



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:16 PM UTC

PDB ID : 5CZ2 / pdb_00005cz2
Title : Crystal structure of a two-domain fragment of MMTV integrase
Authors : Cook, N.; Ballandras-Colas, A.; Engelman, A.; Cherepanov, P.
Deposited on : 2015-07-31
Resolution : 2.72 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

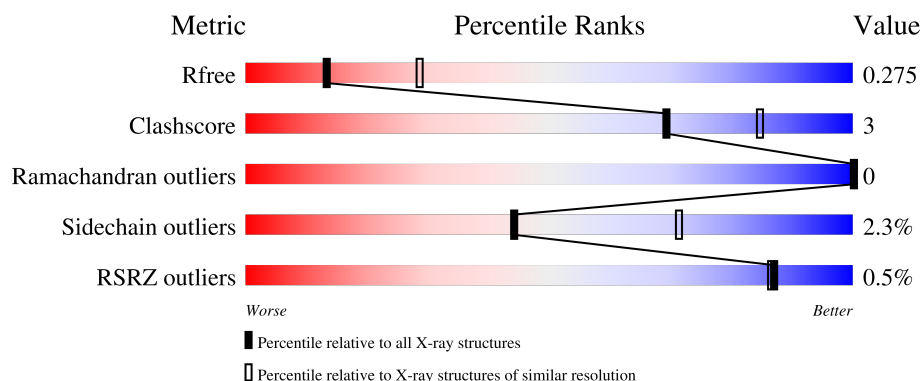
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	210	
1	B	210	
1	C	210	
1	D	210	
1	E	210	

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Mol	Chain	Length	Quality of chain
1	F	210	% 48%7%45%
1	G	210	19%80%
1	H	210	% 19%81%
1	I	210	18%81%
1	J	210	18%80%
1	K	210	17%83%
1	L	210	18%80%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8591 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 Pol polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1214	775	225	211	3			
1	B	142	Total	C	N	O	S	0	0	0
			1150	737	209	201	3			
1	C	152	Total	C	N	O	S	0	0	0
			1207	770	224	210	3			
1	D	139	Total	C	N	O	S	0	0	0
			1098	701	200	194	3			
1	E	153	Total	C	N	O	S	0	0	0
			1215	774	227	211	3			
1	F	115	Total	C	N	O	S	0	0	0
			895	574	163	155	3			
1	G	41	Total	C	N	O	S	0	0	0
			323	200	65	56	2			
1	H	40	Total	C	N	O	S	0	0	0
			291	181	57	51	2			
1	I	39	Total	C	N	O	S	0	0	0
			282	176	56	48	2			
1	J	41	Total	C	N	O	S	0	0	0
			315	195	64	54	2			
1	K	36	Total	C	N	O	S	0	0	0
			270	167	56	45	2			
1	L	41	Total	C	N	O	S	0	0	0
			319	198	65	54	2			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Mg 1	0	0
2	D	1	Total 1	Mg 1	0	0
2	E	1	Total 1	Mg 1	0	0
2	F	1	Total 1	Mg 1	0	0

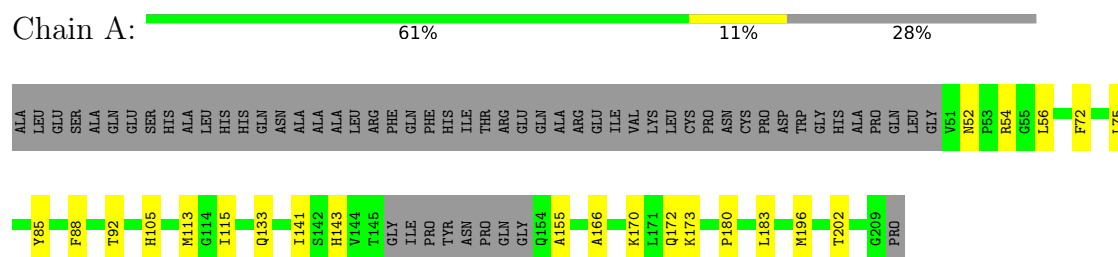
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	I	1	Total 1	Zn 1	0	0
3	J	1	Total 1	Zn 1	0	0
3	K	1	Total 1	Zn 1	0	0
3	L	1	Total 1	Zn 1	0	0

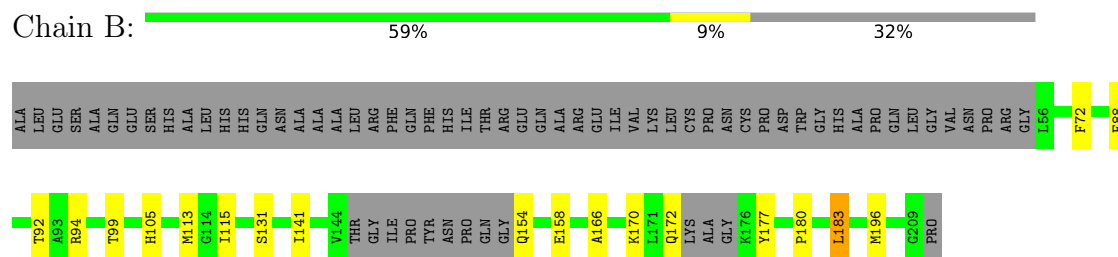
3 Residue-property plots [i](#)

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.

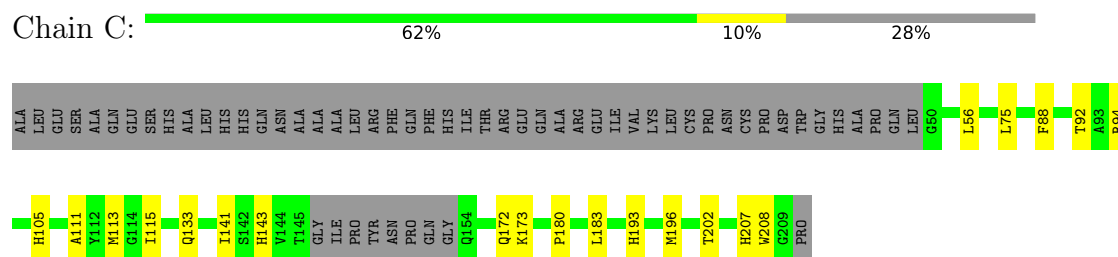
- Molecule 1: Pol polyprotein



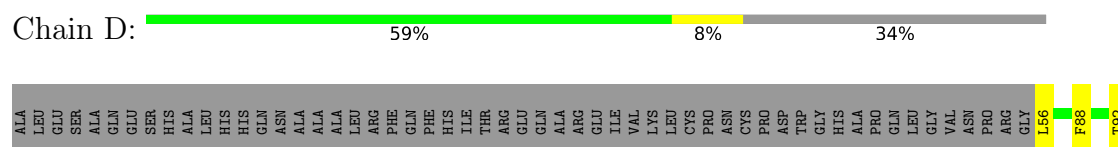
- Molecule 1: Pol polyprotein



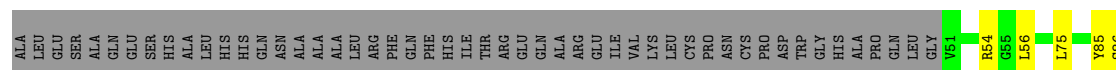
- Molecule 1: Pol polyprotein



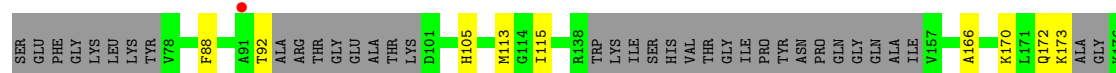
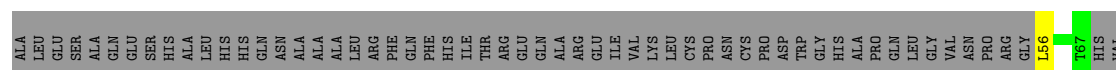
- Molecule 1: Pol polyprotein



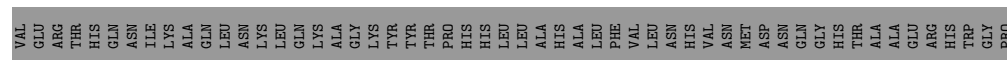
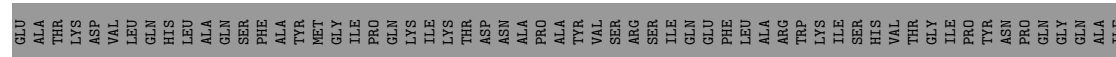
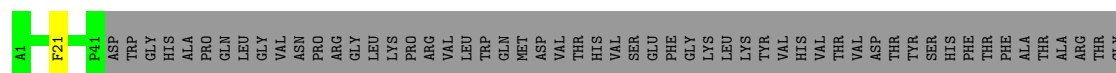
- Molecule 1: Pol polypeptide



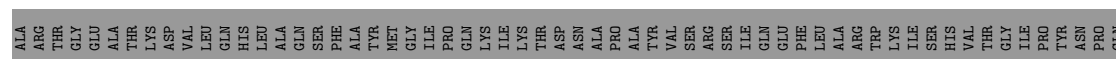
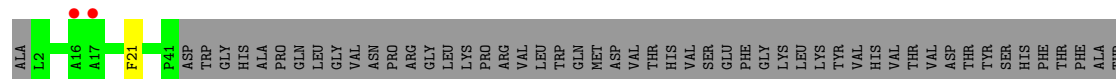
- Molecule 1: Pol polyprotein



- Molecule 1: Pol polypeptide



- Molecule 1: Pol polypeptide



GLY GLN ALA ILE VAL GLU ARG THR THR GLN GLN ASN ILE ILE LYS ALA ALA LEU ASN LYS LEU GLN LYS LYS ALA GLY LYS TYR THR THR PRO THR HIS HIS LEU LEU ALA ALA ALA LEU PHE VAL LEU ASN ASN HIS VAL VAL ASN ASN ASP ASN GLY GLY THR THR ALA ALA GLU ARG HIS TRP GLY PRO

- Molecule 1: Pol polypeptide

Chain I: 18% . 81%

ALA	LEU	E3		A18		F21		P41	ASP	TRP	GLY	HIS	ALA	PRO	GLN	GLY	VAL	ASN	ARG	GLY	LEU	LYS	PRO	ARG	VAL	THR	HIS	VAL	SER	GLU	PHE	GLY	LYS	LEU	LYS	TYR	VAL	HIS	VAL	THR	ASP	THR	TYR	SER	HIS	PHE	THR	PHE	ALA	THR
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ALA ARG THR GLY GLU ALA THR LYS ASP VAL LEU GLN HIS LEU ALA GLN SER PHE ALA TYR MET GLY ILE GLN PRO GLN LYS ILE LYS THR ASP ASN ALA PRO PRO TYR VAL SER ARG SER ILE GLN GLU PHE LEU ALA ARG TRP LYS ILE SER HIS VAL TRP GLY ILE PRO TYR ASN PRO

GLY GLN ALA ALA ILE ILE VAL ARG GLU THR THR GLN GLN ASN ASN ILE ILE LYS ALA ALA LEU LEU ASN ASN LYS LYS LEU LYS LYS ALA ALA GLY LYS TYR TYR THR THR PRO HIS HIS HIS LEU LEU ALA ALA ALA PHE VAL LEU LEU ASN ASN HIS HIS VAL VAL ASN ASN MET MET ASP ASP ASN GLN GLY GLY HIS HIS THR THR ALA ALA GLU GLU ARG ARG HIS HIS TRP TRP PRO PRO

- Molecule 1: Pol polypeptide

Chain J: 18% 80%

[illegible]

THR	ALA	ARG	THR	GLY	GLU	ALA	THR	LYS	ASP	VAL	LEU	GLN	HIS	LEU	ALA	GLN	SER	PHE	ALA	ALA	TYR	MET	GLY	ILE	GLY	PRO	GLN	LYS	ILE	LYS	THR	ASP	ASN	ALA	ALA	ALA	TYR	VAL	SER	ARG	SER	ILE	GLN	GLU	PHE	LEU	ALA	ARG	TRP	LYS	ILE	SER	HIS	VAL	THR	GLY	ILE	PRO	TYR	ASN	PRO
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GLN	GLY	GLN	ALA	ALA	VAL	GLU	ARG	THR	HIS	GLN	ASN	ILE	LYS	ALA	GLN	LEU	LYS	LEU	GLN	LYS	ALA	ALA	GLY	LYS	TYR	TYR	THR	PRO	HIS	HIS	LEU	LEU	ALA	HIS	ASN	VAL	LEU	LEU	ASN	HIS	VAL	HIS	ASN	ASP	ASN	GLN	HIS	GLY	THR	ALA	ALA	ALA	GLU	ARG	HIS	TRP	GLY	PRO
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- Molecule 1: Pol polypeptide

Chain K: 17% 83%

ALA	L2	N15	ALA	ALA	LEU	R21	P41	ASP	TRP	GLY	HIS	ALA	GLN	LEU	GLY	VAL	ASN	PRO	ARG	GLY	LEU	LYS	PRO	ARG	VAL	VAL	TRP	HIS	THR	SER	GLU	PHE	GLY	LYS	LEU	LYS	LYS	THR	VAL	HIS	THR	THR	VAL	ASP	THR	THR	SER	HIS	PHE	THR
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PHE ALA THR ALA ARG ALA GLY GLU GLU ALA THR LYS ASP VAL LEU GLN HIS LEU ALA GLN SER PHE ALA ALA TYR MET GLY ILE PRO PRO LYS LYS ILE THR THR ASP ASN PRO PRO ALA ALA VAL VAL VAL ARG SER SER ILE GLN GLN GLU PHE THR LEU ALA ARG TRP LYS ILE ILE SER HIS VAL THR THR ILE ILE PRO THR

ASN	PRO	GLN	GLY	GLN	ALA	ILE	VAL	GLU	ARG	THR	HIS	GLN	ASN	ILE	LYS	ALA	GLN	LEU	ASN	LYS	LEU	GLN	LYS	ALA	LYS	GLY	LYS	TYR	TYR	THR	THR	PRO	HIS	HIS	HIS	LEU	LEU	ALA	LEU	VAL	LEU	ASN	HIS	ASN	VAL	ASN	MET	ASP	ASN	GLN	GLY	HIS	HIS	THR	ALA	ALA	ALA	GLU	ARG	HIS	TRP	TYR
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PRO

- Molecule 1: Pol polypeptide

Chain L: 18% 2% 80%

[illegible]

THR	ALA	ARG	THR	GLY	GLU	ALA	THR	LYS	ASP	VAL	LEU	GLN	HIS	LEU	ALA	ALA	GLN	SER	PHE	ALA	ALA	TYR	MET	ILE	GLY	ILE	PRO	GLN	LYS	ILE	LYS	THR	ASP	ASN	ALA	ALA	PRO	TYR	ARG	THR	GLY	ILE	PRO	ASN	PRO
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GLN	GLY	GLN	ALA	ILE	VAL	GLU	ARG	THR	HIS	GLN	ASN	ILE	LYS	ALA	GLN	LEU	ASN	LYS	LEU	GLN	LYS	ALA	GLY	LYS	TYR	TYR	THR	PRO	HIS	HIS	LEU	LEU	ALA	HIS	ALA	LEU	PHE	VAL	LEU	ASN	HIS	VAL	ASN	MET	ASP	ASN	GLN	GLY	HIS	THR	ALA	ALA	GLU	ARG	HIS	TRP	GLY	PRO
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.37Å 83.15Å 141.14Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	70.57 – 2.72 70.57 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.3 (70.57-2.72) 98.3 (70.57-2.72)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.241 , 0.280 0.239 , 0.275	Depositor DCC
R_{free} test set	1655 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.116 for h,-k,-l	Xtriage
Reported twinning fraction	0.865 for H, K, L 0.135 for -h,-k,l	Depositor
Outliers	0 of 33771 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8591	wwPDB-VP
Average B, all atoms (Å ²)	67.0	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 22.86 % 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 5.2301e-03.*

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: ZN, 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	0.09	0/1247	0.25	0/1692
1	B	0.08	0/1181	0.24	0/1602
1	C	0.09	0/1239	0.25	0/1682
1	D	0.09	0/1128	0.24	0/1535
1	E	0.09	0/1247	0.25	0/1693
1	F	0.09	0/916	0.24	0/1245
1	G	0.09	0/330	0.26	0/446
1	H	0.08	0/298	0.22	0/407
1	I	0.08	0/289	0.21	0/395
1	J	0.09	0/322	0.26	0/437
1	K	0.09	0/276	0.24	0/374
1	L	0.09	0/326	0.27	0/441
All	All	0.09	0/8799	0.25	0/11949

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	1214	0	1189	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1150	0	1117	10	0
1	C	1207	0	1183	14	0
1	D	1098	0	1032	9	0
1	E	1215	0	1187	7	0
1	F	895	0	847	7	0
1	G	323	0	313	1	0
1	H	291	0	255	1	0
1	I	282	0	249	2	0
1	J	315	0	298	4	0
1	K	270	0	235	1	0
1	L	319	0	309	5	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
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
All	All	8591	0	8214	58	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 3.

All (58) 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:C:196:MET:HE1	1:L:21:PHE:HB2	1.73	0.70
1:E:115:ILE:HD12	1:E:141:ILE:HD11	1.79	0.65
1:E:196:MET:HE1	1:J:21:PHE:HB2	1.78	0.64
1:A:196:MET:HE1	1:G:21:PHE:HB2	1.80	0.62
1:A:115:ILE:HD12	1:A:141:ILE:HD11	1.82	0.61
1:C:115:ILE:HD12	1:C:141:ILE:HD11	1.83	0.61
1:D:196:MET:HE1	1:K:21:PHE:HB2	1.82	0.61
1:F:196:MET:HE1	1:I:21:PHE:HB2	1.85	0.57
1:E:54:ARG:NH2	1:E:85:TYR:O	2.40	0.55
1:A:143:HIS:O	1:L:20:ARG:NH2	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:196:MET:HE2	1:I:18:ALA:HA	1.89	0.53
1:D:92:THR:OG1	1:D:105:HIS:ND1	2.37	0.53
1:C:111:ALA:O	1:D:193:HIS:NE2	2.42	0.52
1:C:92:THR:OG1	1:C:105:HIS:ND1	2.37	0.52
1:A:92:THR:OG1	1:A:105:HIS:ND1	2.42	0.49
1:A:133:GLN:HB3	1:L:26:THR:HG23	1.95	0.48
1:D:94:ARG:HE	1:D:105:HIS:HB2	1.79	0.48
1:C:75:LEU:HD12	1:C:180:PRO:HG2	1.96	0.48
1:C:143:HIS:O	1:J:20:ARG:NH2	2.42	0.47
1:A:75:LEU:HD12	1:A:180:PRO:HG2	1.97	0.47
1:B:115:ILE:HD12	1:B:141:ILE:HD11	1.97	0.47
1:B:196:MET:HE1	1:H:21:PHE:HB2	1.96	0.47
1:E:86:SER:O	1:E:206:ARG:NH2	2.48	0.46
1:B:94:ARG:HE	1:B:105:HIS:HB2	1.81	0.46
1:E:196:MET:HG2	1:E:202:THR:HG22	1.98	0.46
1:D:196:MET:HG2	1:D:202:THR:HG22	1.99	0.45
1:E:75:LEU:HD12	1:E:180:PRO:HG2	1.99	0.44
1:C:207:HIS:HD2	1:C:208:TRP:CE2	2.36	0.43
1:A:54:ARG:NH2	1:A:85:TYR:O	2.51	0.43
1:C:196:MET:HG2	1:C:202:THR:HG22	2.00	0.43
1:B:88:PHE:CD1	1:B:113:MET:HG2	2.53	0.43
1:D:88:PHE:CD1	1:D:113:MET:HG2	2.53	0.43
1:B:99:THR:HG21	1:B:131:SER:HB2	2.01	0.43
1:C:196:MET:HE2	1:L:18:ALA:HA	2.00	0.43
1:F:92:THR:OG1	1:F:105:HIS:ND1	2.46	0.43
1:B:177:TYR:CD2	1:B:183:LEU:HG	2.53	0.43
1:A:72:PHE:CD1	1:A:180:PRO:HB3	2.53	0.42
1:E:196:MET:HE2	1:J:18:ALA:HA	2.01	0.42
1:A:166:ALA:O	1:A:170:LYS:HG3	2.19	0.42
1:A:196:MET:HG2	1:A:202:THR:HG22	2.02	0.42
1:D:166:ALA:O	1:D:170:LYS:HG3	2.20	0.42
1:D:207:HIS:HD2	1:D:208:TRP:CE2	2.37	0.42
1:C:88:PHE:CD1	1:C:113:MET:HG2	2.55	0.41
1:A:115:ILE:HD13	1:A:115:ILE:HA	1.90	0.41
1:A:88:PHE:CD1	1:A:113:MET:HG2	2.55	0.41
1:F:207:HIS:HD2	1:F:208:TRP:CE2	2.38	0.41
1:B:166:ALA:O	1:B:170:LYS:HG3	2.20	0.41
1:F:88:PHE:CD1	1:F:113:MET:HG2	2.56	0.41
1:A:52:ASN:OD1	1:A:155:ALA:N	2.54	0.41
1:B:92:THR:OG1	1:B:105:HIS:ND1	2.46	0.41
1:C:196:MET:HE1	1:L:21:PHE:CB	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ILE:HD13	1:F:115:ILE:HA	1.93	0.41
1:B:72:PHE:CD1	1:B:180:PRO:HB3	2.55	0.41
1:F:166:ALA:O	1:F:170:LYS:HG3	2.21	0.40
1:C:133:GLN:HB3	1:J:26:THR:HG23	2.03	0.40
1:B:154:GLN:O	1:B:158:GLU:HG2	2.21	0.40
1:C:193:HIS:NE2	1:D:111:ALA:O	2.51	0.40
1:C:94:ARG:HE	1:C:105:HIS:HB2	1.85	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	147/210 (70%)	142 (97%)	5 (3%)	0	100	100
1	B	136/210 (65%)	134 (98%)	2 (2%)	0	100	100
1	C	148/210 (70%)	144 (97%)	4 (3%)	0	100	100
1	D	133/210 (63%)	131 (98%)	2 (2%)	0	100	100
1	E	149/210 (71%)	144 (97%)	5 (3%)	0	100	100
1	F	105/210 (50%)	104 (99%)	1 (1%)	0	100	100
1	G	39/210 (19%)	38 (97%)	1 (3%)	0	100	100
1	H	38/210 (18%)	37 (97%)	1 (3%)	0	100	100
1	I	37/210 (18%)	36 (97%)	1 (3%)	0	100	100
1	J	39/210 (19%)	38 (97%)	1 (3%)	0	100	100
1	K	32/210 (15%)	31 (97%)	1 (3%)	0	100	100
1	L	39/210 (19%)	38 (97%)	1 (3%)	0	100	100
All	All	1042/2520 (41%)	1017 (98%)	25 (2%)	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	126/176 (72%)	122 (97%)	4 (3%)	34	62
1	B	120/176 (68%)	118 (98%)	2 (2%)	53	77
1	C	125/176 (71%)	121 (97%)	4 (3%)	34	62
1	D	111/176 (63%)	108 (97%)	3 (3%)	39	68
1	E	125/176 (71%)	122 (98%)	3 (2%)	43	70
1	F	90/176 (51%)	86 (96%)	4 (4%)	25	51
1	G	33/176 (19%)	33 (100%)	0	100	100
1	H	27/176 (15%)	27 (100%)	0	100	100
1	I	26/176 (15%)	26 (100%)	0	100	100
1	J	31/176 (18%)	31 (100%)	0	100	100
1	K	26/176 (15%)	26 (100%)	0	100	100
1	L	32/176 (18%)	32 (100%)	0	100	100
All	All	872/2112 (41%)	852 (98%)	20 (2%)	44	71

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	172	GLN
1	A	173	LYS
1	A	183	LEU
1	B	172	GLN
1	B	183	LEU
1	C	56	LEU
1	C	172	GLN
1	C	173	LYS
1	C	183	LEU
1	D	56	LEU
1	D	172	GLN
1	D	183	LEU
1	E	56	LEU

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Mol	Chain	Res	Type
1	E	172	GLN
1	E	183	LEU
1	F	56	LEU
1	F	172	GLN
1	F	173	LYS
1	F	183	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	133	GLN
1	A	181	HIS
1	B	108	GLN
1	C	104	GLN
1	C	108	GLN
1	C	181	HIS
1	E	181	HIS
1	I	39	ASN
1	L	24	HIS
1	L	39	ASN

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 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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	151/210 (71%)	-0.79	0 100 100	30, 53, 100, 129	0
1	B	142/210 (67%)	-0.80	0 100 100	32, 57, 87, 102	0
1	C	152/210 (72%)	-0.78	0 100 100	33, 57, 91, 106	0
1	D	139/210 (66%)	-0.56	0 100 100	41, 72, 112, 155	0
1	E	153/210 (72%)	-0.68	0 100 100	35, 61, 105, 137	0
1	F	115/210 (54%)	-0.37	3 (2%) 57 54	52, 74, 116, 150	0
1	G	41/210 (19%)	-0.99	0 100 100	44, 53, 81, 120	0
1	H	40/210 (19%)	-0.33	2 (5%) 34 31	52, 83, 129, 166	0
1	I	39/210 (18%)	-0.42	0 100 100	50, 70, 115, 133	0
1	J	41/210 (19%)	-0.46	0 100 100	65, 79, 107, 133	0
1	K	36/210 (17%)	-0.38	0 100 100	72, 96, 113, 131	0
1	L	41/210 (19%)	-0.80	0 100 100	40, 57, 81, 91	0
All	All	1090/2520 (43%)	-0.65	5 (0%) 87 86	30, 64, 108, 166	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	191	LEU	2.6
1	F	179	THR	2.3
1	F	91	ALA	2.1
1	H	16	ALA	2.1
1	H	17	ALA	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(Å ²)	Q<0.9
2	MG	F	301	1/1	0.97	0.09	53,53,53,53	0
2	MG	A	301	1/1	0.98	0.04	52,52,52,52	0
2	MG	C	301	1/1	0.99	0.04	65,65,65,65	0
2	MG	D	301	1/1	0.99	0.04	81,81,81,81	0
2	MG	B	301	1/1	0.99	0.02	52,52,52,52	0
3	ZN	H	301	1/1	0.99	0.04	86,86,86,86	0
3	ZN	I	301	1/1	0.99	0.04	83,83,83,83	0
2	MG	E	301	1/1	1.00	0.02	46,46,46,46	0
3	ZN	G	301	1/1	1.00	0.01	55,55,55,55	0
3	ZN	J	301	1/1	1.00	0.02	57,57,57,57	0
3	ZN	K	301	1/1	1.00	0.03	64,64,64,64	0
3	ZN	L	301	1/1	1.00	0.02	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.