

Full wwPDB X-ray Structure Validation Report (i)

Jan 20, 2024 - 07:01 pm GMT

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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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	Similar resolution
	(#Entries)	(#Entries, resolution range(A))
R_{free}	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 >=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 <=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	2% 90%			9% •	1
1	DDD	517	2% 9 0%			9% •	il.
2	BBB	757	3% 	8%	•	18%	ł
2	EEE	757	5% 72%	8%	•	19%	1



Conti	nued fron	n previous	page					
Mol	Chain	Length			Qı	ality of	chain	
3	CCC	147	10%	4.49/			E 40/	
0	000	147	5%	44%		•	54%	
3	FFF	147	10/	46%		•	52%	
4	JJJ	28	329	%	•		64%	
4	KKK	28	29%		11%		61%	
5	UUU	12	8%				83%	
5	VVV	12	8%			75	%	8%

 $\overline{}$ 1 0



2 Entry composition (i)

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		At	oms			ZeroOcc	AltConf	Trace
1	AAA	514	Total 4133	C 2617	N 702	0 784	S 30	0	0	0
1	DDD	514	Total 4133	C 2617	N 702	0 784	S 30	0	0	0

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		At	oms			ZeroOcc	AltConf	Trace
2	BBB	622	Total 5010	C 3162	N 866	0 944	S 38	0	8	0
2	EEE	615	Total 4892	C 3088	N 847	0 921	S 36	0	0	0

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

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

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



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 $X5F4\overline{27}$

• 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 79	C 47	N 10	O 21	Р 1	0	0	0



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	KKK	11	Total 87	$\begin{array}{c} \mathrm{C} \\ 53 \end{array}$	N 11	O 22	Р 1	0	0	0

• 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	TITIT	19	Total	С	Ν	Ο	Р	0	0	0
5 00	000	12	262	117	52	81	12	0	0	0
F	WWW	12	Total	С	Ν	Ο	Р	0	0	0
Э	VVV		262	117	52	81	12	0		

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

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



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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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



TYR SER PRO THR SEP PRO PRO PRO S7 111	316 PRO PRO SER SER SER PRO PRO PRO PRO SER SER SER			
• Molecule 4:	SER-TYR-SER-P	RO-THR-SEP-I	PRO-SER-TYR-	SER
Chain KKK:	29%	11%	61%	
Y8 T11 S12 P13 F13 SEP PR0 SER	TYR SER PRO THR SEP SER SER PRO PRO SER SER			
• Molecule 5:	RNA $(5'-R(P*AP))$	*GP*UP*AP*C	P*UP*AP*AP*	CP*AP*AP*G)-3')
Chain UUU:	8%		83%	
A1 G2 U3 A7 A10 A11	6 13			
• Molecule 5:	RNA $(5'-R(P*AP))$	*GP*UP*AP*C	P*UP*AP*AP*	CP*AP*AP*G)-3')
Chain VVV:	8% 17%		5%	8%
A1 G2 G2 U6 A7 A1 C9 C9 C9 A11	612			



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	76.47Å 144.13Å 336.20Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution (Å)	49.21 - 3.41	Depositor
Resolution (A)	49.16 - 3.41	EDS
% Data completeness	73.2 (49.21-3.41)	Depositor
(in resolution range)	73.3(49.16-3.41)	EDS
R_{merge}	0.28	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.44 (at 3.40 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
B B.	0.220 , 0.273	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.221 , 0.269	DCC
R_{free} test set	1852 reflections $(4.88%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	73.0	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31 , 64.0	EDS
L-test for $twinning^2$	$ < L >=0.47, < L^2>=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 $(Å^2)$	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.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: SEP, MG

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).

Mal	Chain	Bo	nd lengths	Bond angles			
MOI	Unam	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		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
5	UUU	1	A	OP3-P	-7.42	1.52	1.61
5	VVV	1	А	OP3-P	-7.28	1.52	1.61

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	UUU	9	С	P-O3'-C3'	-6.75	111.61	119.70
5	VVV	9	С	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	А	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 (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	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	$\operatorname{contacts}$	within	the same	asymmetric	unit	are	listed	below,	sorted	$\mathbf{b}\mathbf{y}$	their	clash
magnitud	le.												

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	



Atom-1	Atom-2	Interatomic	Clash
	Atom-2	distance (Å)	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



Atom-1	Atom-2	Interatomic	Clash
	1100111-2	distance (Å)	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



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	Perce	entiles
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



Continuea from precious page							
Mol	Chain	\mathbf{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 (i)

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 side chain 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	\mathbf{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:

IVIOI	Unain	Res	Type
1	AAA	342	LEU



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



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 (i)

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	А
5	UUU	8	А
5	UUU	11	А
5	UUU	12	G
5	VVV	6	U
5	VVV	7	А
5	VVV	8	А
5	VVV	11	А
5	VVV	12	G

There are no RNA pucker outliers to report.

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

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).

Mal	Type	Chain	Dec	Tink	B	ond leng	gths	B	ond ang	gles
IVIOI	туре	Unain	nes		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.



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

All (3) torsion outliers are listed below:

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	$\langle RSRZ \rangle$	#RSRZ>2	$OWAB(Å^2)$	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	10 (1%) 66 66	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	108 (4%) 34 34	28, 92, 137, 179	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	FFF	83	ASP	5.3
3	FFF	86	SER	4.7
3	FFF	84	ALA	4.5
3	FFF	82	ASN	4.5
3	CCC	85	GLY	4.5
1	AAA	379	VAL	4.3
3	CCC	86	SER	4.2
2	EEE	156	THR	4.2
2	EEE	398	ASP	4.0
3	CCC	83	ASP	4.0
5	UUU	12	G	3.9
3	CCC	59	ALA	3.9
2	EEE	292	ASN	3.8



7Z4O

Mol	Chain Res 7		Type	RSRZ
5	VVV	12	G	3.7
1	DDD	390	LEU	3.7
2	BBB	150	PHE	3.7
3	CCC	84	ALA	3.6
3	CCC	87	ASP	3.6
2	EEE	291	THR	3.6
1	DDD	383	ASP	3.5
2	BBB	181	ILE	3.4
2	BBB	154	GLY	3.4
2	EEE	164	ILE	3.3
3	CCC	58	THR	3.3
2	BBB	146	THR	3.3
1	AAA	382	GLU	3.3
3	FFF	87	ASP	3.2
2	BBB	246	MET	3.2
2	BBB	211	ARG	3.2
2	BBB	159	GLU	3.1
2	EEE	437	TRP	3.1
2	EEE	296	THR	3.1
1	DDD	556	GLN	3.1
4	JJJ	7	SER	3.1
2	EEE	152	SER	3.1
2	BBB	274	GLY	3.1
2	EEE	293	SER	3.0
2	EEE	399	GLY	3.0
2	BBB	182	THR	3.0
2	EEE	151	ARG	3.0
1	AAA	383	ASP	3.0
2	EEE	367	GLN	2.9
2	BBB	152	SER	2.9
2	BBB	145	ASN	2.8
3	CCC	65	GLU	2.8
2	EEE	135	ARG	2.8
2	EEE	397	ILE	2.8
3	CCC	60	ASP	2.8
3	CCC	82	ASN	2.8
2	BBB	362	MET	2.8
2	EEE	137	GLN	2.7
1	AAA	390	LEU	2.7
1	AAA	380	ASP	2.7
3	CCC	88	ARG	2.7
3	CCC	63	ILE	2.7



Mol	Chain	Res	Type	RSRZ
2	BBB	179	MET	2.7
2	EEE	400	THR	2.6
2	BBB	209	LYS	2.6
2	BBB	180	GLU	2.6
3	FFF	81	THR	2.6
2	EEE	356	MET	2.6
2	BBB	633	SER	2.6
2	EEE	129	TYR	2.5
1	AAA	381	PHE	2.5
2	EEE	290	MET	2.5
3	FFF	108	THR	2.5
2	EEE	389	ILE	2.5
2	EEE	148	GLU	2.5
1	DDD	382	GLU	2.5
2	EEE	130	ASP	2.5
2	EEE	123	THR	2.5
2	BBB	148	GLU	2.5
2	EEE	141	THR	2.5
1	DDD	393	TYR	2.5
2	EEE	133	LEU	2.4
2	EEE	298	LEU	2.4
2	EEE	358	GLU	2.4
1	DDD	625	PRO	2.4
2	BBB	383	LYS	2.3
3	FFF	85	GLY	2.3
1	DDD	381	PHE	2.3
1	AAA	384	CYS	2.3
2	EEE	150	PHE	2.3
2	EEE	363	LYS	2.3
2	EEE	295	ASP	2.3
2	EEE	368	VAL	2.3
2	EEE	115	GLN	2.2
2	BBB	360	LYS	2.2
2	BBB	156	THR	2.2
1	DDD	260	PHE	2.2
2	EEE	157	ALA	2.2
2	EEE	131	TRP	2.2
2	BBB	210	GLN	2.2
2	BBB	359	SER	2.2
2	BBB	665	SER	2.2
2	EEE	159	GLU	2.1
3	CCC	107	SER	2.1



Mol	Chain	Res	Type	RSRZ
2	EEE	380	TYR	2.1
1	DDD	321	ASN	2.1
2	EEE	294	GLN	2.1
2	BBB	631	PHE	2.1
2	EEE	162	ARG	2.1
2	EEE	670	ARG	2.1
3	CCC	64	MET	2.1
2	EEE	451	VAL	2.0
1	AAA	391	LYS	2.0
1	DDD	478	ASP	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^{th} 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	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	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^{th} 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	$B-factors(Å^2)$	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.

