



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:41 PM UTC

PDB ID : 2YI8 / pdb_00002yi8
Title : Structure of the RNA polymerase VP1 from Infectious Pancreatic Necrosis Virus
Authors : Graham, S.C.; Sarin, L.P.; Bahar, M.W.; Myers, R.A.; Stuart, D.I.; Bamford, D.H.; Grimes, J.M.
Deposited on : 2011-05-11
Resolution : 2.30 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
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

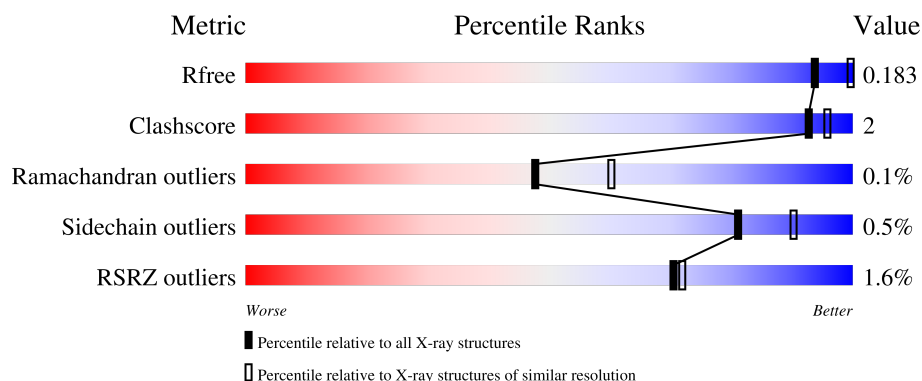
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	799	3% 91% 5%
1	B	799	% 92% 5%
1	C	799	2% 92% 5%
1	D	799	2% 91% 5%
1	E	799	% 91% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33471 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 RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	771	Total	C	N	O	S	0	6	0
			6054	3845	1021	1161	27			
1	B	771	Total	C	N	O	S	0	7	0
			6054	3843	1021	1163	27			
1	C	771	Total	C	N	O	S	0	7	0
			6061	3849	1022	1163	27			
1	D	771	Total	C	N	O	S	0	8	0
			6063	3850	1022	1164	27			
1	E	771	Total	C	N	O	S	0	9	0
			6085	3865	1024	1169	27			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	791	LYS	-	expression tag	UNP P22173
A	792	THR	-	expression tag	UNP P22173
A	793	GLY	-	expression tag	UNP P22173
A	794	HIS	-	expression tag	UNP P22173
A	795	HIS	-	expression tag	UNP P22173
A	796	HIS	-	expression tag	UNP P22173
A	797	HIS	-	expression tag	UNP P22173
A	798	HIS	-	expression tag	UNP P22173
A	799	HIS	-	expression tag	UNP P22173
B	791	LYS	-	expression tag	UNP P22173
B	792	THR	-	expression tag	UNP P22173
B	793	GLY	-	expression tag	UNP P22173
B	794	HIS	-	expression tag	UNP P22173
B	795	HIS	-	expression tag	UNP P22173
B	796	HIS	-	expression tag	UNP P22173
B	797	HIS	-	expression tag	UNP P22173
B	798	HIS	-	expression tag	UNP P22173
B	799	HIS	-	expression tag	UNP P22173
C	791	LYS	-	expression tag	UNP P22173

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Chain	Residue	Modelled	Actual	Comment	Reference
C	792	THR	-	expression tag	UNP P22173
C	793	GLY	-	expression tag	UNP P22173
C	794	HIS	-	expression tag	UNP P22173
C	795	HIS	-	expression tag	UNP P22173
C	796	HIS	-	expression tag	UNP P22173
C	797	HIS	-	expression tag	UNP P22173
C	798	HIS	-	expression tag	UNP P22173
C	799	HIS	-	expression tag	UNP P22173
D	791	LYS	-	expression tag	UNP P22173
D	792	THR	-	expression tag	UNP P22173
D	793	GLY	-	expression tag	UNP P22173
D	794	HIS	-	expression tag	UNP P22173
D	795	HIS	-	expression tag	UNP P22173
D	796	HIS	-	expression tag	UNP P22173
D	797	HIS	-	expression tag	UNP P22173
D	798	HIS	-	expression tag	UNP P22173
D	799	HIS	-	expression tag	UNP P22173
E	791	LYS	-	expression tag	UNP P22173
E	792	THR	-	expression tag	UNP P22173
E	793	GLY	-	expression tag	UNP P22173
E	794	HIS	-	expression tag	UNP P22173
E	795	HIS	-	expression tag	UNP P22173
E	796	HIS	-	expression tag	UNP P22173
E	797	HIS	-	expression tag	UNP P22173
E	798	HIS	-	expression tag	UNP P22173
E	799	HIS	-	expression tag	UNP P22173

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0
3	E	2	Total 2	Cl 2	0	0

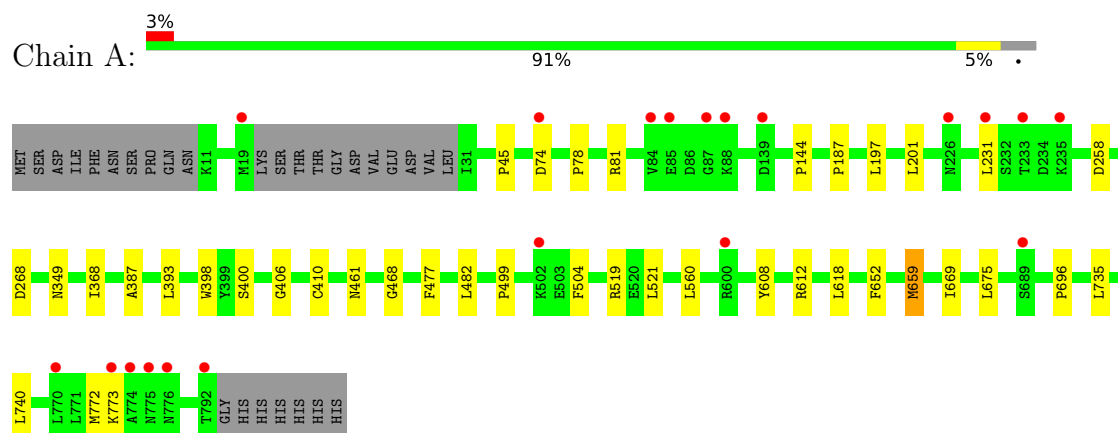
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	563	Total 563	O 563	0	0
4	B	622	Total 622	O 622	0	0
4	C	611	Total 611	O 611	0	0
4	D	637	Total 637	O 637	0	0
4	E	710	Total 710	O 710	0	0

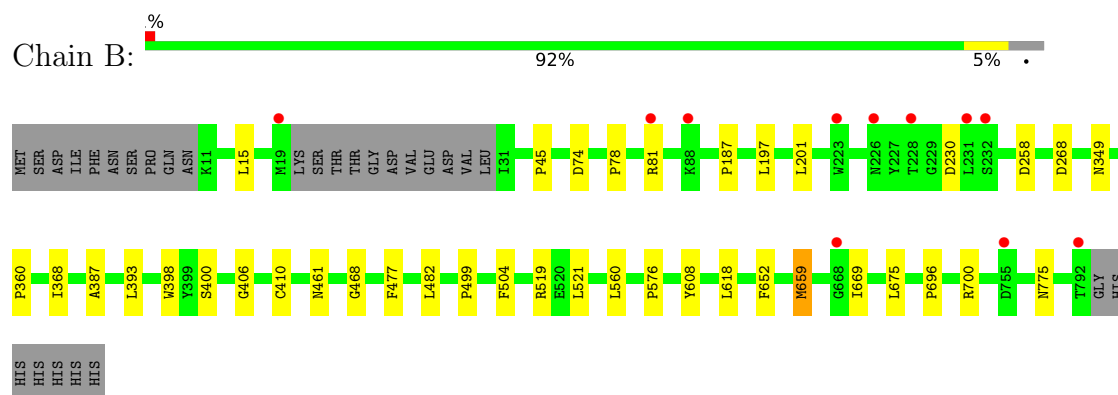
3 Residue-property plots [i](#)

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.

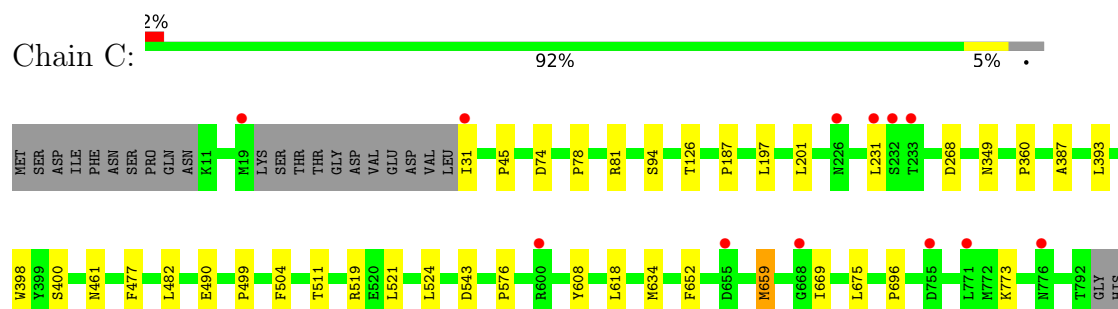
• Molecule 1: RNA-DIRECTED RNA POLYMERASE



• Molecule 1: RNA-DIRECTED RNA POLYMERASE

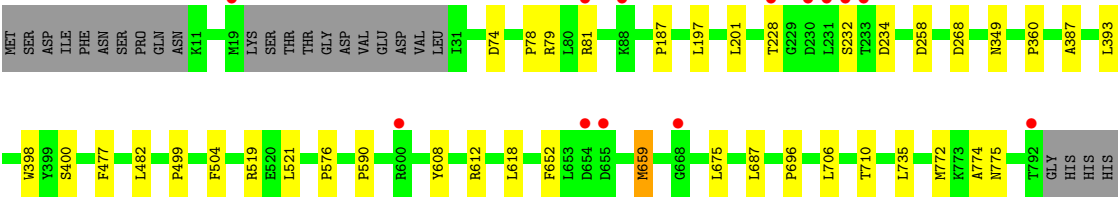
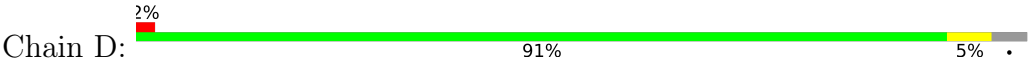


• Molecule 1: RNA-DIRECTED RNA POLYMERASE



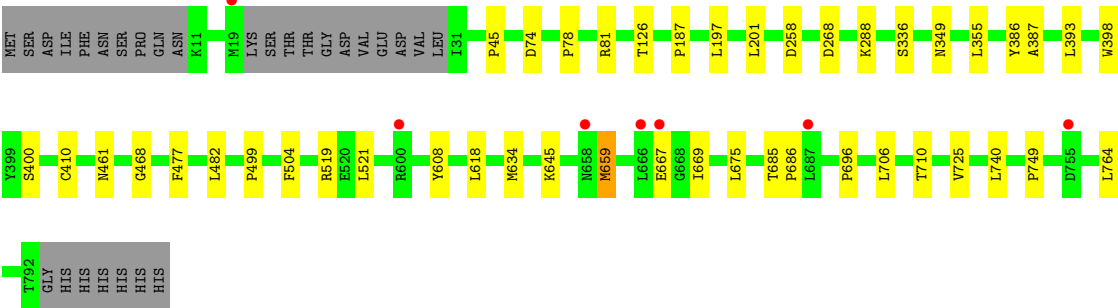
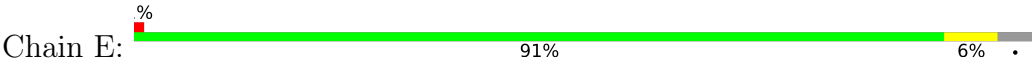
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● Molecule 1: RNA-DIRECTED RNA POLYMERASE



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● Molecule 1: RNA-DIRECTED RNA POLYMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	134.05Å 183.87Å 244.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.33 – 2.30 90.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (90.33-2.30) 100.0 (90.33-2.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.166 , 0.187 0.163 , 0.183	Depositor DCC
R_{free} test set	2655 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	12.0	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33471	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: K, 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	0.84	1/6207 (0.0%)	1.16	5/8448 (0.1%)
1	B	0.87	1/6210 (0.0%)	1.15	4/8453 (0.0%)
1	C	0.87	1/6217 (0.0%)	1.16	6/8461 (0.1%)
1	D	0.87	1/6222 (0.0%)	1.15	5/8468 (0.1%)
1	E	0.91	1/6247 (0.0%)	1.16	5/8498 (0.1%)
All	All	0.87	5/31103 (0.0%)	1.16	25/42328 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	659	MET	SD-CE	-8.94	1.57	1.79
1	C	659	MET	SD-CE	-8.25	1.58	1.79
1	E	659	MET	SD-CE	-7.36	1.61	1.79
1	A	659	MET	SD-CE	-6.71	1.62	1.79
1	D	659	MET	SD-CE	-6.11	1.64	1.79

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	667	GLU	N-CA-C	10.03	123.25	111.71
1	C	773	LYS	N-CA-C	-7.05	103.34	112.23
1	D	652	PHE	CA-CB-CG	5.84	119.64	113.80
1	B	268	ASP	CA-CB-CG	5.81	118.41	112.60
1	E	268	ASP	CA-CB-CG	5.77	118.37	112.60
1	C	268	ASP	CA-CB-CG	5.68	118.28	112.60
1	A	268	ASP	CA-CB-CG	5.57	118.17	112.60
1	D	268	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	773	LYS	N-CA-C	-5.51	105.35	111.36
1	C	652	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	652	PHE	CA-CB-CG	5.42	119.22	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	774	ALA	CA-C-N	5.38	127.49	120.28
1	D	774	ALA	C-N-CA	5.38	127.49	120.28
1	B	652	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	230	ASP	CA-CB-CG	5.29	117.89	112.60
1	E	336	SER	N-CA-C	5.25	117.81	111.40
1	B	258	ASP	CA-CB-CG	5.19	117.79	112.60
1	D	258	ASP	CA-CB-CG	5.17	117.78	112.60
1	E	258	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	740	LEU	N-CA-C	5.07	116.80	111.28
1	E	740	LEU	N-CA-C	5.03	116.77	111.28
1	C	524	LEU	CA-C-N	5.02	127.31	120.54
1	C	524	LEU	C-N-CA	5.02	127.31	120.54
1	A	258	ASP	CA-CB-CG	5.02	117.62	112.60
1	C	543	ASP	CA-CB-CG	5.00	117.60	112.60

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	6054	0	6023	19	0
1	B	6054	0	6014	20	0
1	C	6061	0	6034	17	0
1	D	6063	0	6034	17	0
1	E	6085	0	6078	22	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
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
3	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	563	0	0	2	0
4	B	622	0	0	2	0
4	C	611	0	0	0	0
4	D	637	0	0	0	0
4	E	710	0	0	2	0
All	All	33471	0	30183	93	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 2.

All (93) 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:E:288:LYS:HE2	4:E:2350:HOH:O	1.69	0.91
1:B:187:PRO:HB3	1:B:197:LEU:HD11	1.78	0.66
1:C:187:PRO:HB3	1:C:197:LEU:HD11	1.78	0.64
1:E:706:LEU:O	1:E:710[B]:THR:HG23	1.97	0.64
1:D:187:PRO:HB3	1:D:197:LEU:HD11	1.78	0.64
1:E:187:PRO:HB3	1:E:197:LEU:HD11	1.79	0.64
1:A:187:PRO:HB3	1:A:197:LEU:HD11	1.80	0.62
1:A:735:LEU:HD21	1:A:772:MET:HG2	1.85	0.58
1:D:74:ASP:HB2	1:D:81:ARG:HG2	1.89	0.55
1:C:74:ASP:HB2	1:C:81:ARG:HG2	1.88	0.55
1:A:201:LEU:HD11	1:A:482[A]:LEU:HD13	1.90	0.54
1:C:201:LEU:HD11	1:C:482[A]:LEU:HD13	1.89	0.54
1:E:201:LEU:HD11	1:E:482[A]:LEU:HD13	1.90	0.54
1:B:74:ASP:HB2	1:B:81:ARG:HG2	1.89	0.54
1:D:201:LEU:HD11	1:D:482[A]:LEU:HD13	1.90	0.54
1:D:590:PRO:HB2	1:D:612:ARG:HD2	1.88	0.54
1:E:618:LEU:HG	1:E:675:LEU:HD12	1.91	0.53
1:E:74:ASP:HB2	1:E:81:ARG:HG2	1.89	0.53
1:B:700:ARG:NH2	4:B:2412:HOH:O	2.37	0.53
1:D:618:LEU:HG	1:D:675:LEU:HD12	1.91	0.53
1:A:74:ASP:HB2	1:A:81:ARG:HG2	1.90	0.53
1:B:618:LEU:HG	1:B:675:LEU:HD12	1.90	0.53
1:B:201:LEU:HD11	1:B:482[A]:LEU:HD13	1.90	0.52
1:C:618:LEU:HG	1:C:675:LEU:HD12	1.92	0.52
1:A:618:LEU:HG	1:A:675:LEU:HD12	1.91	0.51
1:C:608:TYR:HB2	1:C:659:MET:HE3	1.95	0.49
1:D:706:LEU:O	1:D:710[B]:THR:HG23	2.12	0.49
1:D:349:ASN:O	1:D:696:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:SER:HB3	1:D:519:ARG:HB3	1.96	0.48
1:A:400:SER:HB3	1:A:519:ARG:HB3	1.96	0.48
1:C:398:TRP:HB3	1:C:521:LEU:HB3	1.95	0.48
1:E:349:ASN:O	1:E:696:PRO:HD2	2.13	0.48
1:D:78:PRO:O	1:D:81:ARG:HG3	2.14	0.47
1:D:398:TRP:HB3	1:D:521:LEU:HB3	1.97	0.47
1:E:398:TRP:HB3	1:E:521:LEU:HB3	1.96	0.47
1:B:398:TRP:HB3	1:B:521:LEU:HB3	1.96	0.47
1:A:349:ASN:O	1:A:696:PRO:HD2	2.15	0.47
1:A:387:ALA:HB2	1:A:477:PHE:CD2	2.50	0.47
1:A:608:TYR:HB2	1:A:659:MET:HE3	1.96	0.47
1:A:612:ARG:HG2	4:A:2473:HOH:O	2.15	0.47
1:C:387:ALA:HB2	1:C:477:PHE:CD2	2.50	0.47
1:A:398:TRP:HB3	1:A:521:LEU:HB3	1.96	0.47
1:E:749:PRO:HG2	1:E:764:LEU:CD1	2.45	0.47
1:B:608:TYR:HB2	1:B:659:MET:HE3	1.97	0.46
1:A:78:PRO:O	1:A:81:ARG:HG3	2.16	0.46
1:B:400:SER:HB3	1:B:519:ARG:HB3	1.97	0.46
1:B:387:ALA:HB2	1:B:477:PHE:CD2	2.51	0.46
1:E:400:SER:HB3	1:E:519:ARG:HB3	1.96	0.46
1:B:499:PRO:HA	1:B:504:PHE:CG	2.51	0.46
1:B:775:ASN:ND2	4:B:2611:HOH:O	2.49	0.46
1:E:387:ALA:HB2	1:E:477:PHE:CD2	2.50	0.46
1:B:349:ASN:O	1:B:696:PRO:HD2	2.16	0.45
1:E:78:PRO:O	1:E:81:ARG:HG3	2.16	0.45
1:D:608:TYR:HA	1:D:659:MET:HE2	1.99	0.45
1:C:499:PRO:HA	1:C:504:PHE:CG	2.51	0.45
1:D:387:ALA:HB2	1:D:477:PHE:CD2	2.51	0.45
1:A:612:ARG:CG	4:A:2473:HOH:O	2.64	0.45
1:B:78:PRO:O	1:B:81:ARG:HG3	2.16	0.45
1:C:78:PRO:O	1:C:81:ARG:HG3	2.17	0.45
1:C:349:ASN:O	1:C:696:PRO:HD2	2.15	0.45
1:E:499:PRO:HA	1:E:504:PHE:CG	2.52	0.44
1:A:499:PRO:HA	1:A:504:PHE:CG	2.51	0.44
1:D:499:PRO:HA	1:D:504:PHE:CG	2.53	0.44
1:D:735:LEU:HD21	1:D:772:MET:HG2	1.99	0.43
1:E:725:VAL:HG23	4:E:2654:HOH:O	2.17	0.43
1:A:144:PRO:HG3	1:E:645:LYS:HA	2.00	0.42
1:C:400:SER:HB3	1:C:519:ARG:HB3	1.99	0.42
1:B:187:PRO:CB	1:B:197:LEU:HD11	2.46	0.42
1:D:360:PRO:HB2	1:D:576:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:THR:HG22	1:C:634:MET:HE3	2.01	0.42
1:D:608:TYR:HB2	1:D:659:MET:HE3	2.02	0.42
1:E:126:THR:HG22	1:E:634:MET:HE3	2.01	0.41
1:C:608:TYR:HA	1:C:659:MET:HE2	2.02	0.41
1:A:45:PRO:HB3	1:A:461:ASN:OD1	2.21	0.41
1:C:490:GLU:HG3	1:C:511:THR:HG22	2.01	0.41
1:B:15:LEU:HD21	1:D:234:ASP:HB3	2.03	0.41
1:C:45:PRO:HB3	1:C:461:ASN:OD1	2.21	0.41
1:B:360:PRO:HB2	1:B:576:PRO:HB3	2.03	0.41
1:B:608:TYR:HA	1:B:659:MET:HE2	2.03	0.41
1:E:685:THR:HA	1:E:686:PRO:HD3	2.00	0.41
1:A:608:TYR:HA	1:A:659:MET:HE2	2.03	0.41
1:E:608:TYR:HB2	1:E:659:MET:HE3	2.02	0.41
1:B:368:ILE:HG21	1:B:560:LEU:HD22	2.03	0.41
1:A:410:CYS:O	1:A:468:GLY:HA2	2.21	0.40
1:C:187:PRO:CB	1:C:197:LEU:HD11	2.47	0.40
1:C:360:PRO:HB2	1:C:576:PRO:HB3	2.03	0.40
1:E:608:TYR:HA	1:E:659:MET:HE2	2.03	0.40
1:E:45:PRO:HB3	1:E:461:ASN:OD1	2.21	0.40
1:E:355:LEU:HB2	1:E:386:TYR:HB2	2.04	0.40
1:A:368:ILE:HG21	1:A:560:LEU:HD22	2.04	0.40
1:B:45:PRO:HB3	1:B:461:ASN:OD1	2.22	0.40
1:B:410:CYS:O	1:B:468:GLY:HA2	2.22	0.40
1:E:410:CYS:O	1:E:468:GLY:HA2	2.22	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	773/799 (97%)	756 (98%)	16 (2%)	1 (0%)	48 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	774/799 (97%)	758 (98%)	15 (2%)	1 (0%)	48	60
1	C	774/799 (97%)	758 (98%)	16 (2%)	0	100	100
1	D	775/799 (97%)	757 (98%)	18 (2%)	0	100	100
1	E	776/799 (97%)	761 (98%)	15 (2%)	0	100	100
All	All	3872/3995 (97%)	3790 (98%)	80 (2%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLY
1	B	406	GLY

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	660/692 (95%)	657 (100%)	3 (0%)	81	90
1	B	660/692 (95%)	658 (100%)	2 (0%)	86	93
1	C	662/692 (96%)	657 (99%)	5 (1%)	73	86
1	D	662/692 (96%)	656 (99%)	6 (1%)	70	84
1	E	668/692 (96%)	666 (100%)	2 (0%)	86	93
All	All	3312/3460 (96%)	3294 (100%)	18 (0%)	81	90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	LEU
1	A	393	LEU
1	A	669	ILE
1	B	393	LEU
1	B	669	ILE
1	C	31	ILE

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Mol	Chain	Res	Type
1	C	94	SER
1	C	231	LEU
1	C	393	LEU
1	C	669	ILE
1	D	79	ARG
1	D	228	THR
1	D	232	SER
1	D	393	LEU
1	D	687	LEU
1	D	775	ASN
1	E	393	LEU
1	E	669	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	389	ASN
1	A	429	ASN
1	A	580	ASN
1	A	775	ASN
1	B	429	ASN
1	B	775	ASN
1	C	226	ASN
1	C	240	HIS
1	D	226	ASN
1	D	429	ASN
1	D	767	GLN
1	E	226	ASN
1	E	429	ASN
1	E	678	GLN
1	E	769	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 11 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 [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	771/799 (96%)	-0.35	20 (2%) 57 59	5, 17, 46, 72	6 (0%)
1	B	771/799 (96%)	-0.47	11 (1%) 73 75	3, 14, 41, 63	7 (0%)
1	C	771/799 (96%)	-0.46	12 (1%) 70 72	4, 14, 39, 58	7 (0%)
1	D	771/799 (96%)	-0.47	13 (1%) 69 70	3, 13, 39, 70	8 (1%)
1	E	771/799 (96%)	-0.57	7 (0%) 81 82	2, 10, 33, 56	9 (1%)
All	All	3855/3995 (96%)	-0.46	63 (1%) 70 72	2, 14, 40, 72	37 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	687	LEU	5.8
1	D	231	LEU	5.3
1	D	232	SER	4.8
1	D	228	THR	4.7
1	A	231	LEU	4.4
1	D	233	THR	4.4
1	D	230	ASP	4.2
1	D	792	THR	4.2
1	D	19	MET	3.9
1	C	231	LEU	3.8
1	A	774	ALA	3.6
1	E	19	MET	3.5
1	B	231	LEU	3.5
1	A	792	THR	3.3
1	C	19	MET	3.2
1	A	776	ASN	3.2
1	A	19	MET	3.2
1	B	232	SER	3.1
1	B	228	THR	2.9
1	C	668	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	600	ARG	2.9
1	B	19	MET	2.8
1	C	776	ASN	2.8
1	D	600	ARG	2.8
1	C	232	SER	2.6
1	A	600	ARG	2.6
1	E	600	ARG	2.6
1	B	88	LYS	2.6
1	A	139	ASP	2.5
1	E	755	ASP	2.5
1	D	655	ASP	2.5
1	A	88	LYS	2.4
1	D	668	GLY	2.4
1	A	235	LYS	2.4
1	A	773	LYS	2.4
1	E	667	GLU	2.4
1	A	74	ASP	2.3
1	D	88	LYS	2.3
1	C	233	THR	2.3
1	A	85	GLU	2.3
1	A	775	ASN	2.3
1	A	770	LEU	2.3
1	E	666	LEU	2.3
1	A	226	ASN	2.3
1	C	755	ASP	2.2
1	C	771	LEU	2.2
1	B	792	THR	2.2
1	B	81	ARG	2.2
1	B	755	ASP	2.2
1	C	226	ASN	2.2
1	A	689	SER	2.2
1	A	87	GLY	2.2
1	C	655	ASP	2.1
1	B	668	GLY	2.1
1	E	658	ASN	2.1
1	D	81	ARG	2.1
1	B	223	TRP	2.1
1	A	502	LYS	2.1
1	A	84	VAL	2.1
1	A	233	THR	2.0
1	B	226	ASN	2.0
1	D	654	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	31	ILE	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 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
2	K	A	1002	1/1	0.99	0.07	14,14,14,14	0
2	K	C	1002	1/1	0.99	0.06	12,12,12,12	0
2	K	E	1002	1/1	0.99	0.04	10,10,10,10	0
3	CL	C	1003	1/1	0.99	0.05	17,17,17,17	0
3	CL	E	1003	1/1	0.99	0.05	14,14,14,14	0
3	CL	E	1005	1/1	0.99	0.05	14,14,14,14	0
3	CL	B	1003	1/1	1.00	0.04	14,14,14,14	0
2	K	D	1002	1/1	1.00	0.04	10,10,10,10	0
3	CL	D	1003	1/1	1.00	0.04	16,16,16,16	0
2	K	B	1002	1/1	1.00	0.01	12,12,12,12	0
3	CL	A	1003	1/1	1.00	0.06	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.