



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2022 – 03:07 pm BST

PDB ID : 7Z4O  
Title : Influenza A/H7N9 polymerase core dimer with Pol II pSer5 CTD peptide mimic bound in site 2A  
Authors : Cusack, S.; Pflug, A.  
Deposited on : 2022-03-04  
Resolution : 3.41 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.28.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.28.1

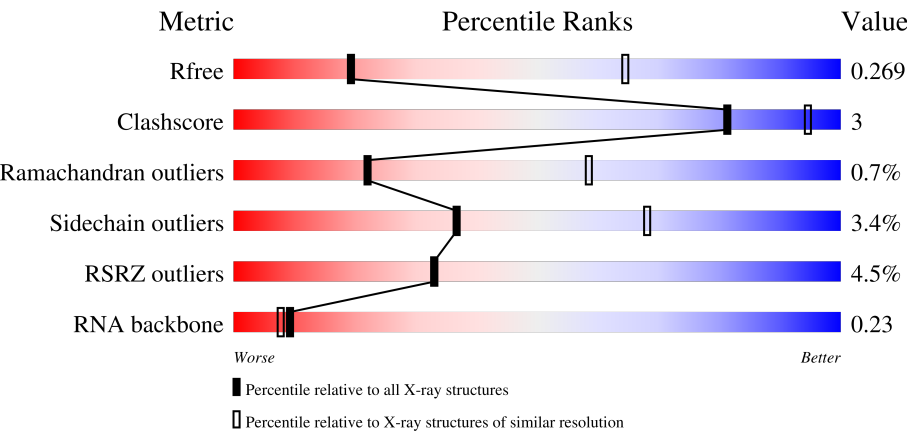


1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.41 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)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1486 (3.50-3.34)
Clashscore	141614	1572 (3.50-3.34)
Ramachandran outliers	138981	1534 (3.50-3.34)
Sidechain outliers	138945	1535 (3.50-3.34)
RSRZ outliers	127900	1395 (3.50-3.34)
RNA backbone	3102	1012 (3.88-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AAA	517	<div><div>2%</div><div>90%</div><div>9%</div><div></div></div>
1	DDD	517	<div><div>2%</div><div>90%</div><div>9%</div><div></div></div>
2	BBB	757	<div><div>3%</div><div>73%</div><div>8%</div><div>18%</div></div>
2	EEE	757	<div><div>5%</div><div>72%</div><div>8%</div><div>19%</div></div>

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Mol	Chain	Length	Quality of chain
3	CCC	147	
3	FFF	147	
4	JJJ	28	
4	KKK	28	
5	UUU	12	
5	VVV	12	



## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19969 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	AAA	514	Total	C	N	O	S	0	0	0
			4133	2617	702	784	30			
1	DDD	514	Total	C	N	O	S	0	0	0
			4133	2617	702	784	30			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	200	MET	-	initiating methionine	UNP M9TI86
DDD	200	MET	-	initiating methionine	UNP M9TI86

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	622	Total	C	N	O	S	0	8	0
			5010	3162	866	944	38			
2	EEE	615	Total	C	N	O	S	0	0	0
			4892	3088	847	921	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	CCC	68	Total	C	N	O	S	0	0	0
			545	341	99	98	7			
3	FFF	71	Total	C	N	O	S	0	0	0
			564	353	102	102	7			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CCC	129	SER	-	expression tag	UNP X5F427
CCC	130	GLY	-	expression tag	UNP X5F427

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	131	SER	-	expression tag	UNP X5F427
CCC	132	GLU	-	expression tag	UNP X5F427
CCC	133	ASN	-	expression tag	UNP X5F427
CCC	134	LEU	-	expression tag	UNP X5F427
CCC	135	TYR	-	expression tag	UNP X5F427
CCC	136	PHE	-	expression tag	UNP X5F427
CCC	137	GLN	-	expression tag	UNP X5F427
CCC	138	GLY	-	expression tag	UNP X5F427
CCC	139	SER	-	expression tag	UNP X5F427
CCC	140	HIS	-	expression tag	UNP X5F427
CCC	141	HIS	-	expression tag	UNP X5F427
CCC	142	HIS	-	expression tag	UNP X5F427
CCC	143	HIS	-	expression tag	UNP X5F427
CCC	144	HIS	-	expression tag	UNP X5F427
CCC	145	HIS	-	expression tag	UNP X5F427
CCC	146	HIS	-	expression tag	UNP X5F427
CCC	147	HIS	-	expression tag	UNP X5F427
FFF	129	SER	-	expression tag	UNP X5F427
FFF	130	GLY	-	expression tag	UNP X5F427
FFF	131	SER	-	expression tag	UNP X5F427
FFF	132	GLU	-	expression tag	UNP X5F427
FFF	133	ASN	-	expression tag	UNP X5F427
FFF	134	LEU	-	expression tag	UNP X5F427
FFF	135	TYR	-	expression tag	UNP X5F427
FFF	136	PHE	-	expression tag	UNP X5F427
FFF	137	GLN	-	expression tag	UNP X5F427
FFF	138	GLY	-	expression tag	UNP X5F427
FFF	139	SER	-	expression tag	UNP X5F427
FFF	140	HIS	-	expression tag	UNP X5F427
FFF	141	HIS	-	expression tag	UNP X5F427
FFF	142	HIS	-	expression tag	UNP X5F427
FFF	143	HIS	-	expression tag	UNP X5F427
FFF	144	HIS	-	expression tag	UNP X5F427
FFF	145	HIS	-	expression tag	UNP X5F427
FFF	146	HIS	-	expression tag	UNP X5F427
FFF	147	HIS	-	expression tag	UNP X5F427

- Molecule 4 is a protein called SER-TYR-SER-PRO-THR-SEP-PRO-SER-TYR-SER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	JJJ	10	Total	C	N	O	P	0	0	0
			79	47	10	21	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	KKK	11	Total	C	N	O	P	0	0	0
			87	53	11	22	1			

- Molecule 5 is a RNA chain called RNA (5'-R(P\*AP\*GP\*UP\*AP\*GP\*UP\*AP\*AP\*CP\*AP\*AP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	UUU	12	Total	C	N	O	P	0	0	0
			262	117	52	81	12			
5	VVV	12	Total	C	N	O	P	0	0	0
			262	117	52	81	12			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	BBB	1	Total	Mg	0	0
			1	1		
6	EEE	1	Total	Mg	0	0
			1	1		





- Molecule 1: Polymerase acidic protein





- Molecule 2: RNA-directed RNA polymerase catalytic subunit

ASP  
ALA  
ARG  
ILE  
ASP  
PHE  
GLU  
SER  
GLY  
ARG  
ILE  
LYS  
LYS  
GLU  
GLU  
PHE  
ALA  
GLU  
ILE  
MET  
LYS  
ILE  
CYS  
SER  
THR  
ILE  
GLU  
GLU  
LEU  
ARG  
ARG  
GLN  
LYS

- Molecule 3: Polymerase basic protein 2

S107 THR VAL HIS TYR PRO LYS VAL TYR LYS THR TYR PHE GLU GLU VAL VAL GLU ARG LEU LYS HIS HIS SER SER GLY GLY GLN ASN LEU TYR PHE GLN GLY SER HIS HIS HIS HIS HIS HIS HIS

- Molecule 3: Polymerase basic protein 2

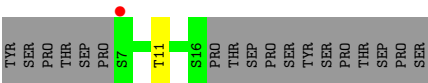
TYR	LYS	THR	TYR	PHE	GLU	LYS	VAL	GLU	ARG	LEU	LYS	HIS	GLY	SER	GLY	SER	GLU	ASN	LEU	TYR	PHE	GLN	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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- Molecule 4: SER-TYR-SER-PRO-THR-SEP-PRO-SER-TYR-SER

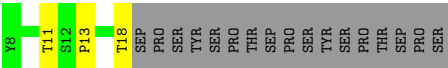


WORLD WIDE  
PDB  
PROTEIN DATA BANK

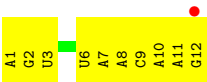




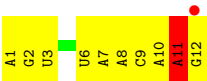
• Molecule 4: SER-TYR-SER-PRO-THR-SEP-PRO-SER-TYR-SER



• Molecule 5: RNA (5'-R(P\*AP\*GP\*UP\*AP\*GP\*UP\*AP\*AP\*CP\*AP\*AP\*G)-3')



• Molecule 5: RNA (5'-R(P\*AP\*GP\*UP\*AP\*GP\*UP\*AP\*AP\*CP\*AP\*AP\*G)-3')





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.47Å 144.13Å 336.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 3.41 49.16 – 3.41	Depositor EDS
% Data completeness (in resolution range)	73.2 (49.21-3.41) 73.3 (49.16-3.41)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.220 , 0.273 0.221 , 0.269	Depositor DCC
$R_{free}$ test set	1852 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	73.0	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	19969	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 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, SEP

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	AAA	0.66	0/4222	0.72	0/5700
1	DDD	0.66	0/4222	0.71	0/5700
2	BBB	0.67	0/5111	0.72	0/6905
2	EEE	0.67	0/4993	0.72	0/6747
3	CCC	0.66	0/558	0.73	0/755
3	FFF	0.66	0/577	0.71	0/782
4	JJJ	0.66	0/71	0.67	0/95
4	KKK	0.62	0/80	0.66	0/109
5	UUU	0.98	1/294 (0.3%)	1.27	3/455 (0.7%)
5	VVV	0.98	1/294 (0.3%)	1.25	4/455 (0.9%)
All	All	0.68	2/20422 (0.0%)	0.74	7/27703 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	UUU	1	A	OP3-P	-7.42	1.52	1.61
5	VVV	1	A	OP3-P	-7.28	1.52	1.61

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	UUU	9	C	P-O3'-C3'	-6.75	111.61	119.70
5	VVV	9	C	P-O3'-C3'	-6.37	112.05	119.70
5	VVV	2	G	P-O3'-C3'	-5.82	112.72	119.70
5	UUU	2	G	P-O3'-C3'	-5.78	112.76	119.70
5	VVV	11	A	P-O3'-C3'	-5.35	113.28	119.70
5	VVV	3	U	P-O3'-C3'	-5.32	113.32	119.70
5	UUU	3	U	P-O3'-C3'	-5.14	113.53	119.70

There are no chirality outliers.



There are no planarity outliers.

## 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	AAA	4133	0	4103	23	0
1	DDD	4133	0	4103	23	0
2	BBB	5010	0	4984	35	0
2	EEE	4892	0	4862	29	0
3	CCC	545	0	543	2	0
3	FFF	564	0	561	1	0
4	JJJ	79	0	61	0	0
4	KKK	87	0	70	1	0
5	UUU	262	0	131	1	0
5	VVV	262	0	131	2	0
6	BBB	1	0	0	0	0
6	EEE	1	0	0	0	0
All	All	19969	0	19549	101	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 3.

All (101) 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:BBB:507[B]:MET:SD	2:BBB:508[B]:GLU:N	2.54	0.81
2:BBB:252:VAL:HG11	2:BBB:411:MET:HG2	1.64	0.78
1:DDD:607:LEU:O	1:DDD:611:PHE:HB2	1.84	0.76
2:BBB:503[B]:ALA:HB1	2:BBB:505[B]:PHE:CE2	2.23	0.73
2:BBB:411:MET:SD	2:BBB:411:MET:N	2.64	0.70
1:DDD:217:GLN:OE1	2:EEE:59:THR:HG22	1.94	0.67
2:BBB:507[A]:MET:O	2:BBB:508[A]:GLU:HB2	1.97	0.64
1:AAA:508:ARG:NH2	5:VVV:11:A:OP2	2.32	0.62
3:CCC:60:ASP:OD2	3:CCC:62:ARG:NH2	2.32	0.61
2:BBB:28:PRO:HB2	2:BBB:231:ALA:HA	1.88	0.55
2:EEE:28:PRO:HB2	2:EEE:231:ALA:HA	1.89	0.55
1:AAA:370:LEU:HD13	1:AAA:507:GLY:HA2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:450:VAL:HG13	1:AAA:641:LEU:HD22	1.89	0.54
1:DDD:450:VAL:HG13	1:DDD:641:LEU:HD22	1.89	0.54
1:DDD:370:LEU:HD13	1:DDD:507:GLY:HA2	1.89	0.54
1:AAA:511:LEU:HD11	1:AAA:518:VAL:HG23	1.91	0.53
2:EEE:114:VAL:HA	2:EEE:254:PHE:CE1	2.45	0.52
1:DDD:673:ARG:NH1	1:DDD:714:ALA:O	2.43	0.52
1:DDD:378:LYS:HA	2:EEE:365:ARG:HG3	1.92	0.52
1:DDD:511:LEU:HD11	1:DDD:518:VAL:HG23	1.92	0.51
2:BBB:114:VAL:HA	2:BBB:254:PHE:CE1	2.45	0.51
1:DDD:559:ARG:HG2	1:DDD:560:PRO:HD2	1.93	0.51
1:AAA:375:ALA:HB2	5:VVV:10:A:H3'	1.93	0.51
2:BBB:92:MET:SD	2:BBB:321:MET:HG2	2.51	0.51
2:BBB:393:ARG:N	2:BBB:394:PRO:HD2	2.27	0.50
2:EEE:393:ARG:N	2:EEE:394:PRO:HD2	2.27	0.50
2:BBB:531:LYS:HD2	2:BBB:535:ILE:HD11	1.92	0.50
2:EEE:92:MET:SD	2:EEE:321:MET:HG2	2.52	0.49
2:BBB:526:GLY:HA3	2:BBB:551:PHE:CE1	2.48	0.49
2:EEE:526:GLY:HA3	2:EEE:551:PHE:CE1	2.48	0.49
2:BBB:177:GLU:HA	2:BBB:214:LYS:HB2	1.95	0.49
2:EEE:69:ILE:HD12	2:EEE:316:ARG:HB2	1.95	0.48
2:EEE:339:ILE:HA	2:EEE:342:ILE:HG12	1.95	0.47
2:BBB:333:PHE:CZ	2:BBB:337:LEU:HD11	2.50	0.47
1:AAA:648:SER:HA	2:BBB:26:GLY:HA3	1.94	0.47
2:BBB:507[A]:MET:O	2:BBB:508[A]:GLU:CB	2.62	0.47
2:EEE:333:PHE:CZ	2:EEE:337:LEU:HD11	2.49	0.47
1:AAA:378:LYS:HA	2:BBB:365:ARG:HG3	1.97	0.46
1:AAA:596:ILE:HG12	1:AAA:611:PHE:CD2	2.49	0.46
1:DDD:427:GLU:N	1:DDD:427:GLU:OE1	2.48	0.46
2:BBB:669:LYS:CE	3:CCC:58:THR:HG22	2.46	0.46
2:BBB:69:ILE:HD12	2:BBB:316:ARG:HB2	1.96	0.46
2:BBB:427:GLY:HA3	2:BBB:438:TRP:CD1	2.51	0.46
1:AAA:427:GLU:OE1	1:AAA:427:GLU:N	2.48	0.46
1:AAA:612:PHE:HA	1:AAA:633:ILE:HG21	1.97	0.46
2:BBB:302:ILE:HG23	2:BBB:449:LEU:HB3	1.98	0.45
2:EEE:427:GLY:HA3	2:EEE:438:TRP:CD1	2.52	0.45
2:EEE:503:ALA:HB1	2:EEE:505:PHE:CE2	2.51	0.45
1:AAA:590:GLN:HE21	2:BBB:506[A]:SER:H	1.64	0.45
1:AAA:322:ILE:HD13	1:AAA:331:ASN:HB3	1.99	0.45
2:BBB:503[B]:ALA:HB1	2:BBB:505[B]:PHE:CD2	2.52	0.44
1:DDD:375:ALA:HB2	5:UUU:10:A:H3'	2.00	0.44
1:DDD:459:ILE:O	1:DDD:463:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:348:MET:HA	2:BBB:402:SER:HA	2.00	0.44
2:EEE:35:GLY:HA3	2:EEE:228:THR:OG1	2.18	0.44
2:BBB:24:TYR:HB2	2:BBB:507[B]:MET:SD	2.59	0.43
2:BBB:35:GLY:HA3	2:BBB:228:THR:OG1	2.18	0.43
1:AAA:549:LEU:HD21	1:AAA:556:GLN:HG3	2.00	0.43
2:EEE:663:THR:HG21	3:FFF:99:TRP:CD1	2.53	0.43
1:AAA:264:THR:N	1:AAA:265:PRO:CD	2.81	0.43
2:BBB:24:TYR:CE2	2:BBB:233:ARG:HG3	2.53	0.43
2:EEE:348:MET:HA	2:EEE:402:SER:HA	1.99	0.43
1:AAA:459:ILE:O	1:AAA:463:VAL:HG23	2.18	0.43
2:EEE:302:ILE:HG23	2:EEE:449:LEU:HB3	1.99	0.43
1:DDD:476:ALA:HB1	1:DDD:479:ASP:HB2	2.01	0.43
1:AAA:559:ARG:HG2	1:AAA:560:PRO:HD2	2.01	0.42
1:DDD:385:LYS:O	2:EEE:380:TYR:OH	2.34	0.42
1:DDD:697:ASP:HA	1:DDD:698:PRO:HD2	1.93	0.42
1:DDD:264:THR:N	1:DDD:265:PRO:CD	2.82	0.42
2:BBB:508[B]:GLU:OE2	2:BBB:508[B]:GLU:HA	2.20	0.42
1:DDD:322:ILE:HD13	1:DDD:331:ASN:HB3	2.02	0.42
2:EEE:507:MET:O	2:EEE:507:MET:HG3	2.20	0.42
2:BBB:219:ILE:O	2:BBB:223:THR:OG1	2.38	0.42
1:DDD:446:PHE:CZ	1:DDD:450:VAL:HG21	2.55	0.42
1:DDD:460:MET:HE1	1:DDD:488:LYS:O	2.19	0.42
1:AAA:450:VAL:HG11	1:AAA:585:LEU:HD23	2.02	0.42
1:DDD:214:LEU:HD11	2:EEE:218:LEU:HD21	2.01	0.42
2:EEE:24:TYR:CE2	2:EEE:233:ARG:HG3	2.54	0.42
1:AAA:446:PHE:CZ	1:AAA:450:VAL:HG21	2.54	0.41
2:BBB:149:VAL:HG11	2:BBB:181:ILE:HD13	2.02	0.41
2:EEE:519:GLU:OE2	2:EEE:664:HIS:ND1	2.54	0.41
2:EEE:219:ILE:O	2:EEE:223:THR:OG1	2.38	0.41
1:AAA:707:PHE:CE1	1:AAA:711:LEU:HD13	2.55	0.41
1:AAA:486:ILE:HA	1:AAA:499:ASN:O	2.21	0.41
2:EEE:592:SER:HB2	2:EEE:664:HIS:CE1	2.56	0.41
1:AAA:548:MET:CE	4:KKK:13:PRO:HG2	2.50	0.41
1:AAA:590:GLN:HE21	2:BBB:506[A]:SER:N	2.17	0.41
2:BBB:404:SER:N	2:BBB:405:PRO:HD2	2.36	0.41
2:BBB:519:GLU:OE2	2:BBB:664:HIS:ND1	2.54	0.41
1:DDD:322:ILE:HA	1:DDD:543:LEU:HD23	2.03	0.41
2:EEE:350:ARG:NH2	2:EEE:371:GLU:OE2	2.53	0.41
2:EEE:598:LEU:HD12	2:EEE:612:LYS:HG2	2.03	0.41
2:BBB:340:ALA:HB3	2:BBB:341:PRO:HD3	2.03	0.40
1:DDD:639:THR:HG22	2:EEE:3:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:404:SER:N	2:BBB:405:PRO:CD	2.84	0.40
2:EEE:310:ASN:O	2:EEE:407:MET:HB2	2.21	0.40
2:EEE:404:SER:N	2:EEE:405:PRO:CD	2.85	0.40
2:BBB:592:SER:HB2	2:BBB:664:HIS:CE1	2.56	0.40
1:AAA:445:TYR:O	1:AAA:448:ALA:HB3	2.22	0.40
1:DDD:648:SER:HA	2:EEE:26:GLY:HA3	2.03	0.40
1:DDD:486:ILE:HA	1:DDD:499:ASN:O	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 X-ray entries followed by that with respect to entries of similar resolution.

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	AAA	512/517 (99%)	477 (93%)	33 (6%)	2 (0%)	34 69
1	DDD	512/517 (99%)	479 (94%)	31 (6%)	2 (0%)	34 69
2	BBB	624/757 (82%)	571 (92%)	46 (7%)	7 (1%)	14 49
2	EEE	609/757 (80%)	560 (92%)	44 (7%)	5 (1%)	19 56
3	CCC	66/147 (45%)	65 (98%)	1 (2%)	0	100 100
3	FFF	69/147 (47%)	67 (97%)	1 (1%)	1 (1%)	11 43
4	JJJ	7/28 (25%)	4 (57%)	3 (43%)	0	100 100
4	KKK	8/28 (29%)	8 (100%)	0	0	100 100
All	All	2407/2898 (83%)	2231 (93%)	159 (7%)	17 (1%)	22 58

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	614	ASN
1	DDD	614	ASN
1	DDD	617	GLU

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Mol	Chain	Res	Type
3	FFF	107	SER
2	BBB	19	SER
2	BBB	409	MET
2	EEE	409	MET
2	EEE	19	SER
1	AAA	299	GLY
2	BBB	127	GLN
2	BBB	249	ARG
2	BBB	508[A]	GLU
2	BBB	508[B]	GLU
2	EEE	127	GLN
2	EEE	249	ARG
2	BBB	23	PRO
2	EEE	23	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 X-ray entries followed by that with respect to entries of similar resolution.

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	AAA	461/464 (99%)	448 (97%)	13 (3%)	43	73
1	DDD	461/464 (99%)	447 (97%)	14 (3%)	41	71
2	BBB	551/668 (82%)	531 (96%)	20 (4%)	35	66
2	EEE	538/668 (80%)	518 (96%)	20 (4%)	34	65
3	CCC	59/134 (44%)	58 (98%)	1 (2%)	60	82
3	FFF	61/134 (46%)	60 (98%)	1 (2%)	62	82
4	JJJ	9/24 (38%)	8 (89%)	1 (11%)	6	27
4	KKK	10/24 (42%)	8 (80%)	2 (20%)	1	5
All	All	2150/2580 (83%)	2078 (97%)	72 (3%)	37	69

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	342	LEU

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Mol	Chain	Res	Type
1	AAA	352	GLU
1	AAA	405	CYS
1	AAA	451	SER
1	AAA	460	MET
1	AAA	506	LYS
1	AAA	512	ARG
1	AAA	539	LYS
1	AAA	548	MET
1	AAA	566	ARG
1	AAA	611	PHE
1	AAA	666	LEU
1	AAA	675	ASN
2	BBB	19	SER
2	BBB	28	PRO
2	BBB	92	MET
2	BBB	115	GLN
2	BBB	116	GLN
2	BBB	227	MET
2	BBB	228	THR
2	BBB	276	ASN
2	BBB	277	GLU
2	BBB	281	LYS
2	BBB	297	GLU
2	BBB	350	ARG
2	BBB	411	MET
2	BBB	445	ASP
2	BBB	456	HIS
2	BBB	520	SER
2	BBB	546	MET
2	BBB	592	SER
2	BBB	660	VAL
2	BBB	667	ILE
3	CCC	76	THR
1	DDD	286	ASP
1	DDD	292	ILE
1	DDD	352	GLU
1	DDD	451	SER
1	DDD	460	MET
1	DDD	506	LYS
1	DDD	508	ARG
1	DDD	512	ARG
1	DDD	566	ARG

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Mol	Chain	Res	Type
1	DDD	595	MET
1	DDD	611	PHE
1	DDD	619	TRP
1	DDD	666	LEU
1	DDD	675	ASN
2	EEE	19	SER
2	EEE	59	THR
2	EEE	92	MET
2	EEE	116	GLN
2	EEE	227	MET
2	EEE	228	THR
2	EEE	276	ASN
2	EEE	297	GLU
2	EEE	350	ARG
2	EEE	411	MET
2	EEE	445	ASP
2	EEE	456	HIS
2	EEE	507	MET
2	EEE	520	SER
2	EEE	546	MET
2	EEE	582	GLN
2	EEE	592	SER
2	EEE	660	VAL
2	EEE	667	ILE
2	EEE	669	LYS
3	FFF	76	THR
4	JJJ	11	THR
4	KKK	11	THR
4	KKK	18	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	UUU	11/12 (91%)	5 (45%)	0
5	VVV	11/12 (91%)	5 (45%)	0
All	All	22/24 (91%)	10 (45%)	0

All (10) RNA backbone outliers are listed below:



Mol	Chain	Res	Type
5	UUU	6	U
5	UUU	7	A
5	UUU	8	A
5	UUU	11	A
5	UUU	12	G
5	VVV	6	U
5	VVV	7	A
5	VVV	8	A
5	VVV	11	A
5	VVV	12	G

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
4	SEP	KKK	12	4	8,9,10	0.59	0	8,12,14	0.67	0
4	SEP	JJJ	12	4	8,9,10	0.58	0	8,12,14	0.68	0

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
4	SEP	KKK	12	4	-	1/5/8/10	-
4	SEP	JJJ	12	4	-	2/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.



All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	KKK	12	SEP	N-CA-CB-OG
4	JJJ	12	SEP	N-CA-CB-OG
4	JJJ	12	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	AAA	514/517 (99%)	-0.17	8 (1%) 72 71	28, 58, 111, 149	0
1	DDD	514/517 (99%)	0.13	11 (2%) 63 63	59, 99, 130, 160	0
2	BBB	622/757 (82%)	0.20	24 (3%) 39 39	32, 88, 133, 167	0
2	EEE	615/757 (81%)	0.44	41 (6%) 17 20	47, 107, 146, 179	0
3	CCC	68/147 (46%)	1.02	14 (20%) 1 1	92, 125, 174, 178	0
3	FFF	71/147 (48%)	0.43	8 (11%) 5 7	58, 93, 146, 161	0
4	JJJ	9/28 (32%)	0.35	1 (11%) 5 7	88, 96, 121, 130	0
4	KKK	10/28 (35%)	-0.20	0 100 100	63, 71, 115, 121	0
5	UUU	12/12 (100%)	0.68	1 (8%) 11 14	112, 119, 131, 161	0
5	VVV	12/12 (100%)	0.27	1 (8%) 11 14	58, 78, 123, 152	0
All	All	2447/2922 (83%)	0.20	109 (4%) 33 33	28, 92, 137, 179	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	FFF	83	ASP	5.3
3	FFF	86	SER	4.7
3	FFF	82	ASN	4.6
3	FFF	84	ALA	4.4
3	CCC	85	GLY	4.4
1	AAA	379	VAL	4.3
2	EEE	156	THR	4.2
3	CCC	86	SER	4.2
3	CCC	83	ASP	4.0
2	EEE	398	ASP	4.0
5	UUU	12	G	3.9
2	EEE	292	ASN	3.8
1	DDD	390	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	BBB	150	PHE	3.7
3	CCC	59	ALA	3.7
5	VVV	12	G	3.7
3	CCC	84	ALA	3.7
2	EEE	291	THR	3.6
3	CCC	87	ASP	3.6
1	DDD	383	ASP	3.4
2	BBB	181	ILE	3.4
2	EEE	164	ILE	3.4
3	CCC	58	THR	3.4
2	BBB	146	THR	3.3
2	BBB	154	GLY	3.3
2	BBB	159	GLU	3.2
2	BBB	246	MET	3.2
2	BBB	211	ARG	3.2
1	AAA	382	GLU	3.2
3	FFF	87	ASP	3.2
1	DDD	556	GLN	3.2
2	BBB	274	GLY	3.2
4	JJJ	7	SER	3.1
2	EEE	296	THR	3.1
2	EEE	152	SER	3.1
2	EEE	437	TRP	3.1
2	EEE	293	SER	3.1
2	BBB	182	THR	3.0
2	EEE	399	GLY	3.0
2	EEE	151	ARG	2.9
1	AAA	383	ASP	2.9
2	EEE	367	GLN	2.9
2	BBB	152	SER	2.8
3	CCC	65	GLU	2.8
2	EEE	135	ARG	2.8
2	BBB	145	ASN	2.8
3	CCC	82	ASN	2.8
2	BBB	362	MET	2.8
2	EEE	137	GLN	2.8
2	EEE	397	ILE	2.8
1	AAA	380	ASP	2.7
3	CCC	60	ASP	2.7
3	CCC	63	ILE	2.7
1	AAA	390	LEU	2.7
3	CCC	88	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	EEE	400	THR	2.6
2	BBB	209	LYS	2.6
2	BBB	180	GLU	2.6
2	EEE	123	THR	2.6
2	BBB	179	MET	2.6
2	BBB	633	SER	2.6
3	FFF	108	THR	2.6
2	EEE	129	TYR	2.6
2	EEE	130	ASP	2.6
2	EEE	148	GLU	2.6
2	EEE	356	MET	2.5
1	AAA	381	PHE	2.5
2	EEE	290	MET	2.5
3	FFF	81	THR	2.5
2	EEE	389	ILE	2.5
2	BBB	148	GLU	2.5
1	DDD	382	GLU	2.5
2	EEE	298	LEU	2.4
2	EEE	133	LEU	2.4
2	EEE	358	GLU	2.4
2	EEE	141	THR	2.4
1	DDD	393	TYR	2.4
3	FFF	85	GLY	2.4
1	DDD	381	PHE	2.4
1	AAA	384	CYS	2.3
2	EEE	295	ASP	2.3
2	EEE	150	PHE	2.3
2	BBB	383	LYS	2.3
2	EEE	363	LYS	2.3
1	DDD	625	PRO	2.3
2	BBB	360	LYS	2.2
2	BBB	156	THR	2.2
2	EEE	115	GLN	2.2
2	EEE	157	ALA	2.2
2	BBB	359	SER	2.2
2	EEE	368	VAL	2.2
2	BBB	210	GLN	2.2
2	EEE	131	TRP	2.2
2	EEE	294	GLN	2.2
1	DDD	260	PHE	2.2
1	DDD	321	ASN	2.2
2	BBB	665	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	BBB	631	PHE	2.1
2	EEE	159	GLU	2.1
2	EEE	380	TYR	2.1
2	EEE	162	ARG	2.1
3	CCC	107	SER	2.1
3	CCC	64	MET	2.1
2	EEE	670	ARG	2.0
1	DDD	478	ASP	2.0
2	EEE	451	VAL	2.0
1	AAA	391	LYS	2.0
1	DDD	557	VAL	2.0
2	EEE	364	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SEP	JJJ	12	10/11	0.95	0.12	85,88,97,97	0
4	SEP	KKK	12	10/11	0.98	0.13	52,56,62,62	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	EEE	801	1/1	0.95	0.10	18,18,18,18	0
6	MG	BBB	801	1/1	0.97	0.25	19,19,19,19	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.