE1	2:D:545:LYS:NZ	2.36	0.48
1:A:421:PRO:HA	2:B:559:LYS:HZ2	1.78	0.48
2:C:549:LYS:O	2:C:553:ILE:HG12	2.14	0.48
2:E:528:ASN:O	2:E:531:MET:HG3	2.13	0.48
1:A:408:ARG:HG2	1:A:413:GLY:HA2	1.96	0.48
1:A:25:LYS:NZ	1:A:233:GLU:OE1	2.47	0.48
1:A:328:PHE:O	1:A:334:ARG:NH1	2.45	0.48
2:B:552:SER:OG	2:C:554:ASP:OD2	2.30	0.48
1:A:151:CYS:SG	1:A:152:ARG:N	2.87	0.47
1:A:426:LYS:HE2	1:A:426:LYS:N	2.24	0.47
1:A:16:HIS:CE1	1:A:916:SER:CB	2.96	0.47
1:A:843:HIS:ND1	1:A:845:ASN:OD1	2.47	0.47
1:A:389:TYR:CZ	1:A:393:MET:HG3	2.49	0.47
1:A:1112:ARG:NH2	1:A:1437:GLY:HA3	2.28	0.47
2:D:521:ILE:HG13	2:D:522:ASN:H	1.79	0.47
2:D:548:ASN:O	2:D:551:GLU:HG3	2.14	0.47
2:E:543:ILE:HG13	2:E:544:PRO:HD3	1.97	0.47
1:A:1014:ASP:OD2	1:A:1017:THR:OG1	2.28	0.47
1:A:1176:LEU:C	1:A:1176:LEU:CD2	2.83	0.47
1:A:1237:GLN:O	1:A:1238:ILE:HG12	2.14	0.47
2:D:695:GLN:HG3	2:D:699:ASN:HD21	1.79	0.47
1:A:423:HIS:CG	2:B:555:ARG:HA	2.50	0.47
2:B:551:GLU:O	2:B:555:ARG:HB3	2.13	0.47
2:D:534:ASN:O	2:D:537:GLU:HG3	2.14	0.47
1:A:829:VAL:HG23	1:A:830:GLN:H	1.79	0.47
2:C:555:ARG:HA	2:C:555:ARG:HE	1.78	0.47
1:A:1243:ASN:CG	1:A:1425:LYS:HB3	2.36	0.47
1:A:1323:SER:O	1:A:1323:SER:OG	2.28	0.46
2:C:521:ILE:O	2:C:524:ILE:HG13	2.15	0.46
1:A:1183:ASN:OD1	1:A:1184:ASP:N	2.41	0.46
2:D:532:ARG:HA	2:D:535:HIS:ND1	2.29	0.46
2:D:676:GLU:OE1	2:D:677:LEU:N	2.34	0.46
1:A:142:ARG:HE	1:A:143:ASP:H	1.62	0.46
1:A:1021:ALA:O	1:A:1024:LYS:HG2	2.15	0.46
1:A:1200:ARG:NH1	1:A:1217:GLU:OE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:520:VAL:HA	2:D:523:SER:HB2	1.97	0.46
2:B:525:LYS:HA	2:B:528:ASN:ND2	2.30	0.46
2:C:525:LYS:NZ	2:D:523:SER:HA	2.31	0.46
1:A:17:LEU:C	1:A:17:LEU:CD2	2.84	0.46
1:A:974:ASP:OD1	1:A:974:ASP:N	2.47	0.46
2:B:559:LYS:HA	2:B:562:THR:HG22	1.98	0.46
1:A:59:LYS:HB2	1:A:59:LYS:HE2	1.70	0.46
2:D:547:ILE:HA	2:D:550:LEU:HG	1.98	0.46
2:E:523:SER:O	2:E:527:ILE:HG13	2.16	0.46
1:A:712:PHE:HD1	1:A:844:PRO:HD3	1.81	0.46
1:A:722:ASP:OD1	1:A:724:LYS:HG2	2.15	0.46
1:A:1067:SER:O	1:A:1071:THR:HG23	2.15	0.46
1:A:945:ASN:OD1	1:A:945:ASN:N	2.47	0.46
1:A:426:LYS:H	1:A:426:LYS:CD	2.28	0.45
2:D:537:GLU:HA	2:D:540:VAL:HG22	1.98	0.45
2:B:545:LYS:HA	2:B:548:ASN:OD1	2.16	0.45
1:A:181:ARG:HH12	1:A:920:VAL:HG21	1.81	0.45
1:A:1439:VAL:HG23	1:A:1440:ASP:H	1.82	0.45
2:B:525:LYS:HA	2:B:528:ASN:HD22	1.81	0.45
2:B:555:ARG:HG2	2:B:556:VAL:HG22	1.98	0.45
1:A:864:GLU:OE2	1:A:865:ARG:N	2.50	0.45
2:D:523:SER:O	2:D:527:ILE:HG12	2.17	0.45
1:A:712:PHE:CD1	1:A:844:PRO:HD3	2.51	0.45
1:A:1443:LEU:HD13	1:A:1444:PRO:HD2	1.98	0.45
1:A:1020:LEU:HD13	1:A:1195:LEU:HB3	1.99	0.45
1:A:1176:LEU:HD23	1:A:1176:LEU:C	2.33	0.45
2:C:541:LYS:O	2:C:544:PRO:HD2	2.16	0.45
1:A:1072:ILE:O	1:A:1076:THR:HG23	2.16	0.45
2:D:674:ASP:HB2	2:D:676:GLU:OE1	2.17	0.45
1:A:922:GLU:HB3	1:A:925:SER:OG	2.17	0.45
1:A:1096:LYS:HE2	1:A:1449:THR:HG21	1.99	0.45
1:A:1319:TRP:HA	1:A:1322:ALA:HB3	1.99	0.45
1:A:398:ILE:O	1:A:402:THR:HG22	2.17	0.45
1:A:1148:GLY:O	1:A:1151:LYS:HG2	2.17	0.45
1:A:1243:ASN:ND2	1:A:1425:LYS:HB3	2.32	0.45
1:A:1003:ASN:OD1	1:A:1003:ASN:N	2.43	0.44
2:B:524:ILE:HD12	2:B:525:LYS:H	1.81	0.44
2:D:662:ASP:O	2:D:666:THR:HG23	2.16	0.44
1:A:1435:ASP:OD1	1:A:1436:VAL:N	2.48	0.44
1:A:1327:ASN:ND2	1:A:1331:ASP:OD2	2.51	0.44
2:D:532:ARG:NH1	2:E:533:LEU:HD13	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:673:LYS:O	2:D:678:ARG:NH2	2.51	0.44
2:E:535:HIS:CD2	2:E:539:GLN:HE22	2.35	0.44
1:A:1157:LYS:HE3	1:A:1157:LYS:HB3	1.84	0.44
2:E:544:PRO:HA	2:E:547:ILE:CD1	2.47	0.44
1:A:18:ASP:HA	1:A:544:LYS:NZ	2.32	0.44
2:D:680:GLU:OE1	2:D:681:LEU:HG	2.17	0.44
1:A:331:GLN:HE21	1:A:332:LYS:HG2	1.83	0.44
1:A:20:PRO:HB2	1:A:368:LEU:HD12	2.00	0.43
1:A:384:ASP:OD1	1:A:384:ASP:N	2.49	0.43
1:A:547:LYS:HG3	1:A:550:GLY:H	1.83	0.43
2:B:548:ASN:C	2:B:550:LEU:H	2.22	0.43
2:E:537:GLU:HA	2:E:540:VAL:HG12	2.01	0.43
1:A:1142:LYS:HG2	1:A:1146:ARG:HH21	1.83	0.43
2:C:546:ILE:HD12	2:C:547:ILE:HG23	2.00	0.43
2:E:558:ALA:O	2:E:562:THR:HG22	2.18	0.43
2:E:568:GLU:HG2	2:E:570:HIS:CE1	2.53	0.43
1:A:314:HIS:ND1	1:A:880:THR:O	2.51	0.43
1:A:1312:GLU:HA	1:A:1315:TRP:HB2	2.01	0.43
1:A:1378:ASP:HB2	1:A:1385:LYS:HE3	2.00	0.43
2:D:697:ILE:O	2:D:701:VAL:HG12	2.19	0.43
1:A:17:LEU:HD22	1:A:17:LEU:O	2.18	0.43
1:A:958:GLN:O	1:A:958:GLN:NE2	2.49	0.43
2:B:526:LEU:HA	2:B:529:LEU:HD12	2.00	0.43
1:A:1188:SER:OG	1:A:1189:ASN:ND2	2.52	0.43
1:A:45:ARG:HG3	1:A:774:ASN:HA	1.99	0.43
2:C:564:LEU:HD12	2:C:564:LEU:H	1.84	0.43
1:A:375:GLU:HA	1:A:378:ARG:NH1	2.33	0.43
1:A:425:SER:O	1:A:428:ILE:N	2.51	0.43
1:A:1076:THR:HA	1:A:1079:THR:HG22	2.01	0.42
2:E:546:ILE:HA	2:E:549:LYS:HE3	2.00	0.42
1:A:16:HIS:CE1	1:A:916:SER:CA	3.02	0.42
1:A:233:GLU:OE2	1:A:233:GLU:N	2.50	0.42
1:A:1378:ASP:N	1:A:1380:ARG:HG3	2.28	0.42
2:E:520:VAL:HG23	2:E:521:ILE:H	1.84	0.42
1:A:131:ASN:HD22	1:A:1029:HIS:CE1	2.37	0.42
1:A:719:LEU:HD11	1:A:863:PHE:HB2	2.01	0.42
1:A:1090:LYS:HD3	1:A:1090:LYS:HA	1.79	0.42
1:A:1144:LEU:O	1:A:1147:SER:OG	2.29	0.42
2:D:693:GLU:O	2:D:697:ILE:HG22	2.20	0.42
1:A:1143:GLY:HA2	1:A:1146:ARG:HD2	2.01	0.42
1:A:1233:SER:O	1:A:1234:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:539:GLN:NE2	2:E:540:VAL:HG22	2.35	0.42
1:A:423:HIS:HB3	2:B:554:ASP:OD1	2.20	0.42
1:A:847:PRO:O	1:A:850:VAL:HG22	2.19	0.42
1:A:1172:ILE:O	1:A:1172:ILE:HG22	2.20	0.42
1:A:1225:MET:SD	1:A:1424:VAL:HG23	2.60	0.42
2:E:543:ILE:O	2:E:547:ILE:HG13	2.19	0.42
1:A:1325:ARG:HA	1:A:1325:ARG:HD2	1.79	0.42
1:A:1004:LEU:O	1:A:1007:ILE:HG12	2.19	0.42
1:A:1331:ASP:HB3	1:A:1333:LEU:HD13	2.00	0.42
1:A:66:GLN:HE21	1:A:213:ASN:HD22	1.67	0.42
1:A:426:LYS:H	1:A:426:LYS:NZ	2.15	0.42
1:A:467:LEU:O	1:A:471:MET:HG2	2.20	0.42
1:A:547:LYS:HE2	1:A:550:GLY:N	2.35	0.42
2:C:544:PRO:HA	2:C:547:ILE:CG1	2.50	0.42
2:D:533:LEU:HD11	2:E:533:LEU:HD21	2.02	0.42
1:A:720:THR:HG23	1:A:883:ILE:HB	2.02	0.41
1:A:1332:VAL:HG23	1:A:1332:VAL:O	2.20	0.41
2:D:557:LEU:HA	2:D:560:THR:HG22	2.02	0.41
2:B:533:LEU:HB2	2:E:532:ARG:NH2	2.35	0.41
2:D:539:GLN:HE22	2:E:540:VAL:HG22	1.85	0.41
1:A:141:ARG:HE	1:A:141:ARG:H	1.67	0.41
1:A:291:GLU:H	1:A:291:GLU:CD	2.24	0.41
1:A:1292:LYS:HG2	1:A:1294:LEU:H	1.83	0.41
2:C:525:LYS:HZ1	2:D:523:SER:HA	1.85	0.41
2:D:682:ILE:O	2:D:686:ASN:ND2	2.44	0.41
2:E:541:LYS:HA	2:E:541:LYS:HD2	1.84	0.41
1:A:66:GLN:NE2	1:A:213:ASN:HD22	2.18	0.41
1:A:1163:SER:OG	1:A:1164:HIS:ND1	2.51	0.41
2:B:524:ILE:HD12	2:B:525:LYS:N	2.35	0.41
2:B:539:GLN:NE2	2:C:541:LYS:HD2	2.35	0.41
2:D:535:HIS:HA	2:D:538:GLU:HG3	2.03	0.41
1:A:17:LEU:O	1:A:17:LEU:CD1	2.68	0.41
1:A:1443:LEU:HD22	1:A:1444:PRO:HD2	2.03	0.41
2:D:532:ARG:HH11	2:E:533:LEU:HD13	1.85	0.41
2:D:677:LEU:HA	2:D:680:GLU:HG3	2.03	0.41
1:A:238:TYR:O	1:A:242:LEU:HD12	2.19	0.41
1:A:18:ASP:HA	1:A:544:LYS:HZ1	1.86	0.41
1:A:733:GLU:HB2	2:C:567:ILE:HD11	2.03	0.41
1:A:1262:ARG:HA	1:A:1264:HIS:CE1	2.56	0.41
2:D:571:LEU:HD12	2:D:571:LEU:HA	1.85	0.41
2:D:705:ILE:HG12	2:D:705:ILE:H	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:O	1:A:544:LYS:NZ	2.53	0.41
1:A:1246:TYR:HD2	1:A:1247:GLY:O	2.04	0.41
2:E:547:ILE:HG13	2:E:547:ILE:H	1.76	0.41
1:A:423:HIS:ND1	2:B:555:ARG:HA	2.35	0.41
1:A:425:SER:HA	1:A:426:LYS:NZ	2.36	0.41
1:A:870:LEU:HD23	1:A:870:LEU:HA	1.89	0.41
1:A:1319:TRP:HZ3	1:A:1333:LEU:HG	1.85	0.41
2:E:527:ILE:HD12	2:E:528:ASN:N	2.36	0.41
1:A:453:ILE:HG12	1:A:454:GLN:N	2.36	0.41
1:A:1141:THR:HG23	1:A:1144:LEU:HD23	2.03	0.41
1:A:321:GLN:NE2	1:A:325:GLU:OE1	2.38	0.40
1:A:1125:ASN:O	1:A:1325:ARG:NH2	2.54	0.40
2:E:554:ASP:OD1	2:E:555:ARG:N	2.55	0.40
1:A:1295:ARG:O	1:A:1298:ILE:HG13	2.21	0.40
2:B:534:ASN:H	2:E:532:ARG:HH22	1.69	0.40
1:A:1120:HIS:O	1:A:1121:GLU:HB3	2.20	0.40
2:C:538:GLU:OE1	2:C:539:GLN:HG2	2.20	0.40
1:A:221:ASP:OD1	1:A:222:LYS:N	2.54	0.40
1:A:1384:GLU:H	1:A:1384:GLU:HG3	1.70	0.40
2:E:545:LYS:H	2:E:545:LYS:HD3	1.87	0.40
1:A:300:LEU:HA	1:A:300:LEU:HD23	1.81	0.40
1:A:420:LEU:HD23	1:A:420:LEU:HA	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	1267/2244 (56%)	1166 (92%)	99 (8%)	2 (0%)	44 73
2	B	49/709 (7%)	40 (82%)	9 (18%)	0	100 100
2	C	52/709 (7%)	45 (86%)	7 (14%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	113/709 (16%)	105 (93%)	8 (7%)	0	100 100
2	E	53/709 (8%)	50 (94%)	3 (6%)	0	100 100
All	All	1534/5080 (30%)	1406 (92%)	126 (8%)	2 (0%)	50 77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ILE
1	A	922	GLU

5.3.2 Protein sidechains (i)

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	1144/2046 (56%)	1042 (91%)	102 (9%)	8 26
2	B	47/625 (8%)	37 (79%)	10 (21%)	1 2
2	C	50/625 (8%)	44 (88%)	6 (12%)	4 13
2	D	107/625 (17%)	89 (83%)	18 (17%)	1 5
2	E	51/625 (8%)	43 (84%)	8 (16%)	2 7
All	All	1399/4546 (31%)	1255 (90%)	144 (10%)	8 19

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	59	LYS
1	A	67	SER
1	A	113	LYS
1	A	134	ARG
1	A	139	GLN
1	A	141	ARG
1	A	142	ARG
1	A	146	ILE

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Mol	Chain	Res	Type
1	A	148	ILE
1	A	151	CYS
1	A	205	SER
1	A	211	ASN
1	A	214	LEU
1	A	221	ASP
1	A	240	ASP
1	A	242	LEU
1	A	254	SER
1	A	263	SER
1	A	282	ARG
1	A	305	ARG
1	A	357	PHE
1	A	369	GLU
1	A	426	LYS
1	A	439	THR
1	A	442	ASP
1	A	446	ASN
1	A	451	CYS
1	A	460	GLU
1	A	461	LEU
1	A	462	LYS
1	A	464	ASP
1	A	472	LYS
1	A	477	SER
1	A	489	ARG
1	A	493	SER
1	A	495	THR
1	A	498	LYS
1	A	499	SER
1	A	529	TYR
1	A	573	SER
1	A	713	ASP
1	A	720	THR
1	A	721	THR
1	A	724	LYS
1	A	781	LEU
1	A	787	ASP
1	A	823	THR
1	A	864	GLU
1	A	885	SER
1	A	886	THR

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Mol	Chain	Res	Type
1	A	898	ASP
1	A	914	PHE
1	A	917	GLU
1	A	920	VAL
1	A	945	ASN
1	A	966	SER
1	A	969	GLU
1	A	1003	ASN
1	A	1022	ASP
1	A	1033	THR
1	A	1041	MET
1	A	1082	ARG
1	A	1090	LYS
1	A	1096	LYS
1	A	1108	LEU
1	A	1140	THR
1	A	1149	LEU
1	A	1150	ARG
1	A	1157	LYS
1	A	1160	SER
1	A	1176	LEU
1	A	1181	ARG
1	A	1188	SER
1	A	1197	ARG
1	A	1205	ARG
1	A	1236	CYS
1	A	1239	CYS
1	A	1253	ARG
1	A	1256	GLN
1	A	1260	VAL
1	A	1263	GLU
1	A	1292	LYS
1	A	1302	THR
1	A	1312	GLU
1	A	1314	CYS
1	A	1315	TRP
1	A	1330	LEU
1	A	1340	SER
1	A	1341	THR
1	A	1373	SER
1	A	1379	PHE
1	A	1384	GLU

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Mol	Chain	Res	Type
1	A	1392	TYR
1	A	1394	GLN
1	A	1411	LEU
1	A	1414	ASP
1	A	1439	VAL
1	A	1440	ASP
1	A	1442	GLU
1	A	1443	LEU
1	A	1449	THR
2	B	522	ASN
2	B	528	ASN
2	B	536	ILE
2	B	538	GLU
2	B	541	LYS
2	B	545	LYS
2	B	548	ASN
2	B	549	LYS
2	B	550	LEU
2	B	565	SER
2	C	533	LEU
2	C	542	GLU
2	C	549	LYS
2	C	554	ASP
2	C	565	SER
2	C	570	HIS
2	D	533	LEU
2	D	538	GLU
2	D	541	LYS
2	D	551	GLU
2	D	555	ARG
2	D	560	THR
2	D	561	ASN
2	D	564	LEU
2	D	568	GLU
2	D	655	MET
2	D	657	ASP
2	D	674	ASP
2	D	676	GLU
2	D	680	GLU
2	D	691	ASP
2	D	693	GLU
2	D	696	GLU

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Mol	Chain	Res	Type
2	D	703	ASP
2	E	530	ASP
2	E	531	MET
2	E	535	HIS
2	E	542	GLU
2	E	545	LYS
2	E	549	LYS
2	E	555	ARG
2	E	570	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	34	GLN
1	A	66	GLN
1	A	135	ASN
1	A	331	GLN
1	A	411	HIS
1	A	446	ASN
1	A	929	ASN
1	A	1029	HIS
1	A	1038	GLN
1	A	1169	GLN
1	A	1189	ASN
1	A	1327	ASN
1	A	1394	GLN
1	A	1417	ASN
2	D	690	ASN
2	D	695	GLN
2	D	699	ASN
2	E	522	ASN
2	E	534	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.