



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:00 AM UTC

PDB ID : 2YIA / pdb_00002yia
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 : 3.02 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

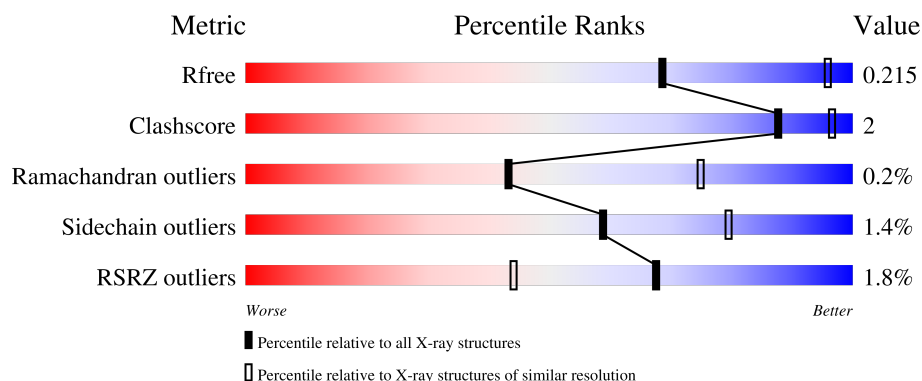
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	% 91% 7% .
1	B	799	% 91% 8% .
1	C	799	3% 90% 9% .
1	D	799	% 91% 8% .
1	E	799	% 90% 8% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	799	90% 8%
1	G	799	88% 7%5%
1	H	799	7% 91% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 49237 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	790	Total	C	N	O	S	0	5	0
			6202	3927	1047	1202	26			
1	B	790	Total	C	N	O	S	0	5	0
			6185	3916	1041	1202	26			
1	C	790	Total	C	N	O	S	0	5	0
			6193	3922	1043	1202	26			
1	D	790	Total	C	N	O	S	0	5	0
			6193	3922	1043	1202	26			
1	E	790	Total	C	N	O	S	0	5	0
			6189	3919	1042	1202	26			
1	F	782	Total	C	N	O	S	0	5	0
			6136	3887	1033	1190	26			
1	G	762	Total	C	N	O	S	0	0	0
			5966	3782	1007	1152	25			
1	H	790	Total	C	N	O	S	0	0	0
			6165	3907	1037	1195	26			

There are 72 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

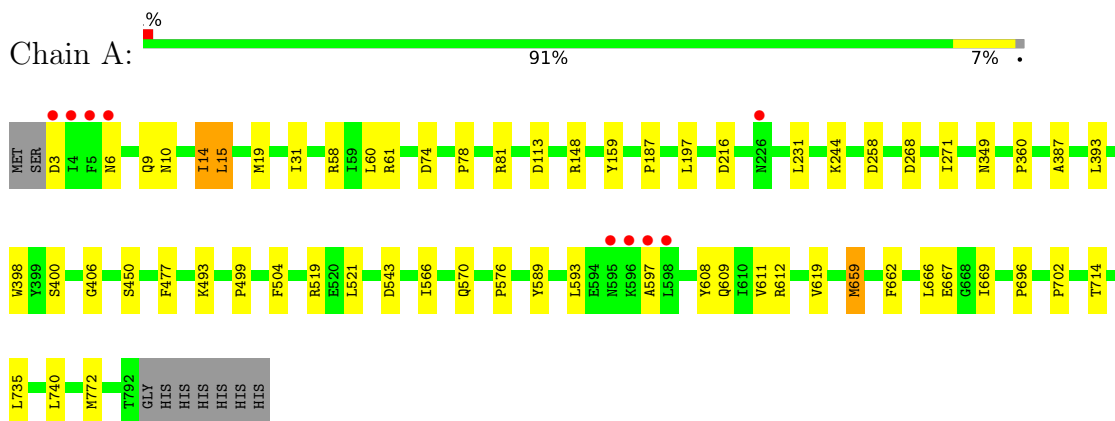
- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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
2	F	1	Total K 1 1	0	0
2	G	1	Total K 1 1	0	0
2	H	1	Total K 1 1	0	0

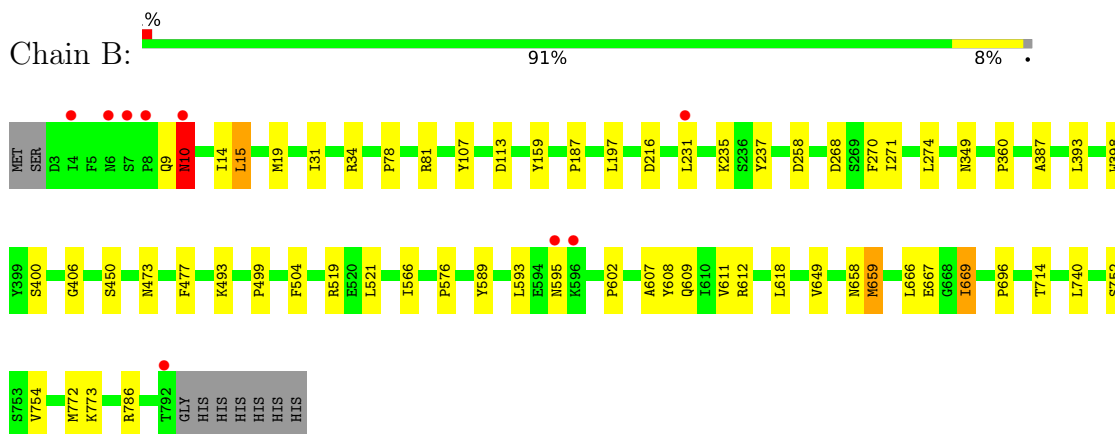
3 Residue-property plots [i](#)

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.

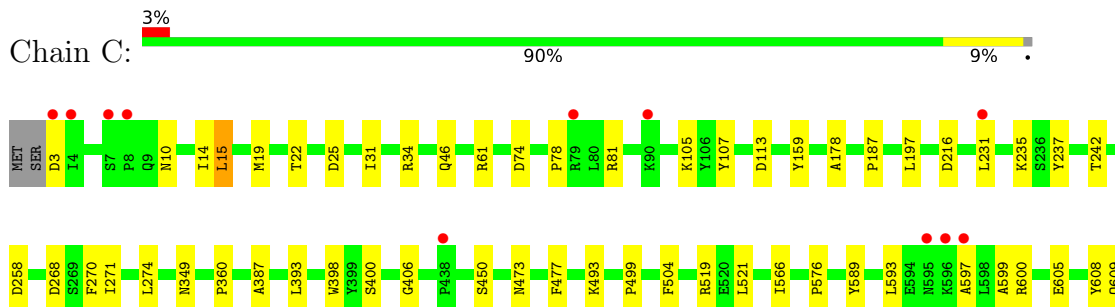
• Molecule 1: RNA-DIRECTED RNA POLYMERASE

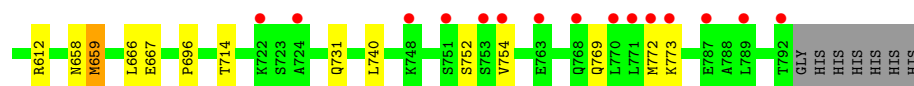


• Molecule 1: RNA-DIRECTED RNA POLYMERASE

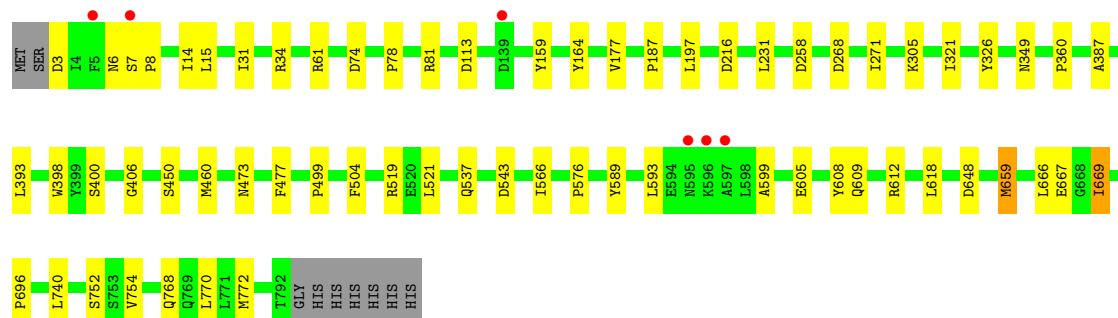
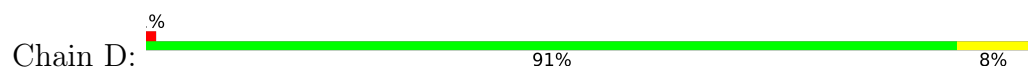


• Molecule 1: RNA-DIRECTED RNA POLYMERASE

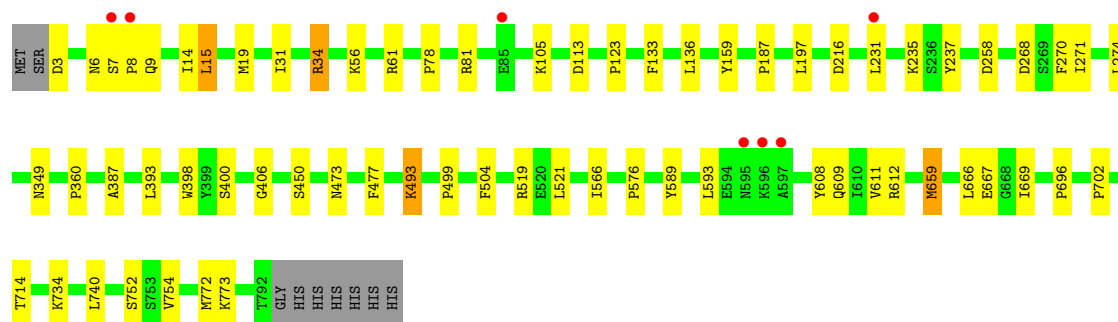
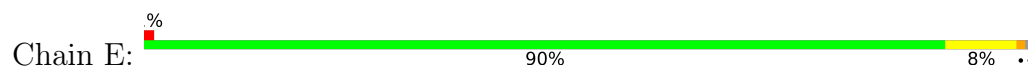




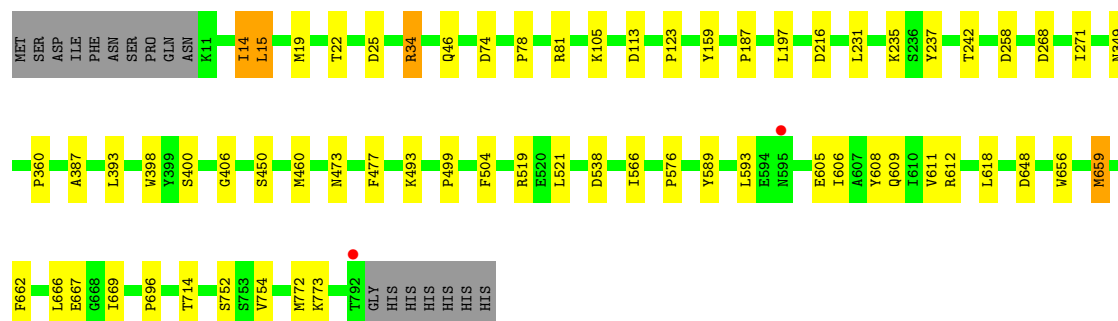
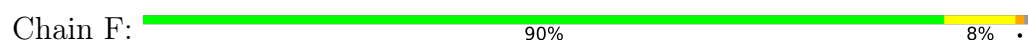
● Molecule 1: RNA-DIRECTED RNA POLYMERASE



● Molecule 1: RNA-DIRECTED RNA POLYMERASE

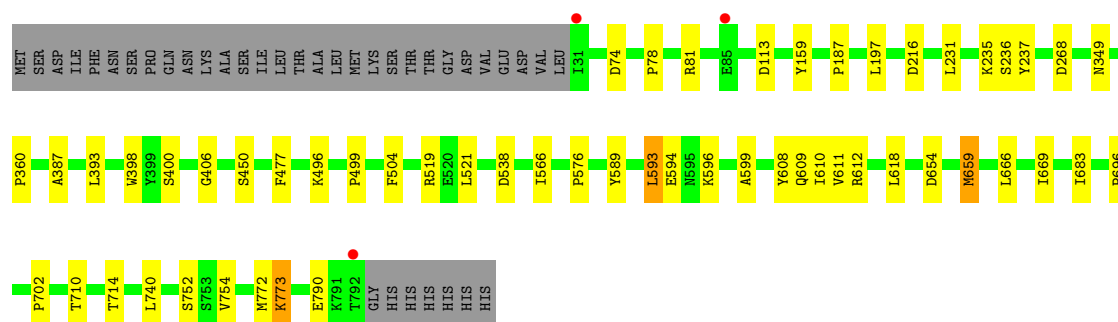


● Molecule 1: RNA-DIRECTED RNA POLYMERASE

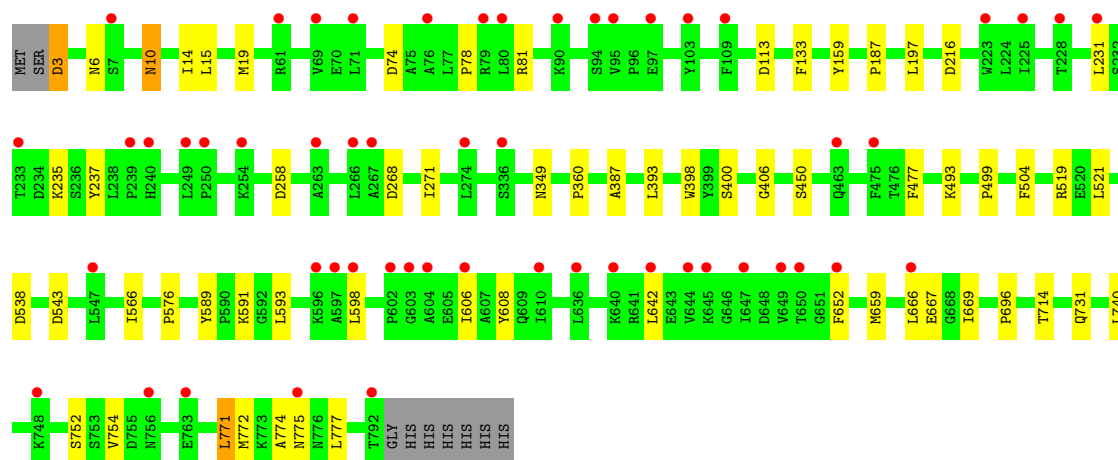
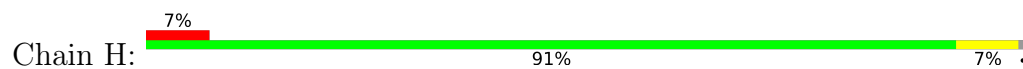


● Molecule 1: RNA-DIRECTED RNA POLYMERASE





● 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	200.94Å 209.47Å 243.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	145.01 – 3.02 145.01 – 3.02	Depositor EDS
% Data completeness (in resolution range)	(Not available) (145.01-3.02) 99.9 (145.01-3.02)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.9.2	Depositor
R, R_{free}	0.187 , 0.216 0.193 , 0.215	Depositor DCC
R_{free} test set	2029 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49237	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 1.78% 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

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	0.88	3/6347 (0.0%)	1.25	13/8643 (0.2%)
1	B	0.89	2/6330 (0.0%)	1.28	12/8625 (0.1%)
1	C	0.86	2/6338 (0.0%)	1.29	14/8633 (0.2%)
1	D	0.90	3/6338 (0.0%)	1.29	13/8633 (0.2%)
1	E	0.88	2/6334 (0.0%)	1.28	15/8629 (0.2%)
1	F	0.90	3/6279 (0.0%)	1.28	12/8550 (0.1%)
1	G	0.89	2/6102 (0.0%)	1.28	19/8310 (0.2%)
1	H	0.81	2/6303 (0.0%)	1.29	12/8585 (0.1%)
All	All	0.88	19/50371 (0.0%)	1.28	110/68608 (0.2%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	659	MET	SD-CE	-8.99	1.57	1.79
1	E	659	MET	SD-CE	-7.61	1.60	1.79
1	C	659	MET	SD-CE	-7.61	1.60	1.79
1	D	659	MET	SD-CE	-7.59	1.60	1.79
1	F	659	MET	SD-CE	-7.29	1.61	1.79
1	A	659	MET	SD-CE	-7.21	1.61	1.79
1	B	659	MET	SD-CE	-7.00	1.62	1.79
1	D	669	ILE	CG1-CD1	-6.29	1.27	1.51
1	H	669	ILE	CG1-CD1	-5.91	1.28	1.51
1	F	460	MET	SD-CE	-5.91	1.64	1.79
1	E	669	ILE	CG1-CD1	-5.68	1.29	1.51
1	H	774	ALA	CA-C	5.53	1.59	1.52
1	A	669	ILE	CG1-CD1	-5.50	1.30	1.51
1	C	605	GLU	CA-C	5.32	1.59	1.52
1	D	326	TYR	CA-C	5.27	1.58	1.52
1	G	496	LYS	CA-C	5.25	1.57	1.53
1	A	14	ILE	CG1-CD1	-5.15	1.31	1.51
1	F	14	ILE	CG1-CD1	-5.02	1.32	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	ILE	CG1-CD1	-5.02	1.32	1.51

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	3	ASP	CA-CB-CG	8.03	120.62	112.60
1	H	775	ASN	CA-C-N	7.88	132.29	120.31
1	H	775	ASN	C-N-CA	7.88	132.29	120.31
1	H	10	ASN	CA-CB-CG	7.82	120.42	112.60
1	C	667	GLU	N-CA-C	6.79	118.68	111.28
1	E	133	PHE	CA-CB-CG	-6.70	107.10	113.80
1	E	773	LYS	N-CA-C	-6.69	105.41	113.97
1	G	772	MET	N-CA-C	6.57	120.91	113.02
1	H	667	GLU	N-CA-C	6.51	118.37	111.28
1	C	10	ASN	CA-CB-CG	6.41	119.01	112.60
1	E	611	VAL	CA-C-N	6.39	129.16	120.54
1	E	611	VAL	C-N-CA	6.39	129.16	120.54
1	D	605	GLU	CA-C-N	6.09	128.23	120.56
1	D	605	GLU	C-N-CA	6.09	128.23	120.56
1	B	113	ASP	CA-CB-CG	6.08	118.68	112.60
1	D	258	ASP	CA-CB-CG	6.06	118.66	112.60
1	F	268	ASP	CA-CB-CG	6.02	118.62	112.60
1	E	113	ASP	CA-CB-CG	6.00	118.60	112.60
1	B	611	VAL	CA-C-N	5.93	128.55	120.54
1	B	611	VAL	C-N-CA	5.93	128.55	120.54
1	D	667	GLU	N-CA-C	5.92	117.73	111.28
1	F	113	ASP	CA-CB-CG	5.91	118.51	112.60
1	G	610	ILE	N-CA-C	-5.89	105.10	110.82
1	D	268	ASP	CA-CB-CG	5.87	118.47	112.60
1	B	216	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	268	ASP	CA-CB-CG	5.86	118.45	112.60
1	A	61	ARG	N-CA-C	-5.83	98.88	109.44
1	E	740	LEU	N-CA-C	5.81	118.36	111.33
1	G	702	PRO	CA-C-N	5.79	128.62	120.28
1	G	702	PRO	C-N-CA	5.79	128.62	120.28
1	H	268	ASP	CA-CB-CG	5.76	118.36	112.60
1	H	133	PHE	CA-CB-CG	-5.76	108.04	113.80
1	H	740	LEU	N-CA-C	5.73	118.27	111.33
1	G	268	ASP	CA-CB-CG	5.73	118.33	112.60
1	F	216	ASP	CA-CB-CG	5.72	118.33	112.60
1	B	773	LYS	N-CA-C	-5.71	106.36	113.38
1	C	3	ASP	CA-CB-CG	5.66	118.26	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	667	GLU	N-CA-C	5.63	117.42	111.28
1	E	473	ASN	CA-CB-CG	5.63	118.23	112.60
1	B	667	GLU	N-CA-C	5.62	117.41	111.28
1	E	702	PRO	CA-C-N	5.61	128.36	120.28
1	E	702	PRO	C-N-CA	5.61	128.36	120.28
1	B	740	LEU	N-CA-C	5.61	118.11	111.33
1	D	473	ASN	CA-CB-CG	5.57	118.17	112.60
1	A	667	GLU	N-CA-C	5.56	117.34	111.28
1	F	667	GLU	N-CA-C	5.55	117.33	111.28
1	B	10	ASN	CA-CB-CG	5.54	118.14	112.60
1	C	268	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	61	ARG	N-CA-C	-5.51	99.46	109.44
1	H	113	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	740	LEU	N-CA-C	5.47	117.94	111.33
1	F	611	VAL	CA-C-N	5.44	128.99	120.82
1	F	611	VAL	C-N-CA	5.44	128.99	120.82
1	B	772	MET	N-CA-C	5.44	119.55	113.02
1	C	113	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	113	ASP	CA-CB-CG	5.43	118.03	112.60
1	G	113	ASP	CA-CB-CG	5.42	118.02	112.60
1	F	648	ASP	CA-CB-CG	5.41	118.01	112.60
1	G	740	LEU	N-CA-C	5.41	117.87	111.33
1	G	596	LYS	CA-C-N	5.40	127.46	120.44
1	G	596	LYS	C-N-CA	5.40	127.46	120.44
1	G	593	LEU	CA-C-N	-5.39	114.00	122.08
1	G	593	LEU	C-N-CA	-5.39	114.00	122.08
1	E	268	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	473	ASN	CA-CB-CG	5.36	117.96	112.60
1	H	538	ASP	N-CA-C	5.35	118.46	109.95
1	C	769	GLN	CA-C-N	5.34	127.87	120.29
1	C	769	GLN	C-N-CA	5.34	127.87	120.29
1	D	740	LEU	N-CA-C	5.34	117.79	111.33
1	A	216	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	268	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	216	ASP	CA-CB-CG	5.31	117.91	112.60
1	G	772	MET	CA-CB-CG	-5.30	103.51	114.10
1	A	3	ASP	CA-CB-CG	5.28	117.88	112.60
1	H	258	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	216	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	113	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	258	ASP	CA-CB-CG	5.21	117.81	112.60
1	F	258	ASP	CA-CB-CG	5.21	117.81	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	538	ASP	N-CA-C	5.20	118.22	109.95
1	G	611	VAL	CA-C-N	5.20	128.62	120.82
1	G	611	VAL	C-N-CA	5.20	128.62	120.82
1	C	258	ASP	CA-CB-CG	5.20	117.80	112.60
1	D	177	VAL	CA-C-N	5.19	127.66	120.29
1	D	177	VAL	C-N-CA	5.19	127.66	120.29
1	C	216	ASP	CA-CB-CG	5.18	117.78	112.60
1	F	662	PHE	CA-C-N	5.18	126.62	120.14
1	F	662	PHE	C-N-CA	5.18	126.62	120.14
1	G	538	ASP	N-CA-C	5.18	118.19	109.95
1	C	740	LEU	N-CA-C	5.17	117.58	111.33
1	G	654	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	773	LYS	N-CA-C	-5.16	105.34	111.69
1	C	178	ALA	N-CA-C	5.13	116.96	111.36
1	C	473	ASN	CA-CB-CG	5.10	117.70	112.60
1	G	594	GLU	N-CA-C	5.09	117.75	110.68
1	A	258	ASP	CA-CB-CG	5.08	117.68	112.60
1	E	258	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	543	ASP	CA-CB-CG	5.07	117.67	112.60
1	E	493	LYS	CG-CD-CE	5.06	122.94	111.30
1	H	216	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	702	PRO	CA-C-N	5.05	127.56	120.28
1	A	702	PRO	C-N-CA	5.05	127.56	120.28
1	G	790	GLU	CB-CG-CD	5.05	121.19	112.60
1	A	611	VAL	CA-C-N	5.04	127.34	120.54
1	A	611	VAL	C-N-CA	5.04	127.34	120.54
1	E	61	ARG	N-CA-C	-5.04	100.32	109.44
1	D	648	ASP	CA-CB-CG	5.04	117.64	112.60
1	G	216	ASP	CA-CB-CG	5.04	117.64	112.60
1	C	61	ARG	N-CA-C	-5.03	100.34	109.44
1	F	473	ASN	CA-CB-CG	5.01	117.61	112.60

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	6202	0	6117	26	0
1	B	6185	0	6075	28	1
1	C	6193	0	6097	28	0
1	D	6193	0	6097	25	0
1	E	6189	0	6086	24	0
1	F	6136	0	6056	26	0
1	G	5966	0	5889	23	0
1	H	6165	0	6085	24	1
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
All	All	49237	0	48502	194	1

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 (194) 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:A:244:LYS:HE3	1:A:597[B]:ALA:HB2	1.39	1.02
1:A:10:ASN:OD1	1:B:658:ASN:ND2	2.10	0.82
1:H:606:ILE:HG21	1:H:642:LEU:HD21	1.60	0.81
1:E:734:LYS:HD3	1:E:772:MET:HE1	1.74	0.70
1:E:3:ASP:OD1	1:E:6:ASN:ND2	2.25	0.69
1:H:493:LYS:HE3	1:H:714:THR:HG22	1.76	0.68
1:G:669:ILE:HG21	1:G:683:ILE:HG22	1.76	0.67
1:A:244:LYS:CE	1:A:597[B]:ALA:HB2	2.23	0.64
1:A:244:LYS:HE3	1:A:597[B]:ALA:CB	2.20	0.64
1:F:493:LYS:HE3	1:F:714:THR:HG22	1.79	0.63
1:H:3:ASP:OD1	1:H:6:ASN:ND2	2.31	0.63
1:C:187:PRO:HB3	1:C:197:LEU:HD11	1.82	0.62
1:C:493:LYS:HE3	1:C:714:THR:HG22	1.84	0.60
1:A:187:PRO:HB3	1:A:197:LEU:HD11	1.84	0.59
1:H:187:PRO:HB3	1:H:197:LEU:HD11	1.85	0.59
1:H:608:TYR:HB2	1:H:659:MET:HE2	1.84	0.58
1:G:593:LEU:HD23	1:G:599:ALA:HA	1.85	0.58
1:E:187:PRO:HB3	1:E:197:LEU:HD11	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:400:SER:HB3	1:F:519:ARG:HB3	1.87	0.56
1:F:187:PRO:HB3	1:F:197:LEU:HD11	1.87	0.56
1:G:398:TRP:HB3	1:G:521:LEU:HB3	1.88	0.56
1:E:398:TRP:HB3	1:E:521:LEU:HB3	1.88	0.56
1:G:187:PRO:HB3	1:G:197:LEU:HD11	1.89	0.55
1:G:618:LEU:HD11	1:G:669:ILE:HD11	1.88	0.55
1:H:598:LEU:HD11	1:H:652:PHE:CE1	2.41	0.55
1:A:608:TYR:HB2	1:A:659:MET:HE2	1.89	0.54
1:A:609:GLN:OE1	1:A:612:ARG:NH2	2.40	0.54
1:D:398:TRP:HB3	1:D:521:LEU:HB3	1.90	0.54
1:C:398:TRP:HB3	1:C:521:LEU:HB3	1.90	0.54
1:H:731:GLN:HG2	1:H:772:MET:SD	2.48	0.54
1:D:400:SER:HB3	1:D:519:ARG:HB3	1.90	0.54
1:B:593:LEU:CD1	1:B:659:MET:HB2	2.37	0.53
1:B:400:SER:HB3	1:B:519:ARG:HB3	1.89	0.53
1:B:398:TRP:HB3	1:B:521:LEU:HB3	1.89	0.53
1:E:593:LEU:CD1	1:E:659:MET:HB2	2.38	0.53
1:B:187:PRO:HB3	1:B:197:LEU:HD11	1.89	0.53
1:C:593:LEU:HD11	1:C:659:MET:HE3	1.89	0.53
1:D:608:TYR:HB2	1:D:659:MET:HE2	1.89	0.53
1:F:398:TRP:HB3	1:F:521:LEU:HB3	1.91	0.53
1:D:187:PRO:HB3	1:D:197:LEU:HD11	1.89	0.53
1:D:609:GLN:OE1	1:D:612:ARG:NH2	2.42	0.53
1:B:608:TYR:HB2	1:B:659:MET:HE2	1.91	0.52
1:A:593:LEU:CD1	1:A:659:MET:HB2	2.39	0.52
1:C:608:TYR:HB2	1:C:659:MET:HE2	1.90	0.52
1:D:3:ASP:OD1	1:D:6:ASN:ND2	2.43	0.52
1:F:609:GLN:OE1	1:F:612:ARG:NH2	2.42	0.52
1:B:609:GLN:OE1	1:B:612:ARG:NH2	2.43	0.52
1:A:398:TRP:HB3	1:A:521:LEU:HB3	1.91	0.52
1:A:400:SER:HB3	1:A:519:ARG:HB3	1.92	0.51
1:H:349:ASN:O	1:H:696:PRO:HD2	2.11	0.51
1:G:593:LEU:CD1	1:G:659:MET:HB2	2.40	0.51
1:G:609:GLN:OE1	1:G:612:ARG:NH2	2.43	0.51
1:E:609:GLN:OE1	1:E:612:ARG:NH2	2.43	0.51
1:F:593:LEU:CD1	1:F:659:MET:HB2	2.40	0.51
1:E:493:LYS:HE3	1:E:714:THR:HG22	1.93	0.50
1:D:593:LEU:CD1	1:D:659:MET:HB2	2.40	0.50
1:H:398:TRP:HB3	1:H:521:LEU:HB3	1.92	0.50
1:C:609:GLN:OE1	1:C:612:ARG:NH2	2.45	0.50
1:E:400:SER:HB3	1:E:519:ARG:HB3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:591:LYS:O	1:H:608:TYR:OH	2.22	0.50
1:E:608:TYR:HB2	1:E:659:MET:HE2	1.93	0.50
1:F:608:TYR:HB2	1:F:659:MET:HE2	1.94	0.50
1:H:771:LEU:HD13	1:H:777:LEU:HD13	1.93	0.50
1:D:537:GLN:OE1	1:F:46:GLN:OE1	2.30	0.49
1:C:400:SER:HB3	1:C:519:ARG:HB3	1.92	0.49
1:G:618:LEU:HD11	1:G:669:ILE:CD1	2.41	0.49
1:H:400:SER:HB3	1:H:519:ARG:HB3	1.94	0.49
1:A:31:ILE:CD1	1:B:602:PRO:HG2	2.43	0.49
1:E:349:ASN:O	1:E:696:PRO:HD2	2.12	0.49
1:A:735:LEU:HD21	1:A:772:MET:HG3	1.93	0.48
1:B:618:LEU:HD11	1:B:669:ILE:HD11	1.95	0.48
1:C:593:LEU:CD1	1:C:659:MET:HB2	2.42	0.48
1:C:349:ASN:O	1:C:696:PRO:HD2	2.14	0.48
1:D:387:ALA:HB2	1:D:477:PHE:CD2	2.48	0.48
1:A:349:ASN:O	1:A:696:PRO:HD2	2.14	0.47
1:B:349:ASN:O	1:B:696:PRO:HD2	2.13	0.47
1:A:58:ARG:NH2	1:A:60:LEU:HD22	2.30	0.47
1:G:400:SER:HB3	1:G:519:ARG:HB3	1.96	0.47
1:F:360:PRO:HB2	1:F:576:PRO:HB3	1.97	0.47
1:H:387:ALA:HB2	1:H:477:PHE:CD2	2.50	0.47
1:C:387:ALA:HB2	1:C:477:PHE:CD2	2.49	0.47
1:C:105:LYS:HD2	1:C:107:TYR:HE1	1.79	0.47
1:G:349:ASN:O	1:G:696:PRO:HD2	2.15	0.47
1:E:136:LEU:HD11	1:F:606:ILE:HG12	1.97	0.47
1:F:349:ASN:O	1:F:696:PRO:HD2	2.15	0.47
1:B:78:PRO:O	1:B:81:ARG:HG3	2.15	0.46
1:A:387:ALA:HB2	1:A:477:PHE:CD2	2.50	0.46
1:B:159:TYR:HB2	1:B:589:TYR:HB3	1.98	0.46
1:G:608:TYR:HB2	1:G:659:MET:HE2	1.97	0.46
1:A:9:GLN:HA	1:B:595[A]:ASN:OD1	2.16	0.46
1:D:78:PRO:O	1:D:81:ARG:HG3	2.16	0.46
1:G:387:ALA:HB2	1:G:477:PHE:CD2	2.51	0.46
1:C:593:LEU:HD23	1:C:599:ALA:HA	1.97	0.46
1:F:78:PRO:O	1:F:81:ARG:HG3	2.16	0.46
1:H:499:PRO:HA	1:H:504:PHE:CG	2.51	0.46
1:D:752:SER:HB2	1:D:754:VAL:HG13	1.98	0.45
1:F:618:LEU:HD11	1:F:669:ILE:HD11	1.98	0.45
1:B:387:ALA:HB2	1:B:477:PHE:CD2	2.51	0.45
1:E:499:PRO:HA	1:E:504:PHE:CG	2.52	0.45
1:G:159:TYR:HB2	1:G:589:TYR:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LYS:HG3	1:A:714:THR:HG21	1.98	0.45
1:B:752:SER:HB2	1:B:754:VAL:HG13	1.99	0.45
1:A:499:PRO:HA	1:A:504:PHE:CG	2.52	0.44
1:H:593:LEU:CD1	1:H:659:MET:HB2	2.47	0.44
1:B:15:LEU:O	1:B:19:MET:HG2	2.17	0.44
1:B:618:LEU:HD11	1:B:669:ILE:CD1	2.47	0.44
1:C:499:PRO:HA	1:C:504:PHE:CG	2.53	0.44
1:G:360:PRO:HB2	1:G:576:PRO:HB3	1.98	0.44
1:F:387:ALA:HB2	1:F:477:PHE:CD2	2.52	0.44
1:A:78:PRO:O	1:A:81:ARG:HG3	2.17	0.44
1:D:593:LEU:HD12	1:D:593:LEU:HA	1.87	0.44
1:E:78:PRO:O	1:E:81:ARG:HG3	2.17	0.44
1:G:618:LEU:HD13	1:G:666:LEU:HD13	1.99	0.44
1:A:15:LEU:O	1:A:19:MET:HG2	2.18	0.44
1:F:15:LEU:O	1:F:19:MET:HG2	2.18	0.44
1:D:519:ARG:HE	1:D:519:ARG:HB2	1.71	0.44
1:B:360:PRO:HB2	1:B:576:PRO:HB3	1.99	0.44
1:F:499:PRO:HA	1:F:504:PHE:CG	2.52	0.44
1:D:349:ASN:O	1:D:696:PRO:HD2	2.18	0.43
1:D:543:ASP:O	1:F:105:LYS:HE2	2.18	0.43
1:D:768:GLN:O	1:D:772:MET:HG3	2.18	0.43
1:F:656:TRP:HE1	1:F:669:ILE:HG13	1.83	0.43
1:E:34:ARG:HD3	1:E:123:PRO:HD2	2.00	0.43
1:B:499:PRO:HA	1:B:504:PHE:CG	2.53	0.43
1:D:360:PRO:HB2	1:D:576:PRO:HB3	2.00	0.43
1:G:499:PRO:HA	1:G:504:PHE:CG	2.53	0.43
1:C:731:GLN:HG2	1:C:772:MET:SD	2.58	0.43
1:E:159:TYR:HB2	1:E:589:TYR:HB3	2.01	0.43
1:E:387:ALA:HB2	1:E:477:PHE:CD2	2.53	0.43
1:B:9:GLN:HB3	1:C:242:THR:HG23	2.00	0.43
1:F:235:LYS:HD3	1:F:237:TYR:CZ	2.54	0.43
1:A:74:ASP:HB2	1:A:81:ARG:HG2	2.00	0.43
1:A:619:VAL:HG11	1:A:662:PHE:CD1	2.54	0.43
1:C:360:PRO:HB2	1:C:576:PRO:HB3	2.00	0.43
1:G:618:LEU:CD1	1:G:669:ILE:HD11	2.48	0.43
1:D:159:TYR:HB2	1:D:589:TYR:HB3	2.01	0.43
1:F:752:SER:HB2	1:F:754:VAL:HG13	2.01	0.43
1:C:78:PRO:O	1:C:81:ARG:HG3	2.18	0.42
1:D:74:ASP:HB2	1:D:81:ARG:HG2	2.00	0.42
1:D:499:PRO:HA	1:D:504:PHE:CG	2.53	0.42
1:E:270:PHE:O	1:E:274:LEU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:THR:HG23	1:F:25:ASP:OD2	2.19	0.42
1:C:752:SER:HB2	1:C:754:VAL:HG13	2.01	0.42
1:D:593:LEU:HD23	1:D:599:ALA:HA	2.02	0.42
1:G:710:THR:O	1:G:714:THR:HG23	2.18	0.42
1:E:360:PRO:HB2	1:E:576:PRO:HB3	2.01	0.42
1:C:15:LEU:O	1:C:19:MET:HG2	2.20	0.42
1:E:752:SER:HB2	1:E:754:VAL:HG13	2.01	0.42
1:F:159:TYR:HB2	1:F:589:TYR:HB3	2.02	0.42
1:B:235:LYS:HD3	1:B:237:TYR:CZ	2.54	0.42
1:B:493:LYS:HE3	1:B:714:THR:HG22	2.02	0.42
1:E:7:SER:HA	1:E:8:PRO:HD3	1.94	0.42
1:E:15:LEU:O	1:E:19:MET:HG2	2.18	0.42
1:H:78:PRO:O	1:H:81:ARG:HG3	2.19	0.42
1:H:360:PRO:HB2	1:H:576:PRO:HB3	2.00	0.42
1:H:593:LEU:HD11	1:H:659:MET:HE3	2.02	0.42
1:A:360:PRO:HB2	1:A:576:PRO:HB3	2.01	0.42
1:F:618:LEU:HD11	1:F:669:ILE:CD1	2.49	0.42
1:G:78:PRO:O	1:G:81:ARG:HG3	2.19	0.42
1:F:74:ASP:HB2	1:F:81:ARG:HG2	2.01	0.42
1:A:187:PRO:CB	1:A:197:LEU:HD11	2.50	0.41
1:B:607:ALA:HB2	1:B:649:VAL:HB	2.02	0.41
1:H:235:LYS:HD3	1:H:237:TYR:CZ	2.55	0.41
1:C:597[A]:ALA:O	1:C:600:ARG:HG2	2.20	0.41
1:H:606:ILE:CG2	1:H:642:LEU:HD21	2.42	0.41
1:E:9:GLN:HB3	1:F:242:THR:HG23	2.01	0.41
1:A:570:GLN:HG3	1:C:46:GLN:NE2	2.36	0.41
1:B:786:ARG:HG2	1:B:786:ARG:HH11	1.85	0.41
1:B:10:ASN:CG	1:C:658:ASN:HD22	2.29	0.41
1:F:34:ARG:HD3	1:F:123:PRO:HD2	2.03	0.41
1:G:74:ASP:HB2	1:G:81:ARG:HG2	2.02	0.41
1:H:752:SER:HB2	1:H:754:VAL:HG13	2.02	0.41
1:C:74:ASP:HB2	1:C:81:ARG:HG2	2.03	0.41
1:D:164:TYR:CD1	1:D:460:MET:HE2	2.56	0.41
1:G:752:SER:HB2	1:G:754:VAL:HG13	2.02	0.41
1:G:773:LYS:HE2	1:G:773:LYS:HB2	1.95	0.41
1:H:159:TYR:HB2	1:H:589:TYR:HB3	2.02	0.41
1:C:22:THR:HG23	1:C:25:ASP:OD2	2.20	0.41
1:D:618:LEU:HD11	1:D:669:ILE:HD11	2.03	0.41
1:C:270:PHE:O	1:C:274:LEU:HB2	2.21	0.40
1:D:305:LYS:HG3	1:D:321:ILE:HD11	2.03	0.40
1:G:235:LYS:HD3	1:G:237:TYR:CZ	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:PHE:O	1:B:274:LEU:HB2	2.20	0.40
1:D:7:SER:HA	1:D:8:PRO:HD3	1.94	0.40
1:H:74:ASP:HB2	1:H:81:ARG:HG2	2.03	0.40
1:C:159:TYR:HB2	1:C:589:TYR:HB3	2.04	0.40
1:C:235:LYS:HD3	1:C:237:TYR:CZ	2.56	0.40
1:A:159:TYR:HB2	1:A:589:TYR:HB3	2.03	0.40
1:B:593:LEU:HA	1:B:593:LEU:HD12	1.83	0.40
1:B:595[A]:ASN:ND2	1:B:658:ASN:HB3	2.37	0.40
1:C:15:LEU:HD12	1:C:15:LEU:HA	1.91	0.40
1:E:235:LYS:HD3	1:E:237:TYR:CZ	2.56	0.40
1:E:519:ARG:HE	1:E:519:ARG:HB2	1.72	0.40
1:H:15:LEU:O	1:H:19:MET:HG2	2.21	0.40

All (1) 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:B:107:TYR:OH	1:H:543:ASP:O[1_545]	2.13	0.07

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	793/799 (99%)	770 (97%)	21 (3%)	2 (0%)	36	68
1	B	793/799 (99%)	769 (97%)	22 (3%)	2 (0%)	36	68
1	C	793/799 (99%)	772 (97%)	19 (2%)	2 (0%)	36	68
1	D	793/799 (99%)	768 (97%)	23 (3%)	2 (0%)	36	68
1	E	793/799 (99%)	771 (97%)	20 (2%)	2 (0%)	36	68
1	F	785/799 (98%)	764 (97%)	19 (2%)	2 (0%)	36	68
1	G	760/799 (95%)	741 (98%)	18 (2%)	1 (0%)	48	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	788/799 (99%)	766 (97%)	20 (2%)	2 (0%)	36 68
All	All	6298/6392 (98%)	6121 (97%)	162 (3%)	15 (0%)	43 75

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	GLY
1	B	406	GLY
1	C	406	GLY
1	D	406	GLY
1	E	406	GLY
1	F	406	GLY
1	G	406	GLY
1	H	406	GLY
1	A	666	LEU
1	B	666	LEU
1	C	666	LEU
1	D	666	LEU
1	E	666	LEU
1	F	666	LEU
1	H	666	LEU

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	676/692 (98%)	667 (99%)	9 (1%)	61 80
1	B	672/692 (97%)	662 (98%)	10 (2%)	57 79
1	C	674/692 (97%)	665 (99%)	9 (1%)	61 80
1	D	674/692 (97%)	664 (98%)	10 (2%)	57 79
1	E	673/692 (97%)	662 (98%)	11 (2%)	55 78
1	F	668/692 (96%)	657 (98%)	11 (2%)	55 78
1	G	648/692 (94%)	642 (99%)	6 (1%)	70 84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	671/692 (97%)	663 (99%)	8 (1%)	63 81
All	All	5356/5536 (97%)	5282 (99%)	74 (1%)	59 79

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	14	ILE
1	A	15	LEU
1	A	148	ARG
1	A	231	LEU
1	A	271	ILE
1	A	393	LEU
1	A	450	SER
1	A	566	ILE
1	B	10	ASN
1	B	14	ILE
1	B	15	LEU
1	B	31	ILE
1	B	34	ARG
1	B	231	LEU
1	B	271	ILE
1	B	393	LEU
1	B	450	SER
1	B	566	ILE
1	C	14	ILE
1	C	15	LEU
1	C	31	ILE
1	C	34	ARG
1	C	231	LEU
1	C	271	ILE
1	C	393	LEU
1	C	450	SER
1	C	566	ILE
1	D	14	ILE
1	D	15	LEU
1	D	31	ILE
1	D	34	ARG
1	D	231	LEU
1	D	271	ILE
1	D	393	LEU
1	D	450	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	566	ILE
1	D	770	LEU
1	E	14	ILE
1	E	15	LEU
1	E	31	ILE
1	E	34	ARG
1	E	56	LYS
1	E	105	LYS
1	E	231	LEU
1	E	271	ILE
1	E	393	LEU
1	E	450	SER
1	E	566	ILE
1	F	14	ILE
1	F	15	LEU
1	F	34	ARG
1	F	231	LEU
1	F	271	ILE
1	F	393	LEU
1	F	450	SER
1	F	566	ILE
1	F	605	GLU
1	F	772	MET
1	F	773	LYS
1	G	231	LEU
1	G	236	SER
1	G	393	LEU
1	G	450	SER
1	G	566	ILE
1	G	773	LYS
1	H	10	ASN
1	H	14	ILE
1	H	231	LEU
1	H	271	ILE
1	H	393	LEU
1	H	450	SER
1	H	566	ILE
1	H	771	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	226	ASN
1	A	580	ASN
1	A	623	ASN
1	A	658	ASN
1	A	767	GLN
1	B	9	GLN
1	B	149	GLN
1	B	226	ASN
1	B	240	HIS
1	B	362	HIS
1	B	429	ASN
1	B	580	ASN
1	B	623	ASN
1	B	767	GLN
1	C	9	GLN
1	C	46	GLN
1	C	149	GLN
1	C	226	ASN
1	C	362	HIS
1	C	429	ASN
1	C	580	ASN
1	C	623	ASN
1	C	658	ASN
1	C	775	ASN
1	D	130	GLN
1	D	149	GLN
1	D	226	ASN
1	D	362	HIS
1	D	580	ASN
1	D	623	ASN
1	E	149	GLN
1	E	226	ASN
1	E	329	HIS
1	E	362	HIS
1	E	580	ASN
1	E	623	ASN
1	E	767	GLN
1	E	768	GLN
1	F	46	GLN
1	F	149	GLN
1	F	226	ASN
1	F	362	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	580	ASN
1	F	623	ASN
1	F	658	ASN
1	G	149	GLN
1	G	226	ASN
1	G	362	HIS
1	G	429	ASN
1	G	580	ASN
1	G	623	ASN
1	G	731	GLN
1	H	226	ASN
1	H	329	HIS
1	H	362	HIS
1	H	623	ASN
1	H	658	ASN
1	H	775	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 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	790/799 (98%)	-0.39	9 (1%) 78 57	24, 50, 84, 112	5 (0%)
1	B	790/799 (98%)	-0.39	9 (1%) 78 57	29, 51, 87, 121	5 (0%)
1	C	790/799 (98%)	0.28	26 (3%) 49 28	32, 77, 124, 151	5 (0%)
1	D	790/799 (98%)	-0.36	6 (0%) 82 64	32, 50, 84, 114	5 (0%)
1	E	790/799 (98%)	-0.26	7 (0%) 81 61	34, 57, 95, 125	5 (0%)
1	F	782/799 (97%)	-0.39	2 (0%) 90 79	30, 52, 79, 107	5 (0%)
1	G	762/799 (95%)	-0.35	3 (0%) 88 76	35, 55, 80, 106	0
1	H	790/799 (98%)	0.58	54 (6%) 23 12	45, 96, 185, 209	0
All	All	6284/6392 (98%)	-0.16	116 (1%) 67 44	24, 57, 116, 209	30 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	595[A]	ASN	5.2
1	B	4	ILE	4.8
1	D	595[A]	ASN	4.4
1	B	595[A]	ASN	4.3
1	H	647	ILE	4.2
1	B	7	SER	4.2
1	D	597[A]	ALA	4.2
1	E	595[A]	ASN	4.1
1	H	652	PHE	4.1
1	C	4	ILE	3.9
1	D	596[A]	LYS	3.9
1	A	6	ASN	3.9
1	C	595[A]	ASN	3.9
1	B	8	PRO	3.8
1	C	7	SER	3.6
1	H	775	ASN	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	602	PRO	3.5
1	H	606	ILE	3.4
1	H	266	LEU	3.3
1	H	644	VAL	3.2
1	C	231	LEU	3.2
1	H	231	LEU	3.2
1	A	596[A]	LYS	3.1
1	A	597[A]	ALA	3.1
1	H	263	ALA	3.1
1	G	792	THR	3.1
1	A	4	ILE	3.1
1	B	792	THR	3.0
1	H	603	GLY	3.0
1	C	770	LEU	2.9
1	H	640	LYS	2.9
1	D	5	PHE	2.9
1	C	768	GLN	2.8
1	A	3	ASP	2.8
1	C	754	VAL	2.8
1	H	463	GLN	2.8
1	B	6	ASN	2.8
1	C	722	LYS	2.7
1	C	771	LEU	2.7
1	H	249	LEU	2.7
1	C	763	GLU	2.7
1	A	595[A]	ASN	2.7
1	B	10	ASN	2.7
1	C	597[A]	ALA	2.7
1	H	80	LEU	2.7
1	F	792	THR	2.6
1	C	3	ASP	2.6
1	H	598	LEU	2.5
1	E	596[A]	LYS	2.5
1	C	792	THR	2.5
1	H	274	LEU	2.5
1	H	225	ILE	2.5
1	A	5	PHE	2.5
1	H	250	PRO	2.5
1	H	233	THR	2.4
1	H	604	ALA	2.4
1	C	90	LYS	2.4
1	H	223	TRP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	666	LEU	2.4
1	H	94	SER	2.4
1	B	231	LEU	2.3
1	E	85	GLU	2.3
1	C	753	SER	2.3
1	H	228	THR	2.3
1	H	649	VAL	2.3
1	G	31	ILE	2.3
1	H	7	SER	2.3
1	A	226	ASN	2.3
1	E	231	LEU	2.3
1	H	792	THR	2.3
1	H	103	TYR	2.3
1	H	90	LYS	2.3
1	C	724	ALA	2.2
1	E	7	SER	2.2
1	H	95	VAL	2.2
1	C	596[A]	LYS	2.2
1	D	7	SER	2.2
1	H	69	VAL	2.2
1	E	597[A]	ALA	2.2
1	H	239	PRO	2.2
1	C	773	LYS	2.2
1	H	596	LYS	2.2
1	H	650	THR	2.2
1	H	76	ALA	2.2
1	A	598[A]	LEU	2.1
1	H	267	ALA	2.1
1	H	336	SER	2.1
1	C	8	PRO	2.1
1	E	8	PRO	2.1
1	D	139	ASP	2.1
1	H	79	ARG	2.1
1	H	97	GLU	2.1
1	H	475	PHE	2.1
1	C	748	LYS	2.1
1	H	547	LEU	2.1
1	H	610	ILE	2.1
1	H	645	LYS	2.1
1	C	79	ARG	2.1
1	C	772	MET	2.1
1	B	596[A]	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	71	LEU	2.1
1	H	240	HIS	2.1
1	G	85	GLU	2.1
1	H	748	LYS	2.0
1	H	61	ARG	2.0
1	H	597	ALA	2.0
1	C	438	PRO	2.0
1	C	787	GLU	2.0
1	H	763	GLU	2.0
1	C	789	LEU	2.0
1	H	636	LEU	2.0
1	H	642	LEU	2.0
1	C	751	SER	2.0
1	H	756	ASN	2.0
1	H	109	PHE	2.0
1	H	254	LYS	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	C	1002	1/1	0.95	0.06	109,109,109,109	0
2	K	E	1002	1/1	0.96	0.10	85,85,85,85	0
2	K	F	1002	1/1	0.96	0.09	71,71,71,71	0
2	K	B	1002	1/1	0.98	0.06	74,74,74,74	0
2	K	A	1002	1/1	0.98	0.04	71,71,71,71	0
2	K	H	1002	1/1	0.98	0.09	108,108,108,108	0
2	K	G	1002	1/1	0.99	0.05	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K	D	1002	1/1	0.99	0.04	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.