



## Full wwPDB EM Validation Report ⓘ

Oct 28, 2024 – 12:17 PM JST

PDB ID : 8JYS  
EMDB ID : EMD-36730  
Title : SARS-CoV-2 Spike RBD (dimer) in complex with two 2S-1244 nanobodies  
Authors : Yang, Y.; Zhang, C.H.  
Deposited on : 2023-07-03  
Resolution : 4.50 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](mailto: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>.

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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) : 2.39

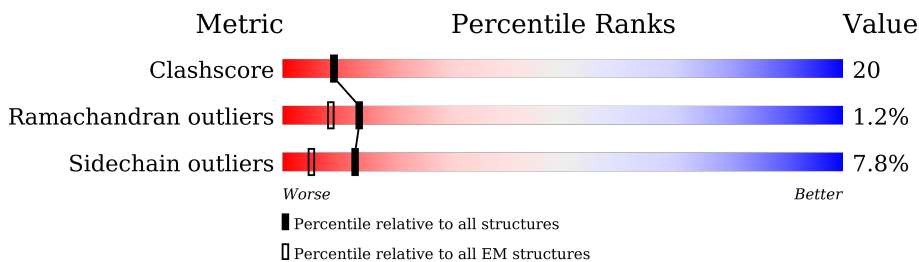
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.50 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  $\geq 3$ , 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	142	19% .. 78%
1	C	142	17% .. 77%
2	B	196	53% 38% 5% .
2	D	196	54% 39% . .

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3522 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 IBT-CoV144 nanobody.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	31	Total	C	N	O	0	0
			241	151	38	52		
1	C	32	Total	C	N	O	0	0
			253	160	39	54		

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	189	Total	C	N	O	S	0	0
			1514	980	255	271	8		
2	D	189	Total	C	N	O	S	0	0
			1514	980	255	271	8		

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
D	339	ASP	GLY	variant	UNP P0DTC2

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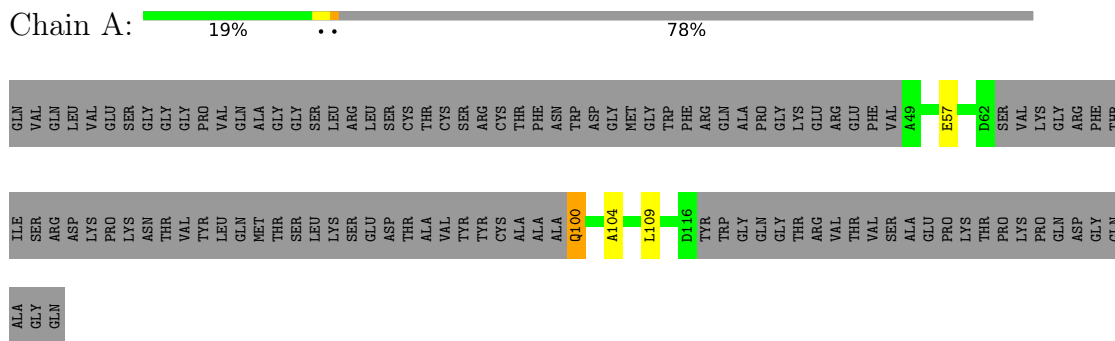
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Chain	Residue	Modelled	Actual	Comment	Reference
D	371	PHE	SER	variant	UNP P0DTC2
D	373	PRO	SER	variant	UNP P0DTC2
D	375	PHE	SER	variant	UNP P0DTC2
D	376	ALA	THR	variant	UNP P0DTC2
D	405	ASN	ASP	variant	UNP P0DTC2
D	408	SER	ARG	variant	UNP P0DTC2
D	417	ASN	LYS	variant	UNP P0DTC2
D	440	LYS	ASN	variant	UNP P0DTC2
D	477	ASN	SER	variant	UNP P0DTC2
D	478	LYS	THR	variant	UNP P0DTC2
D	484	ALA	GLU	variant	UNP P0DTC2
D	493	ARG	GLN	variant	UNP P0DTC2
D	498	ARG	GLN	variant	UNP P0DTC2
D	501	TYR	ASN	variant	UNP P0DTC2
D	505	HIS	TYR	variant	UNP P0DTC2

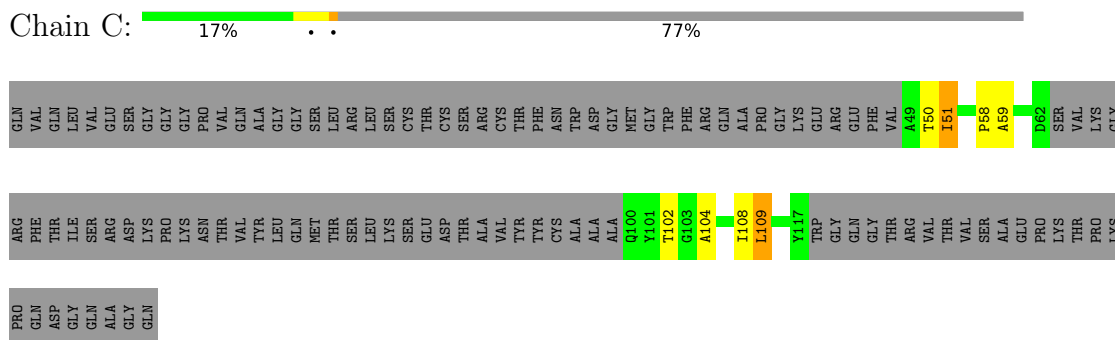
### 3 Residue-property plots [i](#)

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.

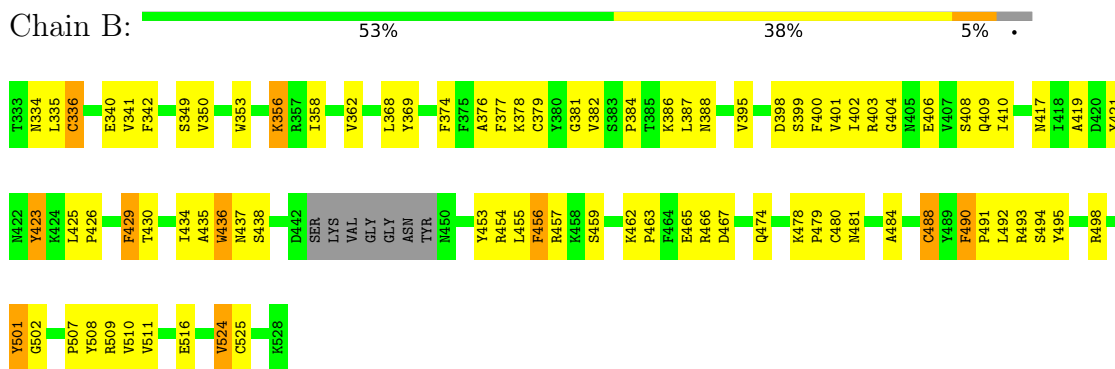
- Molecule 1: IBT-CoV144 nanobody



- Molecule 1: IBT-CoV144 nanobody



- Molecule 2: Spike protein S1

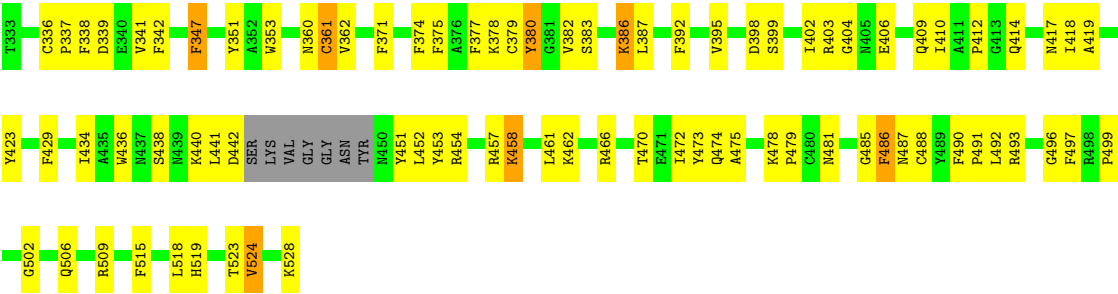


- Molecule 2: Spike protein S1

Chain D: 

54%

39%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	203158	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)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k 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	0.27	0/246	0.57	0/334
1	C	0.27	0/259	0.52	0/352
2	B	0.30	0/1560	0.61	0/2122
2	D	0.29	0/1560	0.63	0/2122
All	All	0.29	0/3625	0.61	0/4930

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	241	0	211	5	0
1	C	253	0	220	7	0
2	B	1514	0	1439	65	0
2	D	1514	0	1439	64	0
All	All	3522	0	3309	137	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 20.

All (137) 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:100:GLN:HE21	1:A:100:GLN:N	1.61	0.97
2:D:475:ALA:HB3	2:D:487:ASN:HB3	1.67	0.76
2:D:383:SER:OG	2:D:386:LYS:NZ	2.20	0.74
2:D:336:CYS:N	2:D:361:CYS:SG	2.60	0.73
2:D:478:LYS:NZ	2:D:479:PRO:O	2.24	0.71
2:D:485:GLY:H	2:D:488:CYS:HB2	1.56	0.69
2:B:501:TYR:HD1	2:B:502:GLY:H	1.42	0.67
1:A:100:GLN:N	1:A:100:GLN:NE2	2.39	0.66
2:B:384:PRO:O	2:B:388:ASN:ND2	2.29	0.65
2:D:360:ASN:HB3	2:D:523:THR:HG21	1.80	0.64
2:B:404:GLY:HA2	2:B:508:TYR:CE2	2.33	0.63
2:B:404:GLY:HA2	2:B:508:TYR:HE2	1.62	0.63
2:B:516:GLU:N	2:B:516:GLU:OE2	2.32	0.62
2:D:347:PHE:HE2	2:D:399:SER:HB3	1.64	0.62
2:B:356:LYS:HA	2:B:356:LYS:HE2	1.81	0.62
2:B:376:ALA:HB3	2:B:435:ALA:HB3	1.79	0.62
2:B:479:PRO:O	2:B:481:ASN:ND2	2.32	0.62
2:D:375:PHE:HA	2:D:436:TRP:HB3	1.80	0.62
2:D:337:PRO:O	2:D:339:ASP:N	2.34	0.61
2:D:518:LEU:HD12	2:D:519:HIS:H	1.66	0.60
2:B:341:VAL:HG13	2:B:342:PHE:HD1	1.67	0.59
2:D:351:TYR:HB2	2:D:454:ARG:HB2	1.85	0.58
2:D:347:PHE:O	2:D:451:TYR:OH	2.20	0.58
2:D:438:SER:OG	2:D:442:ASP:OD1	2.22	0.58
2:D:342:PHE:HE1	2:D:434:ILE:HD11	1.69	0.58
2:D:417:ASN:OD1	2:D:418:ILE:N	2.37	0.57
2:B:453:TYR:N	2:B:493:ARG:O	2.38	0.57
2:D:523:THR:HG23	2:D:524:VAL:HG23	1.85	0.57
2:B:403:ARG:HA	2:B:507:PRO:HA	1.86	0.57
1:C:50:THR:HG23	1:C:109:LEU:HG	1.86	0.56
2:D:412:PRO:O	2:D:414:GLN:NE2	2.35	0.56
2:D:377:PHE:HE1	2:D:379:CYS:HB2	1.70	0.56
2:D:382:VAL:HG13	2:D:387:LEU:HD21	1.86	0.56
2:B:341:VAL:HG13	2:B:342:PHE:CD1	2.41	0.56
2:D:457:ARG:HD2	2:D:458:LYS:H	1.71	0.56
2:D:473:TYR:HE1	2:D:475:ALA:HB2	1.71	0.55
2:D:528:LYS:HE3	2:D:528:LYS:HA	1.88	0.55
2:D:406:GLU:HG3	2:D:418:ILE:HG13	1.89	0.55
2:B:353:TRP:O	2:B:466:ARG:NH2	2.39	0.55
2:B:350:VAL:HG23	2:B:400:PHE:HB2	1.89	0.55
2:B:465:GLU:N	2:B:465:GLU:OE1	2.40	0.55
2:B:436:TRP:HH2	2:B:511:VAL:HG23	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:402:ILE:HD12	2:D:403:ARG:H	1.72	0.54
2:B:382:VAL:HG23	2:B:387:LEU:HD21	1.90	0.54
2:D:461:LEU:HD12	2:D:462:LYS:N	2.23	0.54
2:D:479:PRO:O	2:D:481:ASN:ND2	2.41	0.53
2:B:358:ILE:HB	2:B:395:VAL:HG23	1.89	0.53
2:D:472:ILE:HD11	2:D:488:CYS:HB3	1.91	0.53
1:C:102:THR:O	1:C:102:THR:OG1	2.27	0.53
2:B:402:ILE:HG22	2:B:403:ARG:N	2.23	0.53
2:D:395:VAL:HG12	2:D:515:PHE:HA	1.91	0.53
2:B:400:PHE:HZ	2:B:410:ILE:HD13	1.74	0.52
2:B:398:ASP:OD1	2:B:423:TYR:OH	2.25	0.52
2:D:478:LYS:HD2	2:D:479:PRO:HD2	1.92	0.52
2:D:406:GLU:OE1	2:D:406:GLU:N	2.37	0.51
2:D:361:CYS:SG	2:D:362:VAL:N	2.84	0.50
1:A:104:ALA:HB3	2:B:381:GLY:H	1.76	0.50
2:B:417:ASN:HB2	2:B:421:TYR:CG	2.47	0.50
2:D:383:SER:O	2:D:387:LEU:HG	2.11	0.50
2:B:409:GLN:HB2	2:B:419:ALA:HB3	1.93	0.50
2:B:492:LEU:H	2:B:492:LEU:HD23	1.76	0.49
2:B:401:VAL:HB	2:B:509:ARG:HG2	1.92	0.49
2:B:399:SER:OG	2:B:509:ARG:NH2	2.31	0.49
2:B:494:SER:OG	2:B:495:TYR:N	2.46	0.48
1:C:108:ILE:O	1:C:109:LEU:HG	2.13	0.48
2:D:479:PRO:HB2	2:D:481:ASN:HD22	1.78	0.48
2:D:341:VAL:HG13	2:D:342:PHE:HD2	1.77	0.48
2:D:410:ILE:HD12	2:D:410:ILE:H	1.78	0.48
2:D:462:LYS:HZ3	2:D:462:LYS:H	1.62	0.47
2:B:353:TRP:NE1	2:B:398:ASP:OD1	2.47	0.47
2:B:426:PRO:HD3	2:B:463:PRO:HB3	1.95	0.47
2:B:479:PRO:HB2	2:B:481:ASN:HD22	1.79	0.47
2:D:351:TYR:CE1	2:D:452:LEU:HD12	2.48	0.47
2:D:442:ASP:OD1	2:D:442:ASP:N	2.45	0.47
2:B:406:GLU:HA	2:B:409:GLN:HE22	1.79	0.47
1:C:51:ILE:HA	1:C:59:ALA:H	1.79	0.47
1:A:109:LEU:HD22	2:B:378:LYS:HE3	1.96	0.47
2:B:434:ILE:O	2:B:510:VAL:HA	2.14	0.46
2:D:347:PHE:CE2	2:D:399:SER:HB3	2.49	0.46
2:D:403:ARG:HD2	2:D:404:GLY:N	2.30	0.46
2:D:438:SER:HB2	2:D:509:ARG:HH21	1.80	0.46
2:B:437:ASN:HA	2:B:508:TYR:CB	2.45	0.46
2:D:440:LYS:O	2:D:440:LYS:NZ	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:PRO:HG2	2:B:429:PHE:HB3	1.98	0.46
2:B:353:TRP:HB2	2:B:399:SER:O	2.16	0.46
2:D:341:VAL:HG13	2:D:342:PHE:CD2	2.50	0.46
2:D:486:PHE:HD1	2:D:487:ASN:N	2.13	0.46
2:B:455:LEU:HD11	2:B:456:PHE:CE2	2.51	0.46
2:D:353:TRP:CZ2	2:D:466:ARG:HG2	2.52	0.45
1:C:50:THR:O	1:C:109:LEU:HD11	2.16	0.45
2:D:360:ASN:HA	2:D:524:VAL:HG22	1.98	0.45
2:B:430:THR:O	2:B:430:THR:OG1	2.31	0.45
2:B:340:GLU:OE1	2:B:340:GLU:N	2.47	0.45
2:B:437:ASN:HA	2:B:508:TYR:HB3	1.98	0.45
2:D:491:PRO:O	2:D:492:LEU:HB2	2.17	0.45
1:C:51:ILE:HD12	1:C:58:PRO:HB3	1.98	0.44
2:D:497:PHE:C	2:D:499:PRO:HD3	2.37	0.44
2:B:406:GLU:N	2:B:406:GLU:OE2	2.50	0.44
2:B:484:ALA:HA	2:B:488:CYS:SG	2.58	0.44
2:B:335:LEU:HD12	2:B:335:LEU:H	1.82	0.44
2:B:368:LEU:HG	2:B:377:PHE:HZ	1.83	0.44
2:B:402:ILE:HG21	2:B:406:GLU:HB2	2.00	0.44
2:D:409:GLN:OE1	2:D:419:ALA:N	2.45	0.44
2:B:438:SER:O	2:B:438:SER:OG	2.33	0.44
1:C:104:ALA:HB3	2:D:380:TYR:CD1	2.53	0.44
2:D:402:ILE:HD12	2:D:403:ARG:N	2.31	0.44
2:D:478:LYS:HZ2	2:D:479:PRO:N	2.16	0.44
2:D:387:LEU:HD22	2:D:392:PHE:CZ	2.54	0.43
2:B:480:CYS:HB2	2:B:488:CYS:HB2	1.62	0.43
2:D:441:LEU:H	2:D:441:LEU:HD22	1.83	0.43
2:D:454:ARG:HA	2:D:492:LEU:HD13	1.99	0.43
2:D:382:VAL:CG1	2:D:387:LEU:HD21	2.48	0.43
2:B:334:ASN:O	2:B:334:ASN:ND2	2.52	0.43
2:B:454:ARG:HD2	2:B:454:ARG:HA	1.89	0.42
2:B:478:LYS:HZ2	2:D:496:GLY:H	1.67	0.42
2:B:379:CYS:HB3	2:B:382:VAL:HG11	2.02	0.42
2:B:401:VAL:C	2:B:402:ILE:HD12	2.40	0.42
2:B:524:VAL:HG23	2:B:525:CYS:N	2.35	0.42
2:D:375:PHE:CD1	2:D:375:PHE:O	2.72	0.42
2:B:402:ILE:HG22	2:B:403:ARG:H	1.85	0.42
2:D:470:THR:O	2:D:470:THR:OG1	2.32	0.42
2:B:474:GLN:OE1	2:B:479:PRO:HA	2.19	0.41
2:B:399:SER:HB2	2:B:511:VAL:HG22	2.03	0.41
2:D:378:LYS:HA	2:D:378:LYS:HD2	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:453:TYR:HD2	2:D:493:ARG:HB2	1.86	0.41
2:B:490:PHE:CD1	2:B:491:PRO:HD2	2.56	0.41
2:B:498:ARG:HB2	2:B:501:TYR:HD2	1.86	0.41
2:B:425:LEU:HD13	2:B:426:PRO:HD2	2.03	0.41
2:B:457:ARG:NH1	2:B:467:ASP:OD2	2.52	0.41
1:A:57:GLU:OE1	1:A:57:GLU:N	2.44	0.41
2:B:377:PHE:H	2:B:378:LYS:NZ	2.19	0.41
2:B:455:LEU:HG	2:B:456:PHE:H	1.86	0.41
2:B:462:LYS:HD3	2:B:462:LYS:N	2.36	0.41
2:B:336:CYS:HB2	2:B:362:VAL:C	2.41	0.41
2:D:523:THR:OG1	2:D:524:VAL:N	2.51	0.40
2:D:451:TYR:C	2:D:452:LEU:HD23	2.42	0.40
2:D:502:GLY:O	2:D:506:GLN:HG3	2.22	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	27/142 (19%)	24 (89%)	3 (11%)	0	100	100
1	C	28/142 (20%)	19 (68%)	8 (29%)	1 (4%)	3	20
2	B	185/196 (94%)	164 (89%)	19 (10%)	2 (1%)	12	46
2	D	185/196 (94%)	159 (86%)	24 (13%)	2 (1%)	12	46
All	All	425/676 (63%)	366 (86%)	54 (13%)	5 (1%)	14	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	338	PHE
2	B	524	VAL

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Mol	Chain	Res	Type
1	C	51	ILE
2	B	374	PHE
2	D	524	VAL

### 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	24/114 (21%)	23 (96%)	1 (4%)	25	47
1	C	25/114 (22%)	24 (96%)	1 (4%)	27	48
2	B	162/168 (96%)	148 (91%)	14 (9%)	8	27
2	D	162/168 (96%)	149 (92%)	13 (8%)	10	29
All	All	373/564 (66%)	344 (92%)	29 (8%)	13	29

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
2	B	336	CYS
2	B	349	SER
2	B	356	LYS
2	B	369	TYR
2	B	386	LYS
2	B	408	SER
2	B	423	TYR
2	B	429	PHE
2	B	436	TRP
2	B	456	PHE
2	B	459	SER
2	B	488	CYS
2	B	490	PHE
2	B	501	TYR
1	C	109	LEU
2	D	347	PHE
2	D	361	CYS

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Mol	Chain	Res	Type
2	D	371	PHE
2	D	374	PHE
2	D	380	TYR
2	D	386	LYS
2	D	398	ASP
2	D	423	TYR
2	D	429	PHE
2	D	458	LYS
2	D	474	GLN
2	D	486	PHE
2	D	490	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	388	ASN
2	B	481	ASN
2	D	481	ASN

### 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.