



Full wwPDB EM Validation Report ⓘ

Jul 16, 2025 – 02:01 AM JST

PDB ID : 8YOT / pdb_00008yot
EMDB ID : EMD-39457
Title : Nanobody in complex with LILRB3
Authors : Jin, C.; Shi, Y.
Deposited on : 2024-03-13
Resolution : 2.48 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 : 4-5-2 with Phenix2.0rc1
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) : 2.44

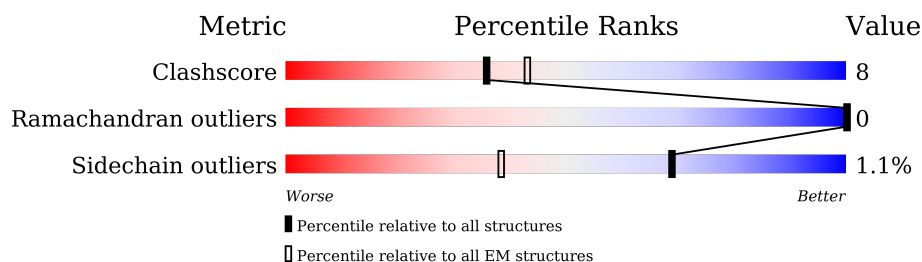
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.48 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	124	
1	C	124	
2	B	476	
2	D	476	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7738 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 nanobody.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	115	Total	C	N	O	S	0	0
			879	557	151	167	4		
1	C	115	Total	C	N	O	S	0	0
			879	557	151	167	4		

- Molecule 2 is a protein called LILRB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	386	Total	C	N	O	S	0	0
			2990	1897	518	558	17		
2	D	386	Total	C	N	O	S	0	0
			2990	1897	518	558	17		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	444	LEU	-	expression tag	UNP U5XHC3
B	445	GLU	-	expression tag	UNP U5XHC3
B	446	GLY	-	expression tag	UNP U5XHC3
B	447	SER	-	expression tag	UNP U5XHC3
B	448	ASP	-	expression tag	UNP U5XHC3
B	449	GLU	-	expression tag	UNP U5XHC3
B	450	VAL	-	expression tag	UNP U5XHC3
B	451	ASP	-	expression tag	UNP U5XHC3
B	452	ALA	-	expression tag	UNP U5XHC3
B	453	GLY	-	expression tag	UNP U5XHC3
B	454	SER	-	expression tag	UNP U5XHC3
B	455	HIS	-	expression tag	UNP U5XHC3
B	456	HIS	-	expression tag	UNP U5XHC3
B	457	HIS	-	expression tag	UNP U5XHC3
B	458	HIS	-	expression tag	UNP U5XHC3
B	459	HIS	-	expression tag	UNP U5XHC3
B	460	HIS	-	expression tag	UNP U5XHC3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	461	HIS	-	expression tag	UNP U5XHC3
B	462	HIS	-	expression tag	UNP U5XHC3
B	463	HIS	-	expression tag	UNP U5XHC3
B	464	HIS	-	expression tag	UNP U5XHC3
B	465	GLY	-	expression tag	UNP U5XHC3
B	466	SER	-	expression tag	UNP U5XHC3
B	467	VAL	-	expression tag	UNP U5XHC3
B	468	GLU	-	expression tag	UNP U5XHC3
B	469	ASP	-	expression tag	UNP U5XHC3
B	470	TYR	-	expression tag	UNP U5XHC3
B	471	LYS	-	expression tag	UNP U5XHC3
B	472	ASP	-	expression tag	UNP U5XHC3
B	473	ASP	-	expression tag	UNP U5XHC3
B	474	ASP	-	expression tag	UNP U5XHC3
B	475	ASP	-	expression tag	UNP U5XHC3
B	476	LYS	-	expression tag	UNP U5XHC3
D	444	LEU	-	expression tag	UNP U5XHC3
D	445	GLU	-	expression tag	UNP U5XHC3
D	446	GLY	-	expression tag	UNP U5XHC3
D	447	SER	-	expression tag	UNP U5XHC3
D	448	ASP	-	expression tag	UNP U5XHC3
D	449	GLU	-	expression tag	UNP U5XHC3
D	450	VAL	-	expression tag	UNP U5XHC3
D	451	ASP	-	expression tag	UNP U5XHC3
D	452	ALA	-	expression tag	UNP U5XHC3
D	453	GLY	-	expression tag	UNP U5XHC3
D	454	SER	-	expression tag	UNP U5XHC3
D	455	HIS	-	expression tag	UNP U5XHC3
D	456	HIS	-	expression tag	UNP U5XHC3
D	457	HIS	-	expression tag	UNP U5XHC3
D	458	HIS	-	expression tag	UNP U5XHC3
D	459	HIS	-	expression tag	UNP U5XHC3
D	460	HIS	-	expression tag	UNP U5XHC3
D	461	HIS	-	expression tag	UNP U5XHC3
D	462	HIS	-	expression tag	UNP U5XHC3
D	463	HIS	-	expression tag	UNP U5XHC3
D	464	HIS	-	expression tag	UNP U5XHC3
D	465	GLY	-	expression tag	UNP U5XHC3
D	466	SER	-	expression tag	UNP U5XHC3
D	467	VAL	-	expression tag	UNP U5XHC3
D	468	GLU	-	expression tag	UNP U5XHC3
D	469	ASP	-	expression tag	UNP U5XHC3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	470	TYR	-	expression tag	UNP U5XHC3
D	471	LYS	-	expression tag	UNP U5XHC3
D	472	ASP	-	expression tag	UNP U5XHC3
D	473	ASP	-	expression tag	UNP U5XHC3
D	474	ASP	-	expression tag	UNP U5XHC3
D	475	ASP	-	expression tag	UNP U5XHC3
D	476	LYS	-	expression tag	UNP U5XHC3

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.

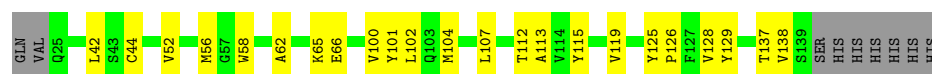
- Molecule 1: nanobody

Chain A: 



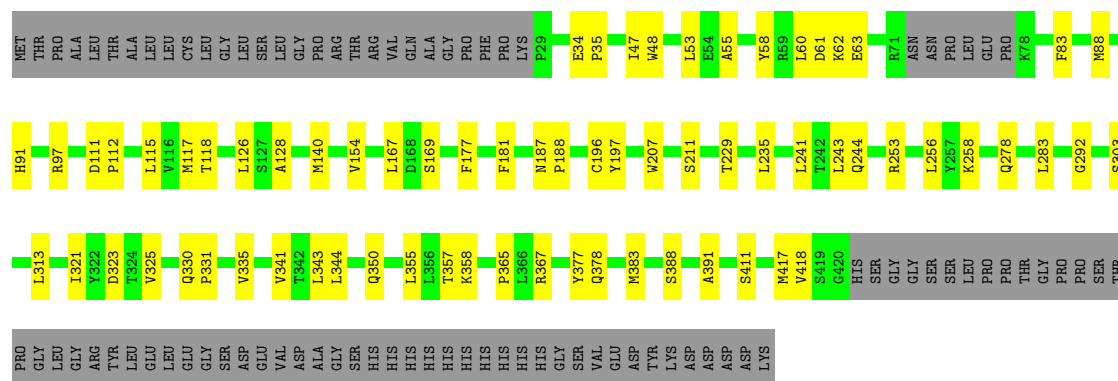
- Molecule 1: nanobody

Chain C: 



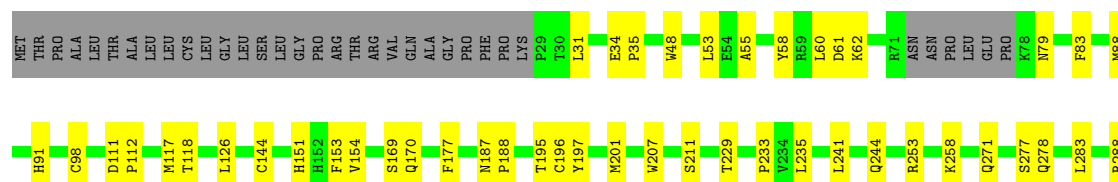
- Molecule 2: LILRB3

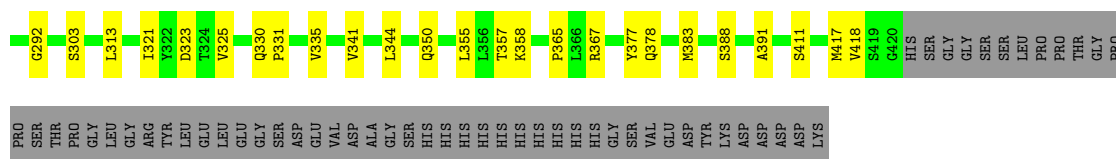
Chain B: 



- Molecule 2: LILRB3

Chain D: 





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1992467	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.14	0/898	0.38	0/1218
1	C	0.14	0/898	0.38	0/1218
2	B	0.15	0/3088	0.34	0/4209
2	D	0.15	0/3088	0.33	0/4209
All	All	0.15	0/7972	0.35	0/10854

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	879	0	857	16	0
1	C	879	0	857	15	0
2	B	2990	0	2826	44	0
2	D	2990	0	2826	40	0
All	All	7738	0	7366	112	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 8.

All (112) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:LEU:HD13	2:B:181:PHE:CE1	1.55	1.39
2:B:167:LEU:CD1	2:B:181:PHE:CE1	2.46	0.99
2:B:167:LEU:HD13	2:B:181:PHE:CD1	2.16	0.81
2:B:167:LEU:HD13	2:B:181:PHE:CZ	2.18	0.75
2:B:253:ARG:NH2	2:B:303:SER:O	2.26	0.69
1:C:125:TYR:OH	2:D:288:ARG:CZ	2.41	0.68
1:C:112:THR:HG23	1:C:137:THR:HA	1.76	0.68
1:A:112:THR:HG23	1:A:137:THR:HA	1.76	0.68
2:D:253:ARG:NH2	2:D:303:SER:O	2.27	0.66
2:D:244:GLN:NE2	2:D:278:GLN:OE1	2.29	0.65
1:A:88:ARG:NH2	1:A:111:ASP:OD2	2.33	0.61
2:B:358:LYS:NZ	2:B:391:ALA:O	2.34	0.61
2:B:88:MET:HG3	2:B:117:MET:HG3	1.84	0.59
1:C:62:ALA:HB3	1:C:65:LYS:HB2	1.84	0.59
2:D:417:MET:HE2	2:D:417:MET:HA	1.85	0.58
2:B:388:SER:HA	2:B:418:VAL:HG21	1.85	0.58
2:D:88:MET:HG3	2:D:117:MET:HG3	1.85	0.57
1:A:62:ALA:HB3	1:A:65:LYS:HB2	1.85	0.57
2:D:62:LYS:NZ	2:D:91:HIS:O	2.35	0.56
2:B:62:LYS:NZ	2:B:91:HIS:O	2.34	0.56
2:B:63:GLU:OE1	2:B:97:ARG:NH2	2.39	0.56
2:D:388:SER:HA	2:D:418:VAL:HG21	1.88	0.55
1:A:42:LEU:HG	1:A:104:MET:HE2	1.89	0.55
2:B:229:THR:HB	2:B:313:LEU:HD21	1.88	0.55
2:B:330:GLN:HB3	2:B:331:PRO:HD3	1.88	0.54
2:B:154:VAL:HB	2:B:197:TYR:HB2	1.88	0.54
2:D:330:GLN:HB3	2:D:331:PRO:HD3	1.89	0.54
2:D:358:LYS:NZ	2:D:391:ALA:O	2.40	0.54
1:C:42:LEU:HG	1:C:104:MET:HE2	1.90	0.54
2:D:335:VAL:HG21	2:D:341:VAL:HG21	1.90	0.53
2:D:355:LEU:HG	2:D:367:ARG:HG3	1.91	0.53
2:D:154:VAL:HB	2:D:197:TYR:HB2	1.90	0.53
1:C:107:LEU:HB3	1:C:138:VAL:HG11	1.90	0.52
2:D:229:THR:HB	2:D:313:LEU:HD21	1.92	0.52
1:A:128:VAL:HG11	1:A:130:TRP:CE2	2.45	0.51
2:B:335:VAL:HG21	2:B:341:VAL:HG21	1.92	0.51
2:B:417:MET:HA	2:B:417:MET:HE2	1.93	0.51
2:D:258:LYS:HE2	2:D:292:GLY:HA3	1.94	0.50
2:B:128:ALA:HB1	2:B:140:MET:HE1	1.91	0.50
1:A:107:LEU:HB3	1:A:138:VAL:HG11	1.93	0.49
2:B:258:LYS:HE2	2:B:292:GLY:HA3	1.94	0.48
2:D:169:SER:OG	2:D:177:PHE:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ALA:HB3	1:A:115:TYR:HE1	1.80	0.47
2:B:34:GLU:HB2	2:B:35:PRO:HD3	1.96	0.47
2:D:196:CYS:H	2:D:211:SER:HB3	1.78	0.47
2:B:140:MET:HE3	2:B:140:MET:HB2	1.75	0.47
2:B:325:VAL:HG23	2:B:411:SER:HB3	1.95	0.47
1:C:113:ALA:HB3	1:C:115:TYR:HE1	1.79	0.47
1:A:56:MET:HB2	1:A:100:VAL:HG21	1.96	0.47
1:A:125:TYR:CD1	1:A:126:PRO:HA	2.48	0.47
2:B:167:LEU:CD1	2:B:181:PHE:CD1	2.88	0.47
1:A:119:VAL:HB	1:A:129:TYR:HB2	1.96	0.47
1:A:44:CYS:HB2	1:A:58:TRP:CH2	2.50	0.47
2:B:350:GLN:HB3	2:B:377:TYR:CZ	2.50	0.46
2:B:196:CYS:H	2:B:211:SER:HB3	1.79	0.46
2:B:169:SER:OG	2:B:177:PHE:HB3	2.15	0.46
2:B:47:ILE:HD11	2:B:115:LEU:HD22	1.98	0.46
2:D:53:LEU:O	2:D:53:LEU:HD13	2.15	0.46
1:C:44:CYS:HB2	1:C:58:TRP:CH2	2.50	0.46
2:B:355:LEU:HG	2:B:367:ARG:HG3	1.98	0.45
2:D:55:ALA:HB3	2:D:58:TYR:HE1	1.82	0.45
2:D:350:GLN:HB3	2:D:377:TYR:CZ	2.52	0.45
1:C:56:MET:HB2	1:C:100:VAL:HG21	1.96	0.45
2:D:344:LEU:HD11	2:D:378:GLN:HG3	1.98	0.45
1:A:107:LEU:HD12	1:A:138:VAL:HG21	1.98	0.45
2:B:126:LEU:HD13	2:B:196:CYS:SG	2.57	0.44
2:D:126:LEU:HD13	2:D:196:CYS:SG	2.58	0.44
2:D:187:ASN:HA	2:D:188:PRO:HD3	1.87	0.44
1:C:113:ALA:HB3	1:C:115:TYR:CE1	2.53	0.44
1:C:125:TYR:CZ	2:D:288:ARG:NE	2.86	0.44
2:D:53:LEU:HA	2:D:79:ASN:HB3	2.00	0.44
2:B:344:LEU:HD11	2:B:378:GLN:HG3	1.98	0.44
2:D:235:LEU:HD11	2:D:241:LEU:HD13	2.00	0.44
2:B:61:ASP:N	2:B:61:ASP:OD1	2.51	0.44
2:B:235:LEU:HD11	2:B:241:LEU:HD13	2.00	0.44
1:A:128:VAL:HG12	1:A:129:TYR:N	2.33	0.44
2:D:271:GLN:HG2	2:D:277:SER:HB3	2.00	0.43
2:D:118:THR:HG22	2:D:207:TRP:HB2	2.01	0.43
1:C:119:VAL:HB	1:C:129:TYR:HB2	2.00	0.43
2:D:34:GLU:HB2	2:D:35:PRO:HD3	1.99	0.43
2:B:391:ALA:HB2	2:B:418:VAL:HG22	2.01	0.43
2:D:31:LEU:HD13	2:D:98:CYS:HB2	2.01	0.43
2:D:61:ASP:N	2:D:61:ASP:OD1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:TYR:CD1	1:C:126:PRO:HA	2.54	0.42
2:B:111:ASP:OD1	2:B:112:PRO:HD2	2.20	0.42
1:A:113:ALA:HB3	1:A:115:TYR:CE1	2.54	0.42
2:B:357:THR:HG22	2:B:365:PRO:HB3	2.01	0.42
2:B:34:GLU:HG2	2:B:48:TRP:CD1	2.54	0.42
2:B:118:THR:HG22	2:B:207:TRP:HB2	2.01	0.42
2:D:60:LEU:HB2	2:D:83:PHE:CE2	2.55	0.42
2:B:244:GLN:HE21	2:B:278:GLN:CD	2.27	0.41
2:D:34:GLU:HG2	2:D:48:TRP:CD1	2.55	0.41
1:A:78:ASN:OD1	1:A:78:ASN:N	2.52	0.41
2:B:55:ALA:HB3	2:B:58:TYR:HE1	1.86	0.41
2:D:151:HIS:NE2	2:D:201:MET:HE3	2.36	0.41
2:B:60:LEU:HB2	2:B:83:PHE:CE2	2.56	0.41
2:D:144:CYS:HB3	2:D:153:PHE:CD1	2.55	0.41
2:B:187:ASN:HA	2:B:188:PRO:HD3	1.88	0.41
2:D:321:ILE:HG22	2:D:323:ASP:H	1.85	0.41
2:B:241:LEU:HD23	2:B:283:LEU:HD12	2.02	0.41
1:C:125:TYR:CE1	2:D:288:ARG:CD	3.03	0.41
1:A:104:MET:HB2	1:A:107:LEU:HD21	2.03	0.41
2:B:243:LEU:HD12	2:B:256:LEU:HD21	2.03	0.41
1:C:58:TRP:CD1	1:C:102:LEU:HD22	2.56	0.41
1:C:100:VAL:HG12	1:C:101:TYR:N	2.35	0.41
2:D:111:ASP:OD1	2:D:112:PRO:HD2	2.21	0.41
2:B:343:LEU:HD12	2:B:383:MET:HE1	2.03	0.41
2:B:321:ILE:HG22	2:B:323:ASP:H	1.86	0.40
2:B:355:LEU:HD11	2:B:367:ARG:NH1	2.36	0.40
2:D:241:LEU:HD23	2:D:283:LEU:HD12	2.04	0.40
2:D:325:VAL:HG23	2:D:411:SER:HB3	2.02	0.40
2:D:233:PRO:HB3	2:D:365:PRO:HD3	2.03	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	113/124 (91%)	108 (96%)	5 (4%)	0	100	100
1	C	113/124 (91%)	108 (96%)	5 (4%)	0	100	100
2	B	382/476 (80%)	369 (97%)	13 (3%)	0	100	100
2	D	382/476 (80%)	372 (97%)	10 (3%)	0	100	100
All	All	990/1200 (82%)	957 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/101 (91%)	91 (99%)	1 (1%)	70	86
1	C	92/101 (91%)	89 (97%)	3 (3%)	33	56
2	B	323/404 (80%)	322 (100%)	1 (0%)	91	96
2	D	323/404 (80%)	319 (99%)	4 (1%)	67	84
All	All	830/1010 (82%)	821 (99%)	9 (1%)	69	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	GLU
2	B	53	LEU
1	C	52	VAL
1	C	66	GLU
1	C	128	VAL
2	D	170	GLN
2	D	195	THR
2	D	357	THR
2	D	383	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	147	GLN
2	B	151	HIS
2	B	152	HIS
2	B	161	HIS
2	B	173	HIS
2	B	209	HIS
2	B	300	HIS
2	B	320	GLN
2	B	375	HIS
1	C	103	GLN
2	D	92	HIS
2	D	147	GLN
2	D	170	GLN
2	D	173	HIS
2	D	209	HIS
2	D	293	GLN
2	D	300	HIS
2	D	375	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.