

Full wwPDB X-ray Structure Validation Report (i)

Jul 19, 2021 - 09:03 am BST

:	7OM6
:	Thosea asigna virus RdRP domain in complex with RNA
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:	2021-05-21
:	2.18 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as 541 be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.22
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)	:	2.22

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.18 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		
	$(\# \mathbf{Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	6864 (2.20-2.16)		
Clashscore	141614	7689 (2.20-2.16)		
Ramachandran outliers	138981	7564 (2.20-2.16)		
Sidechain outliers	138945	7564 (2.20-2.16)		
RSRZ outliers	127900	6738 (2.20-2.16)		
RNA backbone	3102	1052 (2.60-1.76)		

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	А	684	83%	9% 8%
1	В	684	3%	8% 7%
2	С	8	75%	25%
2	D	8	62% 12%	25%



Mol	Chain	\mathbf{Length}	Quality of chain	
			12%	
2	E	8	75%	12% 12%
2	F	8	75%	25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	В	701	-	-	Х	-



70M6

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11170 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	630	Total 4991	C 3164	N 865	O 936	S 26	0	0	0
1	В	634	Total 5022	C 3184	N 870	0 942	S 26	0	0	0

• Molecule 1 is a protein called RNA-dependent RNA polymerase.

Residue	Modelled	Actual	$\mathbf{Comment}$	Reference
-12	MET	-	initiating methionine	UNP Q6A562
-11	GLY	-	expression tag	UNP Q6A562
-10	SER	-	expression tag	UNP Q6A562
-9	SER	-	expression tag	UNP Q6A562
-8	HIS	-	expression tag	UNP Q6A562
-7	HIS	-	expression tag	UNP Q6A562
-6	HIS	-	expression tag	UNP Q6A562
-5	HIS	-	expression tag	UNP Q6A562
-4	HIS	-	expression tag	UNP Q6A562
-3	HIS	-	expression tag	UNP Q6A562
-2	SER	-	expression tag	UNP Q6A562
-1	GLN	-	expression tag	UNP Q6A562
0	ASP	-	expression tag	UNP Q6A562
1	LEU	-	expression tag	UNP Q6A562
2	GLU	-	expression tag	UNP Q6A562
3	ASN	-	expression tag	UNP Q6A562
4	LEU	-	expression tag	UNP Q6A562
5	TYR	-	expression tag	UNP Q6A562
6	PHE	-	expression tag	UNP Q6A562
7	GLN	-	expression tag	UNP Q6A562
8	GLY	-	expression tag	UNP Q6A562
9	GLY	-	expression tag	UNP Q6A562
10	SER	-	expression tag	UNP Q6A562
-12	MET	-	initiating methionine	UNP Q6A562
-11	GLY	-	expression tag	UNP Q6A562
	Residue -12 -11 -10 -9 -8 -7 -6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6 7 8 9 10 -12 -11	Residue Modelled -12 MET -11 GLY -10 SER -9 SER -9 SER -8 HIS -7 HIS -6 HIS -5 HIS -4 HIS -3 HIS -1 GLN 0 ASP 1 LEU 2 GLU 3 ASN 4 LEU 5 TYR 6 PHE 7 GLN 8 GLY 9 GLY 10 SER -12 MET -11 GLY	Residue Modelled Actual -12 MET - -11 GLY - -10 SER - -9 SER - -9 SER - -8 HIS - -7 HIS - -6 HIS - -5 HIS - -4 HIS - -3 HIS - -4 HIS - -3 HIS - -1 GLN - 0 ASP - 1 LEU - 2 GLU - 3 ASN - 4 LEU - 5 TYR - 6 PHE - 7 GLN - 8 GLY - 9 GLY - <tr tbl=""> 10 SER<td>ResidueModelledActualComment-12MET-initiating methionine-11GLY-expression tag-10SER-expression tag-9SER-expression tag-8HIS-expression tag-7HIS-expression tag-6HIS-expression tag-5HIS-expression tag-3HIS-expression tag-3HIS-expression tag-3HIS-expression tag-1GLN-expression tag1LEU-expression tag3ASP-expression tag3ASN-expression tag3GLU-expression tag5TYR-expression tag6PHE-expression tag7GLN-expression tag7GLN-expression tag10SER-expression tag9GLY-expression tag10SER-expression tag-11GLY-expression tag-11GLY-expression tag</td></tr>	ResidueModelledActualComment-12MET-initiating methionine-11GLY-expression tag-10SER-expression tag-9SER-expression tag-8HIS-expression tag-7HIS-expression tag-6HIS-expression tag-5HIS-expression tag-3HIS-expression tag-3HIS-expression tag-3HIS-expression tag-1GLN-expression tag1LEU-expression tag3ASP-expression tag3ASN-expression tag3GLU-expression tag5TYR-expression tag6PHE-expression tag7GLN-expression tag7GLN-expression tag10SER-expression tag9GLY-expression tag10SER-expression tag-11GLY-expression tag-11GLY-expression tag
ResidueModelledActualComment-12MET-initiating methionine-11GLY-expression tag-10SER-expression tag-9SER-expression tag-8HIS-expression tag-7HIS-expression tag-6HIS-expression tag-5HIS-expression tag-3HIS-expression tag-3HIS-expression tag-3HIS-expression tag-1GLN-expression tag1LEU-expression tag3ASP-expression tag3ASN-expression tag3GLU-expression tag5TYR-expression tag6PHE-expression tag7GLN-expression tag7GLN-expression tag10SER-expression tag9GLY-expression tag10SER-expression tag-11GLY-expression tag-11GLY-expression tag				

There are 46 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual Comment		Reference
В	-10	SER	-	expression tag	UNP Q6A562
В	-9	SER	-	expression tag	UNP Q6A562
В	-8	HIS	-	expression tag	UNP Q6A562
В	-7	HIS	-	expression tag	UNP Q6A562
В	-6	HIS	-	expression tag	UNP Q6A562
В	-5	HIS	-	expression tag	UNP Q6A562
В	-4	HIS	-	expression tag	UNP Q6A562
В	-3	HIS	-	expression tag	UNP Q6A562
В	-2	SER	-	expression tag	UNP Q6A562
В	-1	GLN	-	expression tag	UNP Q6A562
В	0	ASP	-	expression tag	UNP Q6A562
В	1	LEU	-	expression tag	UNP Q6A562
В	2	GLU	-	expression tag	UNP Q6A562
В	3	ASN	-	expression tag	UNP Q6A562
В	4	LEU	-	expression tag	UNP Q6A562
В	5	TYR	-	expression tag	UNP Q6A562
В	6	PHE	-	expression tag	UNP Q6A562
В	7	GLN	-	expression tag	UNP Q6A562
В	8	GLY	-	expression tag	UNP Q6A562
В	9	GLY	-	expression tag	UNP Q6A562
В	10	SER	-	expression tag	UNP Q6A562

• Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	С	Ν	Ο	Р	0	0	0
	U	0	126	57	21	42	6	0	0	0
2	П	6	Total	С	Ν	Ο	Р	0	0	0
		0	126	57	21	42	6	0		
0	F	8	Total	С	Ν	Ο	Р	0	0	0
	2 E		168	76	29	55	8	0	0	
0	2 F	8	Total	С	Ν	Ο	Р	0	0	0
			168	76	29	55	8			U

• Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
3	В	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	191	Total O 191 191	0	0
4	В	309	Total O 309 309	0	0
4	С	12	Total O 12 12	0	0
4	D	10	Total O 10 10	0	0
4	Е	22	TotalO2222	0	0
4	F	11	Total O 11 11	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: RNA-dependent RNA polymerase





• Molecule	2: RNA $(5'-R(P*AP*AP*AP*UP*UP*U)-3')$		
Chain C:	75%	2!	5%
C ¥ <mark>¥</mark> ₽ C			
• Molecule	2: RNA $(5'-R(P*AP*AP*AP*UP*UP*U)-3')$		
Chain D:	62% 12%	25	%
C A U U B B B B B B B B B B B B B B B B B			
• Molecule	2: RNA $(5'-R(P*AP*AP*AP*UP*UP*U)-3')$		
Chain E:	75%	12%	12%
C1 A4 U8			
• Molecule	2: RNA $(5'-R(P*AP*AP*AP*UP*UP*U)-3')$		
Chain F:	75%	25	5%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	65.64Å 204.03Å 70.08Å	Depositor
a, b, c, α , β , γ	90.00° 97.19° 90.00°	Depositor
$Bosolution(\AA)$	49.30 - 2.18	Depositor
Resolution (A)	49.30 - 2.18	EDS
% Data completeness	99.0(49.30-2.18)	Depositor
(in resolution range)	99.1 (49.30 - 2.18)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.88 (at 2.18 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
D D.	0.229 , 0.241	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.227 , 0.239	DCC
R_{free} test set	4526 reflections $(4.81%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	41.1	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.32 , 35.7	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11170	wwPDB-VP
Average B, all atoms $(Å^2)$	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.07% 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.



 $^{^1 {\}rm Intensities}$ 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: PEG

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	Bond lengths		Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.57	0/5099	0.76	0/6902	
1	В	0.57	0/5130	0.76	0/6943	
2	С	0.21	0/140	0.68	0/215	
2	D	0.44	0/140	0.69	0/215	
2	Е	0.47	0/187	0.85	1/288~(0.3%)	
2	F	0.31	0/187	0.70	0/288	
All	All	0.56	0/10883	0.76	1/14851~(0.0%)	

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Ε	1	С	N1-C1'-C2'	6.26	122.14	114.00

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	4991	0	4948	73	0
1	В	5022	0	4982	62	0
2	С	126	0	64	0	0
2	D	126	0	64	1	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Ε	168	0	86	1	0
2	F	168	0	86	1	0
3	А	7	0	10	0	0
3	В	7	0	10	5	0
4	А	191	0	0	1	1
4	В	309	0	0	2	1
4	С	12	0	0	0	0
4	D	10	0	0	0	0
4	Е	22	0	0	0	0
4	F	11	0	0	1	0
All	All	11170	0	10250	125	1

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 (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:278:LYS:NZ	3:B:701:PEG:H21	1.66	1.07	
1:A:351:ASP:HA	1:A:373:MET:HE1	1.32	1.06	
1:B:577:GLU:OE1	1:B:580:ARG:NH2	1.91	1.04	
1:A:370:PHE:HD2	1:A:373:MET:HE2	1.24	1.01	
1:B:370:PHE:CE1	1:B:487:ILE:HD13	1.99	0.96	
1:A:370:PHE:CD2	1:A:373:MET:HE2	1.99	0.96	
1:A:370:PHE:HD2	1:A:373:MET:CE	1.80	0.94	
1:A:351:ASP:HA	1:A:373:MET:CE	1.99	0.93	
1:B:278:LYS:HZ1	3:B:701:PEG:H21	1.29	0.91	
1:B:370:PHE:CE1	1:B:487:ILE:CD1	2.57	0.87	
1:A:370:PHE:CE1	1:A:487:ILE:HD13	2.13	0.82	
1:B:87:GLU:HB2	1:B:431:MET:SD	2.20	0.81	
1:A:668:ARG:CG	1:B:399:THR:HG22	2.11	0.80	
1:A:370:PHE:CE1	1:A:487:ILE:CD1	2.63	0.80	
1:B:366:ILE:HG22	1:B:368:PRO:HG3	1.65	0.79	
1:B:278:LYS:HZ2	3:B:701:PEG:H21	1.46	0.78	
1:A:668:ARG:HG2	1:B:399:THR:HG22	1.65	0.76	
1:A:370:PHE:CD1	1:A:487:ILE:HD13	2.23	0.74	
1:A:370:PHE:HE1	1:A:487:ILE:CD1	2.00	0.73	
1:A:668:ARG:HD3	1:B:399:THR:HG21	1.69	0.73	
1:A:366:ILE:HG22	1:A:368:PRO:HG3	1.71	0.73	
1:A:370:PHE:HB2	1:A:373:MET:HE3	1.70	0.72	
1:B:370:PHE:CD1	1:B:487:ILE:HD13	2.25	0.71	



	Interatomic Clash								
Atom-1	Atom-2	distance (Å)	overlap (Å)						
1:A:370:PHE:HE1	1:A:487:ILE:HD11	1.56	0.71						
1:B:577:GLU:OE2	4:B:801:HOH:O	2.08	0.70						
1:A:366:ILE:CG2	1:A:368:PRO:HG3	2.22	0.68						
1:B:366:ILE:CG2	1:B:368:PRO:HG3	2.23	0.68						
1:B:370:PHE:HE1	1:B:487:ILE:CD1	2.05	0.66						
2:F:7:U:OP1	4:F:102:HOH:O	2.13	0.66						
1:B:366:ILE:HD11	1:B:494:PRO:HG3	1.78	0.64						
1:A:370:PHE:CD2	1:A:373:MET:CE	2.68	0.64						
1:A:668:ARG:HB3	1:B:399:THR:HG22	1.80	0.63						
1:A:370:PHE:HB2	1:A:373:MET:CE	2.28	0.63						
1:B:373:MET:CE	1:B:447:ASP:O	2.46	0.63						
1:A:668:ARG:CB	1:B:399:THR:HG22	2.30	0.61						
1:B:373:MET:CE	1:B:451:SER:HB2	2.31	0.61						
1:B:370:PHE:CE1	1:B:487:ILE:HD11	2.36	0.60						
1:A:668:ARG:CD	1:B:399:THR:HG21	2.31	0.60						
1:A:366:ILE:HD11	1:A:494:PRO:HG3	1.85	0.59						
1:A:477:GLU:HG3	1:A:481:ASN:ND2	2.17	0.58						
1:A:519:VAL:CG1	1:A:526:LYS:HB3	2.34	0.58						
1:A:477:GLU:CG	1:A:481:ASN:ND2	2.67	0.57						
1:A:351:ASP:CB	1:A:373:MET:HE3	2.35	0.56						
1:A:106:PRO:HB2	1:A:109:THR:CG2	2.35	0.56						
1:B:373:MET:HE1	1:B:447:ASP:O	2.05	0.56						
1:A:477:GLU:HG3	1:A:481:ASN:HD21	1.71	0.55						
1:B:13:LEU:HD23	1:B:18:MET:HG3	1.89	0.55						
1:A:351:ASP:CA	1:A:373:MET:CE	2.79	0.54						
1:B:366:ILE:CD1	1:B:494:PRO:HG3	2.38	0.54						
1:A:366:ILE:HG22	1:A:368:PRO:CG	2.37	0.54						
1:B:366:ILE:HG22	1:B:368:PRO:CG	2.37	0.54						
1:A:368:PRO:HA	1:A:491:THR:HB	1.89	0.54						
1:B:351:ASP:HA	1:B:373:MET:SD	2.48	0.54						
1:A:370:PHE:CE1	1:A:487:ILE:HD11	2.37	0.54						
1:A:668:ARG:HD3	1:B:399:THR:CG2	2.37	0.53						
1:A:106:PRO:HB2	1:A:109:THR:HG22	1.90	0.53						
1:B:373:MET:HE3	1:B:451:SER:HB2	1.91	0.52						
1:A:477:GLU:HG2	1:A:481:ASN:HD22	1.73	0.52						
1:A:54:ARG:HG2	1:A:58:GLN:HE21	1.74	0.52						
1:A:668:ARG:CD	1:B:399:THR:CG2	2.88	0.52						
1:B:472:GLU:HG3	1:B:492:TRP:HB3	1.91	0.52						
1:A:477:GLU:HG2	4:A:876:HOH:O	2.09	0.51						
1:B:373:MET:HE2	1:B:447:ASP:O	2.10	0.51						
1:A:116:VAL:HG21	1:A:257:GLU:HG3	1.92	0.51						



	to as pagen	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:205:VAL:O	1:A:208:ILE:HG13	2.11	0.51
1:A:519:VAL:HG13	1:A:526:LYS:HB3	1.93	0.51
1:B:143:LEU:HA	1:B:146:GLU:OE2	2.10	0.50
1:B:205:VAL:O	1:B:208:ILE:HG13	2.11	0.50
1:B:370:PHE:HE1	1:B:487:ILE:HD11	1.71	0.50
1:B:332:TRP:O	1:B:335:GLN:HG2	2.11	0.50
1:A:668:ARG:CG	1:B:399:THR:CG2	2.86	0.49
1:B:391:ASP:HA	1:B:394:VAL:HG22	1.93	0.49
1:B:98:LEU:HD23	1:B:103:PRO:HA	1.95	0.49
1:B:87:GLU:CB	1:B:431:MET:SD	2.97	0.49
1:B:373:MET:HE1	1:B:451:SER:HB2	1.93	0.49
1:B:278:LYS:HZ2	3:B:701:PEG:C2	2.23	0.49
1:A:532:LEU:HB2	1:A:537:TRP:CE2	2.48	0.49
1:A:106:PRO:O	1:A:109:THR:HG22	2.14	0.48
1:B:355:ILE:HD11	1:B:455:TYR:CE1	2.48	0.48
1:B:55:GLU:HA	1:B:58:GLN:HE21	1.79	0.47
1:B:371:LYS:HG3	3:B:701:PEG:H12	1.97	0.47
1:A:218:PRO:HG3	1:A:221:TRP:CZ2	2.49	0.47
1:A:320:SER:O	1:A:325:GLY:HA3	2.15	0.47
1:A:351:ASP:CB	1:A:373:MET:CE	2.93	0.46
1:A:391:ASP:HA	1:A:394:VAL:HG22	1.97	0.46
1:A:351:ASP:HB3	1:A:373:MET:HE3	1.97	0.46
1:A:650:PHE:HB2	1:A:653:ALA:HB2	1.97	0.45
1:A:571:THR:HG21	2:D:6:U:H4'	1.99	0.45
1:A:197:VAL:HG21	1:A:393:HIS:HB3	1.99	0.44
1:A:515:LEU:HD22	1:A:530:PRO:HB2	1.99	0.44
1:A:218:PRO:HA	1:A:219:PRO:HA	1.80	0.43
1:B:116:VAL:HG21	1:B:257:GLU:HG3	2.00	0.43
1:B:366:ILE:CG1	1:B:494:PRO:HG3	2.47	0.43
1:A:68:LEU:HD11	1:A:272:VAL:HG21	2.00	0.43
1:B:345:ARG:HD3	1:B:345:ARG:HA	1.83	0.43
1:B:395:LYS:HD3	1:B:395:LYS:HA	1.83	0.43
1:B:532:LEU:HB2	1:B:537:TRP:CE2	2.53	0.43
1:A:506:LEU:HD23	1:A:518:LYS:HB2	2.00	0.43
1:A:69:LYS:HE3	1:A:69:LYS:HB3	1.88	0.43
1:B:218:PRO:HG3	1:B:221:TRP:CZ2	2.53	0.43
1:B:320:SER:O	1:B:325:GLY:HA3	2.19	0.43
2:E:1:C:H2'	2:E:1:C:O2	2.19	0.43
1:A:366:ILE:HD13	1:A:492:TRP:CE2	2.54	0.42
1:B:30:LEU:HD21	1:B:555:THR:HG21	2.01	0.42
1:A:366:ILE:CD1	1:A:494:PRO:HG3	2.48	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:A:13:LEU:HD23	1:A:18:MET:HG3	2.00	0.42
1:A:668:ARG:HG2	1:B:399:THR:CG2	2.43	0.42
1:A:366:ILE:HG22	1:A:368:PRO:CD	2.49	0.42
1:B:374:ASP:HB3	4:B:876:HOH:O	2.20	0.42
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.90	0.42
1:B:366:ILE:HD13	1:B:492:TRP:CE2	2.54	0.42
1:B:559:ARG:HH22	1:B:625:SER:HB3	1.85	0.42
1:A:68:LEU:HD12	1:A:68:LEU:HA	1.92	0.41
1:A:206:LEU:HA	1:B:15:LEU:HB2	2.01	0.41
1:A:106:PRO:HB2	1:A:109:THR:HG21	2.02	0.41
1:A:668:ARG:HB3	1:B:399:THR:CG2	2.47	0.41
1:B:574:VAL:HG21	1:B:631:TYR:HA	2.01	0.41
1:A:477:GLU:HG2	1:A:481:ASN:ND2	2.32	0.41
1:A:174:VAL:HG11	1:A:482:LYS:O	2.21	0.41
1:B:164:ARG:NH2	1:B:278:LYS:HE3	2.36	0.41
1:A:56:SER:O	1:A:60:GLN:HG3	2.21	0.40
1:A:345:ARG:HD3	1:A:345:ARG:HA	1.94	0.40
1:A:366:ILE:HG22	1:A:368:PRO:HD3	2.02	0.40
1:A:370:PHE:HD2	1:A:373:MET:HE1	1.78	0.40
1:B:143:LEU:O	1:B:146:GLU:HG2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1 Atom-2		Interatomic distance (Å)	Clash overlap (Å)
4:A:984:HOH:O	4:B:1072:HOH:O[1_556]	2.13	0.07

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	Percen	tiles
1	А	622/684~(91%)	612~(98%)	10~(2%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}
1	В	626/684~(92%)	616~(98%)	10~(2%)	0	100	100
All	All	1248/1368~(91%)	1228 (98%)	20~(2%)	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 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	А	537/581~(92%)	528~(98%)	9 (2%)	60 72
1	В	540/581~(93%)	536~(99%)	4 (1%)	84 91
All	All	1077/1162~(93%)	1064 (99%)	13 (1%)	71 81

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	52	CYS
1	А	192	GLN
1	А	222	ARG
1	А	287	PHE
1	А	307	MET
1	А	387	ASP
1	А	473	LYS
1	А	518	LYS
1	А	577	GLU
1	В	222	ARG
1	В	307	MET
1	В	349	TYR
1	В	670	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	58	GLN
1	А	110	HIS
1	А	481	ASN
1	А	600	GLN
1	А	663	GLN
1	В	58	GLN
1	В	81	GLN
1	В	175	GLN
1	В	335	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	С	5/8~(62%)	0	0
2	D	5/8~(62%)	0	0
2	Е	7/8~(87%)	1 (14%)	0
2	F	7/8~(87%)	1 (14%)	0
All	All	24/32~(75%)	2 (8%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	Ε	4	А
2	F	4	А

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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 Tru	Tune	e Chain Bes		Tink	Link Bond lengths			Bond angles		
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	PEG	А	701	-	6,6,6	0.08	0	$5,\!5,\!5$	0.14	0
3	PEG	В	701	-	6,6,6	0.10	0	$5,\!5,\!5$	0.09	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
3	PEG	А	701	-	-	3/4/4/4	-
3	PEG	В	701	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	701	PEG	O1-C1-C2-O2
3	В	701	PEG	O1-C1-C2-O2
3	В	701	PEG	O2-C3-C4-O4
3	А	701	PEG	O2-C3-C4-O4
3	В	701	PEG	C4-C3-O2-C2
3	А	701	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	PEG	5	0

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, 95^{th} 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	А	630/684~(92%)	0.83	47 (7%) 14 15	29, 52, 81, 112	0
1	В	634/684~(92%)	0.46	19 (2%) 50 51	24, 44, 70, 94	0
2	С	6/8~(75%)	-0.54	0 100 100	32, 34, 42, 66	0
2	D	6/8~(75%)	-0.47	0 100 100	42, 46, 56, 87	0
2	Ε	8/8~(100%)	-0.42	1 (12%) 3 4	37, 41, 60, 94	0
2	F	8/8 (100%)	-0.37	0 100 100	43, 51, 69, 116	0
All	All	1292/1400~(92%)	0.62	67 (5%) 27 28	24, 48, 77, 116	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	126	VAL	8.6
1	А	462	LEU	6.4
1	В	671	ILE	5.2
1	А	11	THR	4.3
1	А	373	MET	4.3
1	А	341	LYS	4.1
1	А	467	LEU	4.1
1	А	72	VAL	3.9
1	А	363	LEU	3.8
1	В	464	PHE	3.8
1	А	337	GLY	3.6
1	А	119	LYS	3.3
1	А	13	LEU	3.3
1	А	464	PHE	3.2
1	А	123	ALA	3.2
1	В	547	LYS	3.1
1	А	445	LEU	3.1
1	A	340	GLY	3.0
1	В	602	GLY	3.0



Mol	Chain	Res	Type	RSRZ	
1	А	477	GLU	3.0	
1	А	104	VAL	3.0	
1	В	373	MET	2.9	
1	А	124	ALA	2.8	
1	А	62	ARG	2.8	
1	А	113	ASN	2.8	
1	А	343	PRO	2.8	
1	А	356	TYR	2.7	
1	А	234	CYS	2.7	
1	В	577	GLU	2.7	
1	В	26	ALA	2.7	
1	А	342	LYS	2.6	
1	В	556	MET	2.6	
1	А	513	LEU	2.5	
1	В	126	VAL	2.5	
1	А	474	TYR	2.5	
1	А	275	LEU	2.4	
1	А	360	ASP	2.4	
1	В	238	LEU	2.4	
1	А	106	PRO	2.4	
1	В	601	GLU	2.4	
1	В	24	MET	2.3	
1	В	552	GLU	2.3	
1	А	502	GLY	2.3	
1	А	489	GLU	2.3	
1	А	442	GLY	2.3	
1	А	241	ASP	2.2	
1	В	670	VAL	2.2	
1	А	556	MET	2.2	
1	А	515	LEU	2.2	
1	A	181	LYS	2.2	
1	A	415	ALA	2.2	
1	В	11	THR	2.2	
1	A	334	ARG	2.2	
1	В	203	GLU	2.1	
1	A	466	SER	2.1	
1	В	431	MET	2.1	
1	В	23	ALA	2.1	
2	E	1	C	2.1	
1	А	111	ASN	2.1	
1	В	669	VAL	2.1	
1	А	362	LYS	2.0	



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Mol	Chain	Res	Type	RSRZ
1	А	490	GLY	2.0
1	А	524	ASN	2.0
1	А	443	THR	2.0
1	А	465	GLY	2.0
1	А	52	CYS	2.0
1	А	339	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	$\mathbf{B} extsf{-}\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	Q<0.9
3	PEG	А	701	7/7	0.70	0.27	$69,\!72,\!76,\!76$	0
3	PEG	В	701	7/7	0.90	0.26	$62,\!65,\!67,\!68$	0

6.5 Other polymers (i)

There are no such residues in this entry.

