



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:03 AM GMT

PDB ID : 3N4Q
Title : Human cytomegalovirus terminase nuclease domain, Mn soaked
Authors : Nadal, M.; Mas, P.J.; Blanco, A.G.; Arnan, C.; Sola, M.; Hart, D.J.; Coll, M.
Deposited on : 2010-05-22
Resolution : 3.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

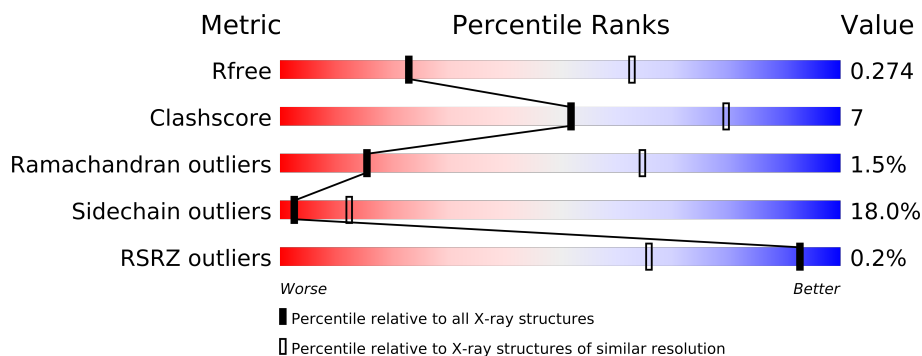
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.20 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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	279	
1	B	279	
1	C	279	
1	D	279	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7056 atoms, of which 0 are hydrogen and 0 are deuterium.

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	221	Total	C	N	O	S	0	0	0
			1775	1137	301	331	6			
1	C	219	Total	C	N	O	S	0	0	0
			1755	1126	293	330	6			
1	D	214	Total	C	N	O	S	0	0	0
			1722	1104	290	322	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 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	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0

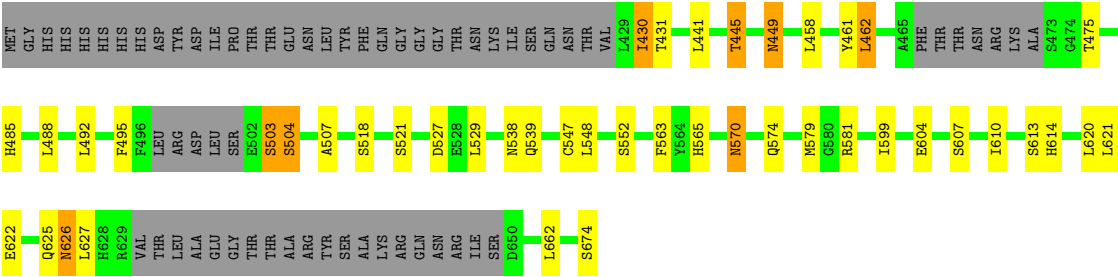
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total 11	O 11	0	0
4	B	17	Total 17	O 17	0	0
4	C	15	Total 15	O 15	0	0
4	D	13	Total 13	O 13	0	0

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.70Å 88.10Å 190.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.05 – 3.20 44.05 – 3.19	Depositor EDS
% Data completeness (in resolution range)	89.6 (44.05-3.20) 89.6 (44.05-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.90 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.207 , 0.283 0.201 , 0.274	Depositor DCC
R_{free} test set	1109 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.820	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.6	EDS
Estimated twinning fraction	0.046 for k,h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 21659 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7056	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.61	0/1770	0.75	1/2399 (0.0%)
1	B	0.58	1/1809 (0.1%)	0.74	2/2452 (0.1%)
1	C	0.58	0/1789	0.74	3/2427 (0.1%)
1	D	0.55	0/1756	0.69	0/2380
All	All	0.58	1/7124 (0.0%)	0.73	6/9658 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	622	GLU	CG-CD	5.10	1.59	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	488	LEU	CA-CB-CG	7.49	132.52	115.30
1	C	458	LEU	CA-CB-CG	6.16	129.46	115.30
1	B	605	LEU	CA-CB-CG	5.69	128.38	115.30
1	C	569	GLN	N-CA-C	-5.46	96.27	111.00
1	B	578	LEU	CA-CB-CG	5.35	127.60	115.30
1	C	462	LEU	CA-CB-CG	5.28	127.43	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1736	0	0	9	0
1	B	1775	0	0	17	0
1	C	1755	0	0	12	0
1	D	1722	0	0	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	11	0	0	0	0
4	B	17	0	0	2	0
4	C	15	0	0	1	0
4	D	13	0	0	1	0
All	All	7056	0	0	50	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (50) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:538:ASN:OD1	1:A:541:ALA:N	2.15	0.79
1:B:664:ASP:CB	4:B:18:HOH:O	2.30	0.78
1:C:583:LYS:NZ	4:C:37:HOH:O	2.27	0.67
1:B:568:ASP:CG	1:B:569:GLN:N	2.49	0.65
1:A:432:ASP:OD1	1:A:432:ASP:N	2.32	0.62
1:C:494:HIS:O	1:C:609:THR:CG2	2.50	0.60
1:B:536:ASN:OD1	1:B:579:MET:N	2.36	0.59
1:D:622:GLU:O	1:D:626:ASN:ND2	2.38	0.56
1:B:483:TYR:OH	1:B:484:ARG:NH1	2.41	0.54
1:B:590:PHE:O	1:B:594:PHE:N	2.44	0.51
1:A:570:ASN:O	1:A:572:ILE:N	2.44	0.51
1:B:615:ASP:O	1:B:616:PRO:C	2.50	0.49
1:B:432:ASP:OD1	1:B:432:ASP:N	2.45	0.49
1:D:503:SER:O	1:D:507:ALA:N	2.46	0.48
1:B:565:HIS:O	1:B:670:ARG:NH2	2.46	0.48
1:D:461:TYR:CD2	1:D:462:LEU:N	2.82	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:576:PHE:C	1:C:576:PHE:CD2	2.87	0.47
1:A:456:LYS:O	1:A:526:LEU:CD2	2.63	0.47
1:C:624:ILE:O	1:C:626:ASN:N	2.47	0.47
1:C:667:HIS:O	1:C:668:ALA:C	2.53	0.46
1:D:570:ASN:OD1	1:D:570:ASN:N	2.48	0.46
1:B:590:PHE:O	1:B:591:ILE:C	2.52	0.46
1:C:536:ASN:ND2	1:C:536:ASN:N	2.63	0.46
1:C:590:PHE:O	1:C:591:ILE:C	2.54	0.45
1:A:553:VAL:O	1:A:556:SER:N	2.50	0.45
1:D:620:LEU:C	1:D:622:GLU:N	2.69	0.45
1:C:459:TYR:N	1:C:480:VAL:O	2.50	0.45
1:A:475:THR:O	1:A:494:HIS:CD2	2.70	0.45
1:B:627:LEU:O	1:B:628:HIS:ND1	2.51	0.44
1:C:568:ASP:OD1	1:C:569:GLN:N	2.51	0.44
1:D:620:LEU:O	1:D:622:GLU:N	2.50	0.44
1:D:492:LEU:O	1:D:607:SER:CB	2.66	0.44
1:D:503:SER:O	1:D:504:SER:C	2.56	0.43
1:D:430:ILE:CD1	1:D:430:ILE:N	2.82	0.43
1:B:582:ASP:O	1:B:583:LYS:C	2.57	0.43
1:D:449:ASN:N	4:D:14:HOH:O	2.51	0.43
1:A:462:LEU:N	1:A:462:LEU:CD2	2.81	0.43
1:B:601:ALA:N	4:B:1:HOH:O	2.52	0.43
1:A:611:LYS:O	1:A:612:LEU:CB	2.66	0.42
1:C:667:HIS:O	1:C:670:ARG:N	2.53	0.42
1:A:456:LYS:CD	1:A:525:TYR:O	2.68	0.41
1:C:452:ASP:N	1:C:452:ASP:OD1	2.54	0.41
1:B:514:HIS:CD2	1:B:608:TYR:CD1	3.09	0.41
1:B:455:GLY:N	1:B:482:ALA:O	2.54	0.41
1:C:662:LEU:C	1:C:664:ASP:N	2.73	0.41
1:D:563:PHE:O	1:D:565:HIS:ND1	2.54	0.41
1:D:445:THR:OG1	1:D:604:GLU:OE1	2.39	0.41
1:B:629:ARG:O	1:B:630:VAL:CB	2.69	0.41
1:B:563:PHE:O	1:B:565:HIS:CD2	2.74	0.40
1:B:451:TYR:O	1:B:453:TYR:N	2.54	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	208/279 (75%)	188 (90%)	15 (7%)	5 (2%)	9	51
1	B	213/279 (76%)	182 (85%)	29 (14%)	2 (1%)	25	76
1	C	213/279 (76%)	179 (84%)	30 (14%)	4 (2%)	12	59
1	D	206/279 (74%)	178 (86%)	26 (13%)	2 (1%)	22	74
All	All	840/1116 (75%)	727 (86%)	100 (12%)	13 (2%)	15	64

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	612	LEU
1	C	569	GLN
1	D	504	SER
1	A	537	THR
1	A	569	GLN
1	C	581	ARG
1	A	571	HIS
1	A	626	ASN
1	B	464	PRO
1	C	625	GLN
1	C	582	ASP
1	B	580	GLY
1	D	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	188/242 (78%)	154 (82%)	34 (18%)	2 12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	192/242 (79%)	160 (83%)	32 (17%)	3	14
1	C	190/242 (78%)	154 (81%)	36 (19%)	2	11
1	D	186/242 (77%)	152 (82%)	34 (18%)	2	12
All	All	756/968 (78%)	620 (82%)	136 (18%)	2	12

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	429	LEU
1	A	431	THR
1	A	432	ASP
1	A	441	LEU
1	A	444	SER
1	A	445	THR
1	A	447	ASN
1	A	462	LEU
1	A	488	LEU
1	A	503	SER
1	A	504	SER
1	A	521	SER
1	A	529	LEU
1	A	537	THR
1	A	547	CYS
1	A	552	SER
1	A	555	SER
1	A	568	ASP
1	A	569	GLN
1	A	572	ILE
1	A	578	LEU
1	A	605	LEU
1	A	610	ILE
1	A	612	LEU
1	A	618	GLU
1	A	620	LEU
1	A	621	LEU
1	A	629	ARG
1	A	649	SER
1	A	653	ILE
1	A	662	LEU
1	A	665	ASP
1	A	666	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	672	ARG
1	B	429	LEU
1	B	430	ILE
1	B	431	THR
1	B	432	ASP
1	B	447	ASN
1	B	456	LYS
1	B	458	LEU
1	B	480	VAL
1	B	488	LEU
1	B	504	SER
1	B	520	LEU
1	B	521	SER
1	B	536	ASN
1	B	537	THR
1	B	539	GLN
1	B	551	GLN
1	B	572	ILE
1	B	574	GLN
1	B	577	TYR
1	B	581	ARG
1	B	583	LYS
1	B	604	GLU
1	B	605	LEU
1	B	648	ILE
1	B	649	SER
1	B	652	LEU
1	B	662	LEU
1	B	663	CYS
1	B	664	ASP
1	B	665	ASP
1	B	666	ILE
1	B	669	ILE
1	C	433	GLN
1	C	452	ASP
1	C	458	LEU
1	C	460	VAL
1	C	462	LEU
1	C	492	LEU
1	C	499	ASP
1	C	500	LEU
1	C	518	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	521	SER
1	C	529	LEU
1	C	536	ASN
1	C	547	CYS
1	C	548	LEU
1	C	551	GLN
1	C	555	SER
1	C	559	ILE
1	C	569	GLN
1	C	570	ASN
1	C	574	GLN
1	C	576	PHE
1	C	581	ARG
1	C	583	LYS
1	C	585	LEU
1	C	592	SER
1	C	593	ARG
1	C	604	GLU
1	C	605	LEU
1	C	613	SER
1	C	617	ILE
1	C	625	GLN
1	C	662	LEU
1	C	663	CYS
1	C	664	ASP
1	C	665	ASP
1	C	672	ARG
1	D	430	ILE
1	D	431	THR
1	D	441	LEU
1	D	445	THR
1	D	449	ASN
1	D	458	LEU
1	D	462	LEU
1	D	475	THR
1	D	485	HIS
1	D	488	LEU
1	D	495	PHE
1	D	503	SER
1	D	518	SER
1	D	521	SER
1	D	527	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	529	LEU
1	D	538	ASN
1	D	539	GLN
1	D	547	CYS
1	D	548	LEU
1	D	552	SER
1	D	570	ASN
1	D	574	GLN
1	D	579	MET
1	D	581	ARG
1	D	599	ILE
1	D	613	SER
1	D	614	HIS
1	D	621	LEU
1	D	625	GLN
1	D	626	ASN
1	D	627	LEU
1	D	662	LEU
1	D	674	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 12 ligands modelled in this entry, 12 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.

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%)	-0.27	1 (0%) 88 46	48, 77, 119, 164	6 (2%)
1	B	221/279 (79%)	-0.33	0 100 100	53, 76, 110, 154	2 (0%)
1	C	219/279 (78%)	-0.26	1 (0%) 88 46	54, 82, 128, 180	4 (1%)
1	D	214/279 (76%)	-0.21	0 100 100	57, 86, 122, 148	12 (5%)
All	All	870/1116 (77%)	-0.27	2 (0%) 93 66	48, 80, 123, 180	24 (2%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	497	LEU	2.2
1	C	571	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MN	D	8	1/1	0.19	-0.31	64,64,64,64	0
3	MG	C	4	1/1	0.15	-1.09	65,65,65,65	0
2	MN	A	1	1/1	0.13	-1.17	58,58,58,58	0
2	MN	A	2	1/1	0.14	-1.31	55,55,55,55	0
2	MN	C	6	1/1	0.06	-1.73	58,58,58,58	0
3	MG	B	2	1/1	0.14	-1.84	40,40,40,40	0
2	MN	D	7	1/1	0.10	-1.94	60,60,60,60	0
2	MN	C	5	1/1	0.06	-2.18	58,58,58,58	0
3	MG	A	675	1/1	0.09	-2.21	29,29,29,29	0
3	MG	D	3	1/1	0.05	-3.26	38,38,38,38	0
2	MN	B	3	1/1	0.05	-3.61	55,55,55,55	0
2	MN	B	4	1/1	0.06	-6.31	52,52,52,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.