



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2020 – 04:11 PM EST

PDB ID : 7KF4  
Title : Crystal structure from SARS-CoV-2 NendoU NSP15  
Authors : Godoy, A.S.; Nakamura, A.M.; Pereira, H.M.; Noske, G.D.; Gawriljuk, V.O.;  
Fernandes, R.S.; Oliveira, K.I.Z.; Oliva, G.  
Deposited on : 2020-10-13  
Resolution : 2.61 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.6  
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) : 2.14.6

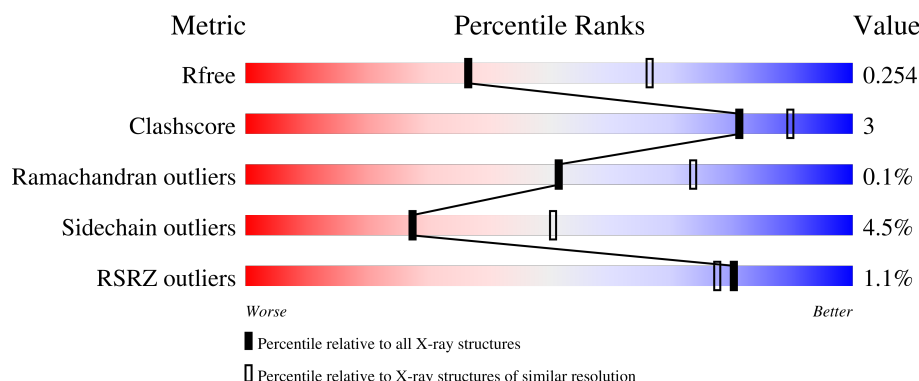
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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 on 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	A	349	<div> <div></div> <div>92% 7% .</div> </div>
1	B	349	<div> <div>2%</div> <div>93% 6% .</div> </div>
1	C	349	<div> <div>%</div> <div>92% 7%</div> </div>
1	D	349	<div> <div>%</div> <div>90% 9% .</div> </div>
1	E	349	<div> <div>%</div> <div>92% 7% .</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	349	<div><div></div><div>3%</div><div>84%</div><div>14%</div><div></div></div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 16984 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 Uridylate-specific endoribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	1	0
			2751	1768	447	526	10			
1	B	348	Total	C	N	O	S	0	1	0
			2754	1770	447	526	11			
1	C	348	Total	C	N	O	S	0	1	0
			2742	1763	446	522	11			
1	D	348	Total	C	N	O	S	0	1	0
			2738	1759	444	524	11			
1	E	348	Total	C	N	O	S	0	1	0
			2750	1767	446	526	11			
1	F	348	Total	C	N	O	S	0	1	0
			2742	1763	446	522	11			

There are 18 discrepancies between the modelled and reference sequences:

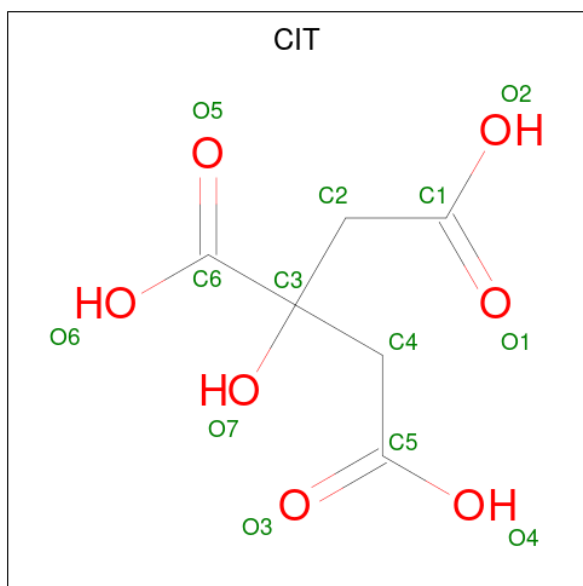
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P0DTD1
A	-1	ALA	-	expression tag	UNP P0DTD1
A	0	MET	-	expression tag	UNP P0DTD1
B	-2	GLY	-	expression tag	UNP P0DTD1
B	-1	ALA	-	expression tag	UNP P0DTD1
B	0	MET	-	expression tag	UNP P0DTD1
C	-2	GLY	-	expression tag	UNP P0DTD1
C	-1	ALA	-	expression tag	UNP P0DTD1
C	0	MET	-	expression tag	UNP P0DTD1
D	-2	GLY	-	expression tag	UNP P0DTD1
D	-1	ALA	-	expression tag	UNP P0DTD1
D	0	MET	-	expression tag	UNP P0DTD1
E	-2	GLY	-	expression tag	UNP P0DTD1
E	-1	ALA	-	expression tag	UNP P0DTD1
E	0	MET	-	expression tag	UNP P0DTD1
F	-2	GLY	-	expression tag	UNP P0DTD1
F	-1	ALA	-	expression tag	UNP P0DTD1

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	MET	-	expression tag	UNP P0DTD1

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula:  $C_6H_8O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		
2	F	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	77	Total	O	0	0
			77	77		
3	C	59	Total	O	0	0
			59	59		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	71	Total 71	O 71	0	0
3	E	61	Total 61	O 61	0	0
3	F	71	Total 71	O 71	0	0

### 3 Residue-property plots [i](#)

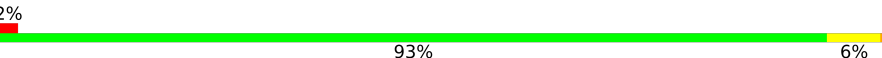
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Uridylate-specific endoribonuclease

Chain A: 

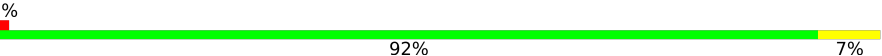


- Molecule 1: Uridylate-specific endoribonuclease

Chain B: 




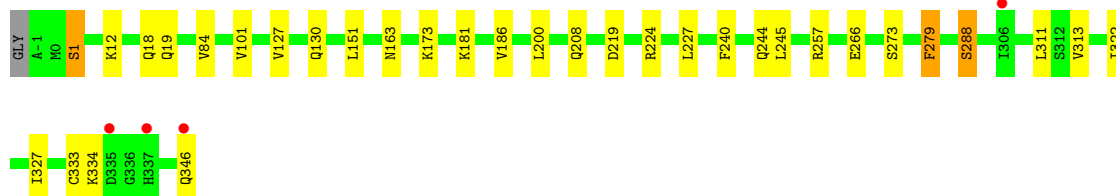
- Molecule 1: Uridylate-specific endoribonuclease

Chain C: 



- Molecule 1: Uridylate-specific endoribonuclease

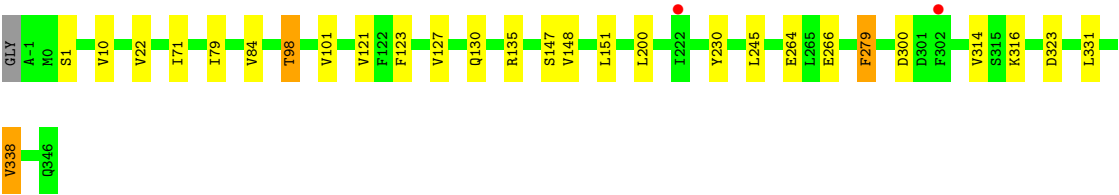
Chain D: 



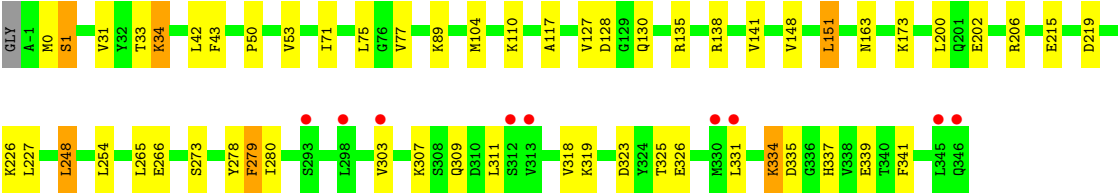
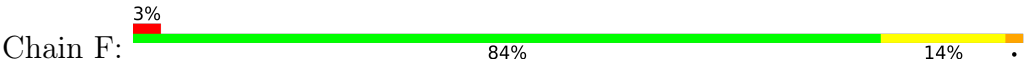
- Molecule 1: Uridylate-specific endoribonuclease

Chain E: 





● Molecule 1: Uridylate-specific endoribonuclease



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.12Å 151.16Å 199.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.16 – 2.61 49.16 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.16-2.61) 99.7 (49.16-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.22 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.219 , 0.246 0.230 , 0.254	Depositor DCC
$R_{free}$ test set	4004 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.42 % 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 1.3252e-04. 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: CIT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.48	0/2811	0.60	0/3814
1	B	0.49	0/2814	0.61	0/3817
1	C	0.50	0/2802	0.68	0/3803
1	D	0.51	0/2798	0.68	0/3800
1	E	0.51	0/2810	0.68	0/3813
1	F	0.52	0/2802	0.72	0/3803
All	All	0.50	0/16837	0.66	0/22850

There are no bond length outliers.

There are no bond angle outliers.

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	2751	0	2742	14	0
1	B	2754	0	2749	11	0
1	C	2742	0	2730	10	0
1	D	2738	0	2712	12	0
1	E	2750	0	2738	14	0
1	F	2742	0	2730	28	0
2	A	13	0	5	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	0	5	1	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	0	0
3	A	90	0	0	1	0
3	B	77	0	0	0	0
3	C	59	0	0	0	0
3	D	71	0	0	0	0
3	E	61	0	0	0	0
3	F	71	0	0	2	0
All	All	16984	0	16431	83	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 (83) 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)
1:A:322:ILE:HB	1:A:327:ILE:HD13	1.60	0.84
1:C:322:ILE:HB	1:C:327:ILE:HD13	1.60	0.83
1:D:322:ILE:HB	1:D:327:ILE:HD13	1.62	0.80
1:C:1:SER:HB2	1:D:1:SER:HB2	1.68	0.75
1:F:265:LEU:HD23	1:F:280:ILE:HG12	1.67	0.75
1:B:148:VAL:HG13	1:B:151:LEU:HB2	1.74	0.70
1:E:230:TYR:HA	1:E:338:VAL:HG13	1.74	0.69
1:E:316:LYS:HE3	1:E:331:LEU:HD23	1.74	0.69
1:F:117:ALA:HB1	1:F:138:ARG:HE	1.59	0.68
1:D:151:LEU:HD22	1:D:186:VAL:HG11	1.77	0.66
1:A:104:MET:HE3	1:F:34:LYS:HD2	1.78	0.65
1:F:77:VAL:HG22	1:F:141:VAL:HG11	1.79	0.64
1:B:1:SER:HB2	1:E:1:SER:HB2	1.81	0.63
1:F:148:VAL:HG13	1:F:151:LEU:HB2	1.81	0.63
1:D:244:GLN:HA	1:D:288:SER:O	2.01	0.61
1:D:240:PHE:CZ	1:D:257:ARG:HD2	2.38	0.58
1:F:50:PRO:HD2	1:F:53:VAL:CG1	2.34	0.57
1:A:1:SER:HB2	1:F:1:SER:HB2	1.85	0.57
1:F:248:LEU:HD11	1:F:254:LEU:HG	1.87	0.57
1:E:98:THR:CG2	1:E:101:VAL:HB	2.35	0.56
1:F:318:VAL:HG11	1:F:341:PHE:HE1	1.70	0.56
1:F:77:VAL:CG2	1:F:141:VAL:HG11	2.37	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:VAL:O	1:D:333:CYS:HB2	2.08	0.54
1:A:322:ILE:HB	1:A:327:ILE:CD1	2.36	0.54
1:E:98:THR:HG23	1:E:101:VAL:HB	1.91	0.53
1:B:127:VAL:HB	1:B:130:GLN:HG3	1.91	0.51
1:E:127:VAL:HB	1:E:130:GLN:HG3	1.92	0.51
1:F:127:VAL:HB	1:F:130:GLN:HG3	1.91	0.51
1:A:127:VAL:HB	1:A:130:GLN:HG3	1.91	0.51
1:C:127:VAL:HB	1:C:130:GLN:HG3	1.91	0.51
1:C:240:PHE:CZ	1:C:257:ARG:HD2	2.46	0.51
1:F:319:LYS:HB3	1:F:326:GLU:HG2	1.92	0.50
1:A:300:ASP:HA	1:A:303:VAL:HG22	1.94	0.50
1:D:127:VAL:HB	1:D:130:GLN:HG3	1.93	0.50
1:F:135:ARG:HH21	1:F:148:VAL:HG22	1.75	0.50
1:F:31:VAL:HG23	1:F:42:LEU:HB2	1.92	0.50
1:C:266:GLU:HB3	1:C:279:PHE:HB3	1.94	0.49
1:F:337:HIS:HB3	3:F:843:HOH:O	2.11	0.49
1:D:266:GLU:HB3	1:D:279:PHE:HB3	1.94	0.49
1:A:266:GLU:HB3	1:A:279:PHE:HB3	1.95	0.48
1:C:207:SER:O	1:C:211:ILE:HG12	2.13	0.48
1:F:303:VAL:O	1:F:307:LYS:HB2	2.13	0.48
1:F:50:PRO:HD2	1:F:53:VAL:HG11	1.95	0.48
1:B:266:GLU:HB3	1:B:279:PHE:HB3	1.97	0.47
1:C:79:ILE:HG12	1:C:99:ILE:HD12	1.96	0.46
1:B:148:VAL:HG12	1:B:179:TYR:CZ	2.50	0.46
1:E:71:ILE:HD13	1:E:323:ASP:HB3	1.97	0.46
1:E:135:ARG:HH21	1:E:148:VAL:HG12	1.81	0.46
1:F:200:LEU:HD11	1:F:254:LEU:HB3	1.98	0.46
1:F:265:LEU:HD22	1:F:278:TYR:CG	2.51	0.46
1:D:322:ILE:HB	1:D:327:ILE:CD1	2.40	0.45
1:B:226:LYS:O	1:B:226:LYS:HG3	2.17	0.45
1:E:266:GLU:HB3	1:E:279:PHE:HB3	1.99	0.45
1:F:71:ILE:HD13	1:F:323:ASP:HB3	1.99	0.45
1:A:300:ASP:O	1:A:303:VAL:HG22	2.17	0.44
1:B:246:GLY:HA2	2:B:700:CIT:O1	2.18	0.44
1:A:34:LYS:HD3	1:F:104:MET:HE3	2.00	0.44
1:B:71:ILE:HD13	1:B:323:ASP:HB3	2.00	0.44
1:D:12:LYS:HE3	1:D:18:GLN:HE21	1.83	0.44
1:B:226:LYS:CG	1:B:226:LYS:O	2.65	0.44
1:D:163:ASN:ND2	1:E:279:PHE:CZ	2.86	0.44
1:F:266:GLU:HB3	1:F:279:PHE:HB3	1.99	0.43
1:F:31:VAL:HG22	1:F:43:PHE:HB3	1.99	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:VAL:CG1	1:F:341:PHE:HE1	2.31	0.43
1:A:246:GLY:HA2	2:A:700:CIT:O2	2.18	0.43
1:C:12:LYS:HE3	1:C:18:GLN:HG3	2.00	0.43
1:A:12:LYS:HE3	1:A:18:GLN:HG3	2.00	0.43
1:F:334:LYS:HD3	1:F:334:LYS:HA	1.83	0.43
1:F:0:MET:HA	3:F:844:HOH:O	2.17	0.43
1:C:322:ILE:HB	1:C:327:ILE:CD1	2.39	0.42
1:F:75:LEU:HD13	1:F:141:VAL:HG21	2.01	0.42
1:E:121:VAL:HG22	1:E:123:PHE:CZ	2.55	0.42
1:E:10:VAL:HG21	1:E:22:VAL:HG11	1.99	0.42
1:E:79:ILE:HG23	1:E:121:VAL:HB	2.01	0.42
1:B:84:VAL:CG2	1:B:101:VAL:HG11	2.50	0.42
1:F:248:LEU:CD1	1:F:254:LEU:HG	2.50	0.42
1:A:0:MET:HA	3:A:846:HOH:O	2.20	0.41
1:A:330:MET:O	1:A:341:PHE:HA	2.20	0.41
1:D:84:VAL:CG2	1:D:101:VAL:HG11	2.51	0.41
1:E:84:VAL:CG2	1:E:101:VAL:HG11	2.51	0.41
1:B:232:PHE:O	1:B:236:VAL:HG22	2.21	0.41
1:C:84:VAL:CG2	1:C:101:VAL:HG11	2.51	0.41
1:A:84:VAL:CG2	1:A:101:VAL:HG11	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	A	347/349 (99%)	342 (99%)	5 (1%)	0	100	100
1	B	347/349 (99%)	343 (99%)	4 (1%)	0	100	100
1	C	347/349 (99%)	334 (96%)	13 (4%)	0	100	100
1	D	347/349 (99%)	335 (96%)	11 (3%)	1 (0%)	41	62

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	347/349 (99%)	338 (97%)	9 (3%)	0	100	100
1	F	347/349 (99%)	338 (97%)	8 (2%)	1 (0%)	41	62
All	All	2082/2094 (99%)	2030 (98%)	50 (2%)	2 (0%)	51	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	226	LYS
1	D	334	LYS

### 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	A	309/309 (100%)	299 (97%)	10 (3%)	39	63
1	B	310/309 (100%)	297 (96%)	13 (4%)	30	53
1	C	307/309 (99%)	297 (97%)	10 (3%)	38	62
1	D	306/309 (99%)	291 (95%)	15 (5%)	25	46
1	E	309/309 (100%)	299 (97%)	10 (3%)	39	63
1	F	307/309 (99%)	283 (92%)	24 (8%)	12	24
All	All	1848/1854 (100%)	1766 (96%)	82 (4%)	27	52

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	147	SER
1	A	148	VAL
1	A	151	LEU
1	A	173	LYS
1	A	200	LEU
1	A	201	GLN
1	A	261	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	279	PHE
1	A	345	LEU
1	B	1	SER
1	B	38	VAL
1	B	89	LYS
1	B	147	SER
1	B	151	LEU
1	B	188	GLN
1	B	200	LEU
1	B	201	GLN
1	B	202	GLU
1	B	226	LYS
1	B	244	GLN
1	B	279	PHE
1	B	300	ASP
1	C	34	LYS
1	C	96	ILE
1	C	147	SER
1	C	148	VAL
1	C	200	LEU
1	C	261	SER
1	C	279	PHE
1	C	313	VAL
1	C	315	SER
1	C	344	LYS
1	D	1	SER
1	D	19	GLN
1	D	173	LYS
1	D	181	LYS
1	D	200	LEU
1	D	208	GLN
1	D	219	ASP
1	D	224	ARG
1	D	227	LEU
1	D	245	LEU
1	D	273	SER
1	D	279	PHE
1	D	288	SER
1	D	311	LEU
1	D	346	GLN
1	E	98	THR
1	E	147	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	151	LEU
1	E	200	LEU
1	E	245	LEU
1	E	264	GLU
1	E	279	PHE
1	E	300	ASP
1	E	314	VAL
1	E	338	VAL
1	F	1	SER
1	F	33	THR
1	F	34	LYS
1	F	89	LYS
1	F	110	LYS
1	F	128	ASP
1	F	151	LEU
1	F	163	ASN
1	F	173	LYS
1	F	202	GLU
1	F	206	ARG
1	F	215	GLU
1	F	219	ASP
1	F	227	LEU
1	F	248	LEU
1	F	273	SER
1	F	279	PHE
1	F	309	GLN
1	F	311	LEU
1	F	325	THR
1	F	331	LEU
1	F	334	LYS
1	F	335	ASP
1	F	339	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	201	GLN
1	D	18	GLN
1	D	244	GLN
1	D	337	HIS
1	F	244	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

6 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	CIT	F	700	-	3,12,12	0.52	0	3,17,17	0.73	0
2	CIT	D	700	-	3,12,12	0.51	0	3,17,17	0.87	0
2	CIT	B	700	-	3,12,12	0.47	0	3,17,17	0.73	0
2	CIT	E	700	-	3,12,12	0.53	0	3,17,17	0.88	0
2	CIT	C	700	-	3,12,12	0.44	0	3,17,17	0.93	0
2	CIT	A	700	-	3,12,12	0.54	0	3,17,17	0.95	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
2	CIT	F	700	-	-	0/6/16/16	-
2	CIT	D	700	-	-	0/6/16/16	-
2	CIT	B	700	-	-	0/6/16/16	-
2	CIT	E	700	-	-	0/6/16/16	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CIT	C	700	-	-	0/6/16/16	-
2	CIT	A	700	-	-	0/6/16/16	-

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	700	CIT	1	0
2	A	700	CIT	1	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

### 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	A	348/349 (99%)	-0.09	0	100	100	43, 65, 93, 149	0
1	B	348/349 (99%)	-0.02	7 (2%)	65	60	43, 67, 105, 210	0
1	C	348/349 (99%)	0.04	2 (0%)	89	88	51, 74, 97, 160	0
1	D	348/349 (99%)	-0.02	4 (1%)	80	78	51, 69, 96, 170	0
1	E	348/349 (99%)	-0.10	2 (0%)	89	88	41, 68, 98, 238	0
1	F	348/349 (99%)	0.24	9 (2%)	56	50	50, 82, 133, 212	0
All	All	2088/2094 (99%)	0.01	24 (1%)	80	78	41, 71, 105, 238	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	346	GLN	3.7
1	F	313	VAL	3.5
1	F	330	MET	3.4
1	C	335	ASP	3.2
1	F	331	LEU	3.0
1	B	230	TYR	3.0
1	F	312	SER	2.9
1	F	303	VAL	2.7
1	D	346	GLN	2.5
1	F	345	LEU	2.5
1	D	335	ASP	2.4
1	C	346	GLN	2.3
1	B	346	GLN	2.3
1	B	227	LEU	2.2
1	B	338	VAL	2.2
1	B	202	GLU	2.1
1	D	306	ILE	2.1
1	B	335	ASP	2.1
1	D	337	HIS	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	E	302	PHE	2.1
1	F	293	SER	2.0
1	F	298	LEU	2.0
1	E	222	ILE	2.0
1	B	36[A]	ASP	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<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
2	CIT	E	700	13/13	0.87	0.26	106,111,117,119	0
2	CIT	D	700	13/13	0.89	0.21	100,104,107,107	0
2	CIT	C	700	13/13	0.89	0.16	99,102,104,105	0
2	CIT	B	700	13/13	0.91	0.17	123,125,126,127	0
2	CIT	F	700	13/13	0.92	0.25	110,115,124,124	0
2	CIT	A	700	13/13	0.93	0.20	80,87,91,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.