



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:18 am BST

PDB ID : 6EY7  
Title : Human cytomegalovirus terminase nuclease domain, Mn soaked, inhibitor bound  
Authors : Bongarzone, S.; Nadal, M.; Kaczmarska, Z.; Machon, C.; Alvarez, M.; Albericio, F.; Coll, M.  
Deposited on : 2017-11-10  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

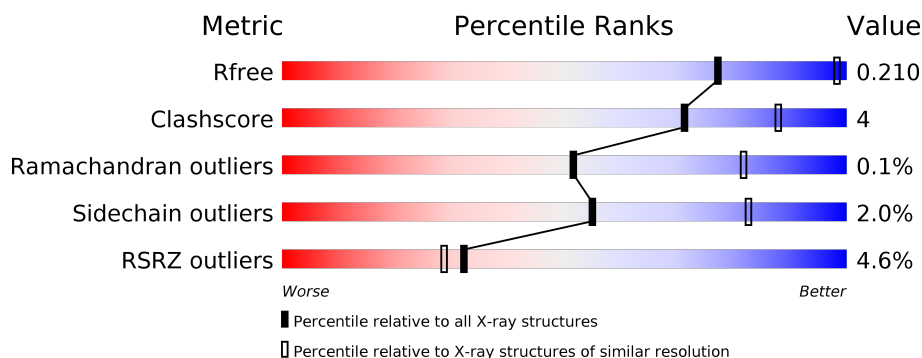
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	279	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>8%</div> <div>19%</div> </div> </div>
1	B	279	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>8%</div> <div>19%</div> </div> </div>
1	C	279	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>7%</div> <div>21%</div> </div> </div>
1	D	279	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>5%</div> <div>23%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6928 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 UL89 HCMV terminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	1	0	0
			1724	1110	294	314	6			
1	B	227	Total	C	N	O	S	1	1	0
			1775	1143	303	323	6			
1	C	221	Total	C	N	O	S	1	0	0
			1688	1086	281	315	6			
1	D	214	Total	C	N	O	S	0	0	0
			1633	1048	275	304	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	MET	-	initiating methionine	UNP P16732
A	397	GLY	-	expression tag	UNP P16732
A	398	HIS	-	expression tag	UNP P16732
A	399	HIS	-	expression tag	UNP P16732
A	400	HIS	VAL	conflict	UNP P16732
A	401	HIS	ARG	conflict	UNP P16732
A	402	HIS	LYS	conflict	UNP P16732
A	403	HIS	THR	conflict	UNP P16732
A	404	ASP	ALA	conflict	UNP P16732
A	405	TYR	ASN	conflict	UNP P16732
A	406	ASP	MET	conflict	UNP P16732
A	407	ILE	PHE	conflict	UNP P16732
A	408	PRO	MET	conflict	UNP P16732
A	409	THR	PRO	conflict	UNP P16732
A	410	THR	GLY	conflict	UNP P16732
A	411	GLU	ALA	conflict	UNP P16732
A	412	ASN	PHE	conflict	UNP P16732
A	413	LEU	MET	conflict	UNP P16732
A	414	TYR	ASP	conflict	UNP P16732
A	415	PHE	GLU	conflict	UNP P16732
A	416	GLN	ILE	conflict	UNP P16732

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Chain	Residue	Modelled	Actual	Comment	Reference
A	417	GLY	ILE	conflict	UNP P16732
B	396	MET	-	initiating methionine	UNP P16732
B	397	GLY	-	expression tag	UNP P16732
B	398	HIS	-	expression tag	UNP P16732
B	399	HIS	-	expression tag	UNP P16732
B	400	HIS	VAL	conflict	UNP P16732
B	401	HIS	ARG	conflict	UNP P16732
B	402	HIS	LYS	conflict	UNP P16732
B	403	HIS	THR	conflict	UNP P16732
B	404	ASP	ALA	conflict	UNP P16732
B	405	TYR	ASN	conflict	UNP P16732
B	406	ASP	MET	conflict	UNP P16732
B	407	ILE	PHE	conflict	UNP P16732
B	408	PRO	MET	conflict	UNP P16732
B	409	THR	PRO	conflict	UNP P16732
B	410	THR	GLY	conflict	UNP P16732
B	411	GLU	ALA	conflict	UNP P16732
B	412	ASN	PHE	conflict	UNP P16732
B	413	LEU	MET	conflict	UNP P16732
B	414	TYR	ASP	conflict	UNP P16732
B	415	PHE	GLU	conflict	UNP P16732
B	416	GLN	ILE	conflict	UNP P16732
B	417	GLY	ILE	conflict	UNP P16732
C	396	MET	-	initiating methionine	UNP P16732
C	397	GLY	-	expression tag	UNP P16732
C	398	HIS	-	expression tag	UNP P16732
C	399	HIS	-	expression tag	UNP P16732
C	400	HIS	VAL	conflict	UNP P16732
C	401	HIS	ARG	conflict	UNP P16732
C	402	HIS	LYS	conflict	UNP P16732
C	403	HIS	THR	conflict	UNP P16732
C	404	ASP	ALA	conflict	UNP P16732
C	405	TYR	ASN	conflict	UNP P16732
C	406	ASP	MET	conflict	UNP P16732
C	407	ILE	PHE	conflict	UNP P16732
C	408	PRO	MET	conflict	UNP P16732
C	409	THR	PRO	conflict	UNP P16732
C	410	THR	GLY	conflict	UNP P16732
C	411	GLU	ALA	conflict	UNP P16732
C	412	ASN	PHE	conflict	UNP P16732
C	413	LEU	MET	conflict	UNP P16732
C	414	TYR	ASP	conflict	UNP P16732

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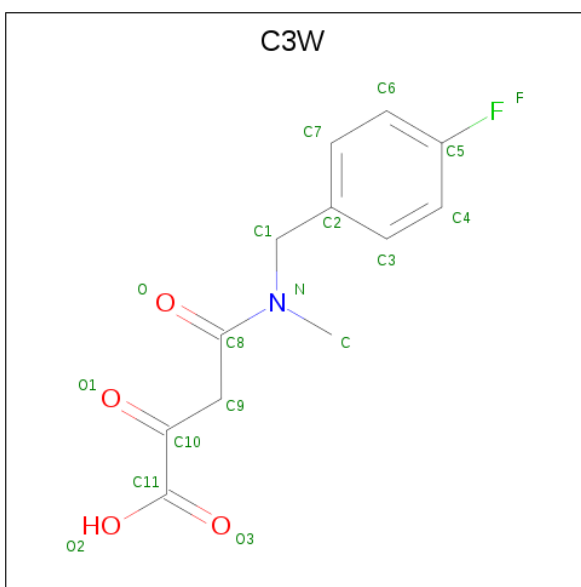
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Chain	Residue	Modelled	Actual	Comment	Reference
C	415	PHE	GLU	conflict	UNP P16732
C	416	GLN	ILE	conflict	UNP P16732
C	417	GLY	ILE	conflict	UNP P16732
D	396	MET	-	initiating methionine	UNP P16732
D	397	GLY	-	expression tag	UNP P16732
D	398	HIS	-	expression tag	UNP P16732
D	399	HIS	-	expression tag	UNP P16732
D	400	HIS	VAL	conflict	UNP P16732
D	401	HIS	ARG	conflict	UNP P16732
D	402	HIS	LYS	conflict	UNP P16732
D	403	HIS	THR	conflict	UNP P16732
D	404	ASP	ALA	conflict	UNP P16732
D	405	TYR	ASN	conflict	UNP P16732
D	406	ASP	MET	conflict	UNP P16732
D	407	ILE	PHE	conflict	UNP P16732
D	408	PRO	MET	conflict	UNP P16732
D	409	THR	PRO	conflict	UNP P16732
D	410	THR	GLY	conflict	UNP P16732
D	411	GLU	ALA	conflict	UNP P16732
D	412	ASN	PHE	conflict	UNP P16732
D	413	LEU	MET	conflict	UNP P16732
D	414	TYR	ASP	conflict	UNP P16732
D	415	PHE	GLU	conflict	UNP P16732
D	416	GLN	ILE	conflict	UNP P16732
D	417	GLY	ILE	conflict	UNP P16732

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mn 2 2	0	0
2	A	3	Total Mn 3 3	0	0
2	D	2	Total Mn 2 2	0	0
2	C	3	Total Mn 3 3	0	0

- Molecule 3 is 4-[(4-fluorophenyl)methyl-methyl-amino]-2,4-bis(oxidanylidene)butanoic acid (three-letter code: C3W) (formula: C<sub>12</sub>H<sub>12</sub>FNO<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			18	12	1	1	4		
3	B	1	Total	C	F	N	O	0	0
			18	12	1	1	4		
3	C	1	Total	C	F	N	O	0	0
			18	12	1	1	4		
3	D	1	Total	C	F	N	O	0	0
			18	12	1	1	4		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

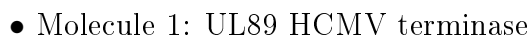
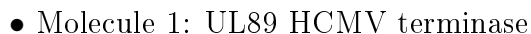
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

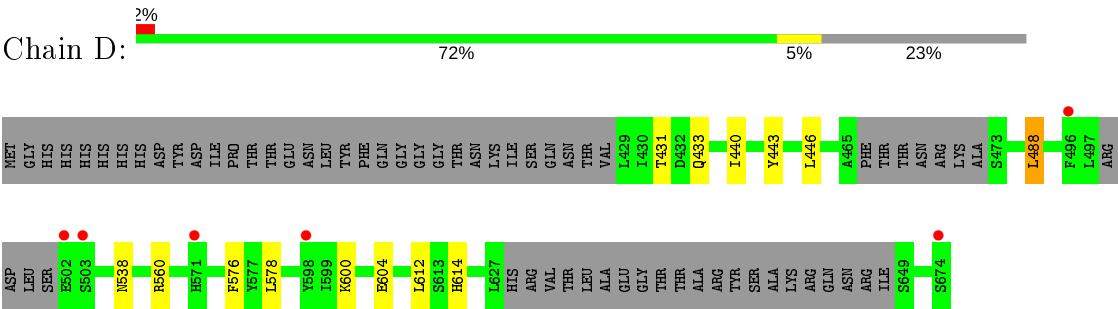
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	12	Total	O	0	0
			12	12		
5	C	3	Total	O	0	0
			3	3		
5	D	4	Total	O	0	0
			4	4		



- Molecule 1: UL89 HCMV terminase



● Molecule 1: UL89 HCMV terminase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.65Å 87.65Å 186.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.90 29.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.87-2.90) 98.9 (29.87-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.10.3, REFMAC	Depositor
R, $R_{free}$	0.175 , 0.198 0.191 , 0.210	Depositor DCC
$R_{free}$ test set	1503 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	84.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 62.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: C3W, MN, CL

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	0.52	0/1760	0.70	0/2394
1	B	0.52	0/1814	0.66	0/2463
1	C	0.51	0/1721	0.68	0/2341
1	D	0.51	0/1664	0.68	0/2262
All	All	0.52	0/6959	0.68	0/9460

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	1724	0	1630	13	0
1	B	1775	0	1717	12	0
1	C	1688	0	1594	17	0
1	D	1633	0	1548	13	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
3	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	18	0	0	0	0
3	C	18	0	0	0	0
3	D	18	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	0	0	0
5	B	12	0	0	1	0
5	C	3	0	0	0	0
5	D	4	0	0	0	0
All	All	6928	0	6489	47	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 4.

All (47) 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:B:566:THR:HG22	1:B:576:PHE:O	1.78	0.82
1:C:440:ILE:CG2	1:D:443:TYR:HD1	1.97	0.78
1:A:664:ASP:HB3	1:A:666:ILE:HD12	1.67	0.76
1:C:440:ILE:HG22	1:D:443:TYR:HD1	1.51	0.75
1:C:669:ILE:H	1:C:669:ILE:HD12	1.61	0.66
1:A:610:ILE:HG22	1:A:611:LYS:H	1.63	0.64
1:D:576:PHE:HE1	1:D:578:LEU:HG	1.67	0.59
1:D:612:LEU:C	1:D:614:HIS:H	2.05	0.59
1:B:607:SER:O	1:B:611:LYS:HB2	2.04	0.58
1:D:443:TYR:CE2	1:D:600:LYS:HB2	2.39	0.57
1:C:607:SER:O	1:C:611:LYS:HB2	2.04	0.57
1:D:446:LEU:HD22	1:D:604:GLU:HG2	1.88	0.56
1:C:440:ILE:CG2	1:D:443:TYR:CD1	2.86	0.54
1:C:467:THR:HG22	1:C:472:ALA:HA	1.88	0.54
1:C:583:LYS:O	1:C:587:VAL:HG23	2.09	0.52
1:C:448:THR:HB	1:D:440:ILE:HG21	1.92	0.52
1:A:443:TYR:CE2	1:A:600:LYS:HB2	2.45	0.51
1:A:443:TYR:HE2	1:A:600:LYS:HB2	1.75	0.51
1:B:464:PRO:HA	1:B:475:THR:HG23	1.92	0.51
1:D:443:TYR:HE2	1:D:600:LYS:HB2	1.75	0.51
1:C:440:ILE:HG22	1:D:443:TYR:CD1	2.39	0.50
1:C:563:PHE:O	1:C:565:HIS:HD2	1.95	0.49
1:D:431:THR:HG22	1:D:433:GLN:H	1.76	0.49
1:C:448:THR:HB	1:D:440:ILE:CG2	2.42	0.49
1:B:588:GLU:HG2	1:C:592:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:PHE:O	1:A:565:HIS:HD2	1.94	0.49
1:C:461:TYR:HD2	1:C:655:ALA:HA	1.78	0.48
1:B:458:LEU:HD11	1:B:479:ALA:HB1	1.95	0.47
1:A:458:LEU:HD11	1:A:479:ALA:HB1	1.96	0.46
1:A:466:PHE:HD1	1:A:537:THR:HG23	1.80	0.46
1:A:488:LEU:HA	1:A:600:LYS:O	2.16	0.46
1:C:621:LEU:O	1:C:625:GLN:HG2	2.16	0.46
1:B:660:THR:O	1:B:663:CYS:HB2	2.17	0.45
1:A:664:ASP:HB3	1:A:666:ILE:CD1	2.44	0.45
1:D:488:LEU:HA	1:D:600:LYS:O	2.17	0.45
1:A:516:ILE:O	1:A:519:VAL:HG22	2.17	0.44
1:B:466:PHE:O	1:B:473:SER:HB3	2.17	0.44
1:C:443:TYR:HB2	1:C:488:LEU:HD21	1.98	0.44
1:B:437:GLU:HG2	1:B:441:LEU:HD12	1.99	0.44
1:B:438:PHE:CE2	1:B:617:ILE:HG23	2.52	0.43
1:A:605:LEU:HD13	1:A:617:ILE:HD11	2.00	0.42
1:B:588:GLU:OE2	1:B:629:ARG:HD3	2.19	0.42
1:B:666:ILE:HA	1:C:666:ILE:HD11	2.02	0.42
1:A:442:ARG:NH1	1:A:617:ILE:HD13	2.35	0.42
1:C:461:TYR:CD2	1:C:655:ALA:HA	2.55	0.41
1:B:654:ILE:HD12	5:B:805:HOH:O	2.19	0.41
1:A:475:THR:HG21	1:A:508:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	219/279 (78%)	211 (96%)	7 (3%)	1 (0%)	29	61
1	B	220/279 (79%)	213 (97%)	7 (3%)	0	100	100
1	C	213/279 (76%)	208 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	206/279 (74%)	196 (95%)	10 (5%)	0	100	100
All	All	858/1116 (77%)	828 (96%)	29 (3%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	610	ILE

### 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	170/242 (70%)	166 (98%)	4 (2%)	49	79
1	B	183/242 (76%)	179 (98%)	4 (2%)	52	81
1	C	169/242 (70%)	166 (98%)	3 (2%)	59	85
1	D	164/242 (68%)	161 (98%)	3 (2%)	59	85
All	All	686/968 (71%)	672 (98%)	14 (2%)	55	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	488	LEU
1	A	547	CYS
1	A	559	ILE
1	A	560	ARG
1	B	592	SER
1	B	651	ASP
1	B	663	CYS
1	B	672	ARG
1	C	499	ASP
1	C	578	LEU
1	C	669	ILE
1	D	488	LEU
1	D	538	ASN

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Mol	Chain	Res	Type
1	D	560	ARG

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

Mol	Chain	Res	Type
1	A	565	HIS
1	B	447	ASN
1	C	565	HIS
1	D	538	ASN
1	D	623	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	$\# Z  > 2$
3	C3W	C	704	2	15,18,18	0.49	0	18,24,24	0.40	0
3	C3W	B	703	2	15,18,18	0.46	0	18,24,24	0.37	0
3	C3W	A	704	2	15,18,18	0.41	0	18,24,24	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	C3W	D	703	2	15,18,18	0.48	0	18,24,24	0.37	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	C3W	C	704	2	-	0/12/16/16	0/1/1/1
3	C3W	B	703	2	-	0/12/16/16	0/1/1/1
3	C3W	A	704	2	-	0/12/16/16	0/1/1/1
3	C3W	D	703	2	-	0/12/16/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	225/279 (80%)	0.19	15 (6%) 17 13	58, 87, 138, 168	1 (0%)
1	B	227/279 (81%)	-0.14	6 (2%) 56 52	55, 80, 123, 154	1 (0%)
1	C	221/279 (79%)	0.08	14 (6%) 20 16	61, 88, 128, 166	1 (0%)
1	D	214/279 (76%)	-0.04	6 (2%) 53 49	60, 85, 126, 153	1 (0%)
All	All	887/1116 (79%)	0.02	41 (4%) 32 29	55, 85, 134, 168	4 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	501	SER	6.6
1	C	571	HIS	4.4
1	C	568	ASP	3.9
1	C	570	ASN	3.5
1	C	503	SER	3.5
1	D	571	HIS	3.3
1	B	569	GLN	3.3
1	C	504	SER	3.1
1	A	571	HIS	3.1
1	A	466	PHE	3.0
1	A	501	SER	3.0
1	C	569	GLN	3.0
1	A	451	TYR	2.9
1	C	612	LEU	2.9
1	C	499	ASP	2.9
1	B	571	HIS	2.8
1	A	502	GLU	2.8
1	A	478	ALA	2.8
1	A	572	ILE	2.8
1	C	572	ILE	2.7
1	D	503	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	466	PHE	2.6
1	C	648	ILE	2.6
1	A	499	ASP	2.6
1	A	570	ASN	2.5
1	D	496	PHE	2.5
1	A	472	ALA	2.4
1	C	449	ASN	2.4
1	C	567	PRO	2.4
1	A	505	GLU	2.4
1	A	629	ARG	2.3
1	D	502	GLU	2.1
1	D	674	SER	2.1
1	A	461	TYR	2.1
1	C	498	ARG	2.1
1	C	479	ALA	2.1
1	B	502	GLU	2.1
1	B	453	TYR	2.0
1	D	598	TYR	2.0
1	A	656	VAL	2.0
1	A	446	LEU	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 carbohydrates 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	MN	C	703	1/1	0.74	0.08	133,133,133,133	0
4	CL	D	704	1/1	0.84	0.17	131,131,131,131	0
2	MN	A	703	1/1	0.89	0.08	140,140,140,140	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C3W	C	704	18/18	0.91	0.21	114,119,127,127	0
3	C3W	B	703	18/18	0.92	0.26	121,127,133,133	0
3	C3W	D	703	18/18	0.94	0.20	119,122,132,132	0
3	C3W	A	704	18/18	0.95	0.21	128,132,138,138	0
2	MN	D	702	1/1	0.95	0.13	91,91,91,91	0
2	MN	C	702	1/1	0.96	0.06	94,94,94,94	0
2	MN	A	701	1/1	0.97	0.16	96,96,96,96	0
2	MN	B	701	1/1	0.98	0.12	80,80,80,80	0
2	MN	B	702	1/1	0.98	0.09	81,81,81,81	0
2	MN	A	702	1/1	0.98	0.13	93,93,93,93	0
2	MN	C	701	1/1	0.99	0.15	87,87,87,87	0
2	MN	D	701	1/1	0.99	0.14	101,101,101,101	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.