



Full wwPDB EM Validation Report ⓘ

Jul 15, 2024 – 12:29 PM JST

PDB ID : 8XZD
EMDB ID : EMD-38793
Title : The structure of fox ACE2 and Omicron BF.7 RBD complex
Authors : sun, J.Q.
Deposited on : 2024-01-21
Resolution : 3.47 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 : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

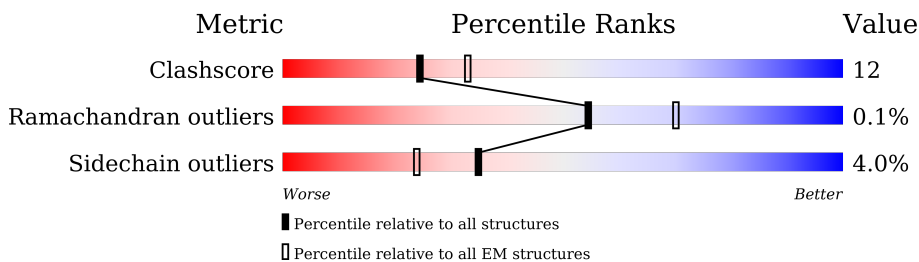
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.47 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	B	247	
2	A	613	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6436 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 Spike protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	195	1550	999	260	283	8	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	301	MET	-	initiating methionine	UNP P0DTC2
B	302	HIS	-	expression tag	UNP P0DTC2
B	303	SER	-	expression tag	UNP P0DTC2
B	304	SER	-	expression tag	UNP P0DTC2
B	305	ALA	-	expression tag	UNP P0DTC2
B	306	LEU	-	expression tag	UNP P0DTC2
B	307	LEU	-	expression tag	UNP P0DTC2
B	308	CYS	-	expression tag	UNP P0DTC2
B	309	CYS	-	expression tag	UNP P0DTC2
B	310	LEU	-	expression tag	UNP P0DTC2
B	311	VAL	-	expression tag	UNP P0DTC2
B	312	LEU	-	expression tag	UNP P0DTC2
B	313	LEU	-	expression tag	UNP P0DTC2
B	314	THR	-	expression tag	UNP P0DTC2
B	315	GLY	-	expression tag	UNP P0DTC2
B	316	VAL	-	expression tag	UNP P0DTC2
B	317	ARG	-	expression tag	UNP P0DTC2
B	318	ALA	-	expression tag	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	346	THR	ARG	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	452	ARG	LEU	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	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	542	HIS	-	expression tag	UNP P0DTC2
B	543	HIS	-	expression tag	UNP P0DTC2
B	544	HIS	-	expression tag	UNP P0DTC2
B	545	HIS	-	expression tag	UNP P0DTC2
B	546	HIS	-	expression tag	UNP P0DTC2
B	547	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	596	4885	3123	810	923	29	0	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
3	A	1	1	1	0

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69826	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	B	0.41	0/1597	0.68	0/2176
2	A	0.94	0/5027	0.80	0/6830
All	All	0.85	0/6624	0.78	0/9006

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	B	1550	0	1479	53	0
2	A	4885	0	4654	99	0
3	A	1	0	0	0	0
All	All	6436	0	6133	147	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 12.

All (147) 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:A:381:TYR:CE2	2:A:385:TYR:HE2	1.44	1.36
2:A:394:ASN:HB2	2:A:562:LYS:HE3	1.20	1.18
2:A:381:TYR:CE2	2:A:385:TYR:CE2	2.31	1.18
2:A:394:ASN:CB	2:A:562:LYS:HE3	1.73	1.15
2:A:336:PRO:HG2	2:A:342:VAL:HG21	1.16	1.14
2:A:381:TYR:OH	2:A:395:GLY:HA2	1.47	1.13
2:A:47:SER:HA	2:A:62:MET:CE	1.80	1.11
1:B:375:PHE:CE1	1:B:508:TYR:CE2	2.39	1.09
2:A:394:ASN:HB2	2:A:562:LYS:CE	1.82	1.08
2:A:47:SER:HA	2:A:62:MET:HE2	1.07	1.06
2:A:455:MET:HE1	2:A:481:LYS:N	1.74	1.01
1:B:396:TYR:HB2	1:B:514:SER:OG	1.61	0.99
2:A:131:LYS:HG2	2:A:143:LEU:HD23	1.40	0.99
1:B:489:TYR:CE1	2:A:31:LYS:HG2	1.98	0.98
1:B:375:PHE:CZ	1:B:508:TYR:CD2	2.51	0.98
1:B:336:CYS:SG	1:B:363:ALA:HB2	2.04	0.98
2:A:455:MET:CE	2:A:481:LYS:HG2	1.96	0.96
2:A:336:PRO:HG2	2:A:342:VAL:CG2	1.95	0.95
1:B:375:PHE:HZ	1:B:508:TYR:HD2	1.16	0.93
2:A:381:TYR:HE2	2:A:385:TYR:HE2	1.14	0.92
2:A:131:LYS:HG2	2:A:143:LEU:CD2	2.00	0.91
2:A:47:SER:CA	2:A:62:MET:HE2	1.98	0.90
1:B:455:LEU:HD21	2:A:34:TYR:HE2	1.34	0.90
1:B:336:CYS:SG	1:B:363:ALA:CB	2.60	0.90
1:B:375:PHE:CZ	1:B:508:TYR:CE2	2.63	0.86
1:B:375:PHE:CZ	1:B:508:TYR:HD2	1.92	0.85
2:A:76:GLN:HE21	2:A:79:LEU:HD12	1.38	0.84
1:B:375:PHE:CE1	1:B:508:TYR:HE2	1.96	0.84
2:A:442:GLN:O	2:A:445:THR:HG22	1.78	0.84
2:A:336:PRO:CG	2:A:342:VAL:HG21	2.05	0.83
1:B:375:PHE:CE1	1:B:508:TYR:CD2	2.69	0.80
2:A:133:CYS:HB3	2:A:141:CYS:SG	2.22	0.80
1:B:379:CYS:HG	1:B:432:CYS:HG	0.92	0.79
2:A:455:MET:HE2	2:A:481:LYS:HG2	1.63	0.79
1:B:468:ILE:O	1:B:468:ILE:HG22	1.82	0.78
2:A:485:VAL:HG12	2:A:485:VAL:O	1.83	0.78
2:A:394:ASN:CB	2:A:562:LYS:CE	2.52	0.77
2:A:76:GLN:NE2	2:A:79:LEU:HD12	2.01	0.74
2:A:393:ARG:O	2:A:394:ASN:OD1	2.05	0.74
1:B:336:CYS:SG	1:B:363:ALA:HA	2.30	0.72
2:A:381:TYR:CD2	2:A:385:TYR:CE2	2.76	0.72
1:B:455:LEU:HD21	2:A:34:TYR:CE2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:526:GLN:NE2	2:A:542:CYS:SG	2.64	0.71
2:A:394:ASN:HB3	2:A:562:LYS:HE3	1.68	0.70
2:A:478:TRP:CD2	2:A:489:GLU:HG3	2.26	0.70
2:A:597:GLU:HG2	2:A:600:ARG:HH22	1.55	0.70
2:A:381:TYR:CD2	2:A:385:TYR:HE2	2.05	0.69
1:B:336:CYS:HB3	1:B:361:CYS:SG	2.31	0.69
1:B:424:LYS:HD3	1:B:463:PRO:HA	1.72	0.69
2:A:197:GLU:HB2	2:A:201:ASP:OD2	1.92	0.68
2:A:50:TYR:HB3	2:A:62:MET:HE3	1.76	0.68
2:A:414:THR:HB	2:A:415:PRO:HD2	1.76	0.67
1:B:336:CYS:SG	1:B:363:ALA:CA	2.84	0.65
2:A:455:MET:CE	2:A:481:LYS:CG	2.73	0.65
2:A:485:VAL:O	2:A:485:VAL:CG1	2.45	0.64
1:B:391:CYS:SG	1:B:525:CYS:HB3	2.36	0.64
2:A:381:TYR:HH	2:A:395:GLY:HA2	1.61	0.63
1:B:375:PHE:HE1	1:B:508:TYR:CE2	2.10	0.63
1:B:468:ILE:O	1:B:468:ILE:CG2	2.48	0.62
2:A:120:LEU:HD21	2:A:183:TYR:CE1	2.35	0.62
2:A:239:HIS:ND1	2:A:599:ASN:ND2	2.47	0.62
2:A:455:MET:HE1	2:A:481:LYS:CA	2.29	0.61
2:A:381:TYR:CD2	2:A:401:HIS:NE2	2.68	0.61
2:A:75:GLU:O	2:A:79:LEU:HG	1.99	0.61
2:A:21:THR:HG22	2:A:25:VAL:HG23	1.82	0.61
2:A:489:GLU:H	2:A:489:GLU:CD	2.03	0.61
2:A:76:GLN:HE21	2:A:79:LEU:CD1	2.10	0.60
2:A:599:ASN:OD1	2:A:599:ASN:C	2.41	0.59
2:A:50:TYR:CB	2:A:62:MET:HE3	2.33	0.58
2:A:50:TYR:HB3	2:A:62:MET:CE	2.34	0.58
2:A:465:LYS:HD2	2:A:467:GLU:HG3	1.86	0.58
1:B:466:ARG:HD3	1:B:468:ILE:HD11	1.85	0.57
2:A:131:LYS:CG	2:A:143:LEU:CD2	2.80	0.56
1:B:477:ASN:OD1	1:B:478:LYS:N	2.38	0.56
1:B:375:PHE:HZ	1:B:508:TYR:CD2	1.95	0.56
2:A:455:MET:HE1	2:A:481:LYS:HG2	1.86	0.56
1:B:489:TYR:CD1	2:A:31:LYS:HE2	2.42	0.55
2:A:455:MET:HE2	2:A:481:LYS:CG	2.35	0.55
2:A:445:THR:HG23	2:A:446:ILE:HG13	1.88	0.54
2:A:131:LYS:CG	2:A:143:LEU:HD23	2.28	0.54
2:A:511:SER:OG	2:A:514:ARG:NH2	2.41	0.54
2:A:555:LEU:HG	2:A:559:LYS:HE3	1.89	0.53
2:A:131:LYS:HG2	2:A:143:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:TRP:HE1	1:B:466:ARG:HB2	1.73	0.53
1:B:376:ALA:HB1	1:B:378:LYS:HG2	1.91	0.52
2:A:394:ASN:HB2	2:A:562:LYS:NZ	2.22	0.52
2:A:455:MET:HE1	2:A:481:LYS:CG	2.39	0.52
1:B:344:ALA:HB3	1:B:347:PHE:HE1	1.75	0.51
1:B:375:PHE:CZ	1:B:508:TYR:HE2	2.20	0.51
2:A:475:LYS:HG2	2:A:479:GLU:OE2	2.11	0.50
2:A:455:MET:HE3	2:A:480:MET:HB3	1.94	0.50
1:B:489:TYR:HD1	2:A:31:LYS:HE2	1.77	0.49
2:A:478:TRP:CE3	2:A:489:GLU:HG3	2.46	0.49
2:A:442:GLN:O	2:A:445:THR:CG2	2.57	0.49
1:B:334:ASN:O	1:B:362:VAL:N	2.41	0.49
1:B:379:CYS:CB	1:B:432:CYS:SG	3.00	0.49
2:A:381:TYR:CE2	2:A:385:TYR:CD2	2.98	0.49
1:B:336:CYS:SG	1:B:338:PHE:CD1	3.02	0.48
2:A:53:ASN:CB	2:A:340:ARG:HD2	2.43	0.48
2:A:487:VAL:HG12	2:A:488:VAL:N	2.27	0.48
2:A:445:THR:HG23	2:A:446:ILE:N	2.28	0.48
1:B:383:SER:H	1:B:387:LEU:HD22	1.78	0.48
2:A:381:TYR:HD1	2:A:558:LEU:HD22	1.78	0.48
2:A:394:ASN:CB	2:A:562:LYS:NZ	2.76	0.47
2:A:394:ASN:HD22	2:A:562:LYS:NZ	2.11	0.47
2:A:264:ALA:HB2	2:A:487:VAL:CG1	2.44	0.47
2:A:342:VAL:HG13	2:A:359:LYS:CE	2.45	0.47
1:B:438:SER:OG	1:B:509:ARG:HG3	2.15	0.47
1:B:421:TYR:HB3	1:B:457:ARG:HE	1.78	0.47
1:B:377:PHE:HE1	1:B:434:ILE:HD11	1.79	0.47
2:A:455:MET:HE3	2:A:480:MET:CB	2.44	0.47
1:B:396:TYR:HB2	1:B:514:SER:HG	1.74	0.46
1:B:412:PRO:HB3	1:B:427:ASP:HA	1.98	0.46
2:A:76:GLN:NE2	2:A:79:LEU:CD1	2.73	0.46
1:B:462:LYS:HA	1:B:462:LYS:HD2	1.41	0.45
2:A:381:TYR:HE2	2:A:385:TYR:CE2	2.02	0.45
1:B:422:ASN:N	1:B:461:LEU:HD11	2.31	0.45
1:B:426:PRO:HG2	1:B:429:PHE:HB2	1.98	0.45
1:B:379:CYS:HB2	1:B:432:CYS:SG	2.57	0.45
2:A:284:PRO:HD3	2:A:440:LEU:HD23	1.98	0.45
2:A:596:LYS:HZ2	2:A:596:LYS:HG2	1.64	0.45
2:A:394:ASN:O	2:A:562:LYS:HG3	2.16	0.45
2:A:418:LEU:HB2	2:A:424:LEU:CD1	2.47	0.45
2:A:455:MET:SD	2:A:481:LYS:HG2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:TYR:C	1:B:461:LEU:HD11	2.38	0.44
1:B:480:CYS:CB	1:B:488:CYS:HG	2.31	0.44
2:A:482:ARG:NH1	2:A:489:GLU:OE2	2.52	0.43
1:B:360:ASN:H	1:B:524:VAL:HG22	1.84	0.43
2:A:251:THR:HG21	2:A:281:LEU:HD22	2.00	0.43
2:A:395:GLY:O	2:A:562:LYS:HE2	2.19	0.43
1:B:421:TYR:CD1	1:B:457:ARG:HB3	2.54	0.43
2:A:131:LYS:CG	2:A:143:LEU:HD21	2.48	0.42
2:A:201:ASP:OD1	2:A:204:ARG:NH2	2.52	0.42
2:A:153:GLU:CD	2:A:154:ASN:OD1	2.57	0.42
2:A:53:ASN:CG	2:A:340:ARG:HD2	2.40	0.42
2:A:120:LEU:HD21	2:A:183:TYR:HE1	1.81	0.42
2:A:455:MET:HE1	2:A:480:MET:C	2.38	0.42
1:B:403:ARG:HG2	1:B:404:GLY:N	2.35	0.42
2:A:381:TYR:OH	2:A:395:GLY:CA	2.39	0.41
1:B:398:ASP:HB2	1:B:512:VAL:HB	2.03	0.41
2:A:335:GLU:HB2	2:A:361:CYS:HB3	2.02	0.41
2:A:53:ASN:HB2	2:A:340:ARG:HD2	2.03	0.41
1:B:383:SER:O	1:B:387:LEU:HB2	2.20	0.41
1:B:439:ASN:HA	1:B:507:PRO:HG2	2.03	0.41
2:A:183:TYR:CE1	2:A:187:LYS:HE3	2.56	0.41
2:A:74:GLU:HG2	2:A:78:LYS:HE3	2.03	0.41
1:B:336:CYS:CB	1:B:361:CYS:SG	3.05	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	B	193/247 (78%)	181 (94%)	12 (6%)	0	100	100
2	A	594/613 (97%)	581 (98%)	12 (2%)	1 (0%)	47	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	787/860 (92%)	762 (97%)	24 (3%)	1 (0%)	54 84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	105	SER

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	B	167/216 (77%)	158 (95%)	9 (5%)	22 53
2	A	530/542 (98%)	511 (96%)	19 (4%)	35 65
All	All	697/758 (92%)	669 (96%)	28 (4%)	35 62

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	455	LEU
1	B	456	PHE
1	B	460	ASN
1	B	462	LYS
1	B	483	VAL
1	B	486	VAL
1	B	492	LEU
1	B	493	GLN
1	B	500	THR
2	A	38	GLU
2	A	55	SER
2	A	210	GLU
2	A	291	ILE
2	A	303	ASP
2	A	309	LYS
2	A	367	ASP
2	A	401	HIS

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Mol	Chain	Res	Type
2	A	402	GLU
2	A	425	PRO
2	A	431	ASP
2	A	471	ASP
2	A	479	GLU
2	A	491	VAL
2	A	541	LYS
2	A	545	SER
2	A	553	LYS
2	A	592	PHE
2	A	607	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	414	GLN
1	B	422	ASN
1	B	474	GLN
2	A	26	ASN
2	A	76	GLN
2	A	238	GLN
2	A	394	ASN
2	A	526	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.