



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:55 AM UTC

PDB ID : 2EC0 / pdb\_00002ec0  
Title : RNA-dependent RNA polymerase of foot-and-mouth disease virus in complex with a template-primer RNA and ATP  
Authors : Ferrer-Orta, C.; Arias, A.; Perez-Luque, R.; Escarmis, C.; Domingo, E.; Verdaguier, N.  
Deposited on : 2007-02-09  
Resolution : 2.75 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

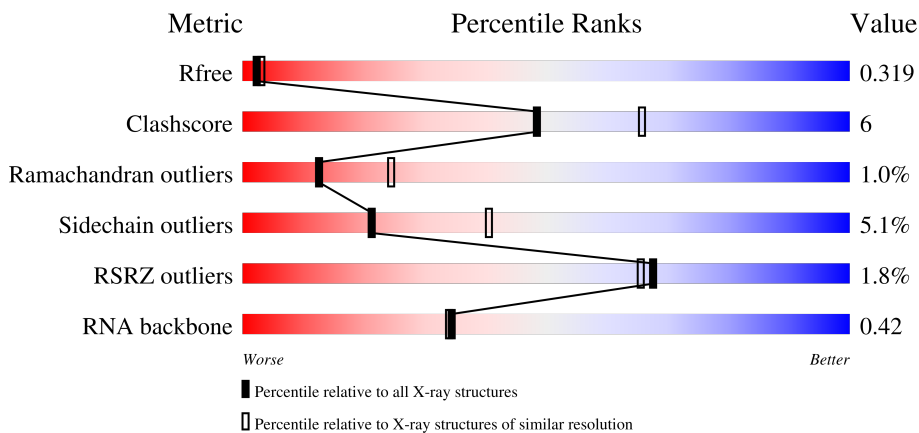
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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.



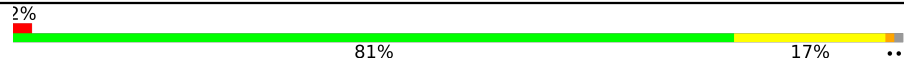

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)
RNA backbone	3983	1179 (3.00-2.52)

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	B	8	 25% 50% 25%
1	E	8	 25% 38% 25% 12%
2	C	7	 43% 57%
2	F	7	 57% 43%

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Mol	Chain	Length	Quality of chain
3	A	476	 2% 81% 17% ..
3	D	476	 2% 84% 14% ..

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8200 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 RNA chain called 5'-R(P\*AP\*UP\*GP\*GP\*GP\*CP\*CP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	8	Total 171	C 76	N 31	O 56	P 8	0	0	0
1	E	8	Total 171	C 76	N 31	O 56	P 8	0	0	0

- Molecule 2 is a RNA chain called 5'-R(\*GP\*GP\*GP\*CP\*CP\*CP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	7	Total 148	C 67	N 29	O 46	P 6	0	0	0
2	F	7	Total 148	C 67	N 29	O 46	P 6	0	0	0

- Molecule 3 is a protein called RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	470	Total 3714	C 2361	N 643	O 689	S 21	0	0	0
3	D	470	Total 3714	C 2361	N 643	O 689	S 21	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	471	ALA	-	cloning artifact	UNP Q0QEE1
A	472	ALA	-	cloning artifact	UNP Q0QEE1
A	473	LEU	-	cloning artifact	UNP Q0QEE1
A	474	GLU	-	cloning artifact	UNP Q0QEE1
A	475	HIS	-	cloning artifact	UNP Q0QEE1
A	476	HIS	-	cloning artifact	UNP Q0QEE1
D	471	ALA	-	cloning artifact	UNP Q0QEE1
D	472	ALA	-	cloning artifact	UNP Q0QEE1

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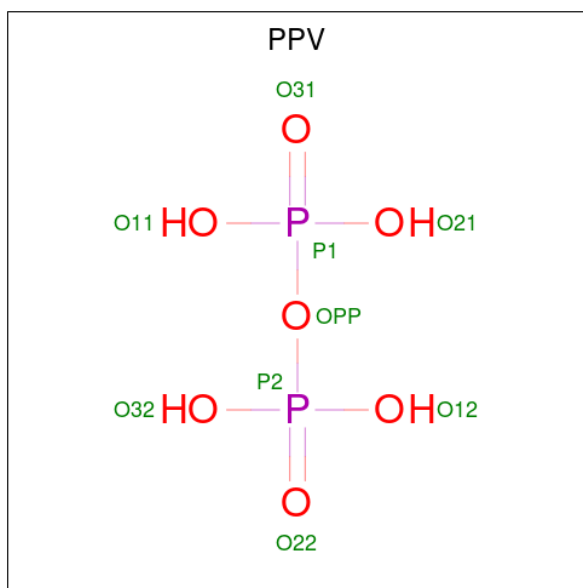
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Chain	Residue	Modelled	Actual	Comment	Reference
D	473	LEU	-	cloning artifact	UNP Q0QEE1
D	474	GLU	-	cloning artifact	UNP Q0QEE1
D	475	HIS	-	cloning artifact	UNP Q0QEE1
D	476	HIS	-	cloning artifact	UNP Q0QEE1

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is PYROPHOSPHATE (CCD ID: PPV) (formula: H<sub>4</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 9 7 2	0	0
5	D	1	Total O P 9 7 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	3	Total O 3 3	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
6	C	2	Total O 2 2	0	0
6	E	4	Total O 4 4	0	0
6	F	1	Total O 1 1	0	0
6	A	49	Total O 49 49	0	0
6	D	55	Total O 55 55	0	0

### 3 Residue-property plots


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.

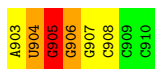
- Molecule 1: 5'-R(P\*AP\*UP\*GP\*GP\*GP\*CP\*CP\*C)-3'

Chain B: 



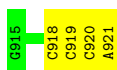
- Molecule 1: 5'-R(P\*AP\*UP\*GP\*GP\*GP\*CP\*CP\*C)-3'

Chain E: 



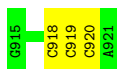
- Molecule 2: 5'-R(\*GP\*GP\*GP\*CP\*CP\*CP\*A)-3'

Chain C: 




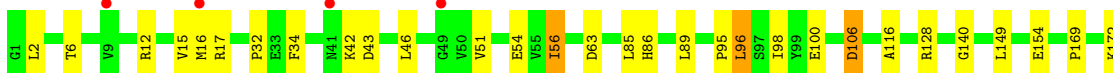
- Molecule 2: 5'-R(\*GP\*GP\*GP\*CP\*CP\*CP\*A)-3'

Chain F: 



- Molecule 3: RNA-dependent RNA polymerase

Chain A: 





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.66Å 95.66Å 201.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.75 20.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	85.5 (20.00-2.75) 99.7 (20.00-2.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.68Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.245 , 0.295 0.276 , 0.319	Depositor DCC
$R_{free}$ test set	1526 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtrriage
Anisotropy	0.118	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8200	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 91.29 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5928e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, PPV

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	B	0.53	0/190	1.08	0/294
1	E	0.55	0/190	1.19	2/294 (0.7%)
2	C	0.43	0/165	0.89	0/256
2	F	0.44	0/165	0.92	0/256
3	A	0.52	0/3803	0.81	4/5149 (0.1%)
3	D	0.57	1/3803 (0.0%)	0.83	5/5149 (0.1%)
All	All	0.54	1/8316 (0.0%)	0.84	11/11398 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	126	LYS	CD-CE	10.94	1.85	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	126	LYS	CG-CD-CE	-6.35	96.70	111.30
3	A	435	GLY	CA-C-N	5.75	125.22	119.24
3	A	435	GLY	C-N-CA	5.75	125.22	119.24
1	E	905	G	O4'-C4'-C3'	-5.30	98.70	104.00
3	D	140	GLY	CA-C-N	5.21	125.01	119.28
3	D	140	GLY	C-N-CA	5.21	125.01	119.28
3	D	112	GLU	CA-C-N	5.20	124.51	118.85
3	D	112	GLU	C-N-CA	5.20	124.51	118.85
3	A	140	GLY	CA-C-N	5.16	124.78	119.05
3	A	140	GLY	C-N-CA	5.16	124.78	119.05
1	E	905	G	C4'-C3'-C2'	-5.05	97.55	102.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	171	0	88	2	0
1	E	171	0	88	4	0
2	C	148	0	79	3	0
2	F	148	0	79	3	0
3	A	3714	0	3642	39	3
3	D	3714	0	3642	39	3
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	9	0	0	0	0
5	D	9	0	0	0	0
6	A	49	0	0	0	0
6	B	3	0	0	0	0
6	C	2	0	0	0	0
6	D	55	0	0	3	0
6	E	4	0	0	0	0
6	F	1	0	0	0	0
All	All	8200	0	7618	87	3

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 (87) 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)
3:D:126:LYS:CD	3:D:126:LYS:CE	1.85	1.50
3:A:85:LEU:HD11	3:A:203:MET:HE1	1.28	1.07
3:D:85:LEU:HD11	3:D:203:MET:HE1	1.37	1.04
3:A:51:VAL:HB	3:A:54:GLU:HG2	1.55	0.87
3:D:126:LYS:CE	3:D:126:LYS:CG	2.62	0.78
3:A:85:LEU:HD11	3:A:203:MET:CE	2.13	0.76
3:D:85:LEU:HD11	3:D:203:MET:CE	2.19	0.70
3:A:56:ILE:HG23	3:A:180:ILE:HG21	1.75	0.68
3:D:464:ASN:HB2	6:D:2969:HOH:O	1.96	0.65
3:D:89:LEU:HD11	3:D:203:MET:HE3	1.78	0.63
3:D:238:ASP:HB2	3:D:383:VAL:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:918:C:H2'	2:F:919:C:C6	2.32	0.62
3:A:321:ARG:HH11	3:A:356:HIS:HD2	1.47	0.62
3:A:300:CYS:SG	3:A:301:SER:O	2.54	0.61
3:A:398:PHE:HE2	3:A:467:CYS:SG	2.24	0.61
3:D:126:LYS:CD	3:D:126:LYS:NZ	2.64	0.60
3:A:89:LEU:HD11	3:A:203:MET:HE3	1.82	0.60
3:A:96:LEU:HG	3:A:100:GLU:HB3	1.84	0.60
2:C:918:C:H2'	2:C:919:C:C6	2.38	0.58
2:C:921:A:HO3'	3:A:338:ASP:CG	2.14	0.56
3:D:51:VAL:HB	3:D:54:GLU:HG2	1.86	0.56
3:D:302:ALA:HA	6:D:2014:HOH:O	2.05	0.55
3:A:238:ASP:HB2	3:A:383:VAL:HG12	1.89	0.55
3:A:43:ASP:HB3	3:A:46:LEU:HG	1.89	0.54
3:D:56:ILE:HG23	3:D:180:ILE:HG21	1.89	0.54
3:A:116:ALA:O	3:A:128:ARG:NH1	2.40	0.54
3:A:85:LEU:CD1	3:A:203:MET:HE1	2.20	0.54
2:F:919:C:H2'	2:F:920:C:C6	2.43	0.53
3:D:244:PHE:HA	3:D:362:GLN:HE22	1.72	0.53
3:A:95:PRO:HG3	3:A:268:HIS:HB2	1.92	0.52
3:A:355:PRO:HA	3:A:358:LYS:HB2	1.91	0.52
3:A:238:ASP:HB3	3:A:367:ALA:HB3	1.91	0.51
3:D:96:LEU:HG	3:D:100:GLU:HB3	1.92	0.51
3:D:355:PRO:HA	3:D:358:LYS:HB2	1.91	0.51
3:A:280:ASN:HD22	3:A:293:GLU:HA	1.76	0.51
3:D:321:ARG:HH11	3:D:356:HIS:HD2	1.58	0.50
3:A:56:ILE:HD11	3:A:178:THR:HB	1.93	0.50
3:A:244:PHE:HA	3:A:362:GLN:HE22	1.76	0.49
3:D:169:PRO:HG2	3:D:172:LYS:HD2	1.95	0.49
3:D:238:ASP:HB3	3:D:367:ALA:HB3	1.94	0.49
3:A:229:HIS:O	3:A:232:GLN:HG2	2.13	0.49
3:D:280:ASN:HD22	3:D:293:GLU:HA	1.78	0.49
3:D:322:HIS:ND1	3:D:356:HIS:HE1	2.10	0.48
3:D:43:ASP:HB3	3:D:46:LEU:HG	1.94	0.48
3:D:95:PRO:HG3	3:D:268:HIS:HB2	1.95	0.48
1:E:904:U:H2'	1:E:905:G:O4'	2.14	0.47
3:D:32:PRO:C	3:D:34:PHE:H	2.22	0.47
3:A:308:THR:HG23	3:A:335:SER:OG	2.13	0.47
3:A:89:LEU:HD11	3:A:203:MET:CE	2.45	0.47
3:A:32:PRO:C	3:A:34:PHE:H	2.22	0.47
2:C:919:C:H2'	2:C:920:C:C6	2.50	0.47
3:A:169:PRO:HG2	3:A:172:LYS:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:12:ARG:HE	3:A:286:GLU:HB3	1.80	0.46
3:A:96:LEU:HB2	3:A:194:MET:HA	1.96	0.46
3:D:467:CYS:O	3:D:467:CYS:SG	2.73	0.46
3:A:322:HIS:ND1	3:A:356:HIS:HE1	2.13	0.46
3:D:85:LEU:CD1	3:D:203:MET:HE1	2.27	0.45
1:B:904:U:H2'	1:B:905:G:O4'	2.16	0.45
1:E:906:G:OP2	3:D:109:ASP:HB2	2.16	0.45
3:D:398:PHE:HE2	3:D:467:CYS:SG	2.39	0.45
3:A:327:GLU:HA	3:A:327:GLU:OE1	2.17	0.45
3:D:96:LEU:HB2	3:D:194:MET:HA	1.99	0.45
3:D:219:PRO:O	3:D:223:TRP:HB2	2.16	0.45
1:B:907:G:H2'	1:B:908:C:O4'	2.17	0.45
3:A:215:VAL:HA	3:A:336:TYR:CE1	2.51	0.45
3:D:215:VAL:HA	3:D:336:TYR:CE1	2.51	0.45
3:D:86:HIS:HE1	3:D:260:VAL:O	1.99	0.45
3:D:184:LEU:HD22	3:D:300:CYS:HB2	1.98	0.44
1:E:907:G:H4'	3:D:218:ASN:HB2	1.99	0.44
3:A:444:GLU:N	3:A:445:PRO:CD	2.80	0.44
3:D:324:GLU:HG3	6:D:2009:HOH:O	2.18	0.44
3:D:56:ILE:HD11	3:D:178:THR:HB	1.99	0.44
3:A:86:HIS:HE1	3:A:260:VAL:O	2.00	0.43
3:A:467:CYS:SG	3:A:467:CYS:O	2.76	0.43
3:D:322:HIS:HB2	3:D:356:HIS:CE1	2.53	0.43
3:D:51:VAL:O	3:D:55:VAL:HG23	2.18	0.43
3:A:298:SER:O	3:A:298:SER:OG	2.36	0.42
1:E:907:G:H2'	1:E:908:C:O4'	2.19	0.42
3:D:152:LYS:HZ1	3:D:154:GLU:HG3	1.84	0.42
3:A:2:LEU:HB2	3:A:63:ASP:N	2.35	0.41
3:A:353:LEU:O	3:A:354:LYS:C	2.62	0.41
3:A:219:PRO:O	3:A:223:TRP:HB2	2.20	0.41
3:D:152:LYS:NZ	3:D:154:GLU:HG3	2.36	0.40
3:D:353:LEU:O	3:D:354:LYS:C	2.62	0.40
2:F:918:C:H2'	2:F:919:C:H6	1.81	0.40
3:A:2:LEU:HB2	3:A:63:ASP:H	1.87	0.40
3:A:188:HIS:HE1	3:A:277:THR:OG1	2.03	0.40

All (3) 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)
3:A:394:TYR:OH	3:D:16:MET:CB[3_664]	1.85	0.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:394:TYR:CE2	3:D:16:MET:SD[3_664]	1.89	0.31
3:A:394:TYR:OH	3:D:17:ARG:N[3_664]	2.10	0.10

### 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	
3	A	468/476 (98%)	444 (95%)	19 (4%)	5 (1%)	11	22
3	D	468/476 (98%)	444 (95%)	20 (4%)	4 (1%)	14	28
All	All	936/952 (98%)	888 (95%)	39 (4%)	9 (1%)	12	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	16	MET
3	D	16	MET
3	A	372	LYS
3	D	372	LYS
3	A	106	ASP
3	A	17	ARG
3	D	17	ARG
3	A	394	TYR
3	D	106	ASP

#### 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	
3	A	395/399 (99%)	373 (94%)	22 (6%)	19	36
3	D	395/399 (99%)	377 (95%)	18 (5%)	24	45
All	All	790/798 (99%)	750 (95%)	40 (5%)	21	40

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	THR
3	A	15	VAL
3	A	42	LYS
3	A	56	ILE
3	A	96	LEU
3	A	98	ILE
3	A	106	ASP
3	A	149	LEU
3	A	154	GLU
3	A	181	VAL
3	A	190	LEU
3	A	205	SER
3	A	221	VAL
3	A	223	TRP
3	A	305	ILE
3	A	324	GLU
3	A	360	LEU
3	A	368	ASP
3	A	384	THR
3	A	417	ARG
3	A	422	GLU
3	A	469	ASP
3	D	41	ASN
3	D	42	LYS
3	D	56	ILE
3	D	114	ASP
3	D	135	GLU
3	D	147	LEU
3	D	149	LEU
3	D	221	VAL
3	D	223	TRP
3	D	225	ARG
3	D	300	CYS
3	D	305	ILE
3	D	324	GLU

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Mol	Chain	Res	Type
3	D	360	LEU
3	D	394	TYR
3	D	417	ARG
3	D	422	GLU
3	D	469	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	60	HIS
3	A	86	HIS
3	A	188	HIS
3	A	254	ASN
3	A	280	ASN
3	A	311	ASN
3	A	356	HIS
3	A	362	GLN
3	A	464	ASN
3	D	60	HIS
3	D	86	HIS
3	D	124	GLN
3	D	188	HIS
3	D	210	GLN
3	D	254	ASN
3	D	280	ASN
3	D	311	ASN
3	D	356	HIS
3	D	362	GLN
3	D	378	HIS
3	D	389	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	8/8 (100%)	3 (37%)	1 (12%)
1	E	8/8 (100%)	3 (37%)	2 (25%)
2	C	6/7 (85%)	0	0
2	F	6/7 (85%)	0	0
All	All	28/30 (93%)	6 (21%)	3 (10%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	904	U
1	B	905	G
1	B	910	C
1	E	904	U
1	E	905	G
1	E	906	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	903	A
1	E	903	A
1	E	905	G

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	$\# Z  > 2$
5	PPV	D	2930	-	6,8,8	0.72	0	12,13,13	0.97	0
5	PPV	A	930	-	6,8,8	1.55	2 (33%)	12,13,13	0.93	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
5	PPV	D	2930	-	-	0/6/6/6	-
5	PPV	A	930	-	-	0/6/6/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	930	PPV	P1-O31	2.41	1.58	1.50
5	A	930	PPV	P2-O22	2.40	1.57	1.50

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	B	8/8 (100%)	0.84	0 <b>100</b> <b>100</b>	44, 52, 65, 69	8 (100%)
1	E	8/8 (100%)	0.71	0 <b>100</b> <b>100</b>	44, 51, 64, 69	8 (100%)
2	C	7/7 (100%)	0.62	0 <b>100</b> <b>100</b>	33, 38, 61, 66	7 (100%)
2	F	7/7 (100%)	0.62	0 <b>100</b> <b>100</b>	34, 38, 61, 66	7 (100%)
3	A	470/476 (98%)	0.14	9 (1%) 66 64	34, 49, 70, 80	0
3	D	470/476 (98%)	0.18	8 (1%) 69 67	33, 49, 70, 80	0
All	All	970/982 (98%)	0.18	17 (1%) 67 65	33, 49, 70, 80	30 (3%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	16	MET	5.7
3	A	394	TYR	4.1
3	A	469	ASP	3.7
3	D	469	ASP	3.3
3	D	49	GLY	2.9
3	A	49	GLY	2.9
3	D	41	ASN	2.9
3	A	468	GLY	2.7
3	D	394	TYR	2.5
3	A	16	MET	2.3
3	D	468	GLY	2.3
3	A	444	GLU	2.2
3	A	9	VAL	2.2
3	A	41	ASN	2.2
3	A	287	ASN	2.1
3	D	132	ILE	2.0
3	D	13	VAL	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 oligosaccharides 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( $\text{\AA}^2$ )	Q<0.9
5	PPV	D	2930	9/9	0.47	0.12	101,102,102,102	9
5	PPV	A	930	9/9	0.66	0.11	129,129,129,129	9
4	MG	D	3990	1/1	0.74	0.18	47,47,47,47	0
4	MG	A	1990	1/1	0.92	0.08	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.