



Full wwPDB EM Model Validation Report ⓘ

Apr 7, 2020 – 10:03 PM EDT

PDB ID : 6T0V
EMDB ID : EMD-10360
Title : Bat Influenza A polymerase elongation complex with incoming UTP analogue
(complete polymerase)
Authors : Wandzik, J.M.; Kouba, T.; Cusack, S.
Deposited on : 2019-10-03
Resolution : 3.02 Å(reported)

This is a Full wwPDB EM 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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.10.1

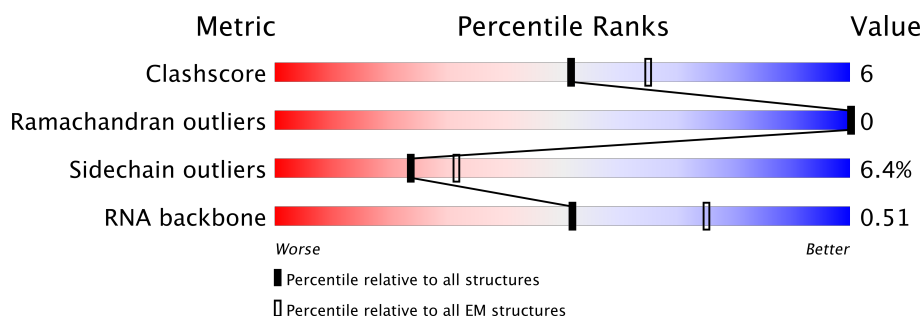
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.02 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

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 on 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	738	
2	B	776	
3	C	809	
4	V	14	
5	R	21	
6	M	26	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 18604 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	705	Total	C	N	O	S	0	0
			5746	3653	970	1086	37		

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP H6QM92
A	-12	SER	-	expression tag	UNP H6QM92
A	-11	HIS	-	expression tag	UNP H6QM92
A	-10	HIS	-	expression tag	UNP H6QM92
A	-9	HIS	-	expression tag	UNP H6QM92
A	-8	HIS	-	expression tag	UNP H6QM92
A	-7	HIS	-	expression tag	UNP H6QM92
A	-6	HIS	-	expression tag	UNP H6QM92
A	-5	HIS	-	expression tag	UNP H6QM92
A	-4	HIS	-	expression tag	UNP H6QM92
A	-3	GLY	-	expression tag	UNP H6QM92
A	-2	SER	-	expression tag	UNP H6QM92
A	-1	GLY	-	expression tag	UNP H6QM92
A	0	SER	-	expression tag	UNP H6QM92
A	714	GLY	-	expression tag	UNP H6QM92
A	715	SER	-	expression tag	UNP H6QM92
A	716	GLY	-	expression tag	UNP H6QM92
A	717	SER	-	expression tag	UNP H6QM92
A	718	GLY	-	expression tag	UNP H6QM92
A	719	GLU	-	expression tag	UNP H6QM92
A	720	ASN	-	expression tag	UNP H6QM92
A	721	LEU	-	expression tag	UNP H6QM92
A	722	TYR	-	expression tag	UNP H6QM92
A	723	PHE	-	expression tag	UNP H6QM92
A	724	GLN	-	expression tag	UNP H6QM92

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	745	Total	C	N	O	S	0	0
			5950	3740	1058	1113	39		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP H6QM91
B	-7	SER	-	expression tag	UNP H6QM91
B	-6	GLY	-	expression tag	UNP H6QM91
B	-5	SER	-	expression tag	UNP H6QM91
B	-4	GLY	-	expression tag	UNP H6QM91
B	-3	SER	-	expression tag	UNP H6QM91
B	-2	GLY	-	expression tag	UNP H6QM91
B	-1	SER	-	expression tag	UNP H6QM91
B	0	GLY	-	expression tag	UNP H6QM91
B	757	GLY	-	expression tag	UNP H6QM91
B	758	SER	-	expression tag	UNP H6QM91
B	759	GLY	-	expression tag	UNP H6QM91
B	760	SER	-	expression tag	UNP H6QM91
B	761	GLY	-	expression tag	UNP H6QM91
B	762	GLU	-	expression tag	UNP H6QM91
B	763	ASN	-	expression tag	UNP H6QM91
B	764	LEU	-	expression tag	UNP H6QM91
B	765	TYR	-	expression tag	UNP H6QM91
B	766	PHE	-	expression tag	UNP H6QM91
B	767	GLN	-	expression tag	UNP H6QM91

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	740	Total	C	N	O	S	0	0
			5878	3708	1040	1098	32		

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP H6QM90
C	-7	SER	-	expression tag	UNP H6QM90
C	-6	GLY	-	expression tag	UNP H6QM90
C	-5	SER	-	expression tag	UNP H6QM90
C	-4	GLY	-	expression tag	UNP H6QM90
C	-3	SER	-	expression tag	UNP H6QM90
C	-2	GLY	-	expression tag	UNP H6QM90

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP H6QM90
C	0	GLY	-	expression tag	UNP H6QM90
C	761	GLY	-	expression tag	UNP H6QM90
C	762	TRP	-	expression tag	UNP H6QM90
C	763	SER	-	expression tag	UNP H6QM90
C	764	HIS	-	expression tag	UNP H6QM90
C	765	PRO	-	expression tag	UNP H6QM90
C	766	GLN	-	expression tag	UNP H6QM90
C	767	PHE	-	expression tag	UNP H6QM90
C	768	GLU	-	expression tag	UNP H6QM90
C	769	LYS	-	expression tag	UNP H6QM90
C	770	GLY	-	expression tag	UNP H6QM90
C	771	GLY	-	expression tag	UNP H6QM90
C	772	GLY	-	expression tag	UNP H6QM90
C	773	SER	-	expression tag	UNP H6QM90
C	774	GLY	-	expression tag	UNP H6QM90
C	775	GLY	-	expression tag	UNP H6QM90
C	776	GLY	-	expression tag	UNP H6QM90
C	777	SER	-	expression tag	UNP H6QM90
C	778	GLY	-	expression tag	UNP H6QM90
C	779	GLY	-	expression tag	UNP H6QM90
C	780	SER	-	expression tag	UNP H6QM90
C	781	ALA	-	expression tag	UNP H6QM90
C	782	TRP	-	expression tag	UNP H6QM90
C	783	SER	-	expression tag	UNP H6QM90
C	784	HIS	-	expression tag	UNP H6QM90
C	785	PRO	-	expression tag	UNP H6QM90
C	786	GLN	-	expression tag	UNP H6QM90
C	787	PHE	-	expression tag	UNP H6QM90
C	788	GLU	-	expression tag	UNP H6QM90
C	789	LYS	-	expression tag	UNP H6QM90
C	790	GLY	-	expression tag	UNP H6QM90
C	791	ARG	-	expression tag	UNP H6QM90
C	792	SER	-	expression tag	UNP H6QM90
C	793	GLY	-	expression tag	UNP H6QM90
C	794	GLY	-	expression tag	UNP H6QM90
C	795	GLU	-	expression tag	UNP H6QM90
C	796	ASN	-	expression tag	UNP H6QM90
C	797	LEU	-	expression tag	UNP H6QM90
C	798	TYR	-	expression tag	UNP H6QM90
C	799	PHE	-	expression tag	UNP H6QM90
C	800	GLN	-	expression tag	UNP H6QM90

- Molecule 4 is a RNA chain called 5' vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	14	Total	C	N	O	P	0	0
			307	137	62	94	14		

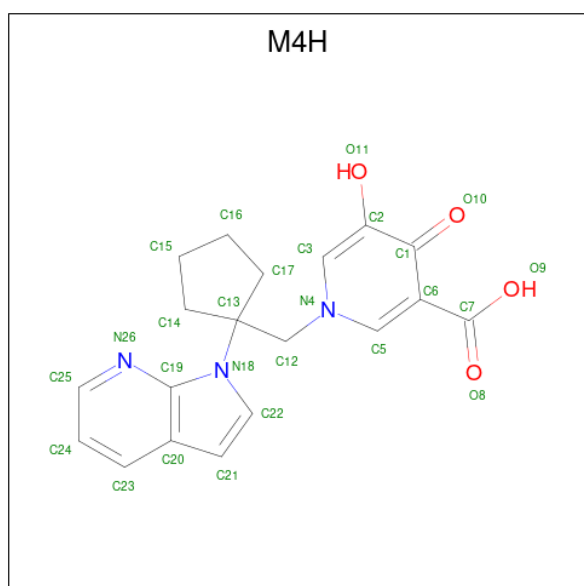
- Molecule 5 is a RNA chain called 3' vRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	18	Total	C	N	O	P	0	0
			367	166	54	130	17		

- Molecule 6 is a RNA chain called Capped mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	M	12	Total	C	N	O	P	0	0
			296	130	63	89	14		

- Molecule 7 is 5-oxidanyl-4-oxidanylidene-1-[(1-pyrrolo[2,3-b]pyridin-1-ylcyclopentyl)methyl]pyridine-3-carboxylic acid (three-letter code: M4H) (formula: C₁₉H₁₉N₃O₄).

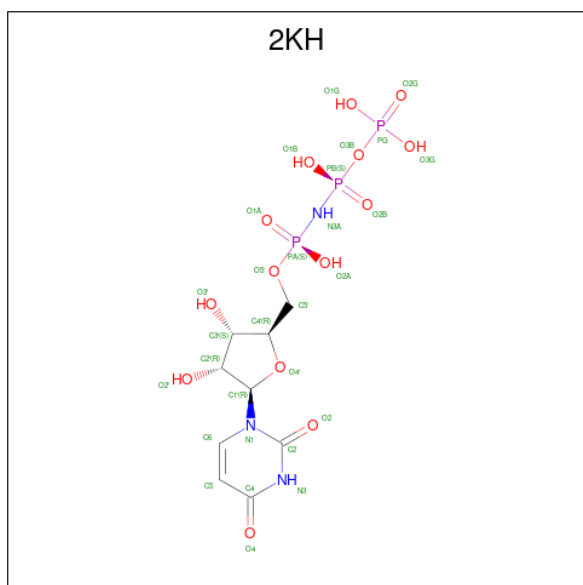


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			26	19	3	4	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
8	B	3	Total Mg 3 3	0
8	A	2	Total Mg 2 2	0

- Molecule 9 is 5'-O-[(S)-hydroxy{[(S)-hydroxy(phosphonooxy)phosphoryl]amino}phosphoryl]uridine (three-letter code: 2KH) (formula: C₉H₁₆N₃O₁₄P₃).

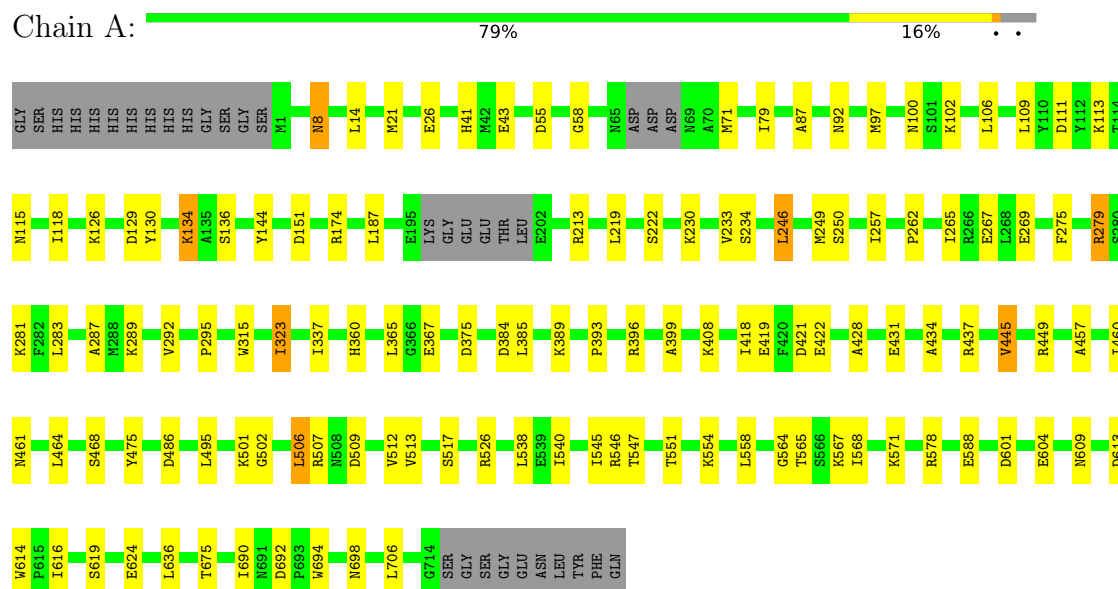


Mol	Chain	Residues	Atoms					AltConf
9	B	1	Total	C	N	O	P	0
			29	9	3	14	3	

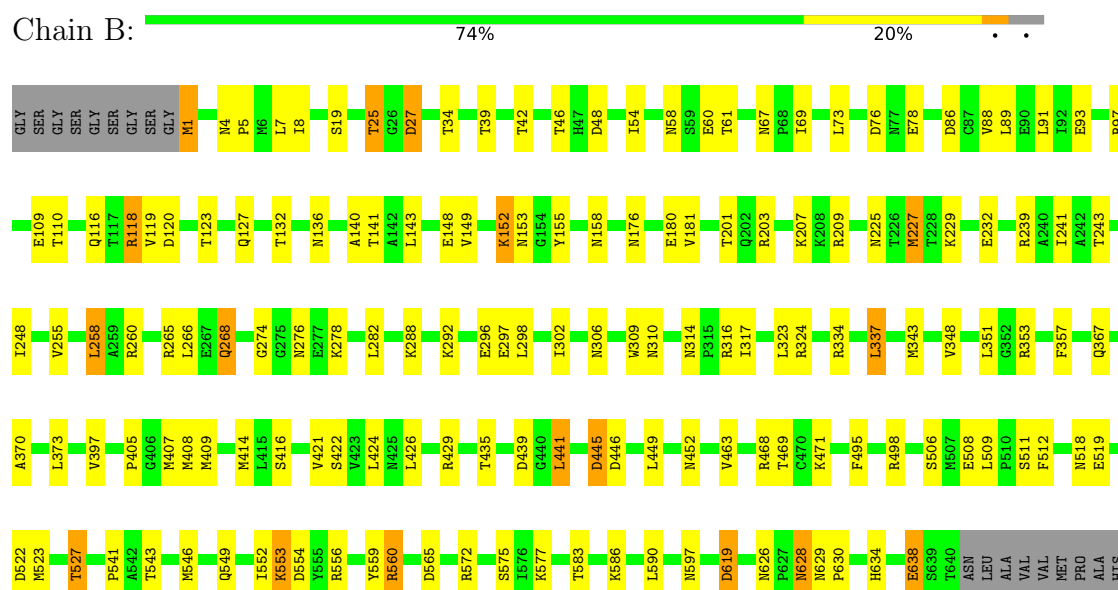
3 Residue-property plots

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: Polymerase acidic protein



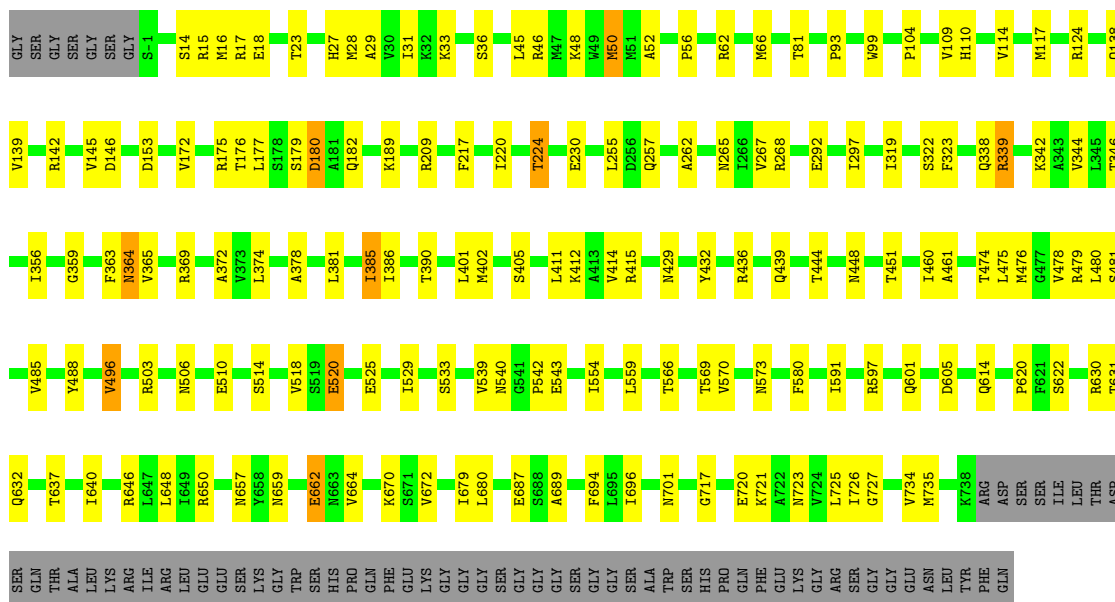
• Molecule 2: RNA-directed RNA polymerase catalytic subunit





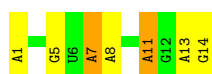
• Molecule 3: Polymerase basic protein 2

Chain C: 72% 19% 9%



• Molecule 4: 5' vRNA

Chain V: 50% 36% 14%



• Molecule 5: 3' vRNA

Chain R: 57% 24% 5% 14%



• Molecule 6: Capped mRNA

Chain M: 46% 54%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	65071	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 2KH, M4H, GTG

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	0.35	0/5868	0.48	0/7901
2	B	0.35	0/6064	0.50	0/8179
3	C	0.32	0/5980	0.50	0/8074
4	V	0.82	1/345 (0.3%)	0.93	1/535 (0.2%)
5	R	0.48	0/406	0.88	0/628
6	M	0.56	0/274	0.82	0/424
All	All	0.36	1/18937 (0.0%)	0.53	1/25741 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1	A	OP3-P	-11.17	1.47	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	V	7	A	O4'-C1'-N9	6.14	113.11	108.20

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	5746	0	5663	73	0
2	B	5950	0	5955	113	0
3	C	5878	0	5995	83	0
4	V	307	0	153	2	0
5	R	367	0	192	6	0
6	M	296	0	149	0	0
7	A	26	0	0	1	0
8	A	2	0	0	0	0
8	B	3	0	0	0	0
9	B	29	0	14	3	0
All	All	18604	0	18121	231	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 6.

All (231) 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:660:VAL:HG21	3:C:114:VAL:HG21	1.69	0.75
1:A:249:MET:HG3	2:B:73:LEU:HB3	1.78	0.65
2:B:58:ASN:HD22	2:B:61:THR:H	1.44	0.64
3:C:461:ALA:HB3	3:C:480:LEU:HB3	1.82	0.62
1:A:111:ASP:O	1:A:115:ASN:HA	2.01	0.61
2:B:629:ASN:OD1	2:B:630:PRO:HD2	2.02	0.60
2:B:628:ASN:ND2	2:B:628:ASN:H	2.00	0.60
3:C:374:LEU:HD11	3:C:381:LEU:HD11	1.84	0.60
2:B:268:GLN:NE2	2:B:439:ASP:OD1	2.35	0.59
2:B:660:VAL:HG22	3:C:110:HIS:HB2	1.84	0.59
2:B:560:ARG:HH11	3:C:52:ALA:HA	1.67	0.58
1:A:694:TRP:O	1:A:698:ASN:ND2	2.34	0.58
2:B:296:GLU:HA	3:C:727:GLY:HA2	1.84	0.58
3:C:381:LEU:HD13	3:C:405:SER:HB3	1.85	0.58
2:B:629:ASN:O	2:B:634:HIS:NE2	2.37	0.57
2:B:306:ASN:ND2	2:B:445:ASP:O	2.37	0.57
3:C:344:VAL:HG11	3:C:411:LEU:HD13	1.85	0.57
3:C:267:VAL:HG11	3:C:518:VAL:HG21	1.86	0.57
3:C:414:VAL:O	3:C:415:ARG:NH1	2.38	0.57
3:C:15:ARG:NH2	3:C:18:GLU:OE1	2.37	0.56
2:B:560:ARG:HH11	3:C:52:ALA:CA	2.18	0.56
1:A:234:SER:OG	2:B:334:ARG:NH2	2.38	0.56
1:A:571:LYS:HB2	3:C:45:LEU:HD13	1.88	0.56
2:B:239:ARG:HH12	9:B:801:2KH:H2	1.53	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:663:THR:HG21	3:C:99:TRP:CD1	2.41	0.55
2:B:46:THR:HG22	2:B:405:PRO:HG2	1.89	0.55
2:B:180:GLU:OE2	2:B:209:ARG:NH1	2.40	0.55
1:A:275:PHE:O	1:A:396:ARG:NH2	2.40	0.55
1:A:578:ARG:NH2	2:B:512:PHE:O	2.40	0.55
3:C:29:ALA:O	3:C:33:LYS:NZ	2.39	0.55
3:C:374:LEU:HD13	3:C:401:LEU:HD13	1.89	0.55
2:B:260:ARG:NH1	5:R:20:U:OP1	2.41	0.54
1:A:213:ARG:NE	2:B:60:GLU:OE2	2.36	0.54
3:C:117:MET:HE2	3:C:209:ARG:HD3	1.90	0.54
2:B:149:VAL:O	2:B:153:ASN:ND2	2.41	0.54
1:A:337:ILE:HG13	1:A:360:HIS:HD2	1.73	0.53
2:B:583:THR:O	2:B:586:LYS:NZ	2.41	0.53
3:C:28:MET:HA	3:C:31:ILE:HG12	1.89	0.53
3:C:342:LYS:HD2	3:C:356:ILE:HD12	1.90	0.53
3:C:637:THR:HG22	3:C:646:ARG:HG2	1.91	0.53
2:B:88:VAL:HG21	2:B:317:ILE:HD12	1.90	0.53
2:B:229:LYS:NZ	9:B:801:2KH:O4	2.37	0.53
1:A:92:ASN:ND2	3:C:172:VAL:O	2.42	0.53
3:C:138:GLN:O	3:C:670:LYS:NZ	2.40	0.53
2:B:560:ARG:O	2:B:572:ARG:HD3	2.09	0.52
2:B:119:VAL:HG12	2:B:143:LEU:HD21	1.89	0.52
2:B:203:ARG:NH1	4:V:13:A:OP2	2.42	0.52
3:C:319:ILE:HD12	3:C:496:VAL:HG21	1.92	0.52
1:A:257:ILE:HD11	2:B:463:VAL:HG21	1.90	0.52
3:C:180:ASP:OD1	3:C:180:ASP:N	2.41	0.52
3:C:220:ILE:HG21	3:C:224:THR:HG22	1.92	0.52
2:B:78:GLU:O	2:B:471:LYS:NZ	2.42	0.52
1:A:385:LEU:HG	2:B:357:PHE:HB3	1.92	0.52
2:B:590:LEU:HD12	2:B:664:HIS:CD2	2.45	0.52
1:A:421:ASP:OD2	2:B:556:ARG:NH1	2.43	0.51
1:A:509:ASP:HB3	1:A:568:ILE:HG12	1.92	0.51
2:B:266:LEU:HD13	2:B:421:VAL:HG11	1.91	0.51
1:A:437:ARG:NH2	1:A:601:ASP:OD1	2.43	0.51
2:B:276:ASN:OD1	3:C:142:ARG:NH1	2.42	0.51
2:B:310:ASN:O	2:B:407:MET:N	2.39	0.51
3:C:650:ARG:NH1	3:C:687:GLU:OE1	2.43	0.51
1:A:283:LEU:HB2	1:A:287:ALA:HB2	1.92	0.51
1:A:507:ARG:NH1	4:V:11:A:O2'	2.44	0.51
3:C:597:ARG:NH2	3:C:622:SER:O	2.42	0.51
3:C:14:SER:OG	3:C:17:ARG:NH2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:614:GLN:NE2	3:C:689:ALA:O	2.42	0.51
2:B:232:GLU:OE2	2:B:239:ARG:NH2	2.44	0.50
3:C:372:ALA:HB2	3:C:386:ILE:HG23	1.93	0.50
3:C:56:PRO:HD2	3:C:93:PRO:HD3	1.93	0.50
1:A:250:SER:O	2:B:468:ARG:NH2	2.44	0.50
2:B:519:GLU:HB2	2:B:664:HIS:HB3	1.91	0.50
2:B:660:VAL:HG22	3:C:110:HIS:CB	2.41	0.50
3:C:145:VAL:HG11	3:C:220:ILE:HG13	1.93	0.50
2:B:27:ASP:N	2:B:27:ASP:OD1	2.38	0.50
1:A:8:ASN:OD1	1:A:8:ASN:N	2.42	0.50
3:C:124:ARG:NH1	3:C:230:GLU:OE1	2.44	0.50
2:B:498:ARG:NH2	3:C:662:GLU:OE1	2.42	0.50
2:B:421:VAL:HA	2:B:424:LEU:HD12	1.93	0.50
3:C:601:GLN:NE2	3:C:605:ASP:OD1	2.43	0.50
1:A:130:TYR:OH	1:A:134:LYS:HE3	2.12	0.49
2:B:729:ASP:HB3	2:B:735:ILE:HB	1.94	0.49
3:C:139:VAL:HG11	3:C:543:GLU:HB2	1.94	0.49
3:C:631:THR:OG1	3:C:632:GLN:N	2.46	0.49
2:B:136:ASN:ND2	5:R:16:U:OP1	2.45	0.49
2:B:278:LYS:HD2	2:B:495:PHE:HE2	1.76	0.49
2:B:148:GLU:OE1	2:B:152:LYS:NZ	2.43	0.49
2:B:554:ASP:OD1	3:C:48:LYS:NZ	2.44	0.49
2:B:76:ASP:OD1	2:B:76:ASP:N	2.46	0.49
3:C:474:THR:OG1	3:C:475:LEU:N	2.46	0.49
1:A:546:ARG:HA	1:A:551:THR:HG23	1.94	0.48
2:B:523:MET:O	2:B:527:THR:OG1	2.30	0.48
1:A:421:ASP:O	2:B:549:GLN:NE2	2.43	0.48
1:A:540:ILE:HG12	1:A:558:LEU:HB2	1.95	0.48
2:B:619:ASP:OD1	2:B:619:ASP:N	2.40	0.48
3:C:265:ASN:OD1	3:C:268:ARG:NH2	2.44	0.48
3:C:262:ALA:HB2	3:C:529:ILE:HD13	1.96	0.48
1:A:445:VAL:HG22	1:A:636:LEU:HD22	1.96	0.48
1:A:512:VAL:HA	1:A:565:THR:O	2.13	0.48
1:A:111:ASP:O	1:A:115:ASN:CA	2.61	0.48
1:A:129:ASP:OD1	1:A:129:ASP:N	2.45	0.48
3:C:255:LEU:HD11	3:C:297:ILE:HD13	1.96	0.48
1:A:262:PRO:HA	1:A:265:ILE:HG12	1.96	0.48
1:A:457:ALA:O	1:A:461:ASN:ND2	2.44	0.48
2:B:302:ILE:HD12	2:B:449:LEU:HD23	1.95	0.48
1:A:267:GLU:HG3	1:A:706:LEU:HD23	1.96	0.47
1:A:246:LEU:HD23	2:B:468:ARG:HH11	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:LYS:HE3	2:B:682:ILE:HG22	1.95	0.47
3:C:179:SER:HB2	3:C:182:GLN:HG3	1.94	0.47
3:C:569:THR:O	3:C:573:ASN:ND2	2.46	0.47
1:A:281:LYS:NZ	1:A:564:GLY:O	2.40	0.47
3:C:429:ASN:HD22	3:C:432:TYR:HD2	1.63	0.47
3:C:46:ARG:O	3:C:50:MET:HB2	2.15	0.47
2:B:69:ILE:HG13	2:B:316:ARG:HB2	1.97	0.47
1:A:279:ARG:NH2	1:A:692:ASP:OD1	2.48	0.47
3:C:402:MET:O	3:C:405:SER:OG	2.32	0.47
2:B:506:SER:O	2:B:509:LEU:HB2	2.14	0.47
1:A:384:ASP:OD1	1:A:384:ASP:N	2.38	0.47
1:A:434:ALA:HB2	2:B:541:PRO:HB2	1.96	0.47
2:B:229:LYS:HE2	2:B:232:GLU:HB2	1.97	0.47
2:B:736:SER:OG	2:B:739:ASP:OD1	2.32	0.47
3:C:701:ASN:H	3:C:723:ASN:HD21	1.63	0.47
1:A:97:MET:HE2	2:B:728:ILE:HD12	1.98	0.46
1:A:428:ALA:HB3	1:A:431:GLU:HG3	1.98	0.46
3:C:506:ASN:OD1	3:C:510:GLU:N	2.47	0.46
1:A:567:LYS:HB3	3:C:45:LEU:HD21	1.98	0.46
1:A:41:HIS:NE2	7:A:801:M4H:O11	2.47	0.46
2:B:663:THR:HG21	3:C:99:TRP:HD1	1.80	0.46
1:A:275:PHE:HB3	1:A:399:ALA:HB2	1.97	0.46
3:C:657:ASN:ND2	3:C:659:ASN:OD1	2.49	0.46
1:A:102:LYS:NZ	3:C:175:ARG:O	2.48	0.45
3:C:554:ILE:HD12	3:C:672:VAL:HG23	1.98	0.45
1:A:109:LEU:HB3	1:A:118:ILE:HB	1.97	0.45
2:B:324:ARG:O	2:B:324:ARG:NH1	2.42	0.45
1:A:118:ILE:HG23	1:A:144:TYR:HD2	1.82	0.45
1:A:464:LEU:O	1:A:468:SER:OG	2.27	0.45
2:B:91:LEU:HB3	2:B:422:SER:HB2	1.97	0.45
2:B:560:ARG:HH11	3:C:52:ALA:N	2.15	0.45
1:A:408:LYS:HA	1:A:408:LYS:HD3	1.86	0.45
2:B:136:ASN:OD1	2:B:225:ASN:ND2	2.44	0.45
3:C:687:GLU:HB2	3:C:696:ILE:HB	1.99	0.45
1:A:79:ILE:HG22	1:A:87:ALA:HB1	1.99	0.45
3:C:339:ARG:HG2	3:C:339:ARG:H	1.55	0.45
2:B:123:THR:HG22	2:B:140:ALA:HA	1.99	0.45
2:B:426:LEU:HD22	2:B:469:THR:HG21	1.98	0.45
1:A:233:VAL:HG22	2:B:89:LEU:HD11	1.98	0.45
2:B:34:THR:HG22	2:B:353:ARG:HD2	1.97	0.44
2:B:42:THR:O	2:B:46:THR:OG1	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:LYS:HA	1:A:389:LYS:HD3	1.88	0.44
2:B:522:ASP:OD2	2:B:559:TYR:OH	2.23	0.44
2:B:638:GLU:H	2:B:638:GLU:HG3	1.50	0.44
3:C:694:PHE:HB3	3:C:734:VAL:HG13	1.99	0.44
1:A:323:ILE:HD12	1:A:526:ARG:HD3	2.00	0.44
2:B:118:ARG:HD3	2:B:707:ARG:HH22	1.82	0.44
1:A:460:ILE:O	1:A:464:LEU:HB2	2.18	0.44
2:B:560:ARG:NH1	3:C:52:ALA:N	2.65	0.44
2:B:241:ILE:HD12	5:R:17:A:C8	2.53	0.44
1:A:545:ILE:HG13	1:A:554:LYS:HD3	2.00	0.44
2:B:274:GLY:HA2	2:B:278:LYS:HE3	2.00	0.44
2:B:309:TRP:HZ2	2:B:416:SER:HB3	1.82	0.44
3:C:322:SER:OG	3:C:323:PHE:N	2.50	0.44
3:C:542:PRO:HB2	3:C:640:ILE:HG13	1.99	0.43
1:A:422:GLU:HG2	2:B:597:ASN:HB3	1.99	0.43
3:C:520:GLU:H	3:C:520:GLU:HG3	1.60	0.43
1:A:506:LEU:H	1:A:506:LEU:HG	1.63	0.43
2:B:508:GLU:O	2:B:511:SER:OG	2.36	0.43
1:A:365:LEU:HD13	1:A:502:GLY:HA2	1.99	0.43
1:A:624:GLU:HG3	2:B:1:MET:HG3	2.00	0.43
2:B:660:VAL:O	2:B:660:VAL:HG12	2.19	0.43
1:A:588:GLU:OE1	2:B:543:THR:OG1	2.31	0.43
2:B:241:ILE:HG22	2:B:409:MET:HG2	2.00	0.43
9:B:801:2KH:N3	5:R:17:A:N1	2.43	0.43
2:B:626:ASN:ND2	3:C:104:PRO:O	2.52	0.43
1:A:289:LYS:HA	1:A:495:LEU:O	2.18	0.43
2:B:155:TYR:HE2	2:B:176:ASN:HD22	1.65	0.42
2:B:4:ASN:HB3	2:B:7:LEU:HG	2.01	0.42
2:B:132:THR:HG23	2:B:181:VAL:HB	2.00	0.42
2:B:292:LYS:HE2	2:B:292:LYS:HB3	1.87	0.42
2:B:297:GLU:OE2	2:B:429:ARG:NH2	2.47	0.42
3:C:436:ARG:NH1	3:C:439:GLN:OE1	2.43	0.42
3:C:23:THR:HG23	3:C:27:HIS:HB3	2.01	0.42
2:B:268:GLN:HE21	2:B:268:GLN:HB3	1.52	0.42
3:C:721:LYS:HG2	3:C:735:MET:HG3	2.01	0.42
1:A:578:ARG:HG3	2:B:25:THR:HG22	2.02	0.42
2:B:552:ILE:HD13	2:B:552:ILE:HA	1.90	0.42
1:A:393:PRO:HG2	1:A:690:ILE:HG21	2.02	0.42
3:C:374:LEU:HD22	3:C:401:LEU:HD22	2.01	0.42
3:C:66:MET:HB3	3:C:66:MET:HE3	1.89	0.42
1:A:367:GLU:OE1	1:A:475:TYR:OH	2.30	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ILE:HA	1:A:568:ILE:HD13	1.82	0.42
2:B:110:THR:HG21	2:B:258:LEU:HB2	2.01	0.42
3:C:224:THR:OG1	3:C:224:THR:O	2.38	0.42
3:C:717:GLY:N	3:C:720:GLU:OE1	2.53	0.42
2:B:577:LYS:HE3	2:B:577:LYS:HB2	1.90	0.42
3:C:359:GLY:H	3:C:378:ALA:HB2	1.84	0.42
1:A:613:ASP:HB2	1:A:614:TRP:CE3	2.55	0.41
2:B:282:LEU:HD22	2:B:441:LEU:HD13	2.02	0.41
1:A:292:VAL:HG23	1:A:295:PRO:HG3	2.02	0.41
3:C:364:ASN:HD21	3:C:485:VAL:HG11	1.84	0.41
1:A:130:TYR:CZ	1:A:134:LYS:HE3	2.55	0.41
2:B:721:ARG:HD2	2:B:721:ARG:HA	1.87	0.41
2:B:5:PRO:O	2:B:8:ILE:HB	2.20	0.41
3:C:385:ILE:HG22	3:C:481:SER:HB2	2.02	0.41
3:C:475:LEU:HB2	3:C:478:VAL:HB	2.03	0.41
2:B:120:ASP:O	2:B:123:THR:OG1	2.28	0.41
2:B:324:ARG:HA	2:B:324:ARG:HD2	1.89	0.41
3:C:363:PHE:HB2	3:C:374:LEU:HB3	2.01	0.41
1:A:21:MET:HB3	1:A:26:GLU:HG3	2.02	0.41
2:B:298:LEU:O	2:B:452:ASN:ND2	2.53	0.41
2:B:370:ALA:HA	2:B:373:LEU:HG	2.00	0.41
1:A:375:ASP:OD1	2:B:203:ARG:NH2	2.53	0.41
2:B:227:MET:HG2	5:R:15:A:H4'	2.02	0.41
2:B:109:GLU:OE2	2:B:265:ARG:NH2	2.44	0.41
2:B:699:PHE:HE2	2:B:722:ALA:HB2	1.86	0.41
1:A:111:ASP:O	1:A:115:ASN:N	2.54	0.41
2:B:255:VAL:HG22	2:B:337:LEU:HD13	2.02	0.41
3:C:460:ILE:HG23	3:C:479:ARG:HB3	2.03	0.41
3:C:701:ASN:H	3:C:723:ASN:ND2	2.18	0.41
1:A:43:GLU:OE2	1:A:174:ARG:NE	2.53	0.41
3:C:177:LEU:HD22	3:C:182:GLN:HE21	1.86	0.41
1:A:419:GLU:O	2:B:553:LYS:NZ	2.44	0.40
1:A:58:GLY:O	1:A:113:LYS:NZ	2.39	0.40
2:B:93:GLU:OE2	2:B:97:ARG:NH1	2.47	0.40
3:C:189:LYS:HD3	3:C:189:LYS:HA	1.90	0.40
1:A:230:LYS:HG3	2:B:323:LEU:HD22	2.02	0.40
2:B:39:THR:HG21	2:B:351:LEU:HA	2.03	0.40
3:C:365:VAL:N	3:C:372:ALA:O	2.54	0.40
1:A:609:ASN:N	1:A:609:ASN:OD1	2.54	0.40
2:B:54:ILE:HB	2:B:67:ASN:HB3	2.04	0.40
1:A:219:LEU:O	2:B:316:ARG:NH1	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:580:PHE:CD2	3:C:620:PRO:HB2	2.56	0.40
2:B:127:GLN:HB2	5:R:17:A:H5'	2.02	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	699/738 (95%)	664 (95%)	35 (5%)	0	100	100
2	B	741/776 (96%)	721 (97%)	20 (3%)	0	100	100
3	C	738/809 (91%)	687 (93%)	51 (7%)	0	100	100
All	All	2178/2323 (94%)	2072 (95%)	106 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	630/657 (96%)	599 (95%)	31 (5%)	27	64
2	B	654/676 (97%)	608 (93%)	46 (7%)	16	49
3	C	654/706 (93%)	607 (93%)	47 (7%)	16	47
All	All	1938/2039 (95%)	1814 (94%)	124 (6%)	23	53

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	14	LEU
1	A	55	ASP
1	A	71	MET
1	A	100	ASN
1	A	106	LEU
1	A	126	LYS
1	A	134	LYS
1	A	136	SER
1	A	151	ASP
1	A	187	LEU
1	A	222	SER
1	A	246	LEU
1	A	269	GLU
1	A	279	ARG
1	A	315	TRP
1	A	323	ILE
1	A	418	ILE
1	A	445	VAL
1	A	449	ARG
1	A	486	ASP
1	A	501	LYS
1	A	506	LEU
1	A	513	VAL
1	A	517	SER
1	A	538	LEU
1	A	547	THR
1	A	604	GLU
1	A	616	ILE
1	A	619	SER
1	A	675	THR
2	B	1	MET
2	B	19	SER
2	B	25	THR
2	B	27	ASP
2	B	48	ASP
2	B	86	ASP
2	B	116	GLN
2	B	118	ARG
2	B	141	THR
2	B	152	LYS
2	B	158	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	201	THR
2	B	227	MET
2	B	243	THR
2	B	248	ILE
2	B	258	LEU
2	B	268	GLN
2	B	288	LYS
2	B	314	ASN
2	B	337	LEU
2	B	343	MET
2	B	348	VAL
2	B	367	GLN
2	B	397	VAL
2	B	408	MET
2	B	414	MET
2	B	435	THR
2	B	441	LEU
2	B	445	ASP
2	B	446	ASP
2	B	518	ASN
2	B	527	THR
2	B	546	MET
2	B	553	LYS
2	B	560	ARG
2	B	565	ASP
2	B	575	SER
2	B	619	ASP
2	B	628	ASN
2	B	638	GLU
2	B	662	THR
2	B	684	GLU
2	B	707	ARG
2	B	735	ILE
2	B	739	ASP
2	B	742	GLU
3	C	16	MET
3	C	36	SER
3	C	50	MET
3	C	62	ARG
3	C	81	THR
3	C	109	VAL
3	C	146	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	153	ASP
3	C	176	THR
3	C	180	ASP
3	C	217	PHE
3	C	224	THR
3	C	257	GLN
3	C	292	GLU
3	C	338	GLN
3	C	339	ARG
3	C	346	THR
3	C	364	ASN
3	C	369	ARG
3	C	385	ILE
3	C	390	THR
3	C	412	LYS
3	C	444	THR
3	C	448	ASN
3	C	451	THR
3	C	476	MET
3	C	488	TYR
3	C	496	VAL
3	C	503	ARG
3	C	514	SER
3	C	520	GLU
3	C	525	GLU
3	C	533	SER
3	C	539	VAL
3	C	540	ASN
3	C	559	LEU
3	C	566	THR
3	C	570	VAL
3	C	591	ILE
3	C	630	ARG
3	C	648	LEU
3	C	662	GLU
3	C	664	VAL
3	C	679	ILE
3	C	680	LEU
3	C	725	LEU
3	C	726	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	294	ASN
1	A	403	GLN
2	B	58	ASN
2	B	108	GLN
2	B	115	GLN
2	B	116	GLN
2	B	127	GLN
2	B	268	GLN
2	B	377	ASN
2	B	452	ASN
2	B	628	ASN
3	C	13	ASN
3	C	39	GLN
3	C	75	ASN
3	C	160	GLN
3	C	182	GLN
3	C	285	HIS
3	C	383	GLN
3	C	425	ASN
3	C	532	ASN
3	C	581	GLN
3	C	632	GLN
3	C	657	ASN
3	C	659	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	V	13/14 (92%)	5 (38%)	0
5	R	17/21 (80%)	3 (17%)	0
6	M	9/26 (34%)	0	0
All	All	39/61 (63%)	8 (20%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	V	5	G
4	V	7	A
4	V	8	A
4	V	11	A
4	V	14	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	15	A
5	R	29	G
5	R	31	U

There are no RNA pucker outliers to report.

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](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	M4H	A	801	8	25,29,29	1.30	3 (12%)	23,43,43	2.23	9 (39%)
9	2KH	B	801	8	25,30,30	4.02	16 (64%)	30,47,47	1.23	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	M4H	A	801	8	-	1/4/24/24	0/4/4/4
9	2KH	B	801	8	-	4/17/38/38	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	801	2KH	C3'-C2'	-8.21	1.30	1.53
9	B	801	2KH	C6-N1	6.76	1.44	1.35
9	B	801	2KH	O4'-C1'	-6.11	1.32	1.41
9	B	801	2KH	C2-N3	6.11	1.50	1.38
9	B	801	2KH	C4-N3	6.05	1.43	1.33
9	B	801	2KH	C6-C5	5.79	1.50	1.38
9	B	801	2KH	C2'-C1'	5.02	1.61	1.53
9	B	801	2KH	PB-O3B	4.37	1.64	1.59
7	A	801	M4H	C22-N18	-4.16	1.35	1.39
9	B	801	2KH	PA-O1A	3.90	1.52	1.46
9	B	801	2KH	O4'-C4'	3.88	1.53	1.45
9	B	801	2KH	O3'-C3'	3.67	1.51	1.43
9	B	801	2KH	PA-O2A	-3.63	1.47	1.56
7	A	801	M4H	C6-C7	3.35	1.50	1.47
9	B	801	2KH	PB-O1B	-3.31	1.47	1.56
9	B	801	2KH	C5'-C4'	-2.81	1.42	1.51
9	B	801	2KH	PB-N3A	2.54	1.70	1.63
9	B	801	2KH	PA-O5'	2.51	1.67	1.57
7	A	801	M4H	C1-C2	2.09	1.48	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	801	M4H	C22-N18-C13	-5.61	119.92	124.18
7	A	801	M4H	C5-C6-C1	-3.86	118.03	119.97
7	A	801	M4H	C15-C14-C13	3.62	109.48	104.37
9	B	801	2KH	C3'-C2'-C1'	3.22	105.82	100.98
9	B	801	2KH	PG-O3B-PB	-2.94	122.27	132.62
7	A	801	M4H	C25-N26-C19	2.77	120.21	116.77
7	A	801	M4H	C6-C1-C2	-2.72	116.34	120.20
7	A	801	M4H	C16-C17-C13	2.38	107.73	104.37
7	A	801	M4H	C21-C20-C19	2.19	111.53	105.30
7	A	801	M4H	C2-C3-N4	2.14	123.15	120.58
7	A	801	M4H	C21-C20-C23	-2.10	129.38	136.72

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	801	2KH	PB-N3A-PA-O5'
9	B	801	2KH	PA-N3A-PB-O2B

Continued on next page...

Continued from previous page...

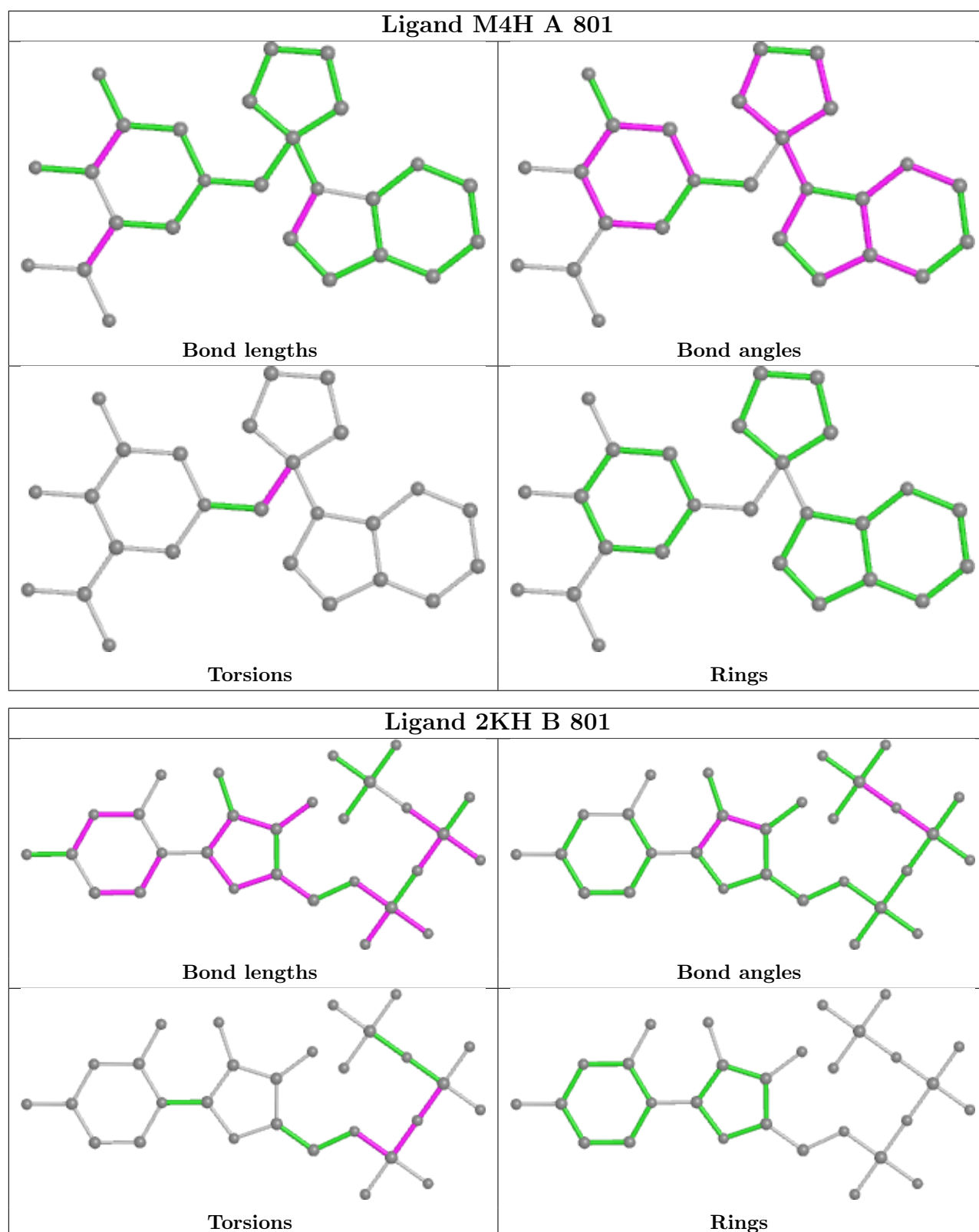
Mol	Chain	Res	Type	Atoms
7	A	801	M4H	N4-C12-C13-C14
9	B	801	2KH	C5'-O5'-PA-O1A
9	B	801	2KH	PB-N3A-PA-O1A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	801	M4H	1	0
9	B	801	2KH	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.