



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 03:14 am BST

PDB ID : 3N4P
Title : Human cytomegalovirus terminase nuclease domain
Authors : Nadal, M.; Mas, P.J.; Blanco, A.G.; Arnan, C.; Sola, M.; Hart, D.J.; Coll, M.
Deposited on : 2010-05-22
Resolution : 2.15 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
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

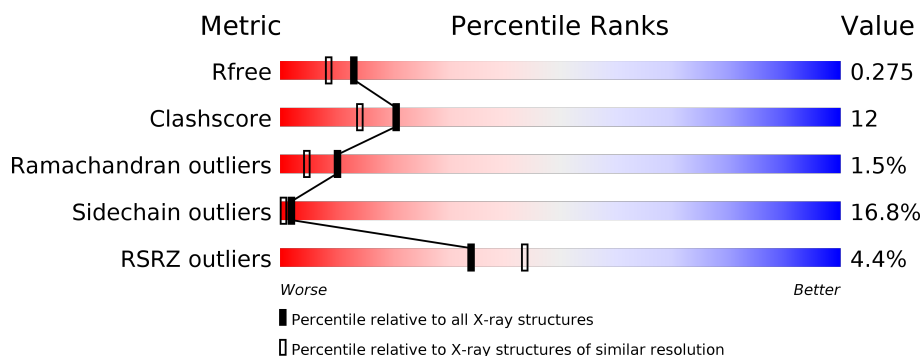
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 ≥ 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>4%</div> <div> <div></div> <div>51%</div> <div>23%</div> <div>• •</div> <div>23%</div> </div> </div>
1	B	279	<div> <div>4%</div> <div> <div></div> <div>53%</div> <div>20%</div> <div>8%</div> <div>19%</div> </div> </div>
1	C	279	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>19%</div> <div>5%</div> <div>22%</div> </div> </div>
1	D	279	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>20%</div> <div>6%</div> <div>•</div> <div>24%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7146 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 Terminase subunit UL89 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1736	1113	292	325	6			
1	B	227	Total	C	N	O	S	0	1	0
			1838	1176	315	341	6			
1	C	218	Total	C	N	O	S	0	0	0
			1747	1120	292	329	6			
1	D	212	Total	C	N	O	S	0	1	0
			1720	1103	290	321	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	MET	-	EXPRESSION TAG	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	-	EXPRESSION TAG	UNP P16732
A	401	HIS	-	EXPRESSION TAG	UNP P16732
A	402	HIS	-	EXPRESSION TAG	UNP P16732
A	403	HIS	-	EXPRESSION TAG	UNP P16732
A	404	ASP	-	EXPRESSION TAG	UNP P16732
A	405	TYR	-	EXPRESSION TAG	UNP P16732
A	406	ASP	-	EXPRESSION TAG	UNP P16732
A	407	ILE	-	EXPRESSION TAG	UNP P16732
A	408	PRO	-	EXPRESSION TAG	UNP P16732
A	409	THR	-	EXPRESSION TAG	UNP P16732
A	410	THR	-	EXPRESSION TAG	UNP P16732
A	411	GLU	-	EXPRESSION TAG	UNP P16732
A	412	ASN	-	EXPRESSION TAG	UNP P16732
A	413	LEU	-	EXPRESSION TAG	UNP P16732
A	414	TYR	-	EXPRESSION TAG	UNP P16732
A	415	PHE	-	EXPRESSION TAG	UNP P16732
A	416	GLN	-	EXPRESSION TAG	UNP P16732

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	417	GLY	-	EXPRESSION TAG	UNP P16732
B	396	MET	-	EXPRESSION TAG	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	-	EXPRESSION TAG	UNP P16732
B	401	HIS	-	EXPRESSION TAG	UNP P16732
B	402	HIS	-	EXPRESSION TAG	UNP P16732
B	403	HIS	-	EXPRESSION TAG	UNP P16732
B	404	ASP	-	EXPRESSION TAG	UNP P16732
B	405	TYR	-	EXPRESSION TAG	UNP P16732
B	406	ASP	-	EXPRESSION TAG	UNP P16732
B	407	ILE	-	EXPRESSION TAG	UNP P16732
B	408	PRO	-	EXPRESSION TAG	UNP P16732
B	409	THR	-	EXPRESSION TAG	UNP P16732
B	410	THR	-	EXPRESSION TAG	UNP P16732
B	411	GLU	-	EXPRESSION TAG	UNP P16732
B	412	ASN	-	EXPRESSION TAG	UNP P16732
B	413	LEU	-	EXPRESSION TAG	UNP P16732
B	414	TYR	-	EXPRESSION TAG	UNP P16732
B	415	PHE	-	EXPRESSION TAG	UNP P16732
B	416	GLN	-	EXPRESSION TAG	UNP P16732
B	417	GLY	-	EXPRESSION TAG	UNP P16732
C	396	MET	-	EXPRESSION TAG	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	-	EXPRESSION TAG	UNP P16732
C	401	HIS	-	EXPRESSION TAG	UNP P16732
C	402	HIS	-	EXPRESSION TAG	UNP P16732
C	403	HIS	-	EXPRESSION TAG	UNP P16732
C	404	ASP	-	EXPRESSION TAG	UNP P16732
C	405	TYR	-	EXPRESSION TAG	UNP P16732
C	406	ASP	-	EXPRESSION TAG	UNP P16732
C	407	ILE	-	EXPRESSION TAG	UNP P16732
C	408	PRO	-	EXPRESSION TAG	UNP P16732
C	409	THR	-	EXPRESSION TAG	UNP P16732
C	410	THR	-	EXPRESSION TAG	UNP P16732
C	411	GLU	-	EXPRESSION TAG	UNP P16732
C	412	ASN	-	EXPRESSION TAG	UNP P16732
C	413	LEU	-	EXPRESSION TAG	UNP P16732
C	414	TYR	-	EXPRESSION TAG	UNP P16732

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	415	PHE	-	EXPRESSION TAG	UNP P16732
C	416	GLN	-	EXPRESSION TAG	UNP P16732
C	417	GLY	-	EXPRESSION TAG	UNP P16732
D	396	MET	-	EXPRESSION TAG	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	-	EXPRESSION TAG	UNP P16732
D	401	HIS	-	EXPRESSION TAG	UNP P16732
D	402	HIS	-	EXPRESSION TAG	UNP P16732
D	403	HIS	-	EXPRESSION TAG	UNP P16732
D	404	ASP	-	EXPRESSION TAG	UNP P16732
D	405	TYR	-	EXPRESSION TAG	UNP P16732
D	406	ASP	-	EXPRESSION TAG	UNP P16732
D	407	ILE	-	EXPRESSION TAG	UNP P16732
D	408	PRO	-	EXPRESSION TAG	UNP P16732
D	409	THR	-	EXPRESSION TAG	UNP P16732
D	410	THR	-	EXPRESSION TAG	UNP P16732
D	411	GLU	-	EXPRESSION TAG	UNP P16732
D	412	ASN	-	EXPRESSION TAG	UNP P16732
D	413	LEU	-	EXPRESSION TAG	UNP P16732
D	414	TYR	-	EXPRESSION TAG	UNP P16732
D	415	PHE	-	EXPRESSION TAG	UNP P16732
D	416	GLN	-	EXPRESSION TAG	UNP P16732
D	417	GLY	-	EXPRESSION TAG	UNP P16732

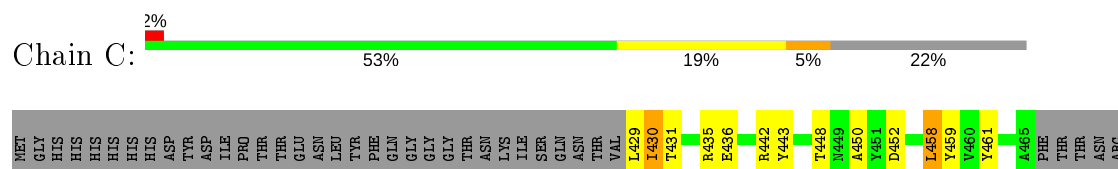
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

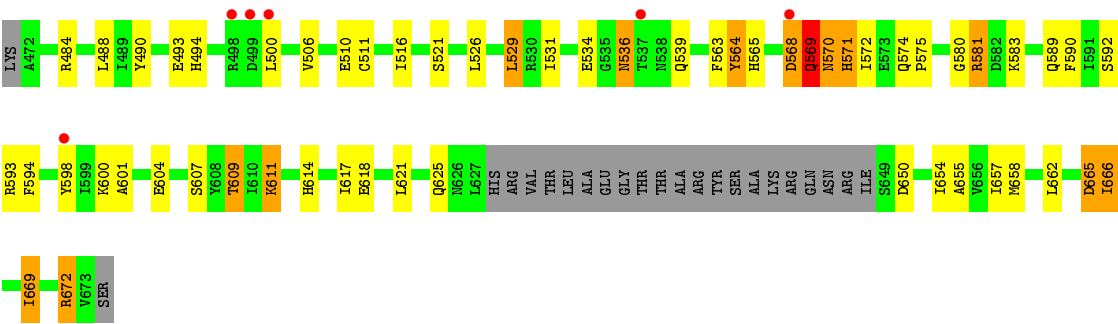
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	1	Total Mg 1 1	0	0
2	D	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0

- Molecule 3 is water.

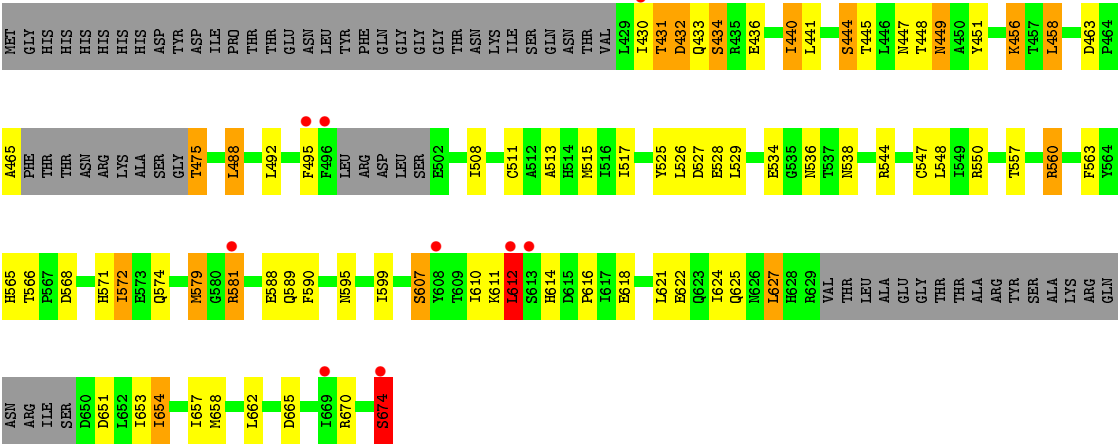
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	25	Total 25	O 25	0	0
3	C	27	Total 27	O 27	0	0
3	D	11	Total 11	O 11	0	0

- Molecule 1: Terminase subunit UL89 protein





● Molecule 1: Terminase subunit UL89 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.86 Å 87.96 Å 188.38 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.15 19.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.99-2.15) 98.7 (19.99-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.15 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.219 , 0.272 0.230 , 0.275	Depositor DCC
R_{free} test set	3760 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7146	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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

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	1.20	5/1770 (0.3%)	1.16	12/2399 (0.5%)
1	B	1.03	5/1875 (0.3%)	1.00	4/2542 (0.2%)
1	C	1.14	5/1781 (0.3%)	1.05	2/2416 (0.1%)
1	D	0.97	1/1754 (0.1%)	1.00	7/2378 (0.3%)
All	All	1.09	16/7180 (0.2%)	1.05	25/9735 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	490	TYR	CD2-CE2	6.67	1.49	1.39
1	A	671	PHE	CE2-CZ	6.45	1.49	1.37
1	A	459	TYR	CD1-CE1	6.36	1.48	1.39
1	B	443	TYR	CD1-CE1	6.03	1.48	1.39
1	C	604	GLU	CB-CG	-5.78	1.41	1.52
1	A	664	ASP	CB-CG	5.68	1.63	1.51
1	A	480	VAL	CB-CG1	5.48	1.64	1.52
1	C	564	TYR	CD1-CE1	5.40	1.47	1.39
1	C	484	ARG	CG-CD	5.35	1.65	1.51
1	B	436	GLU	CB-CG	-5.30	1.42	1.52
1	A	459	TYR	CD2-CE2	5.29	1.47	1.39
1	D	588	GLU	CG-CD	5.28	1.59	1.51
1	B	622	GLU	CG-CD	5.20	1.59	1.51
1	B	459	TYR	CD2-CE2	5.12	1.47	1.39
1	B	599	ILE	CB-CG2	5.01	1.68	1.52
1	C	459	TYR	CZ-OH	5.01	1.46	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	612	LEU	CA-CB-CG	7.74	133.10	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	LEU	CA-CB-CG	7.35	132.20	115.30
1	B	662	LEU	CA-CB-CG	7.12	131.66	115.30
1	A	560	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	662	LEU	CB-CG-CD1	6.53	122.11	111.00
1	A	527	ASP	CB-CG-OD1	6.42	124.07	118.30
1	A	582	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	D	488	LEU	CA-CB-CG	6.06	129.24	115.30
1	A	562	LEU	CB-CG-CD1	-5.86	101.03	111.00
1	B	488	LEU	CB-CG-CD1	-5.74	101.24	111.00
1	A	560	ARG	CG-CD-NE	-5.68	99.88	111.80
1	D	654	ILE	CG1-CB-CG2	-5.67	98.93	111.40
1	A	615	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	669	ILE	CG1-CB-CG2	5.58	123.69	111.40
1	D	674	SER	N-CA-CB	-5.58	102.13	110.50
1	A	582	ASP	CB-CG-OD1	5.57	123.31	118.30
1	D	599	ILE	CB-CA-C	-5.55	100.50	111.60
1	A	589	GLN	CB-CA-C	-5.50	99.40	110.40
1	C	614	HIS	CB-CA-C	-5.32	99.77	110.40
1	B	527	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	605	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	432	ASP	CB-CG-OD1	5.25	123.03	118.30
1	D	515	MET	CG-SD-CE	-5.18	91.92	100.20
1	D	440	ILE	CB-CA-C	-5.12	101.36	111.60
1	C	569	GLN	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1736	0	1707	34	0
1	B	1838	0	1813	51	0
1	C	1747	0	1721	51	0
1	D	1720	0	1688	45	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	35	0	0	2	0
3	B	25	0	0	1	0
3	C	27	0	0	1	0
3	D	11	0	0	0	0
All	All	7146	0	6929	171	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 12.

All (171) 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:D:550:ARG:HD3	1:D:674:SER:HB2	1.14	1.14
1:C:430:ILE:HD11	1:C:435:ARG:HG3	1.25	1.09
1:C:669:ILE:H	1:C:669:ILE:HD12	1.18	1.07
1:A:494:HIS:H	1:A:609:THR:HG21	1.24	1.03
1:C:430:ILE:HD11	1:C:435:ARG:CG	1.91	1.01
1:D:431:THR:HG22	1:D:434:SER:H	1.33	0.93
1:A:611:LYS:O	1:A:612:LEU:HB2	1.66	0.93
1:D:550:ARG:CD	1:D:674:SER:HB2	2.02	0.88
1:B:431:THR:HG22	1:B:434:SER:H	1.37	0.87
1:C:494:HIS:H	1:C:609:THR:CG2	1.87	0.86
1:B:588:GLU:HG2	1:C:592:SER:HA	1.57	0.85
1:C:493:GLU:OE1	1:C:609:THR:HB	1.78	0.83
1:D:440:ILE:HG22	1:D:440:ILE:O	1.80	0.82
1:D:550:ARG:HD3	1:D:674:SER:CB	2.05	0.81
1:B:539:GLN:O	1:B:543:VAL:HG23	1.80	0.81
1:C:669:ILE:H	1:C:669:ILE:CD1	1.89	0.79
1:D:432:ASP:N	1:D:432:ASP:OD1	2.13	0.79
1:D:581:ARG:HH11	1:D:581:ARG:HG3	1.47	0.79
1:D:492:LEU:O	1:D:607:SER:HB3	1.83	0.79
1:C:494:HIS:H	1:C:609:THR:HG21	1.48	0.78
1:D:440:ILE:CG2	1:D:440:ILE:O	2.31	0.78
1:C:581:ARG:HB2	1:C:581:ARG:HH11	1.49	0.77
1:A:494:HIS:H	1:A:609:THR:CG2	1.99	0.76
1:D:448:THR:C	1:D:449:ASN:HD22	1.89	0.76
1:C:581:ARG:HB2	1:C:581:ARG:NH1	2.01	0.76
1:D:449:ASN:N	1:D:449:ASN:HD22	1.80	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:HIS:N	1:A:609:THR:HG21	2.00	0.75
1:B:432:ASP:OD2	1:B:435:ARG:NH1	2.20	0.75
1:D:430:ILE:HD13	1:D:624:ILE:HG23	1.68	0.74
1:B:523:HIS:HE1	3:B:63:HOH:O	1.71	0.73
1:A:431:THR:HG22	1:A:434:SER:H	1.54	0.72
1:D:475:THR:HG23	1:D:495:PHE:O	1.90	0.71
1:C:430:ILE:CD1	1:C:435:ARG:HG3	2.16	0.70
1:C:430:ILE:HD12	1:C:431:THR:O	1.92	0.70
1:D:513:ALA:O	1:D:517:ILE:HG13	1.92	0.70
1:B:445:THR:HG21	1:B:523:HIS:CD2	2.26	0.70
1:B:566:THR:HG23	1:B:576:PHE:O	1.92	0.70
1:B:534:GLU:OE1	1:B:536:ASN:HB3	1.92	0.69
1:D:434:SER:OG	1:D:595:ASN:HA	1.92	0.69
1:A:484:ARG:NH1	1:B:436:GLU:OE1	2.26	0.69
1:C:443:TYR:HE1	1:C:600:LYS:HG3	1.58	0.68
1:C:607:SER:O	1:C:611:LYS:HB2	1.94	0.68
1:A:603:GLN:OE1	1:B:603:GLN:NE2	2.27	0.67
1:D:581:ARG:HH11	1:D:581:ARG:CG	2.08	0.67
1:B:445:THR:HB	1:B:604:GLU:OE2	1.94	0.67
1:A:465:ALA:N	1:A:475:THR:HG22	2.12	0.65
1:A:609:THR:HG23	1:A:610:ILE:HG13	1.77	0.65
1:B:534:GLU:OE1	1:B:536:ASN:CB	2.45	0.64
1:C:669:ILE:O	1:C:672:ARG:NH2	2.31	0.64
1:D:544:ARG:O	1:D:547:CYS:SG	2.53	0.64
1:D:563:PHE:CD1	1:D:674:SER:HB3	2.33	0.64
1:C:443:TYR:HD2	1:D:440:ILE:CG2	2.11	0.63
1:D:432:ASP:O	1:D:436:GLU:HG3	1.98	0.63
1:D:581:ARG:HG3	1:D:581:ARG:NH1	2.11	0.63
1:D:449:ASN:N	1:D:449:ASN:ND2	2.47	0.63
1:C:506:VAL:O	1:C:510:GLU:HG2	1.99	0.62
1:C:494:HIS:N	1:C:609:THR:HG21	2.13	0.62
1:B:536:ASN:C	1:B:536:ASN:HD22	2.02	0.62
1:C:589:GLN:O	1:C:593:ARG:HG3	2.00	0.62
1:B:536:ASN:C	1:B:536:ASN:ND2	2.53	0.61
1:B:568:ASP:CG	1:B:569:GLN:N	2.55	0.60
1:A:465:ALA:H	1:A:475:THR:CG2	2.15	0.58
1:B:444:SER:OG	1:B:603:GLN:OE1	2.22	0.58
1:C:443:TYR:CE1	1:C:600:LYS:HG3	2.39	0.57
1:C:601:ALA:HB1	1:C:617:ILE:HD11	1.86	0.57
1:A:493:GLU:OE1	1:A:609:THR:HG22	2.06	0.56
1:B:660:THR:O	1:B:663:CYS:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:590:PHE:CG	1:C:657:ILE:HG12	2.42	0.55
1:B:588:GLU:HG2	1:C:592:SER:CB	2.37	0.55
1:C:650:ASP:O	1:C:654:ILE:HG13	2.07	0.55
1:C:458:LEU:HG	1:C:526:LEU:HD13	1.89	0.54
1:D:579:MET:HE1	1:D:658:MET:SD	2.48	0.54
1:B:588:GLU:HG2	1:C:592:SER:CA	2.35	0.54
1:B:569:GLN:C	1:B:571:HIS:H	2.10	0.53
1:C:461:TYR:OH	1:C:534:GLU:HG3	2.07	0.53
1:A:455:GLY:HA2	3:A:15:HOH:O	2.09	0.53
1:C:583:LYS:HA	1:C:658:MET:HE1	1.91	0.53
1:A:539:GLN:O	1:A:543:VAL:HG23	2.09	0.53
1:B:445:THR:HG21	1:B:523:HIS:HD2	1.74	0.53
1:B:568:ASP:CG	1:B:569:GLN:H	2.11	0.53
1:C:516:ILE:HG21	1:C:529:LEU:HD11	1.91	0.52
1:D:434:SER:HG	1:D:595:ASN:HA	1.74	0.51
1:A:432:ASP:N	1:A:432:ASP:OD1	2.39	0.51
1:D:444:SER:HB3	1:D:447:ASN:HD22	1.74	0.51
1:C:618:GLU:HG3	3:C:96:HOH:O	2.11	0.50
1:D:611:LYS:HD3	1:D:612:LEU:HD12	1.93	0.50
1:B:536:ASN:HD22	1:B:537:THR:N	2.09	0.50
1:B:563:PHE:CD1	1:B:674:SER:HB3	2.46	0.50
1:C:443:TYR:HD2	1:D:440:ILE:HG22	1.76	0.50
1:C:565:HIS:HA	1:C:574:GLN:O	2.11	0.50
1:C:654:ILE:O	1:C:658:MET:HG2	2.11	0.50
1:A:465:ALA:N	1:A:475:THR:CG2	2.75	0.50
1:A:523:HIS:HB3	1:A:525:TYR:CE1	2.47	0.50
1:C:448:THR:HB	1:C:450:ALA:H	1.76	0.50
1:C:443:TYR:HD2	1:D:440:ILE:HG21	1.76	0.49
1:A:562:LEU:N	1:A:562:LEU:HD12	2.27	0.49
1:B:429:LEU:HD11	1:B:627:LEU:O	2.13	0.49
1:C:669:ILE:N	1:C:669:ILE:HD12	2.04	0.48
1:B:588:GLU:HG2	1:C:592:SER:HB2	1.96	0.48
1:A:462:LEU:N	1:A:462:LEU:HD23	2.28	0.48
1:D:610:ILE:HG22	1:D:610:ILE:O	2.13	0.48
1:B:554:GLN:HE21	1:B:561:VAL:HG23	1.78	0.47
1:A:483:TYR:CZ	1:A:484:ARG:HD2	2.49	0.47
1:C:568:ASP:HB2	1:C:572:ILE:HG23	1.96	0.47
1:D:624:ILE:O	1:D:627:LEU:HB2	2.13	0.47
1:C:534:GLU:OE2	1:C:536:ASN:ND2	2.48	0.47
1:C:430:ILE:HD13	1:C:594:PHE:CE2	2.50	0.47
1:C:621:LEU:O	1:C:625:GLN:HG2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:ARG:NH1	1:C:617:ILE:HD12	2.29	0.47
1:C:593:ARG:HB3	1:C:598:TYR:HB2	1.97	0.47
1:B:513:ALA:HB1	1:B:552:SER:HB2	1.97	0.46
1:A:464:PRO:HA	1:A:475:THR:HG22	1.96	0.46
1:D:563:PHE:HD1	1:D:674:SER:HB3	1.75	0.46
1:B:492:LEU:HB3	1:B:652:LEU:HD21	1.96	0.46
1:D:463:ASP:HA	1:D:534:GLU:HB3	1.98	0.46
1:D:534:GLU:OE2	1:D:536[B]:ASN:CG	2.54	0.46
1:A:488:LEU:HD12	1:A:488:LEU:H	1.81	0.45
1:A:565:HIS:O	1:A:670:ARG:NH1	2.48	0.45
1:A:441:LEU:HD13	1:A:600:LYS:HE2	1.99	0.45
1:B:539:GLN:HG2	1:B:539:GLN:H	1.56	0.45
1:B:458:LEU:HB3	1:B:529:LEU:HD23	1.97	0.45
1:B:560:ARG:HG2	1:B:560:ARG:H	1.55	0.45
1:D:458:LEU:HG	1:D:526:LEU:HD13	1.99	0.45
1:D:566:THR:HA	1:D:670:ARG:HH12	1.82	0.45
1:B:430:ILE:O	1:B:430:ILE:CG2	2.65	0.45
1:D:572:ILE:HG13	1:D:574:GLN:HE21	1.82	0.44
1:B:495:PHE:CZ	1:B:507:ALA:HB1	2.52	0.44
1:B:665:ASP:N	1:B:665:ASP:OD1	2.50	0.44
1:C:564:TYR:O	1:C:575:PRO:HA	2.17	0.44
1:B:605:LEU:O	1:B:611:LYS:NZ	2.51	0.44
1:B:430:ILE:O	1:B:430:ILE:HG23	2.17	0.44
1:C:570:ASN:OD1	1:C:572:ILE:HG22	2.17	0.44
1:A:497:LEU:HD11	1:A:508:ILE:HD11	1.99	0.44
1:B:563:PHE:HD1	1:B:674:SER:HB3	1.82	0.44
1:C:666:ILE:HD12	1:C:666:ILE:HA	1.79	0.44
1:B:620:LEU:HD13	1:B:652:LEU:HD13	2.00	0.43
1:B:629:ARG:O	1:B:630:VAL:HB	2.18	0.43
1:D:590:PHE:CG	1:D:657:ILE:HG12	2.54	0.43
1:C:672:ARG:HE	1:C:672:ARG:HB2	1.53	0.43
1:B:433:GLN:NE2	1:B:437:GLU:OE2	2.39	0.43
1:A:450:ALA:O	1:A:451:TYR:HB2	2.19	0.43
1:C:461:TYR:CD2	1:C:655:ALA:HA	2.54	0.43
1:B:646:ASN:OD1	1:B:646:ASN:N	2.51	0.43
1:D:444:SER:CB	1:D:447:ASN:HD22	2.32	0.42
1:B:458:LEU:HG	1:B:526:LEU:HD13	2.00	0.42
1:D:579:MET:HB2	1:D:579:MET:HE3	1.63	0.42
1:A:502:GLU:HB2	1:A:503:SER:H	1.45	0.42
1:B:588:GLU:HB3	1:C:592:SER:HB2	2.00	0.42
1:A:464:PRO:HA	1:A:475:THR:CG2	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:ILE:HG13	1:A:669:ILE:H	1.62	0.42
1:B:534:GLU:OE1	1:B:536:ASN:HB2	2.19	0.42
1:B:513:ALA:CB	1:B:552:SER:HB2	2.49	0.42
1:B:554:GLN:NE2	1:B:561:VAL:HG23	2.34	0.42
1:D:528:GLU:HG3	1:D:560:ARG:HB3	2.02	0.42
1:A:458:LEU:HD11	1:A:479:ALA:HB1	2.01	0.42
1:A:529:LEU:HD12	1:A:561:VAL:HG22	2.02	0.42
1:C:611:LYS:HZ2	1:C:611:LYS:HG2	1.59	0.42
1:D:451:TYR:CE2	1:D:525:TYR:CD1	3.08	0.41
1:C:531:ILE:O	1:C:563:PHE:HA	2.20	0.41
1:A:449:ASN:ND2	3:A:97:HOH:O	2.49	0.41
1:B:627:LEU:HA	1:B:627:LEU:HD23	1.93	0.41
1:D:572:ILE:H	1:D:572:ILE:HG12	1.68	0.41
1:A:611:LYS:O	1:A:612:LEU:CB	2.52	0.41
1:D:565:HIS:HA	1:D:574:GLN:O	2.20	0.41
1:A:544:ARG:O	1:A:548:LEU:HG	2.20	0.41
1:D:465:ALA:H	1:D:475:THR:HB	1.86	0.40
1:A:488:LEU:HD12	1:A:488:LEU:N	2.36	0.40
1:B:650:ASP:OD2	1:B:654:ILE:HD11	2.20	0.40
1:D:456:LYS:HB3	1:D:527:ASP:OD1	2.21	0.40
1:B:624:ILE:HG13	1:B:653:ILE:HD13	2.04	0.40
1:B:572:ILE:HD13	1:B:573:GLU:H	1.87	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	208/279 (75%)	196 (94%)	9 (4%)	3 (1%)	11	5
1	B	222/279 (80%)	206 (93%)	13 (6%)	3 (1%)	11	5
1	C	212/279 (76%)	204 (96%)	3 (1%)	5 (2%)	6	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	205/279 (74%)	190 (93%)	13 (6%)	2 (1%)	15	9
All	All	847/1116 (76%)	796 (94%)	38 (4%)	13 (2%)	10	5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	GLN
1	A	612	LEU
1	B	467	THR
1	C	571	HIS
1	C	569	GLN
1	C	580	GLY
1	D	612	LEU
1	A	537	THR
1	B	468	THR
1	C	568	ASP
1	C	665	ASP
1	D	571	HIS
1	B	570	ASN

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	188/242 (78%)	156 (83%)	32 (17%)	2	0
1	B	199/242 (82%)	165 (83%)	34 (17%)	2	0
1	C	189/242 (78%)	166 (88%)	23 (12%)	5	2
1	D	186/242 (77%)	147 (79%)	39 (21%)	1	0
All	All	762/968 (79%)	634 (83%)	128 (17%)	2	0

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	429	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	431	THR
1	A	432	ASP
1	A	441	LEU
1	A	448	THR
1	A	452	ASP
1	A	462	LEU
1	A	488	LEU
1	A	501	SER
1	A	502	GLU
1	A	504	SER
1	A	510	GLU
1	A	515	MET
1	A	537	THR
1	A	552	SER
1	A	555	SER
1	A	568	ASP
1	A	579	MET
1	A	583	LYS
1	A	602	SER
1	A	605	LEU
1	A	612	LEU
1	A	617	ILE
1	A	618	GLU
1	A	621	LEU
1	A	627	LEU
1	A	629	ARG
1	A	653	ILE
1	A	662	LEU
1	A	665	ASP
1	A	669	ILE
1	A	672	ARG
1	B	431	THR
1	B	444	SER
1	B	445	THR
1	B	452	ASP
1	B	458	LEU
1	B	468	THR
1	B	470	ARG
1	B	471	LYS
1	B	473	SER
1	B	485	HIS
1	B	488	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	497	LEU
1	B	511	CYS
1	B	534	GLU
1	B	536	ASN
1	B	537	THR
1	B	539	GLN
1	B	560	ARG
1	B	561	VAL
1	B	572	ILE
1	B	578	LEU
1	B	579	MET
1	B	581	ARG
1	B	583	LYS
1	B	605	LEU
1	B	611	LYS
1	B	621	LEU
1	B	625	GLN
1	B	627	LEU
1	B	646	ASN
1	B	652	LEU
1	B	662	LEU
1	B	665	ASP
1	B	674	SER
1	C	429	LEU
1	C	430	ILE
1	C	436	GLU
1	C	452	ASP
1	C	458	LEU
1	C	488	LEU
1	C	500	LEU
1	C	511	CYS
1	C	521	SER
1	C	529	LEU
1	C	536	ASN
1	C	539	GLN
1	C	569	GLN
1	C	570	ASN
1	C	571	HIS
1	C	581	ARG
1	C	609	THR
1	C	611	LYS
1	C	662	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	665	ASP
1	C	666	ILE
1	C	669	ILE
1	C	672	ARG
1	D	431	THR
1	D	432	ASP
1	D	433	GLN
1	D	434	SER
1	D	441	LEU
1	D	444	SER
1	D	445	THR
1	D	449	ASN
1	D	456	LYS
1	D	458	LEU
1	D	475	THR
1	D	488	LEU
1	D	508	ILE
1	D	511	CYS
1	D	529	LEU
1	D	538	ASN
1	D	548	LEU
1	D	557	THR
1	D	560	ARG
1	D	568	ASP
1	D	572	ILE
1	D	579	MET
1	D	581	ARG
1	D	589	GLN
1	D	607	SER
1	D	612	LEU
1	D	614	HIS
1	D	616	PRO
1	D	618	GLU
1	D	621	LEU
1	D	622	GLU
1	D	625	GLN
1	D	627	LEU
1	D	651	ASP
1	D	653	ILE
1	D	654	ILE
1	D	662	LEU
1	D	665	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	674	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	449	ASN
1	A	551	GLN
1	A	570	ASN
1	A	589	GLN
1	B	469	ASN
1	B	523	HIS
1	B	536	ASN
1	B	539	GLN
1	B	554	GLN
1	B	565	HIS
1	B	574	GLN
1	B	646	ASN
1	C	447	ASN
1	C	539	GLN
1	C	625	GLN
1	D	447	ASN
1	D	449	ASN
1	D	538	ASN
1	D	554	GLN
1	D	625	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	216/279 (77%)	0.54	11 (5%) 28 36	28, 53, 94, 132	2 (0%)
1	B	227/279 (81%)	0.64	12 (5%) 26 35	36, 62, 112, 137	2 (0%)
1	C	218/279 (78%)	0.52	6 (2%) 53 62	31, 63, 101, 138	1 (0%)
1	D	212/279 (75%)	0.64	9 (4%) 36 45	39, 73, 108, 139	6 (2%)
All	All	873/1116 (78%)	0.59	38 (4%) 34 43	28, 62, 104, 139	11 (1%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	497	LEU	12.9
1	C	500	LEU	8.9
1	D	612	LEU	8.2
1	B	469	ASN	6.7
1	B	471	LYS	6.0
1	B	468	THR	5.9
1	A	612	LEU	5.5
1	B	467	THR	5.4
1	A	502	GLU	5.1
1	D	674	SER	4.8
1	B	466	PHE	4.8
1	B	470	ARG	4.2
1	B	472	ALA	4.0
1	D	496	PHE	3.8
1	A	501	SER	3.8
1	D	495	PHE	3.3
1	B	674	SER	3.3
1	D	613	SER	3.2
1	C	598	TYR	3.1
1	A	450	ALA	2.9
1	B	497	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	498	ARG	2.5
1	C	537	THR	2.5
1	C	568	ASP	2.5
1	A	568	ASP	2.5
1	A	610	ILE	2.4
1	B	630	VAL	2.4
1	B	648	ILE	2.3
1	D	608	TYR	2.2
1	A	496	PHE	2.2
1	A	571	HIS	2.2
1	B	485	HIS	2.2
1	D	430	ILE	2.1
1	D	669	ILE	2.1
1	A	570	ASN	2.1
1	D	581	ARG	2.1
1	A	651	ASP	2.0
1	C	499	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	B	1	1/1	0.41	0.31	151,151,151,151	0
2	MG	C	2	1/1	0.45	0.35	130,130,130,130	0
2	MG	A	4	1/1	0.54	0.39	100,100,100,100	0
2	MG	C	7	1/1	0.55	0.23	102,102,102,102	0
2	MG	B	5	1/1	0.77	0.21	96,96,96,96	0
2	MG	D	6	1/1	0.81	0.40	130,130,130,130	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	D	3	1/1	0.82	0.24	122,122,122,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.