



Full wwPDB EM Validation Report ⓘ

Jul 9, 2025 – 01:37 PM JST

PDB ID : 9ILY / pdb_00009ily
EMDB ID : EMD-60676
Title : The Cryo-EM structure of MPXV E5 in the apo state
Authors : Cheng, Y.X.; Han, P.; Wang, H.
Deposited on : 2024-07-01
Resolution : 3.33 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

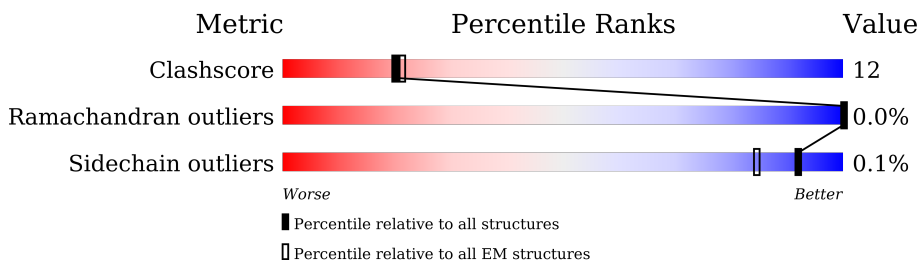
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	785	38% 15% 46%
1	B	785	38% 15% 46%
1	C	785	39% 14% 47%
1	D	785	38% 16% 46%
1	E	785	41% 13% 46%
1	F	785	38% 16% 46%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 20595 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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.

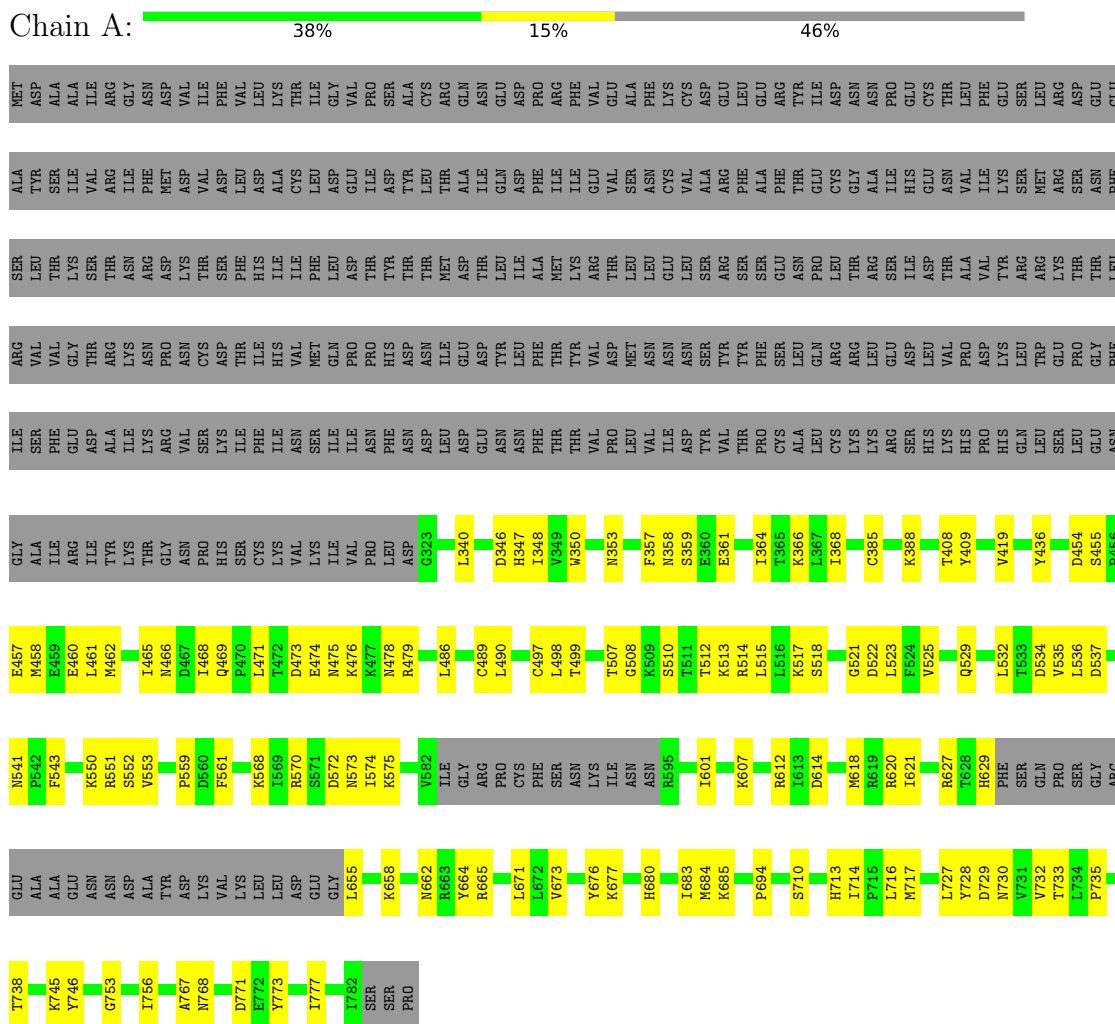
- Molecule 1 is a protein called Primase D5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	423	Total	C	N	O	S	0	0
			3441	2214	575	636	16		
1	F	423	Total	C	N	O	S	0	0
			3441	2214	575	636	16		
1	E	423	Total	C	N	O	S	0	0
			3441	2214	575	636	16		
1	D	423	Total	C	N	O	S	0	0
			3441	2214	575	636	16		
1	C	417	Total	C	N	O	S	0	0
			3390	2181	568	625	16		
1	B	423	Total	C	N	O	S	0	0
			3441	2214	575	636	16		

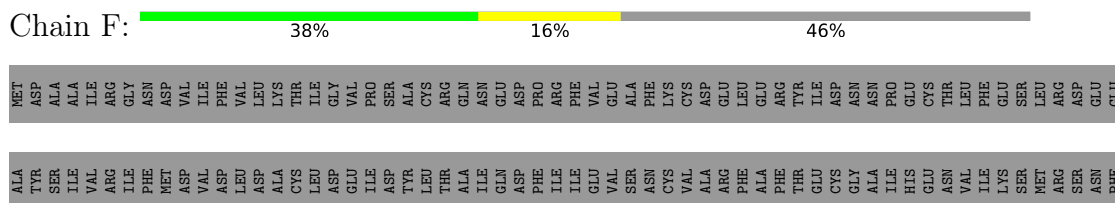
3 Residue-property plots

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. 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. 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: Primase D5



• Molecule 1: Primase D5



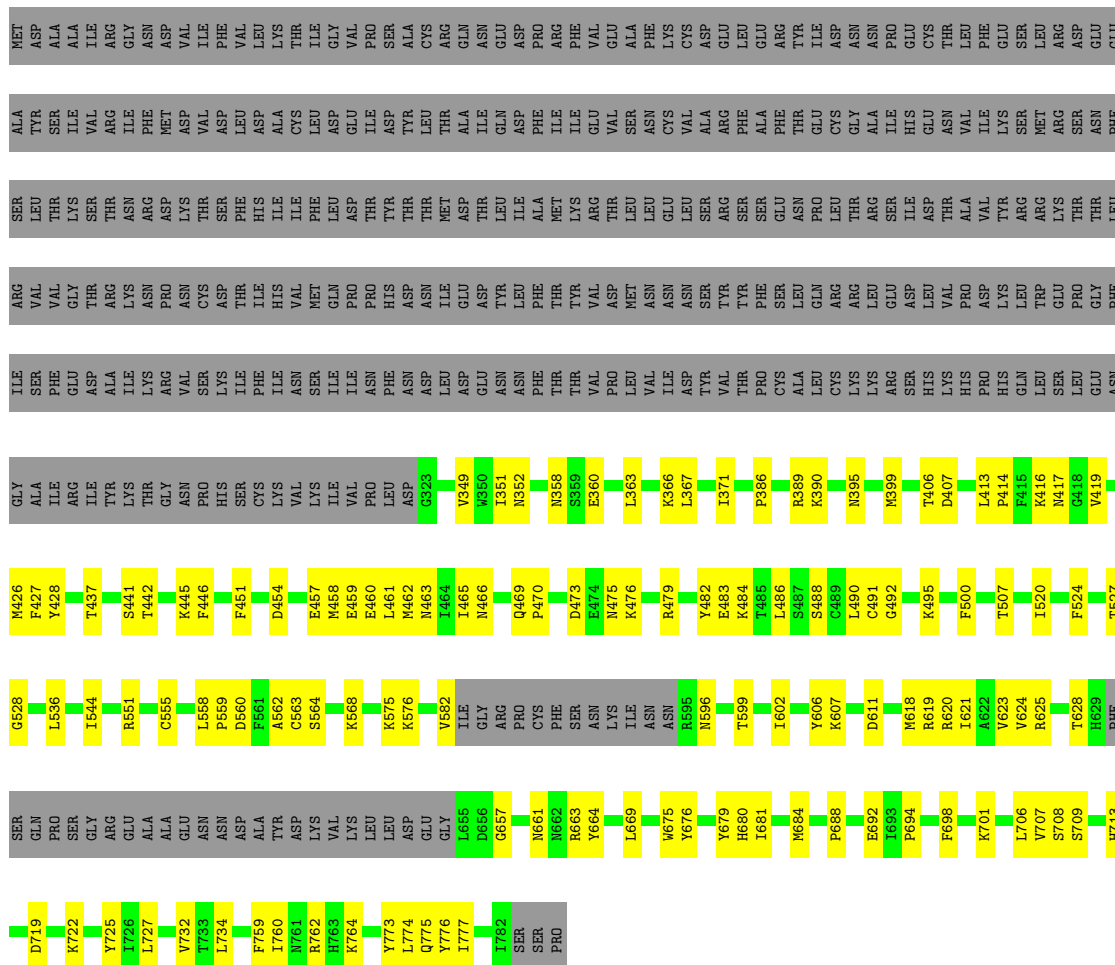
ILE	GLY	E393	F524	D614	K685	SR
ALA	ALA	E993	V525	N615	L686	LEU
ILE	ILE	R397	E528	A616	Y687	THR
ARG	ARG	S403	T527	L617	P688	LYS
ASP	ILE	S403	G528	M618	M717	THR
THR	ALA	L413	T533	R619	T718	ASN
LYS	LYS	P414	P542	E620	S721	ARG
ASN	THR	G418	N546	A622	T733	ASN
ARG	LYS	Y428	M547	V623	L734	ARG
PRO	VAL	D431	K550	R625	R750	LYS
ASN	ASN	D447	R551	F626	H754	THR
LYS	PRO	D454	V553	E627	D755	ASN
CYS	HIS	M458	S556	T628	I756	GLY
THR	LYS	L461	D560	H629	E757	VAL
ASN	VAL	N462	F561	PHE	I760	ASN
THR	ILE	N465	S566	GLN	N761	PRO
ASP	ASP	M466	K567	PRO	R762	THR
THR	ASP	N469	K568	SER	H764	THR
MET	LEU	Q469	I569	ASN	K765	THR
ILE	GLU	D473	S571	ARG	D771	THR
ALA	ASN	E474	D572	ASP	E772	THR
LYS	ASN	M475	N573	ALA	L774	LYS
ARG	THR	K476	I574	TYR	Q775	ARG
THR	PRO	T336	K575	ASP	I782	GLU
LEU	LEU	E343	T578	VAL	SR	ALA
GLU	ILE	D346	E579	LYS	SR	ALA
SER	ASP	V349	P580	LEU	SR	LYS
ARG	TYR	P362	C581	LEU	PRO	CYS
GLU	THR	L367	V582	ASP	GLY	ASP
ASN	PRO	I371	ILE	GLY	L655	GLU
LEU	ARG	Q374	ARG	GLY	A667	ASP
ILE	ASP	K377	PRO	LYS	F668	THR
THR	VAL	E378	CYS	ASN	Y670	ASN
ALA	PRO	E382	PHE	ASN	V673	THR
VAL	PRO	C385	SR	R595	K674	THR
LYS	LYS	T511	ASN	N596	Y675	ALA
ARG	GLN	R387	Y606	K607	K678	VAL
TRP	LEU	K513	P608	I681	E679	LYS
GLY	SR	I520	R612	I682	H680	THR
THR	LEU	T391	I613	I683	Y682	LYS
LEU	ASN	V392		M684	P684	THR

• Molecule 1: Primase D5

Chain E:										41%										13%										46%																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
S564	S565	S566	S567	S568	S569	S570	S571	S575	S582	S586	S596	S597	T602	D614	M618	M619	R620	R625	M629	PHE	SER	GLN	PRO	SER	GLY	ARG	GLU	ALA	GLY	THR	LEU	LEU	GLU	ALA	PHE	ASN	GLY	THR	ARG	ILE	PHE	ILE	GLY	VAL	GLU	GLU	ASN	ASP	PRO	ASP	GLN	ASN	ILE	ASP	ALA	GLN	THR	ARG	CYS	ALA	THR	ASP	ILE	THR	PRO	VAL	GLY	ILE	THR	LYS	ALA	CYS	ILE	THR	LYS	LEU	VAL	ASP	LEU	THR	ASP	ASN	ASP	THR	ASP	THR	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR

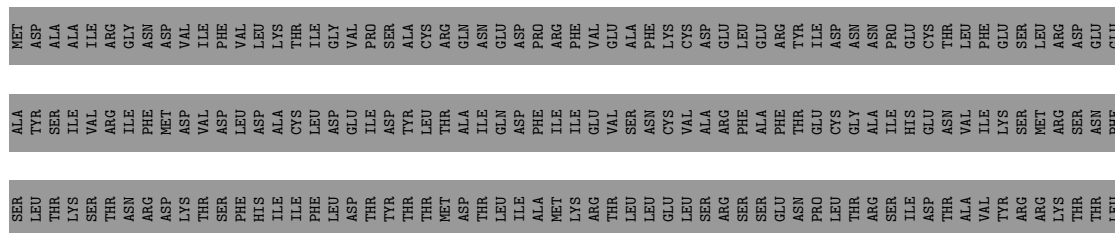
- Molecule 1: Primase D5

Chain D: 38% 16% 46%



- Molecule 1: Primase D5

Chain C: 39% 14% 47%







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94493	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.10	0/3514	0.31	0/4744
1	B	0.11	0/3514	0.35	0/4744
1	C	0.11	0/3461	0.34	0/4669
1	D	0.09	0/3514	0.29	0/4744
1	E	0.10	0/3514	0.33	0/4744
1	F	0.14	0/3514	0.42	2/4744 (0.0%)
All	All	0.11	0/21031	0.34	2/28389 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	F	362	PRO	CA-N-CD	-8.46	100.15	112.00
1	F	462	MET	CA-CB-CG	5.33	124.75	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	489	CYS	Peptide
1	B	490	LEU	Peptide

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	3441	0	3480	89	0
1	B	3441	0	3478	88	0
1	C	3390	0	3429	80	0
1	D	3441	0	3478	87	0
1	E	3441	0	3480	76	0
1	F	3441	0	3478	93	0
All	All	20595	0	20823	499	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 12.

All (499) 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:F:681:ILE:HD12	1:F:682:PRO:HD3	1.54	0.89
1:B:489:CYS:HA	1:B:491:CYS:HB3	1.56	0.87
1:F:568:LYS:HE3	1:F:568:LYS:HA	1.59	0.83
1:B:477:LYS:HA	1:B:480:GLU:HG2	1.64	0.79
1:F:454:ASP:H	1:F:458:MET:HE3	1.50	0.75
1:B:520:ILE:HD12	1:B:523:LEU:HB2	1.71	0.73
1:B:681:ILE:HD12	1:B:681:ILE:H	1.54	0.72
1:A:618:MET:HE2	1:A:618:MET:H	1.55	0.71
1:B:477:LYS:O	1:B:480:GLU:HB2	1.92	0.70
1:E:452:VAL:HG12	1:E:454:ASP:H	1.56	0.70
1:C:501:PHE:HB3	1:C:557:GLU:HA	1.72	0.70
1:C:524:PHE:HE1	1:C:554:PHE:HB2	1.57	0.69
1:F:382:GLU:OE1	1:F:382:GLU:N	2.26	0.68
1:C:458:MET:O	1:C:462:MET:HG2	1.94	0.68
1:E:678:LYS:O	1:E:680:HIS:ND1	2.26	0.68
1:D:363:LEU:HG	1:D:366:LYS:HD2	1.76	0.68
1:E:757:GLU:O	1:E:761:ASN:ND2	2.27	0.68
1:F:678:LYS:O	1:F:680:HIS:ND1	2.23	0.67
1:F:771:ASP:HB2	1:E:750:ARG:HD2	1.76	0.67
1:A:612:ARG:HH12	1:A:614:ASP:HB2	1.60	0.67
1:C:763:HIS:CE1	1:C:765:LYS:HD3	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:618:MET:HE3	1:E:618:MET:H	1.60	0.66
1:B:484:LYS:O	1:B:488:SER:N	2.28	0.66
1:E:492:GLY:O	1:E:597:HIS:ND1	2.24	0.66
1:B:538:LYS:HD2	1:B:541:ASN:HB2	1.76	0.66
1:E:556:SER:HB3	1:E:602:ILE:HG23	1.77	0.65
1:F:618:MET:HE3	1:F:618:MET:H	1.62	0.65
1:B:618:MET:HE1	1:B:690:PRO:HB3	1.79	0.65
1:A:462:MET:O	1:A:466:ASN:ND2	2.30	0.65
1:E:708:SER:HA	1:E:776:TYR:HA	1.79	0.65
1:C:490:LEU:O	1:C:551:ARG:NH1	2.30	0.65
1:E:382:GLU:OE2	1:E:382:GLU:N	2.28	0.64
1:B:579:GLU:HG3	1:B:581:CYS:H	1.61	0.64
1:B:510:SER:OG	1:B:514:ARG:NH2	2.30	0.64
1:D:469:GLN:O	1:D:479:ARG:NH1	2.31	0.64
1:D:708:SER:O	1:C:627:ARG:NH2	2.31	0.64
1:C:451:PHE:HD1	1:C:666:PHE:HB3	1.63	0.64
1:F:765:LYS:NZ	1:E:560:ASP:OD2	2.31	0.64
1:E:421:ASP:O	1:E:425:GLY:N	2.30	0.64
1:C:426:MET:HA	1:C:426:MET:HE2	1.78	0.63
1:C:765:LYS:HE3	1:C:774:LEU:HD22	1.80	0.63
1:E:684:MET:HE2	1:E:684:MET:HA	1.81	0.63
1:C:473:ASP:HA	1:C:476:LYS:HG2	1.80	0.63
1:E:398:ASP:OD2	1:D:389:ARG:NH1	2.32	0.62
1:D:482:TYR:HB2	1:D:624:VAL:HG11	1.79	0.62
1:D:491:CYS:SG	1:D:492:GLY:N	2.72	0.62
1:F:374:GLN:OE1	1:F:374:GLN:N	2.32	0.62
1:C:531:ILE:HG23	1:C:532:LEU:HD22	1.81	0.62
1:A:729:ASP:O	1:A:730:ASN:ND2	2.32	0.62
1:F:619:ARG:O	1:F:619:ARG:NH1	2.31	0.62
1:E:462:MET:HA	1:E:465:ILE:HG12	1.81	0.61
1:B:468:ILE:HG22	1:B:469:GLN:HG2	1.82	0.61
1:F:680:HIS:HB3	1:F:684:MET:HE1	1.83	0.61
1:C:666:PHE:HA	1:C:669:LEU:HD23	1.82	0.61
1:E:547:MET:O	1:E:596:ASN:ND2	2.33	0.61
1:A:732:VAL:HG21	1:A:777:ILE:HG12	1.83	0.60
1:D:607:LYS:HB3	1:D:694:PRO:HG3	1.82	0.60
1:A:768:ASN:OD1	1:F:754:HIS:NE2	2.34	0.60
1:B:488:SER:O	1:B:495:LYS:NZ	2.28	0.60
1:B:497:CYS:H	1:B:620:ARG:HD2	1.66	0.60
1:B:779:ILE:H	1:B:779:ILE:HD12	1.67	0.60
1:A:710:SER:H	1:A:713:HIS:HD2	1.47	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:GLU:HB3	1:F:403:SER:HB2	1.82	0.60
1:A:497:CYS:HA	1:A:620:ARG:HG3	1.82	0.60
1:E:680:HIS:HB3	1:E:684:MET:HE1	1.83	0.59
1:F:491:CYS:HB2	1:F:551:ARG:HH11	1.67	0.59
1:F:393:GLU:OE2	1:F:397:ARG:NH1	2.36	0.59
1:E:660:GLN:O	1:E:662:ASN:ND2	2.36	0.59
1:C:762:ARG:O	1:B:564:SER:OG	2.17	0.59
1:C:553:VAL:HB	1:C:600:ILE:HG12	1.82	0.59
1:C:684:MET:HE2	1:C:684:MET:HA	1.84	0.59
1:A:535:VAL:HG23	1:A:570:ARG:HH11	1.68	0.58
1:C:469:GLN:O	1:C:479:ARG:NH1	2.37	0.58
1:B:765:LYS:HB2	1:B:773:TYR:HB2	1.84	0.58
1:E:765:LYS:HG3	1:D:562:ALA:HB1	1.85	0.58
1:F:333:ILE:O	1:F:336:THR:OG1	2.21	0.58
1:C:580:PRO:HA	1:C:596:ASN:HB3	1.85	0.58
1:A:714:ILE:HA	1:A:717:MET:HE2	1.86	0.58
1:E:426:MET:HA	1:E:426:MET:HE2	1.84	0.58
1:A:514:ARG:HH12	1:A:518:SER:HB3	1.68	0.58
1:B:494:THR:HG21	1:B:580:PRO:HB3	1.85	0.58
1:F:500:PHE:HB2	1:F:621:ILE:HD11	1.84	0.58
1:C:333:ILE:O	1:C:336:THR:OG1	2.22	0.58
1:B:685:LYS:NZ	1:B:686:LEU:O	2.32	0.57
1:D:657:GLY:O	1:D:661:ASN:ND2	2.36	0.57
1:E:734:LEU:HD23	1:E:774:LEU:HB2	1.86	0.57
1:B:680:HIS:ND1	1:B:684:MET:SD	2.77	0.57
1:E:402:ASP:OD1	1:E:402:ASP:N	2.37	0.57
1:A:728:TYR:HD2	1:A:733:THR:HG21	1.70	0.57
1:F:484:LYS:O	1:F:488:SER:N	2.38	0.57
1:A:498:LEU:HB2	1:A:621:ILE:HG22	1.87	0.57
1:A:457:GLU:HA	1:A:460:GLU:HG2	1.85	0.57
1:A:676:TYR:HB3	1:A:680:HIS:CE1	2.39	0.56
1:A:348:ILE:HG22	1:A:357:PHE:HB2	1.86	0.56
1:D:458:MET:O	1:D:458:MET:HE3	2.04	0.56
1:D:358:ASN:ND2	1:D:360:GLU:O	2.39	0.56
1:B:386:PRO:O	1:B:390:LYS:HG2	2.06	0.56
1:F:618:MET:H	1:F:618:MET:CE	2.19	0.56
1:C:503:GLY:HA2	1:C:559:PRO:HA	1.86	0.56
1:D:484:LYS:HE3	1:D:679:TYR:HB3	1.87	0.56
1:C:563:CYS:SG	1:C:564:SER:N	2.79	0.56
1:B:384:LEU:O	1:B:389:ARG:NH2	2.39	0.56
1:F:762:ARG:HH22	1:E:565:GLY:HA3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:479:ARG:NH1	1:E:483:GLU:OE1	2.39	0.56
1:C:617:LEU:H	1:C:617:LEU:HD12	1.70	0.56
1:E:675:TRP:O	1:E:680:HIS:ND1	2.36	0.56
1:C:454:ASP:OD1	1:C:454:ASP:N	2.39	0.55
1:A:515:LEU:O	1:A:518:SER:OG	2.19	0.55
1:B:482:TYR:O	1:B:485:THR:OG1	2.17	0.55
1:B:485:THR:O	1:B:488:SER:HB3	2.06	0.55
1:F:681:ILE:HD12	1:F:682:PRO:CD	2.33	0.55
1:E:618:MET:H	1:E:618:MET:CE	2.19	0.55
1:F:718:THR:O	1:F:721:SER:HB2	2.07	0.55
1:F:500:PHE:N	1:F:622:ALA:O	2.39	0.54
1:A:475:ASN:O	1:A:479:ARG:N	2.32	0.54
1:F:484:LYS:HA	1:F:680:HIS:NE2	2.22	0.54
1:A:521:GLY:O	1:A:523:LEU:N	2.41	0.54
1:E:494:THR:OG1	1:E:596:ASN:O	2.24	0.54
1:C:374:GLN:N	1:C:374:GLN:OE1	2.40	0.54
1:A:671:LEU:H	1:A:671:LEU:HD23	1.73	0.54
1:D:490:LEU:O	1:D:551:ARG:NH1	2.41	0.54
1:D:732:VAL:HG22	1:D:773:TYR:HA	1.89	0.54
1:B:548:HIS:HE2	1:B:582:VAL:HG21	1.72	0.54
1:A:408:THR:HG23	1:A:409:TYR:CD2	2.43	0.54
1:F:675:TRP:O	1:F:680:HIS:ND1	2.40	0.54
1:A:673:VAL:HA	1:A:676:TYR:CD2	2.43	0.54
1:F:367:LEU:O	1:F:371:ILE:HG22	2.08	0.54
1:D:536:LEU:HD12	1:D:576:LYS:HD2	1.89	0.54
1:B:452:VAL:HG23	1:B:453:GLU:H	1.73	0.54
1:D:713:HIS:HB2	1:D:777:ILE:HG21	1.90	0.54
1:B:757:GLU:O	1:B:761:ASN:ND2	2.41	0.54
1:F:418:GLY:HA3	1:F:428:TYR:O	2.07	0.53
1:F:461:LEU:O	1:F:465:ILE:HG22	2.09	0.53
1:D:454:ASP:OD1	1:D:454:ASP:N	2.37	0.53
1:F:670:TYR:HA	1:F:673:VAL:HG12	1.90	0.53
1:F:733:THR:OG1	1:F:734:LEU:N	2.39	0.53
1:E:533:THR:O	1:E:570:ARG:NH1	2.36	0.53
1:F:502:PHE:O	1:F:626:PHE:N	2.38	0.53
1:A:534:ASP:O	1:A:573:ASN:ND2	2.41	0.53
1:A:713:HIS:HA	1:A:716:LEU:HD12	1.91	0.53
1:A:745:LYS:HZ2	1:A:746:TYR:HD2	1.57	0.53
1:A:514:ARG:O	1:A:517:LYS:HB3	2.09	0.53
1:D:419:VAL:HG12	1:D:428:TYR:HB2	1.90	0.53
1:A:340:LEU:HB2	1:A:348:ILE:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:377:LYS:NZ	1:F:378:GLU:OE1	2.42	0.53
1:B:560:ASP:HB3	1:B:563:CYS:HB3	1.91	0.53
1:F:763:HIS:HE1	1:F:765:LYS:HE2	1.73	0.52
1:E:566:SER:O	1:E:568:LYS:NZ	2.42	0.52
1:A:454:ASP:HA	1:A:458:MET:HG2	1.91	0.52
1:C:509:LYS:NZ	1:C:557:GLU:O	2.38	0.52
1:C:547:MET:HA	1:C:550:LYS:HB2	1.91	0.52
1:B:723:LYS:HD3	1:B:725:TYR:HE2	1.75	0.52
1:C:406:THR:OG1	1:C:437:THR:O	2.25	0.52
1:A:525:VAL:HG23	1:A:553:VAL:HG23	1.90	0.52
1:D:507:THR:HA	1:D:628:THR:HB	1.91	0.52
1:B:473:ASP:HA	1:B:476:LYS:HB2	1.92	0.52
1:F:615:ASN:OD1	1:F:616:ALA:N	2.43	0.52
1:E:543:PHE:HA	1:E:546:ASN:HB3	1.91	0.52
1:A:458:MET:HE2	1:A:458:MET:HA	1.92	0.52
1:E:563:CYS:SG	1:E:564:SER:N	2.82	0.52
1:C:468:ILE:HD12	1:C:626:PHE:HZ	1.75	0.52
1:F:612:ARG:HH22	1:F:614:ASP:HB3	1.73	0.52
1:E:514:ARG:O	1:E:517:LYS:HB3	2.10	0.52
1:D:488:SER:HB2	1:D:599:THR:HG21	1.90	0.52
1:C:414:PRO:HB2	1:C:441:SER:HA	1.92	0.52
1:A:574:ILE:HD12	1:A:574:ILE:H	1.75	0.52
1:E:426:MET:SD	1:E:427:PHE:N	2.83	0.52
1:E:421:ASP:O	1:E:425:GLY:CA	2.58	0.51
1:E:482:TYR:CZ	1:E:486:LEU:HD11	2.45	0.51
1:E:742:LYS:HA	1:E:745:LYS:HE2	1.92	0.51
1:A:522:ASP:O	1:A:550:LYS:NZ	2.42	0.51
1:D:461:LEU:O	1:D:465:ILE:HG13	2.10	0.51
1:C:457:GLU:OE1	1:C:663:ARG:NH2	2.43	0.51
1:B:458:MET:O	1:B:462:MET:HG2	2.09	0.51
1:A:489:CYS:O	1:A:552:SER:OG	2.28	0.51
1:C:520:ILE:HG22	1:C:523:LEU:HB2	1.91	0.51
1:B:461:LEU:HD11	1:B:664:TYR:HB3	1.92	0.51
1:B:714:ILE:O	1:B:717:MET:HE1	2.10	0.51
1:D:413:LEU:HD12	1:D:414:PRO:HD2	1.92	0.51
1:C:680:HIS:CG	1:C:684:MET:HE1	2.46	0.51
1:F:717:MET:O	1:F:721:SER:N	2.43	0.51
1:D:395:ASN:O	1:D:399:MET:HG3	2.11	0.51
1:D:759:PHE:HD1	1:D:762:ARG:HH21	1.57	0.51
1:B:511:THR:HA	1:B:514:ARG:HE	1.75	0.51
1:B:580:PRO:HA	1:B:596:ASN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:490:LEU:HD21	1:F:676:TYR:CZ	2.45	0.51
1:E:544:ILE:HG23	1:E:582:VAL:HG11	1.93	0.51
1:F:349:VAL:HG13	1:F:367:LEU:HD22	1.91	0.51
1:F:520:ILE:HB	1:F:524:PHE:HB2	1.93	0.51
1:B:489:CYS:HA	1:B:491:CYS:CB	2.32	0.51
1:B:665:ARG:O	1:B:669:LEU:HD23	2.10	0.51
1:B:607:LYS:HE2	1:B:694:PRO:HD2	1.92	0.51
1:D:582:VAL:HA	1:D:596:ASN:HD21	1.76	0.50
1:C:515:LEU:O	1:C:518:SER:OG	2.29	0.50
1:A:767:ALA:H	1:A:773:TYR:HE1	1.59	0.50
1:D:426:MET:HE1	1:D:428:TYR:CE2	2.46	0.50
1:D:473:ASP:HA	1:D:476:LYS:HE2	1.93	0.50
1:D:367:LEU:O	1:D:371:ILE:HG12	2.11	0.50
1:F:500:PHE:HE2	1:F:502:PHE:HB2	1.77	0.50
1:F:619:ARG:HD2	1:F:688:PRO:HG3	1.93	0.50
1:E:676:TYR:O	1:E:680:HIS:HB2	2.10	0.50
1:C:484:LYS:C	1:C:486:LEU:H	2.19	0.50
1:C:726:ILE:HB	1:C:733:THR:HG22	1.93	0.50
1:D:619:ARG:HA	1:D:688:PRO:HG3	1.94	0.50
1:A:455:SER:H	1:A:458:MET:HB3	1.76	0.50
1:E:418:GLY:HA3	1:E:428:TYR:O	2.11	0.50
1:C:733:THR:OG1	1:C:773:TYR:HA	2.12	0.50
1:A:717:MET:HB3	1:A:727:LEU:HD22	1.93	0.50
1:E:463:ASN:HA	1:E:466:ASN:HB2	1.94	0.50
1:C:490:LEU:HA	1:C:551:ARG:HD2	1.94	0.50
1:F:462:MET:O	1:F:466:ASN:ND2	2.31	0.50
1:F:525:VAL:HB	1:F:553:VAL:HG22	1.94	0.50
1:A:535:VAL:HG12	1:A:537:ASP:H	1.76	0.49
1:E:397:ARG:O	1:D:366:LYS:NZ	2.45	0.49
1:D:520:ILE:HD11	1:D:524:PHE:HB2	1.94	0.49
1:D:706:LEU:HB3	1:D:776:TYR:HB3	1.94	0.49
1:A:529:GLN:HG2	1:A:559:PRO:HB3	1.94	0.49
1:F:560:ASP:HB3	1:F:606:TYR:HD2	1.78	0.49
1:F:667:ALA:HB1	1:F:670:TYR:CE2	2.47	0.49
1:D:568:LYS:HB2	1:D:611:ASP:HB3	1.94	0.49
1:C:453:GLU:O	1:C:458:MET:HG2	2.12	0.49
1:B:708:SER:HA	1:B:776:TYR:HA	1.95	0.49
1:D:460:GLU:HA	1:D:463:ASN:HD21	1.78	0.49
1:A:475:ASN:HB2	1:A:627:ARG:HH12	1.76	0.49
1:A:655:LEU:HA	1:A:658:LYS:HE3	1.94	0.49
1:F:625:ARG:HG2	1:F:627:ARG:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:MET:SD	1:D:427:PHE:N	2.85	0.49
1:F:533:THR:O	1:F:570:ARG:NH2	2.46	0.49
1:E:508:GLY:O	1:E:512:THR:OG1	2.28	0.49
1:B:485:THR:O	1:B:488:SER:CB	2.60	0.49
1:B:529:GLN:NE2	1:B:555:CYS:SG	2.86	0.49
1:E:377:LYS:H	1:E:377:LYS:HD2	1.78	0.49
1:C:458:MET:O	1:C:461:LEU:HD23	2.12	0.49
1:B:489:CYS:CA	1:B:491:CYS:HB3	2.37	0.49
1:A:710:SER:H	1:A:713:HIS:CD2	2.28	0.48
1:E:377:LYS:HD2	1:E:377:LYS:N	2.28	0.48
1:D:416:LYS:HD2	1:D:445:LYS:HG3	1.95	0.48
1:B:555:CYS:SG	1:B:556:SER:N	2.86	0.48
1:C:476:LYS:O	1:C:480:GLU:HG2	2.13	0.48
1:C:763:HIS:HE1	1:B:563:CYS:SG	2.36	0.48
1:B:736:LEU:HD23	1:B:739:PHE:CE2	2.48	0.48
1:A:466:ASN:HB3	1:A:471:LEU:HD11	1.95	0.48
1:D:558:LEU:HD12	1:D:559:PRO:HD2	1.95	0.48
1:C:765:LYS:HD2	1:C:774:LEU:HA	1.95	0.48
1:B:766:PHE:HE1	1:B:772:GLU:HB3	1.79	0.48
1:C:358:ASN:ND2	1:C:360:GLU:O	2.46	0.48
1:B:440:VAL:HG11	1:B:549:LEU:HB3	1.95	0.48
1:F:757:GLU:HA	1:F:760:ILE:HG22	1.95	0.48
1:E:725:TYR:HB3	1:E:732:VAL:HG23	1.95	0.48
1:D:349:VAL:HG23	1:D:367:LEU:HD22	1.96	0.48
1:C:385:CYS:SG	1:C:387:ARG:NH2	2.73	0.48
1:E:460:GLU:HB3	1:E:664:TYR:HE1	1.78	0.48
1:D:563:CYS:SG	1:D:564:SER:N	2.86	0.48
1:A:513:LYS:HD2	1:A:514:ARG:HB2	1.95	0.48
1:E:374:GLN:H	1:E:374:GLN:CD	2.22	0.48
1:F:542:PRO:O	1:F:546:ASN:ND2	2.47	0.48
1:B:548:HIS:ND1	1:B:595:ARG:O	2.46	0.48
1:D:459:GLU:O	1:D:463:ASN:ND2	2.47	0.47
1:D:719:ASP:HA	1:D:722:LYS:HE3	1.95	0.47
1:B:561:PHE:HB3	1:B:568:LYS:HA	1.95	0.47
1:F:447:ASP:OD1	1:F:447:ASP:N	2.45	0.47
1:D:462:MET:SD	1:D:466:ASN:ND2	2.81	0.47
1:D:669:LEU:HD12	1:D:669:LEU:H	1.79	0.47
1:E:520:ILE:HD12	1:E:523:LEU:HB2	1.96	0.47
1:C:402:ASP:OD1	1:C:402:ASP:N	2.43	0.47
1:B:488:SER:OG	1:B:489:CYS:N	2.47	0.47
1:F:431:ASP:OD1	1:F:431:ASP:N	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:458:MET:O	1:F:462:MET:SD	2.73	0.47
1:D:500:PHE:HB2	1:D:623:VAL:HG22	1.96	0.47
1:C:735:PRO:HA	1:C:772:GLU:HB2	1.97	0.47
1:B:462:MET:O	1:B:466:ASN:ND2	2.31	0.47
1:A:346:ASP:OD1	1:A:347:HIS:N	2.48	0.47
1:A:673:VAL:O	1:A:677:LYS:HG2	2.15	0.47
1:F:580:PRO:HA	1:F:596:ASN:CG	2.40	0.47
1:D:462:MET:O	1:D:466:ASN:ND2	2.48	0.47
1:E:571:SER:O	1:E:575:LYS:NZ	2.47	0.47
1:D:457:GLU:OE2	1:D:663:ARG:NH2	2.47	0.47
1:B:529:GLN:HG2	1:B:559:PRO:HD2	1.95	0.47
1:A:535:VAL:HA	1:A:573:ASN:ND2	2.29	0.47
1:D:459:GLU:HA	1:D:462:MET:HB3	1.97	0.47
1:B:515:LEU:O	1:B:519:ALA:N	2.48	0.47
1:B:406:THR:OG1	1:B:437:THR:O	2.33	0.47
1:B:558:LEU:HD21	1:B:561:PHE:CZ	2.50	0.47
1:F:619:ARG:NH2	1:F:686:LEU:O	2.48	0.46
1:D:760:ILE:HA	1:D:764:LYS:HG2	1.98	0.46
1:C:382:GLU:H	1:C:382:GLU:CD	2.21	0.46
1:F:527:THR:O	1:F:556:SER:N	2.46	0.46
1:C:385:CYS:HB3	1:C:388:LYS:HG2	1.98	0.46
1:A:514:ARG:HD2	1:A:517:LYS:HB3	1.97	0.46
1:A:364:ILE:O	1:A:368:ILE:HG12	2.14	0.46
1:A:683:ILE:HD13	1:A:685:LYS:H	1.79	0.46
1:F:390:LYS:HB2	1:F:390:LYS:HE3	1.74	0.46
1:F:669:LEU:HD23	1:F:669:LEU:H	1.80	0.46
1:D:462:MET:HA	1:D:462:MET:HE2	1.98	0.46
1:D:386:PRO:O	1:D:390:LYS:HG2	2.15	0.46
1:D:451:PHE:HE1	1:D:669:LEU:HB2	1.81	0.46
1:F:326:LEU:HD23	1:F:392:VAL:HG23	1.98	0.46
1:E:665:ARG:O	1:E:669:LEU:HG	2.15	0.46
1:A:607:LYS:HE2	1:A:694:PRO:HG2	1.98	0.46
1:F:413:LEU:HD22	1:F:414:PRO:HD2	1.98	0.46
1:C:574:ILE:O	1:C:578:THR:OG1	2.25	0.46
1:C:718:THR:OG1	1:C:719:ASP:N	2.49	0.46
1:D:483:GLU:OE2	1:D:679:TYR:OH	2.33	0.46
1:A:366:LYS:HE2	1:B:401:VAL:HG23	1.98	0.46
1:A:490:LEU:O	1:A:551:ARG:NE	2.49	0.46
1:E:614:ASP:O	1:E:618:MET:HE1	2.16	0.46
1:D:575:LYS:HA	1:D:620:ARG:HH22	1.80	0.46
1:F:561:PHE:HB3	1:F:566:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ILE:HG23	1:B:611:ASP:HB2	1.98	0.46
1:A:461:LEU:HD11	1:A:664:TYR:HB3	1.98	0.45
1:A:486:LEU:HA	1:A:489:CYS:HB2	1.97	0.45
1:E:717:MET:C	1:E:717:MET:HE3	2.42	0.45
1:D:727:LEU:HG	1:D:732:VAL:HG12	1.98	0.45
1:B:711:VAL:HA	1:B:714:ILE:HG12	1.97	0.45
1:E:358:ASN:HB2	1:E:362:PRO:HA	1.98	0.45
1:D:407:ASP:OD1	1:D:407:ASP:N	2.49	0.45
1:E:550:LYS:HA	1:E:550:LYS:HD2	1.60	0.45
1:D:560:ASP:HA	1:D:606:TYR:CE1	2.52	0.45
1:D:698:PHE:HA	1:D:701:LYS:HE3	1.97	0.45
1:A:512:THR:O	1:A:515:LEU:HB3	2.15	0.45
1:D:707:VAL:HG12	1:D:777:ILE:HB	1.99	0.45
1:F:324:ASN:OD1	1:F:327:PHE:N	2.42	0.45
1:E:395:ASN:OD1	1:D:389:ARG:NH2	2.48	0.45
1:E:426:MET:HG3	1:E:428:TYR:CE1	2.51	0.45
1:E:758:SER:HA	1:E:761:ASN:HD21	1.81	0.45
1:D:527:THR:OG1	1:D:528:GLY:N	2.48	0.45
1:A:350:TRP:CZ2	1:A:353:ASN:HA	2.52	0.45
1:A:499:THR:HB	1:A:601:ILE:HG12	1.99	0.45
1:A:561:PHE:O	1:A:568:LYS:NZ	2.48	0.45
1:F:500:PHE:HD2	1:F:623:VAL:HG13	1.82	0.45
1:E:414:PRO:HA	1:E:419:VAL:HG12	1.99	0.45
1:A:455:SER:N	1:A:458:MET:HB3	2.32	0.45
1:A:529:GLN:HA	1:A:532:LEU:HB2	1.98	0.45
1:C:458:MET:HG3	1:C:459:GLU:OE2	2.17	0.45
1:B:747:PHE:HB3	1:B:752:PHE:HD2	1.82	0.45
1:A:507:THR:HA	1:A:629:HIS:HA	1.99	0.44
1:E:464:ILE:HA	1:E:467:ASP:OD2	2.18	0.44
1:B:535:VAL:HB	1:B:570:ARG:HE	1.81	0.44
1:B:675:TRP:HA	1:B:678:LYS:HB3	1.99	0.44
1:B:758:SER:HA	1:B:761:ASN:HD21	1.81	0.44
1:F:572:ASP:OD1	1:F:573:ASN:N	2.50	0.44
1:F:760:ILE:O	1:F:764:LYS:HB3	2.17	0.44
1:E:343:GLU:OE1	1:E:343:GLU:N	2.43	0.44
1:D:441:SER:OG	1:D:442:THR:N	2.49	0.44
1:C:662:ASN:HB3	1:C:665:ARG:HG3	1.99	0.44
1:B:350:TRP:CZ2	1:B:353:ASN:HA	2.52	0.44
1:B:543:PHE:O	1:B:547:MET:HG3	2.17	0.44
1:D:469:GLN:HB3	1:D:479:ARG:HD3	2.00	0.44
1:A:535:VAL:HA	1:A:573:ASN:HD21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:773:TYR:HE2	1:F:775:GLN:HB2	1.83	0.44
1:B:499:THR:HA	1:B:622:ALA:HB3	2.00	0.44
1:A:385:CYS:HB3	1:A:388:LYS:HG2	1.99	0.44
1:D:486:LEU:HD23	1:D:675:TRP:HZ3	1.82	0.44
1:B:486:LEU:HD22	1:B:486:LEU:H	1.82	0.44
1:C:455:SER:O	1:C:458:MET:HB3	2.17	0.44
1:C:499:THR:HA	1:C:622:ALA:HB3	2.00	0.44
1:C:772:GLU:O	1:C:774:LEU:HG	2.18	0.44
1:B:663:ARG:NH2	1:B:664:TYR:OH	2.50	0.44
1:D:351:ILE:HG23	1:D:352:ASN:H	1.82	0.44
1:C:571:SER:OG	1:C:611:ASP:O	2.31	0.44
1:B:597:HIS:O	1:B:597:HIS:ND1	2.47	0.44
1:A:475:ASN:OD1	1:A:478:ASN:ND2	2.50	0.44
1:E:448:ASP:OD1	1:E:448:ASP:N	2.50	0.44
1:A:523:LEU:H	1:A:523:LEU:HD22	1.82	0.44
1:F:575:LYS:HE2	1:F:575:LYS:HB2	1.88	0.44
1:F:734:LEU:HB3	1:F:774:LEU:HB2	2.00	0.44
1:E:515:LEU:HB3	1:E:668:PHE:CZ	2.52	0.44
1:A:462:MET:HA	1:A:465:ILE:HG22	2.00	0.43
1:F:469:GLN:NE2	1:F:475:ASN:OD1	2.51	0.43
1:E:733:THR:HG22	1:E:735:PRO:HD3	2.00	0.43
1:D:709:SER:OG	1:D:775:GLN:O	2.33	0.43
1:C:486:LEU:HD23	1:C:486:LEU:HA	1.85	0.43
1:B:615:ASN:O	1:B:618:MET:HB3	2.18	0.43
1:A:735:PRO:O	1:A:738:THR:OG1	2.22	0.43
1:C:489:CYS:C	1:C:491:CYS:N	2.76	0.43
1:D:625:ARG:NH2	1:D:692:GLU:O	2.52	0.43
1:C:458:MET:HE2	1:C:458:MET:HA	2.00	0.43
1:F:676:TYR:O	1:F:680:HIS:HB2	2.18	0.43
1:E:674:LYS:HA	1:E:674:LYS:HD3	1.79	0.43
1:D:734:LEU:HD23	1:D:774:LEU:HD22	2.00	0.43
1:C:557:GLU:OE1	1:C:557:GLU:N	2.52	0.43
1:D:463:ASN:HA	1:D:466:ASN:HD21	1.83	0.43
1:C:532:LEU:HD22	1:C:532:LEU:H	1.83	0.43
1:D:676:TYR:O	1:D:680:HIS:N	2.52	0.43
1:C:460:GLU:OE1	1:C:664:TYR:OH	2.22	0.43
1:C:510:SER:HA	1:C:513:LYS:HG3	2.00	0.43
1:E:464:ILE:HD13	1:E:467:ASP:OD2	2.19	0.43
1:D:457:GLU:HA	1:D:460:GLU:HB2	2.01	0.43
1:C:608:PRO:HG2	1:C:610:PHE:HE1	1.84	0.43
1:B:618:MET:HE2	1:B:618:MET:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:346:ASP:OD1	1:F:346:ASP:N	2.51	0.43
1:A:680:HIS:CD2	1:A:684:MET:SD	3.12	0.43
1:A:346:ASP:OD2	1:A:359:SER:OG	2.32	0.43
1:A:468:ILE:HG13	1:A:508:GLY:HA3	2.00	0.43
1:A:473:ASP:OD1	1:A:473:ASP:N	2.51	0.43
1:A:662:ASN:OD1	1:A:665:ARG:HB2	2.19	0.43
1:F:547:MET:HA	1:F:550:LYS:HG2	2.00	0.43
1:C:462:MET:HA	1:C:465:ILE:HG12	2.01	0.43
1:B:571:SER:OG	1:B:611:ASP:OD2	2.37	0.43
1:A:534:ASP:HA	1:A:570:ARG:CZ	2.49	0.42
1:A:683:ILE:C	1:A:683:ILE:HD12	2.44	0.42
1:F:473:ASP:O	1:F:476:LYS:HG2	2.19	0.42
1:F:667:ALA:HB1	1:F:670:TYR:HE2	1.84	0.42
1:E:658:LYS:HE3	1:E:658:LYS:HB2	1.91	0.42
1:D:417:ASN:ND2	1:D:446:PHE:O	2.50	0.42
1:D:732:VAL:HG23	1:D:734:LEU:H	1.83	0.42
1:C:340:LEU:HB2	1:C:348:ILE:HG13	2.00	0.42
1:B:717:MET:HE2	1:B:717:MET:N	2.33	0.42
1:A:536:LEU:HD23	1:A:536:LEU:H	1.84	0.42
1:D:460:GLU:HB3	1:D:664:TYR:HE1	1.84	0.42
1:B:566:SER:O	1:B:568:LYS:NZ	2.52	0.42
1:A:753:GLY:HA2	1:A:756:ILE:HD12	2.01	0.42
1:E:502:PHE:HB3	1:E:625:ARG:HD2	1.99	0.42
1:D:575:LYS:HD3	1:D:620:ARG:NH2	2.34	0.42
1:F:329:ILE:O	1:F:333:ILE:HG12	2.19	0.42
1:E:458:MET:C	1:E:458:MET:HE2	2.44	0.42
1:E:732:VAL:HG11	1:E:777:ILE:HG22	2.01	0.42
1:D:618:MET:HE3	1:D:618:MET:N	2.34	0.42
1:C:363:LEU:HD12	1:C:363:LEU:H	1.84	0.42
1:A:572:ASP:HA	1:A:575:LYS:HG2	2.02	0.42
1:F:547:MET:O	1:F:547:MET:HE2	2.20	0.42
1:D:406:THR:O	1:D:437:THR:OG1	2.30	0.42
1:C:329:ILE:HD11	1:C:379:TYR:HB3	2.01	0.42
1:C:477:LYS:HA	1:C:477:LYS:HD3	1.81	0.42
1:A:513:LYS:HE2	1:A:513:LYS:HB3	1.79	0.42
1:F:575:LYS:O	1:F:578:THR:HG22	2.19	0.42
1:F:667:ALA:HA	1:F:670:TYR:HD2	1.85	0.42
1:B:573:ASN:HA	1:B:576:LYS:HG2	2.02	0.42
1:F:494:THR:HG21	1:F:580:PRO:HD3	2.02	0.42
1:F:755:ASP:OD1	1:F:755:ASP:N	2.53	0.42
1:D:495:LYS:HE2	1:D:684:MET:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:MET:SD	1:C:427:PHE:N	2.93	0.42
1:B:426:MET:HE2	1:B:427:PHE:N	2.34	0.42
1:A:513:LYS:C	1:A:515:LEU:H	2.28	0.42
1:F:500:PHE:HB3	1:F:623:VAL:HG22	2.00	0.42
1:A:771:ASP:OD2	1:F:750:ARG:NE	2.53	0.42
1:C:469:GLN:OE1	1:C:475:ASN:ND2	2.43	0.42
1:A:476:LYS:O	1:A:479:ARG:HB3	2.19	0.41
1:A:510:SER:O	1:A:513:LYS:HB3	2.19	0.41
1:F:480:GLU:OE1	1:F:481:LEU:HD22	2.20	0.41
1:D:544:ILE:HD12	1:D:544:ILE:HA	1.95	0.41
1:C:775:GLN:OE1	1:B:563:CYS:HB2	2.19	0.41
1:B:426:MET:HE1	1:B:428:TYR:CG	2.55	0.41
1:B:736:LEU:HD23	1:B:739:PHE:HE2	1.84	0.41
1:E:351:ILE:HD11	1:E:356:LYS:HD2	2.01	0.41
1:E:421:ASP:O	1:E:425:GLY:HA2	2.20	0.41
1:C:612:ARG:HA	1:C:612:ARG:HD2	1.86	0.41
1:C:596:ASN:O	1:C:596:ASN:ND2	2.52	0.41
1:E:498:LEU:N	1:E:620:ARG:O	2.41	0.41
1:C:424:ASP:OD1	1:C:424:ASP:C	2.63	0.41
1:A:518:SER:HB2	1:A:662:ASN:OD1	2.21	0.41
1:A:676:TYR:O	1:A:680:HIS:ND1	2.53	0.41
1:B:494:THR:HA	1:B:597:HIS:HA	2.02	0.41
1:B:535:VAL:HA	1:B:573:ASN:HD21	1.85	0.41
1:B:495:LYS:HE2	1:B:684:MET:HG3	2.02	0.41
1:A:541:ASN:ND2	1:A:543:PHE:HB2	2.36	0.41
1:F:510:SER:HB2	1:F:513:LYS:NZ	2.36	0.41
1:E:693:ILE:HD12	1:E:694:PRO:HD2	2.02	0.41
1:C:619:ARG:HD2	1:C:619:ARG:H	1.85	0.41
1:C:742:LYS:HB3	1:C:746:TYR:CE2	2.56	0.41
1:B:489:CYS:O	1:B:490:LEU:HB2	2.21	0.41
1:A:358:ASN:ND2	1:A:361:GLU:HB3	2.36	0.41
1:A:419:VAL:HG11	1:A:436:TYR:HD2	1.86	0.41
1:F:501:PHE:HB3	1:F:509:LYS:HE3	2.03	0.41
1:E:483:GLU:HG3	1:E:675:TRP:CG	2.56	0.41
1:D:681:ILE:HD13	1:D:681:ILE:HA	1.95	0.41
1:B:456:PRO:O	1:B:460:GLU:HG3	2.21	0.41
1:B:561:PHE:HB3	1:B:568:LYS:HD3	2.02	0.41
1:B:729:ASP:HB3	1:B:731:VAL:HG23	2.03	0.41
1:A:474:GLU:HG2	1:A:475:ASN:N	2.36	0.41
1:D:459:GLU:H	1:D:459:GLU:CD	2.30	0.41
1:F:385:CYS:SG	1:F:387:ARG:NH2	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:508:GLY:O	1:F:511:THR:OG1	2.34	0.40
1:F:528:GLY:HA2	1:F:556:SER:HB2	2.03	0.40
1:E:358:ASN:HB3	1:E:363:LEU:HG	2.04	0.40
1:D:470:PRO:HG2	1:D:475:ASN:HB2	2.03	0.40
1:D:725:TYR:CE1	1:D:732:VAL:HB	2.56	0.40
1:F:596:ASN:OD1	1:F:596:ASN:N	2.54	0.40
1:F:673:VAL:O	1:F:677:LYS:HG2	2.21	0.40
1:F:733:THR:OG1	1:F:774:LEU:N	2.53	0.40
1:E:458:MET:O	1:E:462:MET:SD	2.79	0.40
1:D:555:CYS:HB3	1:D:602:ILE:HD13	2.03	0.40
1:B:472:THR:N	1:B:475:ASN:OD1	2.54	0.40
1:F:607:LYS:HA	1:F:608:PRO:HD3	1.93	0.40
1:E:717:MET:HG3	1:E:727:LEU:HD11	2.03	0.40
1:D:414:PRO:HA	1:D:419:VAL:HG23	2.04	0.40
1:D:621:ILE:HD13	1:D:621:ILE:HA	1.90	0.40
1:B:713:HIS:HE1	1:B:732:VAL:HG21	1.86	0.40
1:A:469:GLN:HG3	1:A:475:ASN:HD21	1.86	0.40
1:F:490:LEU:H	1:F:495:LYS:HE3	1.86	0.40
1:F:491:CYS:O	1:F:551:ARG:NH1	2.54	0.40
1:D:399:MET:HE2	1:D:399:MET:HB3	1.91	0.40
1:D:463:ASN:HA	1:D:466:ASN:ND2	2.37	0.40
1:C:355:TRP:HZ2	1:C:434:LYS:HG3	1.86	0.40
1:C:457:GLU:H	1:C:457:GLU:HG2	1.64	0.40
1:C:612:ARG:NH1	1:C:614:ASP:HB2	2.36	0.40
1:C:348:ILE:HG22	1:C:357:PHE:HB3	2.03	0.40
1:B:371:ILE:HA	1:B:371:ILE:HD12	1.88	0.40
1:B:546:ASN:HB2	1:B:550:LYS:HE3	2.02	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 PDB entries followed by that with respect to all EM entries.

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	417/785 (53%)	393 (94%)	24 (6%)	0	100	100
1	B	417/785 (53%)	378 (91%)	39 (9%)	0	100	100
1	C	409/785 (52%)	360 (88%)	49 (12%)	0	100	100
1	D	417/785 (53%)	390 (94%)	27 (6%)	0	100	100
1	E	417/785 (53%)	397 (95%)	20 (5%)	0	100	100
1	F	417/785 (53%)	389 (93%)	27 (6%)	1 (0%)	44	72
All	All	2494/4710 (53%)	2307 (92%)	186 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	683	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	391/725 (54%)	391 (100%)	0	100	100
1	B	391/725 (54%)	391 (100%)	0	100	100
1	C	385/725 (53%)	384 (100%)	1 (0%)	91	94
1	D	391/725 (54%)	391 (100%)	0	100	100
1	E	391/725 (54%)	391 (100%)	0	100	100
1	F	391/725 (54%)	389 (100%)	2 (0%)	86	91
All	All	2340/4350 (54%)	2337 (100%)	3 (0%)	92	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	462	MET
1	F	755	ASP
1	C	491	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	ASN
1	A	478	ASN
1	F	328	ASN
1	F	469	GLN
1	F	475	ASN
1	E	352	ASN
1	E	353	ASN
1	E	475	ASN
1	E	713	HIS
1	E	748	ASN
1	E	761	ASN
1	D	358	ASN
1	D	596	ASN
1	D	605	ASN
1	C	763	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.