



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 10, 2018 – 10:24 AM EST

PDB ID : 6CE7
EMDB ID: : EMD-7461
Title : Insulin Receptor ectodomain in complex with one insulin molecule
Authors : Scapin, G.; Dandey, V.P.; Zhang, Z.; Strickland, C.; Potter, C.S.; Carragher, B.
Deposited on : 2018-02-11
Resolution : 7.40 Å(reported)

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

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

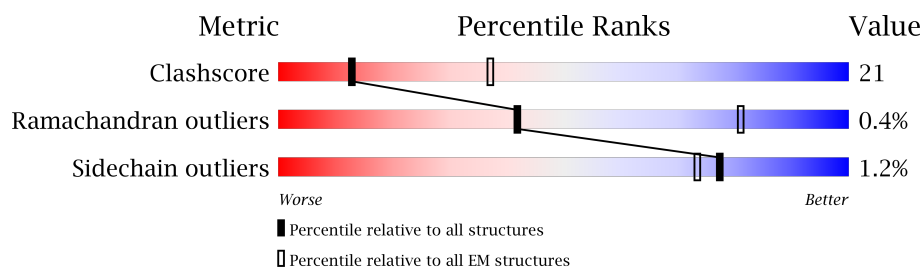
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 7.40 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	929	
1	B	929	
2	N	21	
3	O	30	
4	P	30	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10242 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 Insulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	659	Total	C	N	O	S	0	0
			5321	3373	921	984	43		
1	A	528	Total	C	N	O	S	0	0
			4275	2717	736	786	36		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	144	HIS	TYR	conflict	UNP P06213
A	144	HIS	TYR	conflict	UNP P06213

- Molecule 2 is a protein called Insulin A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	21	Total	C	N	O	S	0	0
			163	99	25	35	4		

- Molecule 3 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	O	30	Total	C	N	O	S	0	0
			240	157	40	41	2		

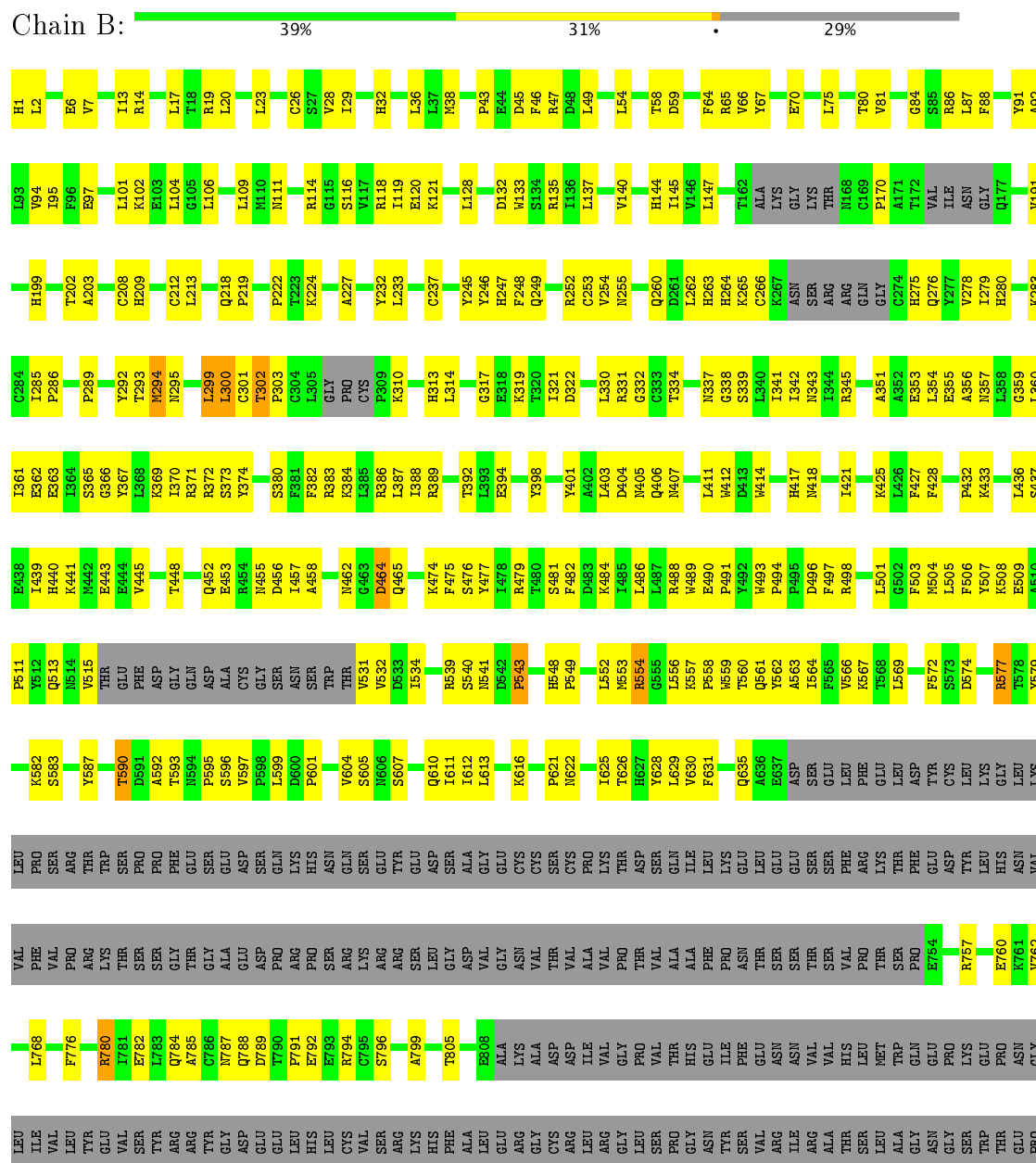
- Molecule 4 is a protein called Insulin receptor subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	P	30	Total	C	N	O	0	0
			243	156	41	46		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: Insulin receptor



- Molecule 3: Insulin B chain

Chain O:  63% 33%



- Molecule 4: Insulin receptor subunit alpha

Chain P:  60% 40%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48315	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 ($e^-/\text{\AA}^2$)	45.5	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.44	0/4371	0.65	0/5912
1	B	0.38	0/5448	0.60	0/7382
2	N	0.46	0/164	0.67	0/220
3	O	0.46	0/247	0.69	0/332
4	P	0.49	0/249	0.72	0/336
All	All	0.41	0/10479	0.63	0/14182

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	4
1	B	0	3
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	ASN	Peptide
1	A	374	TYR	Peptide
1	A	395	ILE	Peptide
1	A	455	ASN	Peptide
1	B	294	MET	Peptide
1	B	455	ASN	Peptide
1	B	792	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4275	0	4182	151	0
1	B	5321	0	5183	251	0
2	N	163	0	150	9	0
3	O	240	0	231	9	0
4	P	243	0	221	10	0
All	All	10242	0	9967	421	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 21.

All (421) 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:B:557:LYS:O	1:B:590:THR:HG21	1.25	1.27
1:B:280:HIS:HB2	1:B:301:CYS:SG	1.79	1.22
1:B:292:TYR:CD2	1:B:301:CYS:HB3	1.78	1.19
1:B:289:PRO:HD2	1:B:301:CYS:SG	1.95	1.07
1:B:557:LYS:O	1:B:590:THR:CG2	2.16	0.94
1:B:292:TYR:HD2	1:B:301:CYS:HB3	1.30	0.94
1:B:292:TYR:CE2	1:B:301:CYS:HB3	2.03	0.93
1:B:280:HIS:CD2	1:B:301:CYS:HB2	2.07	0.90
1:B:559:TRP:N	1:B:590:THR:OG1	2.04	0.90
1:B:280:HIS:CB	1:B:301:CYS:SG	2.61	0.89
1:B:279:ILE:HB	1:B:299:LEU:O	1.72	0.88
1:B:280:HIS:HB2	1:B:301:CYS:HG	1.37	0.88
1:B:289:PRO:CD	1:B:301:CYS:SG	2.62	0.88
1:B:552:LEU:O	1:B:554:ARG:NH1	2.07	0.87
1:B:294:MET:CA	1:B:302:THR:OG1	2.26	0.84
1:B:386:ARG:HH12	1:B:418:ASN:H	1.26	0.84
1:B:559:TRP:N	1:B:590:THR:CB	2.42	0.83
1:B:294:MET:HA	1:B:302:THR:OG1	1.76	0.82
1:B:488:ARG:NH1	1:B:548:HIS:O	2.12	0.81
1:B:559:TRP:H	1:B:590:THR:HB	1.48	0.79
1:B:132:ASP:OD2	1:B:135:ARG:NH1	2.18	0.76
1:B:294:MET:C	1:B:302:THR:OG1	2.23	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ILE:O	1:B:300:LEU:HA	1.85	0.75
1:B:310:LYS:NZ	1:B:331:ARG:O	2.19	0.75
1:B:477:TYR:HB3	1:B:488:ARG:HB2	1.70	0.74
1:B:558:PRO:HA	1:B:590:THR:HB	1.69	0.74
1:A:477:TYR:HB3	1:A:488:ARG:HB2	1.68	0.74
1:B:453:GLU:N	1:B:456:ASP:OD2	2.18	0.73
1:B:559:TRP:N	1:B:590:THR:HB	2.03	0.73
1:B:86:ARG:NH1	1:B:249:GLN:OE1	2.22	0.73
1:A:118:ARG:HG3	1:A:144:HIS:HB3	1.72	0.72
1:B:428:PHE:HB2	1:B:457:ILE:HA	1.72	0.70
1:B:300:LEU:O	1:B:300:LEU:HD12	1.91	0.70
1:B:280:HIS:HD2	1:B:301:CYS:HB2	1.54	0.70
1:B:295:ASN:N	1:B:302:THR:OG1	2.25	0.69
1:B:482:PHE:HB2	1:B:558:PRO:HB3	1.74	0.69
1:B:593:THR:HA	1:B:794:ARG:HD3	1.73	0.69
1:A:99:VAL:HG22	1:A:123:ASN:HD21	1.57	0.69
1:A:73:LYS:HD3	1:A:105:GLY:HA3	1.75	0.69
1:B:559:TRP:H	1:B:590:THR:CB	2.04	0.68
1:B:559:TRP:CE3	1:B:592:ALA:HB2	2.28	0.68
1:B:285:ILE:HD11	1:B:301:CYS:SG	2.34	0.68
1:B:294:MET:C	1:B:302:THR:HG1	1.98	0.67
1:A:476:SER:H	1:A:489:TRP:HA	1.59	0.66
1:A:567:LYS:HA	1:A:582:LYS:HA	1.79	0.65
1:B:498:ARG:HH22	3:O:8:GLY:HA3	1.60	0.65
1:B:479:ARG:HB3	1:B:486:LEU:HB3	1.78	0.65
1:B:366:GLY:HA2	1:B:392:THR:H	1.63	0.64
1:B:119:ILE:HD12	1:B:145:ILE:HG12	1.81	0.63
1:B:484:LYS:HB3	1:B:552:LEU:HD11	1.79	0.63
1:A:505:LEU:HA	1:A:566:VAL:HA	1.79	0.63
1:A:406:GLN:HA	1:A:432:PRO:HD2	1.79	0.62
1:B:293:THR:O	1:B:302:THR:OG1	2.17	0.62
1:A:58:THR:HG22	1:A:83:ARG:HD3	1.81	0.62
1:B:401:TYR:HA	1:B:427:PHE:HB3	1.81	0.62
1:B:494:PRO:HG2	1:B:497:PHE:HA	1.81	0.62
1:B:386:ARG:HH12	1:B:418:ASN:N	1.97	0.62
1:B:398:TYR:HA	1:B:425:LYS:H	1.64	0.62
1:B:278:VAL:HG23	1:B:285:ILE:HG13	1.81	0.61
1:B:593:THR:CA	1:B:794:ARG:HD3	2.29	0.61
1:A:63:LEU:HD12	1:A:95:ILE:HG12	1.83	0.61
1:A:385:LEU:O	1:A:417:HIS:NE2	2.33	0.61
1:A:87:LEU:HD11	1:A:114:ARG:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ILE:HD12	1:B:119:ILE:HG12	1.82	0.61
1:A:365:SER:HA	1:A:389:ARG:HD2	1.83	0.60
1:B:345:ARG:HH21	1:B:372:ARG:HB3	1.66	0.60
1:A:223:THR:HG22	1:A:236:ARG:HG2	1.83	0.60
1:A:311:VAL:HA	1:A:335:VAL:HB	1.82	0.60
1:A:14:ARG:HE	1:A:36:LEU:HD21	1.65	0.60
1:B:622:ASN:O	1:B:787:ASN:ND2	2.34	0.60
1:A:494:PRO:HG2	1:A:497:PHE:HA	1.84	0.60
1:B:369:LYS:HA	1:B:401:TYR:HB3	1.83	0.59
1:B:383:ARG:NH1	1:B:417:HIS:HB2	2.18	0.59
1:A:334:THR:HA	1:A:361:ILE:HA	1.86	0.58
2:N:6:CYS:HB3	3:O:6:LEU:HB2	1.86	0.58
1:B:511:PRO:HA	1:B:561:GLN:HB3	1.85	0.58
1:B:17:LEU:HD12	1:B:45:ASP:HB3	1.84	0.58
1:B:404:ASP:OD1	1:B:406:GLN:NE2	2.36	0.58
1:B:94:VAL:HA	1:B:118:ARG:HB3	1.84	0.58
1:B:247:HIS:HB2	1:B:283:LYS:HG2	1.85	0.58
1:A:213:LEU:HD13	1:A:229:ARG:HG3	1.85	0.58
1:A:380:SER:O	1:A:383:ARG:NH2	2.36	0.58
1:B:218:GLN:OE1	1:B:224:LYS:NZ	2.36	0.58
1:B:476:SER:H	1:B:489:TRP:HA	1.67	0.58
1:B:560:THR:N	1:B:590:THR:H	2.02	0.58
1:B:599:LEU:HB2	1:B:616:LYS:HB2	1.85	0.58
1:A:34:GLN:NE2	1:A:60:TYR:OH	2.37	0.57
1:B:46:PHE:HD1	1:B:75:LEU:HD21	1.69	0.57
1:B:262:LEU:HD23	1:B:265:LYS:HD3	1.86	0.57
1:B:406:GLN:HA	1:B:432:PRO:HD2	1.86	0.57
1:A:100:HIS:H	1:A:124:GLU:HG3	1.68	0.57
1:B:355:GLU:HG3	1:B:359:GLY:HA3	1.86	0.57
1:B:464:ASP:N	1:B:464:ASP:OD1	2.37	0.57
1:A:148:ASN:H	1:A:151:ASP:HB2	1.70	0.57
1:B:292:TYR:CD2	1:B:301:CYS:O	2.57	0.57
1:B:507:TYR:HA	1:B:564:ILE:HA	1.87	0.57
1:A:137:LEU:HD22	1:A:143:ASN:HD21	1.69	0.57
1:A:121:LYS:H	1:A:147:LEU:HB2	1.70	0.57
1:A:84:GLY:O	1:A:114:ARG:NH1	2.35	0.57
1:B:785:ALA:H	1:B:796:SER:HB3	1.68	0.57
1:A:509:GLU:HA	1:A:562:TYR:HA	1.87	0.57
1:B:120:GLU:HG2	1:B:121:LYS:HG3	1.87	0.57
1:A:362:GLU:HA	1:A:385:LEU:HA	1.87	0.56
1:B:331:ARG:HH12	1:B:356:ALA:HB1	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:SER:O	1:B:441:LYS:N	2.34	0.56
1:B:260:GLN:O	1:B:264:HIS:ND1	2.35	0.56
1:A:93:LEU:HB3	1:A:117:VAL:HG22	1.87	0.56
1:B:106:LEU:HD13	1:B:109:LEU:HD22	1.87	0.56
1:B:474:LYS:HE3	1:B:490:GLU:OE2	2.06	0.56
1:B:292:TYR:HB3	1:B:302:THR:O	2.05	0.56
1:B:558:PRO:C	1:B:590:THR:OG1	2.44	0.56
1:A:13:ILE:HB	1:A:35:ILE:HG12	1.87	0.56
1:A:481:SER:HB2	1:A:484:LYS:H	1.69	0.56
1:B:345:ARG:HG2	1:B:374:TYR:H	1.71	0.56
1:A:505:LEU:N	1:A:532:VAL:O	2.37	0.56
1:B:331:ARG:HG3	1:B:357:ASN:HA	1.88	0.56
1:A:469:GLU:HA	1:A:579:TYR:HB3	1.87	0.56
1:B:607:SER:HB3	1:B:610:GLN:H	1.71	0.56
1:B:341:ILE:HA	1:B:369:LYS:HB3	1.88	0.56
1:B:567:LYS:HA	1:B:582:LYS:HA	1.88	0.56
1:B:631:PHE:HB2	1:B:782:GLU:HB3	1.88	0.56
1:B:559:TRP:CZ3	1:B:592:ALA:HB2	2.41	0.55
1:B:541:ASN:HB2	1:B:543:PRO:HD2	1.88	0.55
1:A:216:CYS:HA	1:A:226:VAL:H	1.72	0.55
1:A:34:GLN:HA	1:A:62:LEU:HB3	1.88	0.55
1:A:213:LEU:HB2	1:A:229:ARG:HA	1.89	0.55
1:B:20:LEU:HD23	1:B:49:LEU:HD21	1.89	0.55
1:B:245:TYR:HA	1:B:255:ASN:HA	1.88	0.55
1:B:7:VAL:HA	1:B:28:VAL:HB	1.89	0.55
1:B:199:HIS:HB3	1:B:212:CYS:HB2	1.88	0.54
1:A:401:TYR:HA	1:A:427:PHE:HB3	1.88	0.54
1:B:292:TYR:CB	1:B:302:THR:O	2.56	0.54
1:B:788:GLN:HB3	1:B:794:ARG:H	1.72	0.54
1:A:120:GLU:HG2	1:A:121:LYS:HG3	1.89	0.54
1:A:321:ILE:HB	1:A:342:ILE:HG12	1.89	0.54
1:A:371:ARG:HG2	1:A:372:ARG:HG3	1.87	0.54
1:B:331:ARG:NH1	1:B:356:ALA:HB1	2.23	0.54
1:B:118:ARG:HA	1:B:144:HIS:HB3	1.89	0.54
1:B:407:ASN:HA	1:B:433:LYS:HD2	1.90	0.54
1:B:414:TRP:HB2	1:B:441:LYS:HD3	1.89	0.54
1:A:345:ARG:NH2	4:P:704:THR:OG1	2.31	0.54
1:B:94:VAL:HG13	1:B:118:ARG:HD3	1.90	0.54
1:B:503:PHE:N	1:B:534:ILE:O	2.38	0.54
1:B:425:LYS:HD2	1:B:456:ASP:OD2	2.08	0.54
2:N:18:ASN:HA	4:P:720:ARG:HH12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:O	1:B:133:TRP:NE1	2.41	0.54
2:N:10:ILE:HG21	3:O:3:ASN:HD22	1.72	0.53
1:A:436:LEU:O	1:A:440:HIS:ND1	2.32	0.53
1:B:559:TRP:HA	1:B:590:THR:O	2.08	0.53
1:B:293:THR:N	1:B:302:THR:O	2.42	0.53
1:A:233:LEU:HD13	1:A:253:CYS:HB2	1.90	0.53
1:A:310:LYS:NZ	1:A:331:ARG:O	2.42	0.53
1:B:6:GLU:HB2	1:B:26:CYS:HA	1.90	0.53
1:A:159:CYS:HB2	1:A:162:THR:HG23	1.90	0.53
1:B:407:ASN:HD22	1:B:433:LYS:NZ	2.07	0.53
1:B:448:THR:O	1:B:452:GLN:NE2	2.38	0.53
1:B:43:PRO:HB2	1:B:47:ARG:HH12	1.74	0.53
2:N:14:TYR:O	2:N:18:ASN:N	2.36	0.53
1:A:247:HIS:HB2	1:A:283:LYS:HG2	1.91	0.52
1:B:104:LEU:HD13	1:B:106:LEU:HD12	1.91	0.52
1:B:313:HIS:ND1	1:B:337:ASN:O	2.42	0.52
1:B:496:ASP:OD2	1:B:498:ARG:HB2	2.10	0.52
1:B:757:ARG:NH2	1:B:782:GLU:OE1	2.41	0.52
1:A:429:HIS:HB3	1:A:430:TYR:HD2	1.75	0.52
1:A:428:PHE:HB2	1:A:457:ILE:HA	1.91	0.52
1:A:209:HIS:CD2	1:A:211:GLU:H	2.27	0.52
1:B:572:PHE:HA	1:B:577:ARG:HG3	1.90	0.52
1:A:8:CYS:N	1:A:28:VAL:O	2.43	0.52
1:A:371:ARG:HG3	1:A:403:LEU:HB3	1.92	0.52
1:B:292:TYR:CD2	1:B:301:CYS:CB	2.72	0.52
1:B:505:LEU:O	1:B:532:VAL:N	2.35	0.52
1:A:443:GLU:OE1	1:A:449:LYS:NZ	2.36	0.52
1:A:565:PHE:HB3	1:A:585:ILE:HA	1.92	0.52
1:B:407:ASN:HD22	1:B:433:LYS:HZ2	1.58	0.52
1:B:436:LEU:O	1:B:440:HIS:ND1	2.32	0.52
1:A:398:TYR:HA	1:A:425:LYS:H	1.76	0.51
1:A:508:LYS:HD3	1:A:515:VAL:HG11	1.91	0.51
1:B:481:SER:N	1:B:484:LYS:O	2.43	0.51
1:B:334:THR:O	1:B:362:GLU:N	2.39	0.51
1:B:373:SER:H	1:B:405:ASN:HD22	1.58	0.51
1:A:73:LYS:NZ	1:A:103:GLU:OE2	2.40	0.51
1:A:389:ARG:HB3	1:A:391:GLU:HG3	1.93	0.51
1:A:8:CYS:O	1:A:30:GLU:N	2.43	0.51
1:B:119:ILE:HD13	1:B:128:LEU:HD22	1.93	0.51
1:B:345:ARG:NH2	1:B:372:ARG:HH11	2.09	0.51
1:A:355:GLU:HA	1:A:358:LEU:HB2	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:LEU:HD13	1:B:253:CYS:HB2	1.94	0.50
1:B:635:GLN:HE21	1:B:780:ARG:HB2	1.75	0.50
1:A:321:ILE:HD11	1:A:340:LEU:HD22	1.93	0.50
1:A:211:GLU:O	1:A:229:ARG:N	2.34	0.50
1:A:354:LEU:HG	1:A:358:LEU:HG	1.94	0.50
1:B:561:GLN:HE21	1:B:587:TYR:HB3	1.76	0.50
1:A:119:ILE:HD12	1:A:145:ILE:HG12	1.92	0.50
1:A:552:LEU:O	1:A:554:ARG:NH1	2.44	0.50
1:B:29:ILE:HG13	1:B:54:LEU:HD11	1.94	0.50
1:B:388:ILE:HD12	1:B:421:ILE:HG12	1.94	0.50
1:A:422:THR:O	1:A:451:ARG:NH1	2.44	0.50
1:A:482:PHE:HA	1:A:591:ASP:H	1.77	0.50
1:A:506:PHE:HD1	1:A:531:VAL:HA	1.76	0.49
1:B:289:PRO:HD3	1:B:301:CYS:SG	2.47	0.49
1:A:499:ASP:O	1:A:571:THR:N	2.45	0.49
1:A:485:ILE:HB	1:A:553:MET:HB2	1.93	0.49
1:A:342:ILE:HB	1:A:370:ILE:HG13	1.94	0.49
1:B:515:VAL:O	1:B:587:TYR:OH	2.30	0.49
1:A:295:ASN:ND2	1:A:297:SER:OG	2.45	0.49
1:A:372:ARG:HA	1:A:404:ASP:HB3	1.95	0.49
1:B:506:PHE:HD1	1:B:531:VAL:HA	1.77	0.49
1:B:334:THR:HA	1:B:361:ILE:HA	1.95	0.49
1:B:362:GLU:HG2	1:B:384:LYS:HB3	1.93	0.49
1:A:482:PHE:HA	1:A:590:THR:HB	1.93	0.49
1:B:503:PHE:O	1:B:534:ILE:N	2.37	0.49
1:A:380:SER:HA	1:A:412:TRP:CD1	2.48	0.49
1:A:99:VAL:HG12	1:A:100:HIS:CD2	2.48	0.49
1:B:87:LEU:HD11	1:B:114:ARG:HG2	1.95	0.48
1:B:501:LEU:HB2	1:B:569:LEU:HG	1.95	0.48
2:N:14:TYR:HA	2:N:17:GLU:HB3	1.95	0.48
1:B:300:LEU:C	1:B:300:LEU:HD12	2.33	0.48
1:B:319:LYS:HZ2	1:B:321:ILE:HG12	1.79	0.48
1:B:479:ARG:O	1:B:486:LEU:N	2.46	0.48
1:B:613:LEU:N	1:B:768:LEU:O	2.43	0.48
1:B:776:PHE:N	1:B:805:THR:OG1	2.45	0.48
1:A:501:LEU:HB2	1:A:569:LEU:HG	1.96	0.48
2:N:6:CYS:O	3:O:6:LEU:N	2.46	0.48
1:A:192:CYS:SG	1:A:201:CYS:N	2.85	0.48
1:A:127:TYR:N	1:A:157:ASP:OD1	2.47	0.48
1:B:279:ILE:CB	1:B:299:LEU:O	2.52	0.48
1:B:314:LEU:HD21	1:B:330:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:ARG:HH12	3:O:7:CYS:C	2.17	0.48
1:A:119:ILE:HB	1:A:145:ILE:HA	1.95	0.48
1:A:369:LYS:HA	1:A:401:TYR:HB3	1.96	0.48
1:B:246:TYR:N	1:B:254:VAL:O	2.34	0.48
1:B:292:TYR:CA	1:B:302:THR:O	2.62	0.48
1:A:482:PHE:HB3	1:A:591:ASP:HB2	1.95	0.48
1:B:294:MET:CA	1:B:302:THR:HG1	2.20	0.48
1:B:628:TYR:HB2	1:B:762:VAL:HB	1.94	0.47
1:B:489:TRP:O	1:B:548:HIS:ND1	2.40	0.47
1:B:506:PHE:HA	1:B:531:VAL:HA	1.96	0.47
1:A:568:THR:OG1	1:A:581:ALA:N	2.43	0.47
2:N:9:SER:OG	2:N:10:ILE:N	2.47	0.47
1:A:313:HIS:HA	1:A:337:ASN:HB3	1.96	0.47
1:A:52:PRO:HB3	1:A:77:PRO:HD2	1.96	0.47
1:B:36:LEU:HB2	1:B:64:PHE:HB3	1.94	0.47
1:B:365:SER:HA	1:B:389:ARG:HD2	1.96	0.47
3:O:9:SER:HA	3:O:12:VAL:HB	1.96	0.47
1:A:437:SER:O	1:A:576:ARG:NH1	2.48	0.47
1:B:280:HIS:CD2	1:B:301:CYS:CB	2.92	0.47
1:A:70:GLU:HA	1:A:101:LEU:HA	1.95	0.47
1:B:292:TYR:CE2	1:B:301:CYS:O	2.68	0.47
1:B:353:GLU:O	1:B:357:ASN:ND2	2.47	0.47
1:B:365:SER:HA	1:B:389:ARG:HB2	1.97	0.47
1:B:88:PHE:HB3	1:B:94:VAL:HG21	1.96	0.47
1:A:331:ARG:HG3	1:A:357:ASN:HA	1.97	0.47
1:B:118:ARG:NH2	1:B:120:GLU:OE1	2.48	0.47
1:B:121:LYS:H	1:B:147:LEU:HB2	1.80	0.47
1:A:318:GLU:OE2	1:A:320:THR:OG1	2.33	0.47
1:B:232:TYR:HA	1:B:237:CYS:HA	1.96	0.47
4:P:694:LYS:HG3	4:P:695:GLU:HG3	1.97	0.47
1:B:292:TYR:HD2	1:B:301:CYS:CB	2.14	0.46
1:B:363:GLU:HG2	1:B:387:LEU:HB3	1.96	0.46
1:B:553:MET:HB3	1:B:556:LEU:HD13	1.97	0.46
1:B:566:VAL:O	1:B:583:SER:N	2.47	0.46
1:B:628:TYR:O	1:B:762:VAL:N	2.43	0.46
3:O:27:THR:HB	3:O:30:ALA:HB3	1.96	0.46
4:P:698:GLU:HA	4:P:701:PHE:HB3	1.96	0.46
1:A:503:PHE:O	1:A:534:ILE:N	2.40	0.46
1:B:505:LEU:HA	1:B:566:VAL:HA	1.96	0.46
1:A:89:PHE:HZ	4:P:708:TYR:HB3	1.81	0.46
1:A:119:ILE:HG23	1:A:122:ASN:HD22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ASN:HB2	1:A:324:VAL:HG21	1.98	0.46
2:N:5:GLN:HA	2:N:9:SER:HB3	1.98	0.46
1:B:489:TRP:CE2	1:B:549:PRO:HG2	2.51	0.46
1:A:129:ALA:H	1:A:157:ASP:HB3	1.80	0.46
1:B:458:ALA:O	1:B:462:ASN:ND2	2.49	0.46
1:B:380:SER:HA	1:B:412:TRP:CD1	2.51	0.46
1:B:248:PHE:HE2	1:B:252:ARG:HH21	1.62	0.45
1:B:266:CYS:HB2	1:B:276:GLN:HE21	1.81	0.45
1:A:278:VAL:HG23	1:A:285:ILE:HG13	1.97	0.45
1:B:80:THR:HG22	1:B:81:VAL:HG23	1.98	0.45
1:A:386:ARG:O	1:A:420:THR:N	2.48	0.45
1:A:341:ILE:HG12	1:A:369:LYS:HB3	1.97	0.45
1:A:202:THR:OG1	1:A:203:ALA:N	2.48	0.45
1:A:350:LEU:HG	1:A:350:LEU:H	1.41	0.45
1:B:509:GLU:HA	1:B:562:TYR:HD1	1.81	0.45
1:A:14:ARG:HD3	1:A:37:LEU:HD12	1.98	0.45
1:B:367:TYR:HE2	1:B:369:LYS:HB2	1.80	0.45
1:B:621:PRO:HB3	1:B:625:ILE:HG13	1.98	0.45
1:A:319:LYS:NZ	1:A:329:GLU:OE1	2.48	0.45
1:A:379:LEU:HG	1:A:408:LEU:HD11	1.99	0.45
1:A:428:PHE:O	1:A:458:ALA:N	2.36	0.45
1:B:628:TYR:N	1:B:762:VAL:O	2.44	0.45
1:A:402:ALA:H	1:A:427:PHE:HD2	1.65	0.45
1:A:53:LYS:HE2	1:A:53:LYS:HB2	1.83	0.45
1:B:23:LEU:HA	1:B:26:CYS:HB2	1.98	0.45
1:A:292:TYR:HA	1:A:292:TYR:HD1	1.64	0.44
1:A:321:ILE:N	1:A:341:ILE:O	2.40	0.44
1:B:317:GLY:O	1:B:339:SER:N	2.44	0.44
1:B:386:ARG:HH22	1:B:417:HIS:HA	1.82	0.44
1:B:38:MET:O	1:B:67:TYR:N	2.50	0.44
1:B:558:PRO:HA	1:B:590:THR:CB	2.43	0.44
1:A:505:LEU:HD12	1:A:566:VAL:HG22	1.99	0.44
1:B:414:TRP:HB3	1:B:445:VAL:HG21	1.98	0.44
4:P:700:SER:O	4:P:704:THR:N	2.48	0.44
4:P:697:GLU:O	4:P:701:PHE:N	2.49	0.44
1:A:119:ILE:N	1:A:144:HIS:O	2.41	0.44
1:A:394:GLU:O	1:A:398:TYR:N	2.39	0.44
1:B:504:MET:N	1:B:567:LYS:O	2.47	0.44
1:B:170:PRO:HG2	1:B:191:VAL:HB	2.00	0.44
1:B:604:VAL:HB	1:B:612:ILE:HG13	1.98	0.44
1:A:478:ILE:HA	1:A:487:LEU:HD23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:PRO:HG3	1:B:799:ALA:HB1	2.00	0.44
2:N:2:ILE:HD11	2:N:16:LEU:HD23	2.00	0.44
1:B:70:GLU:HB3	1:B:102:LYS:HG2	1.99	0.43
1:A:232:TYR:N	1:A:251:TRP:O	2.34	0.43
1:A:338:GLY:N	1:A:365:SER:OG	2.51	0.43
1:B:92:ALA:N	1:B:116:SER:O	2.39	0.43
1:A:146:VAL:HG22	1:A:147:LEU:HG	1.99	0.43
1:A:429:HIS:ND1	1:A:458:ALA:HB2	2.33	0.43
1:A:473:LEU:HD21	1:A:492:TYR:HB2	2.00	0.43
1:B:630:VAL:O	1:B:760:GLU:N	2.50	0.43
1:B:626:THR:HB	1:B:789:ASP:HB2	2.00	0.43
1:A:407:ASN:HA	1:A:433:LYS:HD2	2.01	0.43
1:A:58:THR:O	1:A:84:GLY:N	2.51	0.43
1:B:394:GLU:N	1:B:398:TYR:O	2.51	0.43
3:O:26:TYR:HD1	4:P:716:PRO:HG3	1.83	0.43
1:A:241:CYS:H	1:A:247:HIS:CD2	2.37	0.43
1:A:504:MET:N	1:A:567:LYS:O	2.34	0.43
1:A:94:VAL:HG22	1:A:118:ARG:HB3	2.00	0.43
1:B:493:TRP:CD2	1:B:539:ARG:HD3	2.54	0.43
1:B:91:TYR:CG	1:B:118:ARG:HB2	2.53	0.43
1:B:577:ARG:HD3	1:B:579:TYR:HD1	1.84	0.43
1:B:32:HIS:HB3	1:B:59:ASP:HB2	2.01	0.43
1:B:605:SER:HB2	1:B:805:THR:HA	2.01	0.43
3:O:8:GLY:O	3:O:12:VAL:N	2.51	0.43
1:A:493:TRP:CD2	1:A:539:ARG:HD3	2.54	0.43
1:B:202:THR:OG1	1:B:203:ALA:N	2.51	0.43
1:B:332:GLY:HA2	1:B:360:LEU:HD12	2.01	0.43
1:B:382:PHE:HB2	1:B:412:TRP:HZ2	1.84	0.43
1:B:505:LEU:N	1:B:532:VAL:O	2.52	0.43
1:B:491:PRO:HD3	1:B:548:HIS:HA	2.01	0.43
1:A:414:TRP:NE1	1:A:438:GLU:OE1	2.52	0.43
1:A:491:PRO:HB2	1:A:493:TRP:NE1	2.34	0.43
1:A:59:ASP:HB3	1:A:86:ARG:HB2	2.01	0.43
1:B:13:ILE:HG12	1:B:19:ARG:NH1	2.34	0.43
1:B:58:THR:O	1:B:84:GLY:N	2.51	0.43
1:B:1:HIS:CD2	1:B:2:LEU:HD22	2.54	0.42
1:A:310:LYS:HD3	1:A:333:CYS:HA	2.01	0.42
1:A:508:LYS:O	1:A:563:ALA:N	2.41	0.42
1:A:566:VAL:O	1:A:583:SER:N	2.46	0.42
1:A:369:LYS:HG3	1:A:401:TYR:HB3	2.01	0.42
1:A:21:HIS:HA	1:A:51:PHE:HZ	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:HIS:CE1	1:B:299:LEU:CD2	3.02	0.42
1:A:364:ILE:HD12	1:A:388:ILE:HG12	2.02	0.42
1:A:377:VAL:HG23	1:A:409:ARG:HH11	1.84	0.42
1:A:421:ILE:HB	1:A:448:THR:HG21	2.02	0.42
1:B:558:PRO:CA	1:B:590:THR:HB	2.45	0.42
1:B:208:CYS:HA	1:B:219:PRO:HA	2.00	0.42
1:A:263:HIS:ND1	1:A:276:GLN:HB3	2.34	0.42
1:B:343:ASN:HD21	1:B:372:ARG:NH1	2.18	0.42
1:B:595:PRO:HG2	1:B:796:SER:HB2	2.02	0.42
4:P:694:LYS:NZ	4:P:695:GLU:OE2	2.52	0.42
1:A:231:PHE:HB2	1:A:238:VAL:HG23	2.02	0.42
1:A:394:GLU:HB3	1:A:398:TYR:HB2	2.02	0.42
1:B:248:PHE:HD2	1:B:252:ARG:HE	1.66	0.42
1:B:411:LEU:HB2	1:B:414:TRP:HE1	1.85	0.42
1:B:508:LYS:O	1:B:563:ALA:N	2.53	0.42
1:B:567:LYS:HB3	1:B:567:LYS:HE3	1.91	0.42
1:A:386:ARG:HD2	1:A:418:ASN:HB3	2.01	0.42
1:B:275:HIS:HB3	1:B:286:PRO:HB3	2.01	0.42
1:B:319:LYS:NZ	1:B:321:ILE:HG12	2.34	0.42
1:B:365:SER:OG	1:B:366:GLY:N	2.53	0.42
1:B:629:LEU:HB3	1:B:784:GLN:HB2	2.02	0.42
1:A:340:LEU:O	1:A:369:LYS:N	2.52	0.41
1:A:36:LEU:HD22	1:A:62:LEU:HD22	2.01	0.41
1:B:119:ILE:N	1:B:144:HIS:O	2.39	0.41
1:B:213:LEU:N	1:B:227:ALA:O	2.53	0.41
1:B:351:ALA:H	1:B:354:LEU:HD12	1.85	0.41
1:B:338:GLY:N	1:B:365:SER:OG	2.53	0.41
1:B:493:TRP:CG	1:B:539:ARG:NH1	2.88	0.41
1:B:38:MET:HB2	1:B:66:VAL:HG13	2.02	0.41
1:B:70:GLU:HA	1:B:101:LEU:HA	2.01	0.41
1:B:1:HIS:HD2	1:B:2:LEU:HD22	1.85	0.41
4:P:711:ASN:HA	4:P:714:PHE:CE1	2.55	0.41
1:A:100:HIS:N	1:A:124:GLU:HG3	2.34	0.41
1:B:279:ILE:N	1:B:299:LEU:O	2.53	0.41
1:B:567:LYS:HG3	1:B:582:LYS:HB3	2.02	0.41
1:A:404:ASP:HA	1:A:406:GLN:HE21	1.85	0.41
1:B:81:VAL:HG22	1:B:111:ASN:HB3	2.01	0.41
1:B:314:LEU:HD23	1:B:314:LEU:HA	1.87	0.41
1:B:14:ARG:HH21	1:B:36:LEU:HD11	1.86	0.41
1:B:574:ASP:OD1	1:B:574:ASP:N	2.52	0.41
1:A:102:LYS:HG3	1:A:103:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:HIS:CD2	1:B:222:PRO:HB3	2.56	0.41
1:B:475:PHE:CD1	1:B:489:TRP:HB3	2.55	0.41
1:B:491:PRO:HB2	1:B:493:TRP:NE1	2.36	0.41
1:B:65:ARG:HE	1:B:97:GLU:HB3	1.85	0.41
1:B:788:GLN:NE2	1:B:791:PRO:HG2	2.35	0.41
1:B:593:THR:C	1:B:794:ARG:HD3	2.41	0.41
1:A:20:LEU:HD21	1:A:49:LEU:HD21	2.02	0.41
1:B:605:SER:HA	1:B:611:ILE:HG12	2.03	0.41
1:B:91:TYR:CD2	1:B:118:ARG:HB2	2.55	0.41
1:A:568:THR:HG1	1:A:581:ALA:H	1.64	0.41
1:B:137:LEU:HD22	1:B:140:VAL:HG12	2.02	0.41
1:B:343:ASN:HD21	1:B:372:ARG:HH12	1.69	0.41
1:A:29:ILE:HB	1:A:57:ILE:HG12	2.03	0.41
1:B:403:LEU:HB2	1:B:427:PHE:HE2	1.85	0.41
1:A:246:TYR:HE2	1:A:256:PHE:HA	1.86	0.41
1:A:339:SER:OG	1:A:367:TYR:N	2.54	0.41
1:A:436:LEU:HA	1:A:439:ILE:HB	2.03	0.41
1:B:322:ASP:OD1	1:B:322:ASP:N	2.54	0.41
1:B:513:GLN:HE21	1:B:561:GLN:NE2	2.19	0.41
1:A:504:MET:O	1:A:567:LYS:N	2.53	0.40
1:B:342:ILE:HB	1:B:370:ILE:HA	2.02	0.40
1:A:483:ASP:N	1:A:483:ASP:OD1	2.55	0.40
1:B:292:TYR:HA	1:B:303:PRO:HA	2.02	0.40
1:B:371:ARG:HG2	1:B:372:ARG:HG3	2.04	0.40
1:A:470:ASN:OD1	1:A:471:GLU:N	2.54	0.40
1:B:433:LYS:HG2	1:B:465:GLN:O	2.22	0.40
1:B:439:ILE:O	1:B:443:GLU:N	2.37	0.40
1:B:596:SER:OG	1:B:597:VAL:N	2.54	0.40
1:A:336:ILE:HD13	1:A:340:LEU:HD11	2.03	0.40
1:B:425:LYS:NZ	1:B:453:GLU:OE1	2.55	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 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	516/929 (56%)	452 (88%)	62 (12%)	2 (0%)	38	77
1	B	645/929 (69%)	577 (90%)	66 (10%)	2 (0%)	44	81
2	N	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
3	O	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	4	33
4	P	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
All	All	1236/1939 (64%)	1096 (89%)	135 (11%)	5 (0%)	42	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	SER
1	A	539	ARG
1	B	540	SER
3	O	2	VAL
1	B	543	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 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	483/840 (58%)	479 (99%)	4 (1%)	85	92
1	B	603/840 (72%)	595 (99%)	8 (1%)	73	87
2	N	20/20 (100%)	20 (100%)	0	100	100
3	O	25/25 (100%)	23 (92%)	2 (8%)	14	45
4	P	26/30 (87%)	26 (100%)	0	100	100
All	All	1157/1755 (66%)	1143 (99%)	14 (1%)	77	88

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	299	LEU
1	B	300	LEU
1	B	302	THR
1	B	464	ASP
1	B	554	ARG
1	B	577	ARG
1	B	590	THR
1	B	780	ARG
1	A	350	LEU
1	A	358	LEU
1	A	508	LYS
1	A	577	ARG
3	O	3	ASN
3	O	22	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1	HIS
1	B	34	GLN
1	B	187	HIS
1	B	280	HIS
1	B	405	ASN
1	B	407	ASN
1	B	561	GLN
1	B	635	GLN
1	A	15	ASN
1	A	34	GLN
1	A	276	GLN
1	A	406	GLN
1	A	407	ASN
1	A	455	ASN
3	O	3	ASN
4	P	710	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.