



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:51 PM UTC

PDB ID : 4O6H / pdb_00004o6h
Title : 2.8Å crystal structure of Lymphocytic Choriomeningitis Virus Nucleoprotein C-terminal Domain
Authors : West, B.R.; Hastie, K.M.; Sapphire, E.O.
Deposited on : 2013-12-20
Resolution : 2.80 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 types of validation reports are described at

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

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

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

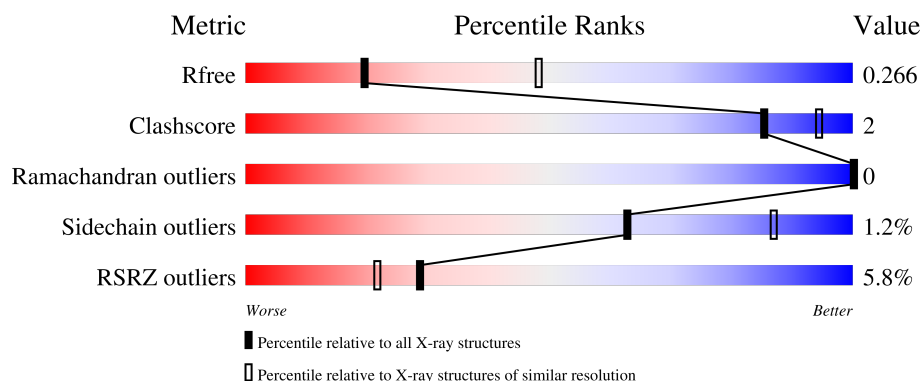
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



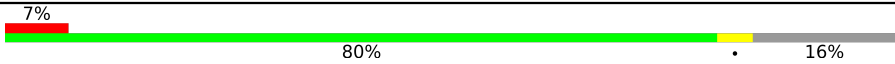
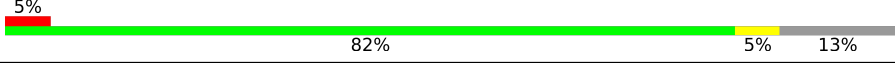
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	233	5% 82% 5% 13%
1	B	233	5% 82% 6% 12%
1	C	233	3% 77% 10% 13%
1	D	233	4% 80% 7% 12%
1	E	233	6% 80% • 16%

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Mol	Chain	Length	Quality of chain
1	F	233	 7%80%16%
1	G	233	 6%82%5%13%
1	H	233	 5%82%5%13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24479 atoms, of which 11980 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 Nucleoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	203	Total	C	H	N	O	S	0	0	0
			3096	1000	1513	270	302	11			
1	B	204	Total	C	H	N	O	S	0	0	0
			3054	994	1488	261	300	11			
1	C	203	Total	C	H	N	O	S	0	0	0
			3129	1007	1543	271	297	11			
1	D	204	Total	C	H	N	O	S	0	0	0
			3133	1009	1543	272	299	10			
1	E	196	Total	C	H	N	O	S	0	0	0
			2924	952	1427	249	286	10			
1	F	195	Total	C	H	N	O	S	0	0	0
			2930	950	1431	252	287	10			
1	G	203	Total	C	H	N	O	S	0	0	0
			3072	996	1503	266	296	11			
1	H	203	Total	C	H	N	O	S	0	0	0
			3085	994	1512	269	299	11			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	MET	-	expression tag	UNP P09992
A	327	ALA	-	expression tag	UNP P09992
A	328	HIS	-	expression tag	UNP P09992
A	329	HIS	-	expression tag	UNP P09992
A	330	HIS	-	expression tag	UNP P09992
A	331	HIS	-	expression tag	UNP P09992
A	332	HIS	-	expression tag	UNP P09992
A	333	HIS	-	expression tag	UNP P09992
A	334	VAL	-	expression tag	UNP P09992
A	335	ASP	-	expression tag	UNP P09992
A	336	ASP	-	expression tag	UNP P09992
A	337	ASP	-	expression tag	UNP P09992
A	338	ASP	-	expression tag	UNP P09992

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Chain	Residue	Modelled	Actual	Comment	Reference
A	339	ARG	-	expression tag	UNP P09992
A	340	MET	-	expression tag	UNP P09992
B	326	MET	-	expression tag	UNP P09992
B	327	ALA	-	expression tag	UNP P09992
B	328	HIS	-	expression tag	UNP P09992
B	329	HIS	-	expression tag	UNP P09992
B	330	HIS	-	expression tag	UNP P09992
B	331	HIS	-	expression tag	UNP P09992
B	332	HIS	-	expression tag	UNP P09992
B	333	HIS	-	expression tag	UNP P09992
B	334	VAL	-	expression tag	UNP P09992
B	335	ASP	-	expression tag	UNP P09992
B	336	ASP	-	expression tag	UNP P09992
B	337	ASP	-	expression tag	UNP P09992
B	338	ASP	-	expression tag	UNP P09992
B	339	ARG	-	expression tag	UNP P09992
B	340	MET	-	expression tag	UNP P09992
C	326	MET	-	expression tag	UNP P09992
C	327	ALA	-	expression tag	UNP P09992
C	328	HIS	-	expression tag	UNP P09992
C	329	HIS	-	expression tag	UNP P09992
C	330	HIS	-	expression tag	UNP P09992
C	331	HIS	-	expression tag	UNP P09992
C	332	HIS	-	expression tag	UNP P09992
C	333	HIS	-	expression tag	UNP P09992
C	334	VAL	-	expression tag	UNP P09992
C	335	ASP	-	expression tag	UNP P09992
C	336	ASP	-	expression tag	UNP P09992
C	337	ASP	-	expression tag	UNP P09992
C	338	ASP	-	expression tag	UNP P09992
C	339	ARG	-	expression tag	UNP P09992
C	340	MET	-	expression tag	UNP P09992
D	326	MET	-	expression tag	UNP P09992
D	327	ALA	-	expression tag	UNP P09992
D	328	HIS	-	expression tag	UNP P09992
D	329	HIS	-	expression tag	UNP P09992
D	330	HIS	-	expression tag	UNP P09992
D	331	HIS	-	expression tag	UNP P09992
D	332	HIS	-	expression tag	UNP P09992
D	333	HIS	-	expression tag	UNP P09992
D	334	VAL	-	expression tag	UNP P09992
D	335	ASP	-	expression tag	UNP P09992

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Chain	Residue	Modelled	Actual	Comment	Reference
D	336	ASP	-	expression tag	UNP P09992
D	337	ASP	-	expression tag	UNP P09992
D	338	ASP	-	expression tag	UNP P09992
D	339	ARG	-	expression tag	UNP P09992
D	340	MET	-	expression tag	UNP P09992
E	326	MET	-	expression tag	UNP P09992
E	327	ALA	-	expression tag	UNP P09992
E	328	HIS	-	expression tag	UNP P09992
E	329	HIS	-	expression tag	UNP P09992
E	330	HIS	-	expression tag	UNP P09992
E	331	HIS	-	expression tag	UNP P09992
E	332	HIS	-	expression tag	UNP P09992
E	333	HIS	-	expression tag	UNP P09992
E	334	VAL	-	expression tag	UNP P09992
E	335	ASP	-	expression tag	UNP P09992
E	336	ASP	-	expression tag	UNP P09992
E	337	ASP	-	expression tag	UNP P09992
E	338	ASP	-	expression tag	UNP P09992
E	339	ARG	-	expression tag	UNP P09992
E	340	MET	-	expression tag	UNP P09992
F	326	MET	-	expression tag	UNP P09992
F	327	ALA	-	expression tag	UNP P09992
F	328	HIS	-	expression tag	UNP P09992
F	329	HIS	-	expression tag	UNP P09992
F	330	HIS	-	expression tag	UNP P09992
F	331	HIS	-	expression tag	UNP P09992
F	332	HIS	-	expression tag	UNP P09992
F	333	HIS	-	expression tag	UNP P09992
F	334	VAL	-	expression tag	UNP P09992
F	335	ASP	-	expression tag	UNP P09992
F	336	ASP	-	expression tag	UNP P09992
F	337	ASP	-	expression tag	UNP P09992
F	338	ASP	-	expression tag	UNP P09992
F	339	ARG	-	expression tag	UNP P09992
F	340	MET	-	expression tag	UNP P09992
G	326	MET	-	expression tag	UNP P09992
G	327	ALA	-	expression tag	UNP P09992
G	328	HIS	-	expression tag	UNP P09992
G	329	HIS	-	expression tag	UNP P09992
G	330	HIS	-	expression tag	UNP P09992
G	331	HIS	-	expression tag	UNP P09992
G	332	HIS	-	expression tag	UNP P09992

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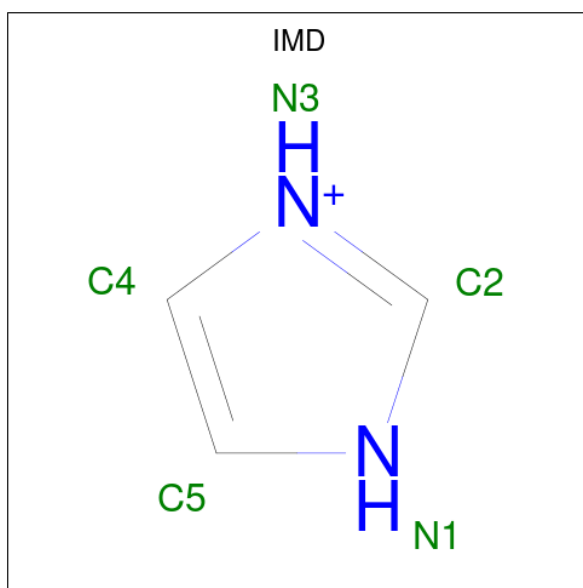
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Chain	Residue	Modelled	Actual	Comment	Reference
G	333	HIS	-	expression tag	UNP P09992
G	334	VAL	-	expression tag	UNP P09992
G	335	ASP	-	expression tag	UNP P09992
G	336	ASP	-	expression tag	UNP P09992
G	337	ASP	-	expression tag	UNP P09992
G	338	ASP	-	expression tag	UNP P09992
G	339	ARG	-	expression tag	UNP P09992
G	340	MET	-	expression tag	UNP P09992
H	326	MET	-	expression tag	UNP P09992
H	327	ALA	-	expression tag	UNP P09992
H	328	HIS	-	expression tag	UNP P09992
H	329	HIS	-	expression tag	UNP P09992
H	330	HIS	-	expression tag	UNP P09992
H	331	HIS	-	expression tag	UNP P09992
H	332	HIS	-	expression tag	UNP P09992
H	333	HIS	-	expression tag	UNP P09992
H	334	VAL	-	expression tag	UNP P09992
H	335	ASP	-	expression tag	UNP P09992
H	336	ASP	-	expression tag	UNP P09992
H	337	ASP	-	expression tag	UNP P09992
H	338	ASP	-	expression tag	UNP P09992
H	339	ARG	-	expression tag	UNP P09992
H	340	MET	-	expression tag	UNP P09992

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	H	1	Total Zn 1 1	0	0

- Molecule 3 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	N	0	0
			10	3	5	2		
3	B	1	Total	C	H	N	0	0
			10	3	5	2		
3	E	1	Total	C	H	N	0	0
			10	3	5	2		
3	F	1	Total	C	H	N	0	0
			10	3	5	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	G	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	K	0	0
			1	1		

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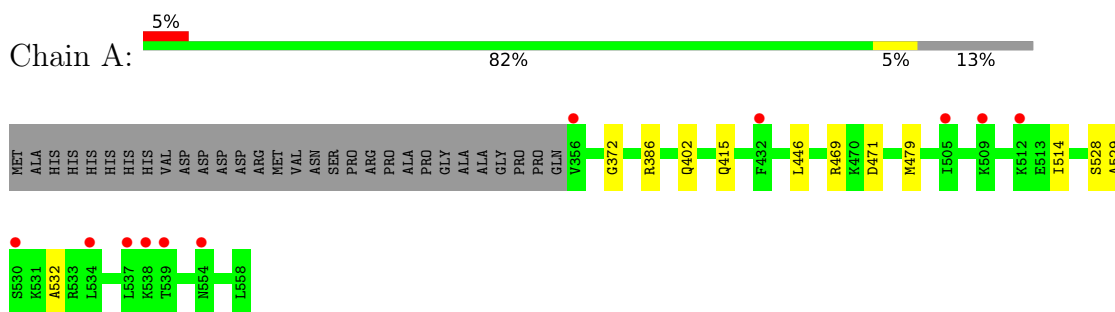
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	K 1	0	0
5	G	1	Total 1	K 1	0	0
5	H	1	Total 1	K 1	0	0

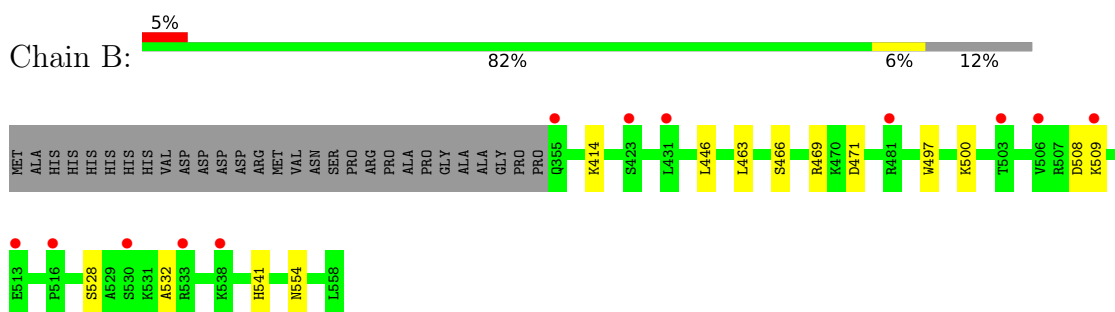
3 Residue-property plots [i](#)

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.

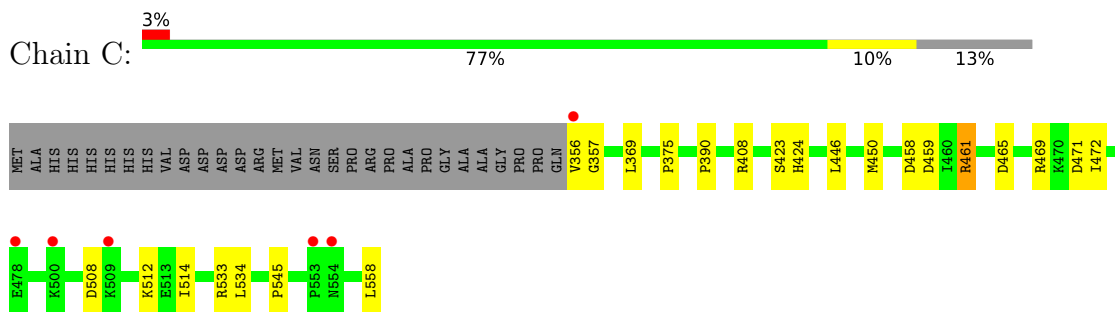
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein

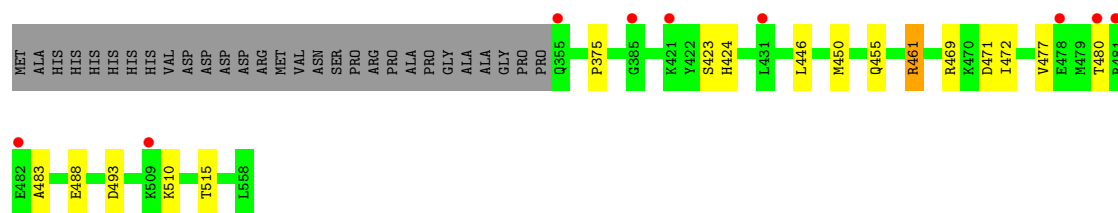


- Molecule 1: Nucleoprotein

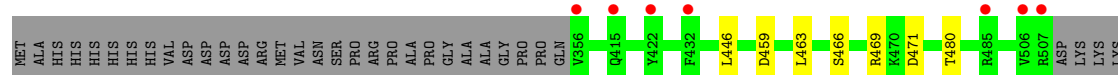
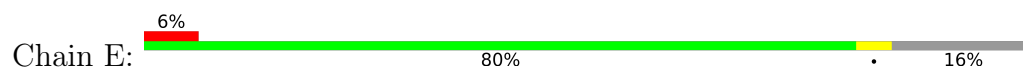


- Molecule 1: Nucleoprotein

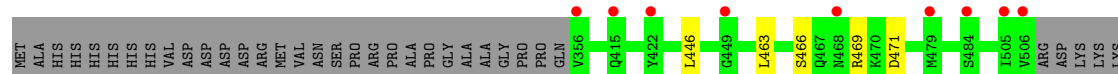
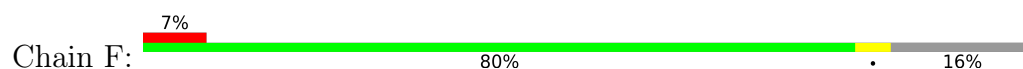




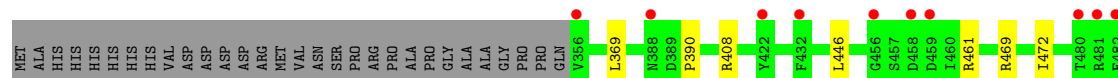
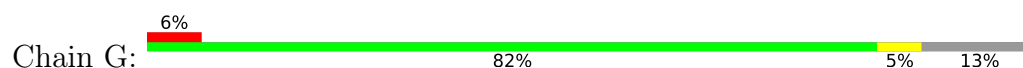
● Molecule 1: Nucleoprotein



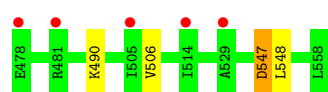
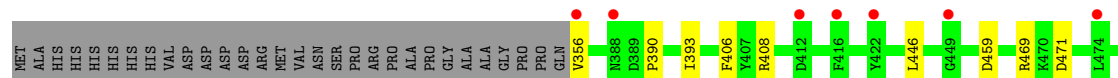
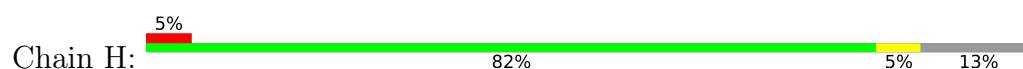
● Molecule 1: Nucleoprotein



● Molecule 1: Nucleoprotein



● Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.86Å 94.40Å 145.12Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	47.26 – 2.80 47.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.26-2.80) 97.2 (47.26-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.227 , 0.261 0.238 , 0.266	Depositor DCC
R_{free} test set	2991 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24479	wwPDB-VP
Average B, all atoms (Å ²)	82.0	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 48.82 % 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 8.1519e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: IMD, ZN, K, 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	0.29	0/1618	0.60	0/2195
1	B	0.29	0/1601	0.59	0/2176
1	C	0.29	0/1621	0.59	0/2195
1	D	0.28	0/1625	0.60	0/2202
1	E	0.28	0/1530	0.60	0/2078
1	F	0.28	0/1532	0.59	0/2079
1	G	0.29	0/1604	0.59	0/2177
1	H	0.28	0/1607	0.59	0/2179
All	All	0.28	0/12738	0.60	0/17281

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	1583	1513	1514	6	0
1	B	1566	1488	1488	7	0
1	C	1586	1543	1543	12	0
1	D	1590	1543	1543	9	0
1	E	1497	1427	1427	4	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1499	1431	1431	5	0
1	G	1569	1503	1503	5	2
1	H	1573	1512	1512	6	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	5	5	5	0	0
3	B	5	5	5	0	0
3	E	5	5	5	0	0
3	F	5	5	5	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
All	All	12499	11980	11981	53	2

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 2.

All (53) 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:461:ARG:NH2	1:D:472:ILE:O	2.17	0.78
1:C:446:LEU:O	1:C:469:ARG:NH2	2.17	0.77
1:C:461:ARG:NH2	1:C:472:ILE:O	2.19	0.75
1:B:446:LEU:O	1:B:469:ARG:NH2	2.22	0.72
1:D:446:LEU:O	1:D:469:ARG:NH2	2.23	0.71
1:A:386:ARG:NH1	1:A:415:GLN:OE1	2.23	0.71
1:H:446:LEU:O	1:H:469:ARG:NH2	2.23	0.70
1:G:446:LEU:O	1:G:469:ARG:NH2	2.25	0.69
1:C:461:ARG:NH1	1:C:465:ASP:OD1	2.26	0.69
1:D:480:THR:OG1	1:D:483:ALA:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:446:LEU:O	1:E:469:ARG:NH2	2.32	0.62
1:A:372:GLY:O	1:A:402:GLN:NE2	2.36	0.58
1:E:463:LEU:O	1:E:466:SER:OG	2.22	0.57
1:E:528:SER:O	1:E:532:ALA:N	2.38	0.57
1:B:497:TRP:O	1:B:500:LYS:NZ	2.39	0.56
1:A:469:ARG:NH1	1:A:471:ASP:OD1	2.39	0.56
1:G:461:ARG:NH1	1:G:472:ILE:O	2.39	0.55
1:E:469:ARG:NH1	1:E:471:ASP:OD1	2.39	0.55
1:B:508:ASP:OD1	1:B:509:LYS:N	2.40	0.54
1:H:547:ASP:N	1:H:547:ASP:OD1	2.41	0.53
1:C:390:PRO:O	1:C:408:ARG:NH1	2.40	0.53
1:H:393:ILE:HD11	1:H:406:PHE:CE2	2.44	0.53
1:F:469:ARG:NH1	1:F:471:ASP:OD1	2.43	0.52
1:A:528:SER:O	1:A:532:ALA:N	2.43	0.51
1:F:463:LEU:O	1:F:466:SER:OG	2.26	0.51
1:F:446:LEU:O	1:F:469:ARG:NH2	2.43	0.51
1:D:455:GLN:NE2	1:D:477:VAL:O	2.44	0.50
1:D:469:ARG:NH1	1:D:471:ASP:OD2	2.44	0.50
1:C:423:SER:OG	1:C:424:HIS:N	2.46	0.49
1:C:469:ARG:NH1	1:C:471:ASP:OD2	2.45	0.48
1:G:390:PRO:O	1:G:408:ARG:NH1	2.41	0.48
1:A:479:MET:SD	1:A:529:ALA:HB3	2.54	0.48
1:D:488:GLU:OE2	1:D:515:THR:HB	2.14	0.48
1:A:446:LEU:O	1:A:469:ARG:NH2	2.48	0.47
1:H:459:ASP:OD2	1:H:459:ASP:N	2.48	0.47
1:C:375:PRO:HA	1:C:450:MET:HE2	1.97	0.47
1:B:463:LEU:O	1:B:466:SER:OG	2.31	0.46
1:B:469:ARG:NH1	1:B:471:ASP:OD2	2.49	0.46
1:B:554:ASN:ND2	1:D:510:LYS:O	2.49	0.46
1:C:508:ASP:OD1	1:C:512:LYS:N	2.48	0.45
1:D:375:PRO:HA	1:D:450:MET:HE2	1.99	0.44
1:G:508:ASP:N	1:G:512:LYS:O	2.46	0.44
1:D:423:SER:OG	1:D:424:HIS:N	2.50	0.44
1:C:458:ASP:OD1	1:C:459:ASP:N	2.48	0.44
1:F:528:SER:O	1:F:532:ALA:N	2.51	0.43
1:H:469:ARG:NH1	1:H:471:ASP:OD1	2.51	0.43
1:G:369:LEU:HD13	1:G:545:PRO:HD3	2.02	0.42
1:B:528:SER:O	1:B:532:ALA:N	2.52	0.42
1:H:390:PRO:O	1:H:408:ARG:NH1	2.49	0.41
1:C:356:VAL:HG22	1:C:357:GLY:H	1.85	0.41
1:C:369:LEU:HD13	1:C:545:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:469:ARG:NH1	1:C:472:ILE:HG13	2.36	0.40
1:F:518:CYS:HB3	1:F:521:MET:HB2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:480:THR:HG1	1:G:547:ASP:OD2[2_555]	1.54	0.06
1:E:480:THR:OG1	1:G:547:ASP:OD2[2_555]	2.17	0.03

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	201/233 (86%)	198 (98%)	3 (2%)	0	100	100
1	B	202/233 (87%)	196 (97%)	6 (3%)	0	100	100
1	C	201/233 (86%)	195 (97%)	6 (3%)	0	100	100
1	D	202/233 (87%)	193 (96%)	9 (4%)	0	100	100
1	E	192/233 (82%)	189 (98%)	3 (2%)	0	100	100
1	F	191/233 (82%)	187 (98%)	4 (2%)	0	100	100
1	G	201/233 (86%)	193 (96%)	8 (4%)	0	100	100
1	H	201/233 (86%)	188 (94%)	13 (6%)	0	100	100
All	All	1591/1864 (85%)	1539 (97%)	52 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	171/205 (83%)	170 (99%)	1 (1%)	78	92
1	B	168/205 (82%)	166 (99%)	2 (1%)	63	87
1	C	172/205 (84%)	167 (97%)	5 (3%)	37	73
1	D	172/205 (84%)	170 (99%)	2 (1%)	63	87
1	E	160/205 (78%)	159 (99%)	1 (1%)	78	92
1	F	162/205 (79%)	162 (100%)	0	100	100
1	G	168/205 (82%)	168 (100%)	0	100	100
1	H	170/205 (83%)	165 (97%)	5 (3%)	37	73
All	All	1343/1640 (82%)	1327 (99%)	16 (1%)	63	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	514	ILE
1	B	414	LYS
1	B	541	HIS
1	C	461	ARG
1	C	514	ILE
1	C	533	ARG
1	C	534	LEU
1	C	558	LEU
1	D	461	ARG
1	D	493	ASP
1	E	459	ASP
1	H	356	VAL
1	H	490	LYS
1	H	506	VAL
1	H	547	ASP
1	H	548	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	455	GLN
1	B	388	ASN
1	B	415	GLN
1	B	467	GLN
1	C	455	GLN
1	D	415	GLN
1	D	541	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 16 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	IMD	E	602	-	5,5,5	0.63	0	5,5,5	0.41	0
3	IMD	F	602	-	5,5,5	0.63	0	5,5,5	0.43	0
3	IMD	A	602	-	5,5,5	0.65	0	5,5,5	0.43	0
3	IMD	B	602	-	5,5,5	0.64	0	5,5,5	0.41	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	IMD	E	602	-	-	-	0/1/1/1
3	IMD	F	602	-	-	-	0/1/1/1
3	IMD	A	602	-	-	-	0/1/1/1
3	IMD	B	602	-	-	-	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, 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	203/233 (87%)	0.48	11 (5%) 31 24	46, 71, 114, 135	0
1	B	204/233 (87%)	0.46	12 (5%) 28 21	46, 74, 112, 130	0
1	C	203/233 (87%)	0.42	6 (2%) 52 42	48, 72, 111, 127	0
1	D	204/233 (87%)	0.31	9 (4%) 39 31	48, 69, 106, 136	0
1	E	196/233 (84%)	0.49	14 (7%) 22 16	57, 84, 118, 128	0
1	F	195/233 (83%)	0.59	16 (8%) 17 13	60, 90, 120, 135	0
1	G	203/233 (87%)	0.58	14 (6%) 23 16	59, 85, 125, 134	0
1	H	203/233 (87%)	0.68	12 (5%) 28 21	63, 93, 128, 143	0
All	All	1611/1864 (86%)	0.50	94 (5%) 29 22	46, 81, 120, 143	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	355	GLN	6.1
1	E	507	ARG	5.1
1	C	553	PRO	5.1
1	C	554	ASN	4.6
1	H	422	TYR	4.5
1	E	538	LYS	4.1
1	G	480	THR	3.8
1	A	505	ILE	3.8
1	C	356	VAL	3.7
1	H	505	ILE	3.7
1	H	478	GLU	3.6
1	E	536	ASP	3.6
1	A	509	LYS	3.5
1	G	514	ILE	3.4
1	A	537	LEU	3.3
1	D	509	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	415	GLN	3.2
1	A	539	THR	3.2
1	F	422	TYR	3.1
1	D	355	GLN	3.1
1	H	356	VAL	3.0
1	B	423	SER	3.0
1	C	478	GLU	3.0
1	E	539	THR	3.0
1	G	482	GLU	2.9
1	G	458	ASP	2.9
1	B	538	LYS	2.8
1	G	356	VAL	2.8
1	F	530	SER	2.8
1	G	422	TYR	2.7
1	B	533	ARG	2.7
1	G	500	LYS	2.7
1	B	516	PRO	2.7
1	F	484	SER	2.7
1	G	484	SER	2.7
1	C	509	LYS	2.7
1	F	539	THR	2.7
1	H	529	ALA	2.7
1	F	479	MET	2.7
1	E	432	PHE	2.6
1	E	554	ASN	2.6
1	A	530	SER	2.6
1	E	356	VAL	2.6
1	F	534	LEU	2.6
1	E	422	TYR	2.6
1	A	356	VAL	2.6
1	B	481	ARG	2.5
1	D	478	GLU	2.5
1	F	537	LEU	2.5
1	E	415	GLN	2.5
1	F	506	VAL	2.5
1	B	513	GLU	2.5
1	E	485	ARG	2.5
1	A	554	ASN	2.4
1	G	432	PHE	2.4
1	H	514	ILE	2.4
1	B	506	VAL	2.4
1	F	356	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	481	ARG	2.4
1	H	474	LEU	2.4
1	C	500	LYS	2.3
1	D	480	THR	2.3
1	D	481	ARG	2.3
1	B	509	LYS	2.3
1	E	533	ARG	2.3
1	E	517	HIS	2.3
1	F	468	ASN	2.2
1	F	533	ARG	2.2
1	G	481	ARG	2.2
1	A	538	LYS	2.2
1	G	459	ASP	2.2
1	F	449	GLY	2.2
1	D	431	LEU	2.2
1	D	421	LYS	2.2
1	D	482	GLU	2.2
1	H	388	ASN	2.2
1	B	530	SER	2.1
1	F	529	ALA	2.1
1	D	385	GLY	2.1
1	E	537	LEU	2.1
1	G	388	ASN	2.1
1	G	535	PRO	2.1
1	F	505	ILE	2.1
1	A	534	LEU	2.1
1	B	431	LEU	2.1
1	A	432	PHE	2.1
1	H	449	GLY	2.1
1	E	506	VAL	2.0
1	H	416	PHE	2.0
1	F	516	PRO	2.0
1	G	456	GLY	2.0
1	B	503	THR	2.0
1	H	412	ASP	2.0
1	A	512	LYS	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
4	MG	H	602	1/1	0.57	0.39	85,85,85,85	0
4	MG	G	602	1/1	0.71	0.28	78,78,78,78	0
3	IMD	E	602	5/5	0.75	0.24	84,95,110,114	0
5	K	H	603	1/1	0.76	0.27	89,89,89,89	0
3	IMD	F	602	5/5	0.77	0.27	88,92,110,111	0
3	IMD	A	602	5/5	0.80	0.20	65,74,81,89	0
5	K	G	603	1/1	0.81	0.25	85,85,85,85	0
5	K	D	603	1/1	0.85	0.23	71,71,71,71	0
3	IMD	B	602	5/5	0.87	0.18	63,75,87,91	0
4	MG	D	602	1/1	0.89	0.21	65,65,65,65	0
5	K	C	603	1/1	0.90	0.20	63,63,63,63	0
4	MG	C	602	1/1	0.91	0.19	70,70,70,70	0
2	ZN	E	601	1/1	0.99	0.03	77,77,77,77	0
2	ZN	F	601	1/1	0.99	0.03	78,78,78,78	0
2	ZN	G	601	1/1	0.99	0.03	72,72,72,72	0
2	ZN	H	601	1/1	0.99	0.02	83,83,83,83	0
2	ZN	A	601	1/1	1.00	0.01	53,53,53,53	0
2	ZN	B	601	1/1	1.00	0.02	61,61,61,61	0
2	ZN	C	601	1/1	1.00	0.02	54,54,54,54	0
2	ZN	D	601	1/1	1.00	0.02	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.