



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:58 AM EDT

PDB ID : 4IGM / pdb\_00004igm  
Title : 2.39 Angstrom X-ray Crystal structure of human ACMSD  
Authors : Liu, F.; Liu, A.  
Deposited on : 2012-12-17  
Resolution : 2.39 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

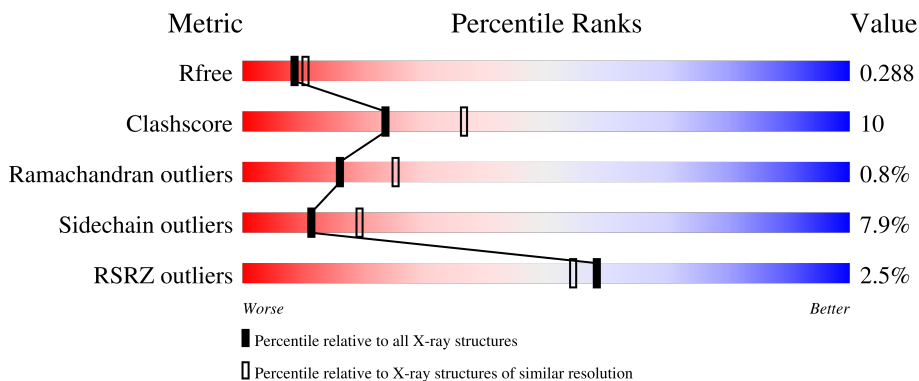
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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  $\geq 3$ , 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	332	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">73%      23%      ..</p>
1	B	332	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 76%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">76%      21%      ..</p>
1	C	332	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">78%      20%      .</p>
1	D	332	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">77%      20%      .</p>
1	E	332	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: red;"></div> </div> <p style="text-align: center; margin-top: 5px;">72%      25%      .</p>

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Mol	Chain	Length	Quality of chain
1	F	332	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into four segments: a small red segment on the left labeled '6%', a large green segment labeled '70%', a yellow segment labeled '25%', and a small orange segment on the far right labeled '5%'.</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16294 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 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	332	Total 2635	C 1703	N 443	O 468	S 21	0	0	0
1	B	332	Total 2635	C 1703	N 443	O 468	S 21	0	0	0
1	C	332	Total 2635	C 1703	N 443	O 468	S 21	0	0	0
1	D	332	Total 2635	C 1703	N 443	O 468	S 21	0	0	0
1	E	332	Total 2635	C 1703	N 443	O 468	S 21	0	0	0
1	F	332	Total 2635	C 1703	N 443	O 468	S 21	0	0	0

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

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

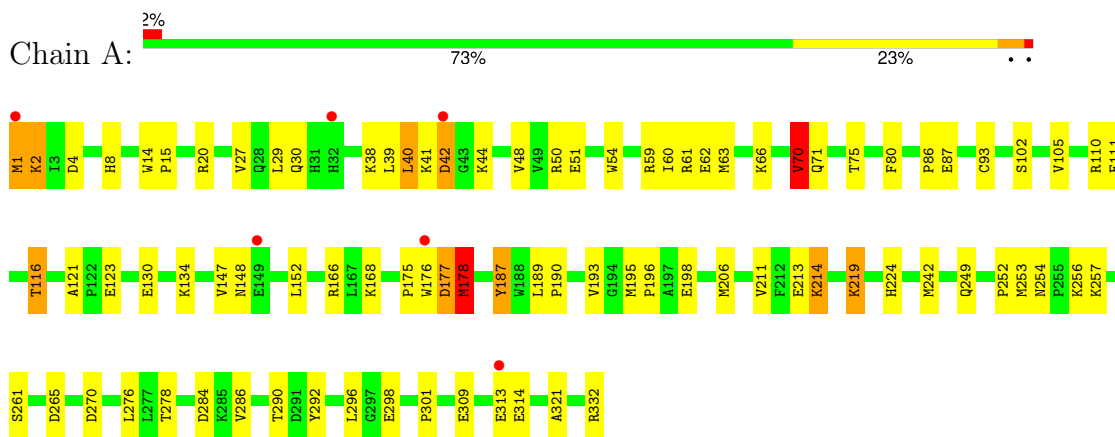
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	78	Total O 78 78	0	0
3	B	101	Total O 101 101	0	0
3	C	79	Total O 79 79	0	0
3	D	93	Total O 93 93	0	0
3	E	73	Total O 73 73	0	0
3	F	54	Total O 54 54	0	0

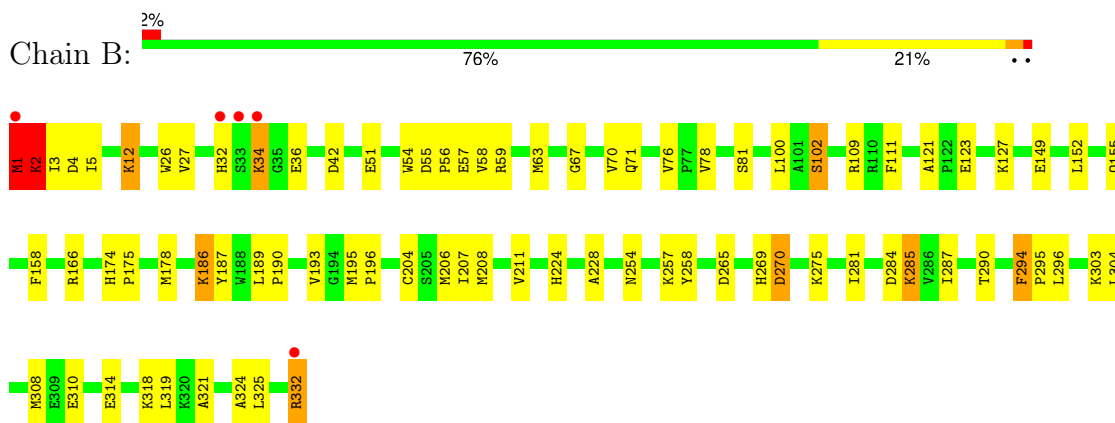
### 3 Residue-property plots [i](#)

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.

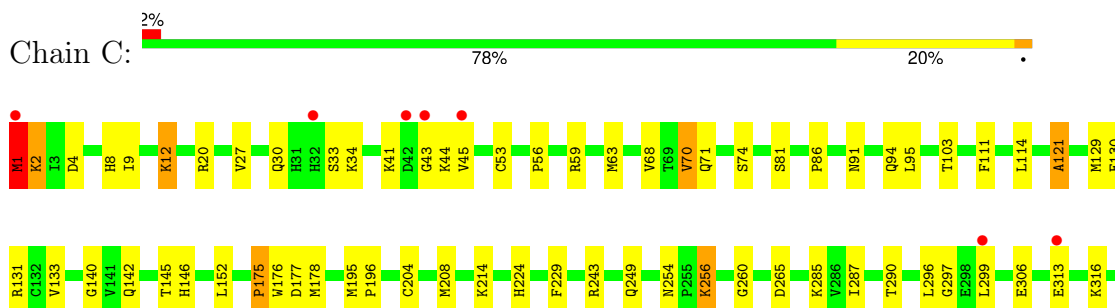
- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

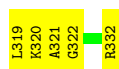


- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

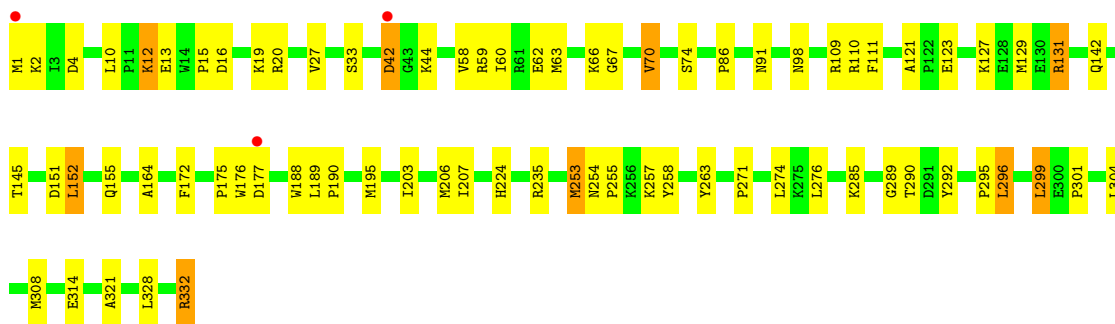
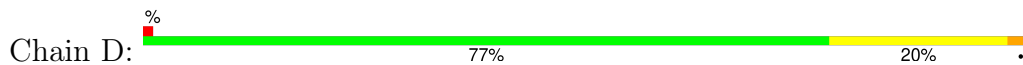


- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase

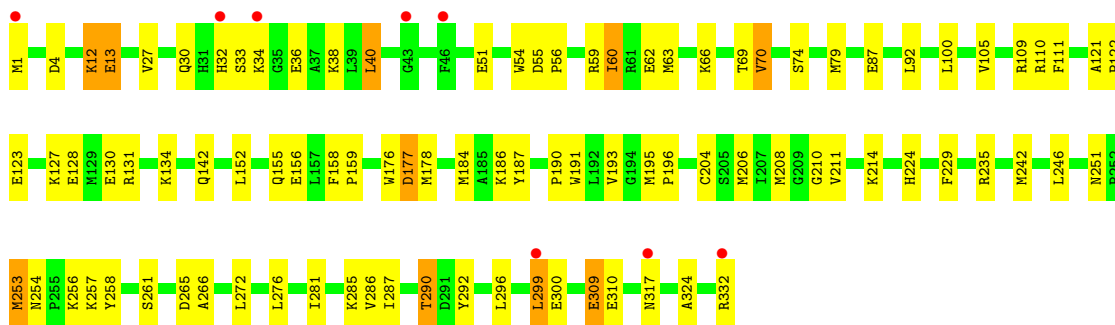




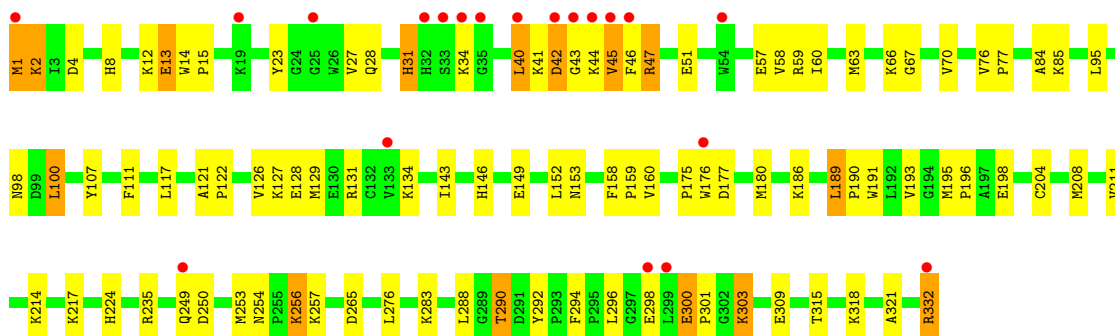
- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase



- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase



- Molecule 1: 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.11Å 101.88Å 233.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.39 45.00 – 2.39	Depositor EDS
% Data completeness (in resolution range)	94.8 (45.00-2.39) 94.9 (45.00-2.39)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.208 , 0.289 0.207 , 0.288	Depositor DCC
$R_{free}$ test set	4033 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtrriage
Anisotropy	0.229	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 24.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	1.09	2/2706 (0.1%)	1.15	6/3662 (0.2%)
1	B	1.08	2/2706 (0.1%)	1.14	9/3662 (0.2%)
1	C	1.06	1/2706 (0.0%)	1.12	12/3662 (0.3%)
1	D	1.01	0/2706	1.06	3/3662 (0.1%)
1	E	0.98	0/2706	1.09	4/3662 (0.1%)
1	F	0.95	0/2706	1.07	5/3662 (0.1%)
All	All	1.03	5/16236 (0.0%)	1.10	39/21972 (0.2%)

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	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	PRO	C-O	9.99	1.35	1.23
1	A	175	PRO	CA-C	6.25	1.60	1.52
1	C	175	PRO	C-O	5.80	1.30	1.23
1	B	54	TRP	CD2-CE2	5.23	1.50	1.41
1	B	26	TRP	CD2-CE2	5.00	1.49	1.41

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	PRO	CA-C-O	-10.07	109.88	121.56
1	E	229	PHE	CA-C-N	-9.46	109.82	120.04
1	E	229	PHE	C-N-CA	-9.46	109.82	120.04
1	C	229	PHE	CA-C-N	-8.23	111.25	119.56
1	C	229	PHE	C-N-CA	-8.23	111.25	119.56
1	C	254	ASN	CA-C-N	7.86	129.66	119.84
1	C	254	ASN	C-N-CA	7.86	129.66	119.84
1	A	177	ASP	N-CA-C	-6.45	97.06	110.80
1	B	121	ALA	CA-C-N	6.37	127.80	119.84
1	B	121	ALA	C-N-CA	6.37	127.80	119.84
1	B	270	ASP	CA-C-N	6.34	125.84	119.24
1	B	270	ASP	C-N-CA	6.34	125.84	119.24
1	F	121	ALA	CA-C-N	6.23	127.63	119.84
1	F	121	ALA	C-N-CA	6.23	127.63	119.84
1	C	2	LYS	N-CA-C	6.15	123.89	110.80
1	B	228	ALA	N-CA-C	-5.96	106.63	114.31
1	A	178	MET	N-CA-C	-5.88	101.81	110.52
1	C	45	VAL	CB-CA-C	-5.70	106.18	112.68
1	C	243	ARG	CA-C-N	-5.66	113.98	119.87
1	C	243	ARG	C-N-CA	-5.66	113.98	119.87
1	E	134	LYS	N-CA-C	5.49	120.13	113.38
1	D	44	LYS	N-CA-C	5.44	117.89	110.55
1	B	294	PHE	CA-C-N	5.38	125.00	119.56
1	B	294	PHE	C-N-CA	5.38	125.00	119.56
1	E	186	LYS	N-CA-C	5.38	117.48	110.53
1	F	189	LEU	CA-C-N	-5.27	113.36	119.47
1	F	189	LEU	C-N-CA	-5.27	113.36	119.47
1	A	70	VAL	CB-CA-C	5.26	118.46	110.62
1	A	14	TRP	CA-C-N	-5.18	114.37	119.92
1	A	14	TRP	C-N-CA	-5.18	114.37	119.92
1	D	10	LEU	CA-C-N	-5.18	114.45	119.78
1	D	10	LEU	C-N-CA	-5.18	114.45	119.78
1	B	166	ARG	CB-CA-C	-5.14	100.80	110.67
1	B	3	ILE	N-CA-C	5.04	115.23	108.17
1	C	322	GLY	N-CA-C	5.01	118.70	112.64
1	F	211	VAL	N-CA-C	5.01	115.23	110.42
1	C	70	VAL	N-CA-C	5.01	115.49	108.17
1	C	121	ALA	CA-C-N	5.00	125.02	119.32
1	C	121	ALA	C-N-CA	5.00	125.02	119.32

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	MET	Peptide
1	C	1	MET	Peptide

## 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	2635	0	2643	59	0
1	B	2635	0	2643	44	0
1	C	2635	0	2643	44	0
1	D	2635	0	2643	60	0
1	E	2635	0	2643	69	0
1	F	2635	0	2643	67	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	A	78	0	0	5	0
3	B	101	0	0	0	0
3	C	79	0	0	1	0
3	D	93	0	0	5	0
3	E	73	0	0	3	0
3	F	54	0	0	2	0
All	All	16294	0	15858	322	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 10.

All (322) 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:1:MET:SD	1:C:2:LYS:NZ	2.32	1.03
1:C:12:LYS:HD3	1:C:12:LYS:H	1.19	1.02
1:E:317:ASN:HB2	3:E:568:HOH:O	1.61	0.99
1:B:63:MET:HE1	1:B:111:PHE:HE1	1.28	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:HA	3:A:506:HOH:O	1.63	0.97
1:D:195:MET:CE	1:E:235:ARG:NH2	2.30	0.94
1:B:63:MET:HE1	1:B:111:PHE:CE1	2.01	0.94
1:C:63:MET:HE1	1:C:111:PHE:CE1	2.03	0.92
1:D:63:MET:HE1	1:D:111:PHE:CE1	2.05	0.92
1:E:290:THR:HG22	1:E:292:TYR:H	1.32	0.92
1:C:175:PRO:HG2	1:C:195:MET:HE3	1.54	0.90
1:B:63:MET:HE2	1:B:71:GLN:CD	1.98	0.89
1:E:309:GLU:H	1:E:309:GLU:CD	1.90	0.80
1:D:63:MET:HE1	1:D:111:PHE:HE1	1.44	0.80
1:F:175:PRO:HG2	1:F:195:MET:CE	2.12	0.80
1:B:1:MET:SD	1:B:2:LYS:NZ	2.53	0.79
1:B:12:LYS:HE3	1:B:12:LYS:H	1.48	0.79
1:B:59:ARG:HB3	1:B:63:MET:HE3	1.65	0.79
1:F:175:PRO:HG2	1:F:195:MET:HE2	1.64	0.79
1:C:63:MET:HE1	1:C:111:PHE:HE1	1.46	0.78
1:A:254:ASN:H	1:A:257:LYS:NZ	1.81	0.78
1:D:195:MET:HE2	1:E:235:ARG:HH21	1.50	0.77
1:C:12:LYS:HD3	1:C:12:LYS:N	2.00	0.77
1:D:235:ARG:NH2	1:E:195:MET:HE2	2.00	0.77
1:F:253:MET:HG3	1:F:257:LYS:HD2	1.64	0.76
1:D:195:MET:HE2	1:E:235:ARG:NH2	1.99	0.76
1:B:2:LYS:HB2	1:B:321:ALA:HB2	1.68	0.75
1:F:63:MET:HE1	1:F:111:PHE:CE1	2.21	0.74
1:C:195:MET:HE2	1:C:224:HIS:NE2	2.03	0.73
1:F:98:ASN:OD1	1:F:131:ARG:NH2	2.20	0.73
1:F:4:ASP:OD2	1:F:290:THR:HB	1.88	0.73
1:B:2:LYS:CB	1:B:321:ALA:HB2	2.19	0.73
1:A:254:ASN:H	1:A:257:LYS:HZ2	1.37	0.71
1:D:109:ARG:HG2	3:D:588:HOH:O	1.91	0.71
1:C:1:MET:O	1:C:68:VAL:HA	1.89	0.71
1:E:74:SER:HB2	1:E:142:GLN:NE2	2.05	0.70
1:D:12:LYS:H	1:D:12:LYS:HD3	1.57	0.70
1:B:1:MET:HG2	1:B:67:GLY:O	1.92	0.69
1:F:63:MET:HE1	1:F:111:PHE:CZ	2.28	0.69
1:E:290:THR:CG2	1:E:292:TYR:HB2	2.22	0.69
1:B:63:MET:HE2	1:B:71:GLN:OE1	1.92	0.68
1:E:290:THR:HG22	1:E:292:TYR:N	2.08	0.67
1:D:235:ARG:HH22	1:E:195:MET:HE2	1.58	0.67
1:D:253:MET:HG3	1:D:257:LYS:HD2	1.76	0.67
1:D:195:MET:CE	1:E:235:ARG:HH22	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LYS:H	1:C:12:LYS:CD	1.99	0.66
1:B:270:ASP:OD2	1:C:256:LYS:NZ	2.24	0.66
1:F:290:THR:HG22	1:F:292:TYR:H	1.61	0.66
1:F:41:LYS:O	1:F:42:ASP:HB3	1.95	0.66
1:F:51:GLU:HG2	1:F:58:VAL:HG21	1.77	0.66
1:C:63:MET:HE2	1:C:71:GLN:CD	2.21	0.66
1:E:309:GLU:CD	1:E:309:GLU:N	2.53	0.66
1:B:206:MET:HE2	1:B:211:VAL:HG11	1.77	0.65
1:D:1:MET:O	1:D:67:GLY:O	2.14	0.65
1:F:204:CYS:HB3	1:F:208:MET:HE3	1.76	0.65
1:A:290:THR:HG22	1:A:292:TYR:H	1.61	0.64
1:A:254:ASN:HB3	1:A:257:LYS:HE3	1.80	0.64
1:A:4:ASP:OD2	1:A:290:THR:HB	1.98	0.64
1:B:12:LYS:H	1:B:12:LYS:CE	2.11	0.63
1:D:254:ASN:H	1:D:257:LYS:HZ1	1.45	0.62
1:E:290:THR:HG21	1:E:292:TYR:HB2	1.81	0.62
1:F:265:ASP:OD1	1:F:265:ASP:C	2.42	0.62
1:B:265:ASP:C	1:B:265:ASP:OD1	2.43	0.62
1:E:299:LEU:HD23	1:E:299:LEU:H	1.65	0.61
1:F:122:PRO:O	1:F:126:VAL:HG23	2.01	0.60
1:F:300:GLU:HB2	1:F:303:LYS:HB2	1.83	0.60
1:C:63:MET:HE2	1:C:71:GLN:OE1	2.02	0.60
1:E:33:SER:OG	1:E:34:LYS:N	2.33	0.60
1:A:63:MET:HE1	1:A:111:PHE:CE1	2.37	0.60
1:A:298:GLU:OE1	1:A:301:PRO:HA	2.03	0.58
1:C:63:MET:HE1	1:C:111:PHE:CZ	2.36	0.58
1:D:63:MET:HE1	1:D:111:PHE:CZ	2.38	0.58
1:A:15:PRO:HG2	1:A:20:ARG:HH21	1.68	0.58
1:F:117:LEU:HD11	1:F:129:MET:HE2	1.84	0.58
1:A:278:THR:HG22	1:A:286:VAL:HG21	1.85	0.58
1:E:128:GLU:OE1	1:E:131:ARG:HD3	2.02	0.58
1:A:41:LYS:O	1:A:42:ASP:C	2.46	0.57
1:F:290:THR:HG22	1:F:292:TYR:N	2.19	0.57
1:C:195:MET:CE	1:C:224:HIS:NE2	2.66	0.57
1:D:271:PRO:HD3	1:D:304:LEU:HD11	1.87	0.57
1:F:2:LYS:HB3	1:F:321:ALA:HB2	1.85	0.57
1:F:28:GLN:HB2	1:F:40:LEU:HD11	1.87	0.57
1:A:63:MET:HE1	1:A:111:PHE:HE1	1.69	0.57
1:B:284:ASP:OD1	1:B:318:LYS:HE3	2.04	0.56
1:A:206:MET:HE3	1:A:211:VAL:HG11	1.87	0.56
1:E:30:GLN:CG	1:E:40:LEU:HD11	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:MET:HE3	1:E:211:VAL:HG11	1.86	0.56
1:A:38:LYS:HE2	1:A:48:VAL:HG22	1.86	0.56
1:E:156:GLU:O	1:E:159:PRO:HD2	2.06	0.56
1:A:80:PHE:HE1	3:A:507:HOH:O	1.89	0.56
1:A:176:TRP:O	1:A:177:ASP:HB3	2.05	0.55
1:A:253:MET:HB3	1:A:257:LYS:HD2	1.88	0.55
1:D:263:TYR:CZ	1:D:285:LYS:HE3	2.41	0.55
1:F:176:TRP:O	1:F:177:ASP:CB	2.54	0.55
1:C:4:ASP:OD2	1:C:290:THR:HB	2.07	0.55
1:F:41:LYS:O	1:F:42:ASP:CB	2.55	0.55
1:A:102:SER:OG	1:B:102:SER:HB3	2.07	0.55
1:D:12:LYS:HG2	1:D:13:GLU:HG3	1.88	0.54
1:F:31:HIS:CD2	1:F:31:HIS:H	2.26	0.54
1:F:1:MET:N	1:F:288:LEU:CD2	2.71	0.54
1:E:251:ASN:OD1	1:E:253:MET:HE2	2.07	0.54
1:E:253:MET:SD	1:E:253:MET:N	2.81	0.54
1:F:12:LYS:HG2	1:F:13:GLU:N	2.22	0.54
1:F:128:GLU:OE1	1:F:131:ARG:HD3	2.07	0.54
1:B:59:ARG:HB3	1:B:63:MET:CE	2.37	0.54
1:E:195:MET:HE3	1:E:224:HIS:NE2	2.23	0.54
1:A:270:ASP:OD2	1:F:256:LYS:NZ	2.37	0.54
1:D:16:ASP:OD2	1:D:19:LYS:HG3	2.07	0.54
1:A:195:MET:HE2	1:F:235:ARG:NH2	2.24	0.53
1:E:184:MET:O	1:E:190:PRO:HD3	2.08	0.53
1:E:210:GLY:O	1:E:214:LYS:HD3	2.07	0.53
1:E:191:TRP:HA	1:E:195:MET:HG3	1.91	0.53
1:E:254:ASN:OD1	1:E:256:LYS:HB2	2.09	0.53
1:A:87:GLU:OE1	1:A:87:GLU:HA	2.09	0.53
1:A:193:VAL:C	1:A:196:PRO:HD2	2.34	0.53
1:C:53:CYS:HB2	3:C:527:HOH:O	2.08	0.53
1:D:295:PRO:HD2	3:D:501:HOH:O	2.09	0.52
1:E:265:ASP:OD1	1:E:265:ASP:C	2.53	0.52
1:D:176:TRP:CG	1:D:177:ASP:H	2.27	0.52
1:E:12:LYS:HE2	1:E:13:GLU:H	1.74	0.52
1:A:284:ASP:HB2	3:A:518:HOH:O	2.10	0.52
1:B:204:CYS:HB3	1:B:208:MET:CE	2.40	0.52
1:C:290:THR:O	1:C:297:GLY:HA3	2.10	0.52
1:D:58:VAL:O	1:D:62:GLU:HG3	2.09	0.52
1:F:46:PHE:O	1:F:47:ARG:HB2	2.09	0.52
1:D:4:ASP:OD2	1:D:290:THR:HB	2.10	0.52
1:E:204:CYS:HB3	1:E:208:MET:CE	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:MET:HE2	1:F:235:ARG:HH22	1.74	0.51
1:C:2:LYS:HB3	1:C:321:ALA:HB2	1.92	0.51
1:F:1:MET:N	1:F:288:LEU:HD21	2.24	0.51
1:C:175:PRO:HG2	1:C:195:MET:CE	2.35	0.51
1:D:176:TRP:CG	1:D:177:ASP:N	2.78	0.51
1:D:195:MET:HE1	1:E:235:ARG:HH22	1.74	0.51
1:A:187:TYR:OH	1:F:153:ASN:ND2	2.44	0.51
1:D:332:ARG:HD2	1:D:332:ARG:C	2.35	0.51
1:C:86:PRO:HB3	1:C:121:ALA:HB2	1.91	0.51
1:A:178:MET:HG3	1:A:198:GLU:HG3	1.92	0.50
1:B:174:HIS:ND1	1:B:175:PRO:HD2	2.27	0.50
1:D:15:PRO:HG2	1:D:20:ARG:HH21	1.76	0.50
1:D:274:LEU:HD22	1:D:304:LEU:HD23	1.94	0.50
1:A:252:PRO:HG2	1:A:253:MET:SD	2.52	0.50
1:C:59:ARG:HB3	1:C:63:MET:HE3	1.92	0.50
1:D:188:TRP:CD1	1:E:246:LEU:HD13	2.47	0.50
1:B:325:LEU:HD13	1:B:332:ARG:HG3	1.94	0.50
1:A:290:THR:HG22	1:A:292:TYR:N	2.26	0.50
1:C:1:MET:SD	1:C:2:LYS:HG2	2.51	0.50
1:C:74:SER:HB2	1:C:142:GLN:NE2	2.25	0.50
1:C:95:LEU:HD23	1:C:95:LEU:C	2.36	0.50
1:D:74:SER:HB2	1:D:142:GLN:OE1	2.12	0.50
1:E:176:TRP:CG	1:E:177:ASP:N	2.80	0.50
1:F:254:ASN:H	1:F:257:LYS:HZ2	1.59	0.50
1:B:4:ASP:OD2	1:B:290:THR:HB	2.12	0.49
1:B:189:LEU:N	1:B:190:PRO:CD	2.75	0.49
1:D:304:LEU:O	1:D:308:MET:HG2	2.12	0.49
1:D:189:LEU:N	1:D:190:PRO:CD	2.76	0.49
1:D:290:THR:HG22	1:D:292:TYR:N	2.27	0.49
1:E:109:ARG:NH2	3:E:508:HOH:O	2.46	0.49
1:A:195:MET:HE3	1:A:224:HIS:NE2	2.28	0.49
1:D:86:PRO:HB3	1:D:121:ALA:HB2	1.94	0.48
1:F:15:PRO:HD2	1:F:95:LEU:HD11	1.95	0.48
1:F:41:LYS:HA	1:F:46:PHE:HE2	1.79	0.48
1:A:86:PRO:HB3	1:A:121:ALA:HB2	1.94	0.48
1:D:299:LEU:O	1:D:301:PRO:HD3	2.13	0.48
1:D:59:ARG:C	1:D:63:MET:HE3	2.38	0.48
1:F:57:GLU:HG3	1:F:107:TYR:OH	2.13	0.48
1:B:12:LYS:H	1:B:12:LYS:CD	2.26	0.48
1:E:30:GLN:HG3	1:E:40:LEU:HD11	1.95	0.48
1:A:59:ARG:C	1:A:63:MET:HE3	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:GLU:O	1:E:66:LYS:HG2	2.13	0.47
1:C:41:LYS:C	1:C:43:GLY:H	2.22	0.47
1:C:145:THR:O	1:C:146:HIS:HB3	2.14	0.47
1:C:204:CYS:HB3	1:C:208:MET:HE3	1.96	0.47
1:B:51:GLU:HG2	1:B:58:VAL:HG21	1.95	0.47
1:F:23:TYR:OH	1:F:85:LYS:HB2	2.14	0.47
1:F:283:LYS:HD3	1:F:315:THR:CG2	2.43	0.47
1:C:8:HIS:HA	1:C:74:SER:O	2.15	0.47
1:E:287:ILE:HG23	1:E:324:ALA:HB2	1.97	0.47
1:F:4:ASP:CG	1:F:290:THR:HB	2.40	0.47
1:E:30:GLN:CG	1:E:40:LEU:CD1	2.92	0.47
1:E:59:ARG:C	1:E:63:MET:HE3	2.39	0.47
1:E:195:MET:HB2	1:E:196:PRO:HD3	1.97	0.47
1:E:266:ALA:HB2	1:E:286:VAL:CG1	2.45	0.47
1:E:242:MET:HE2	1:E:242:MET:HA	1.96	0.47
1:E:63:MET:HE1	1:E:111:PHE:CZ	2.50	0.47
1:F:175:PRO:HG2	1:F:195:MET:HE3	1.95	0.47
1:D:12:LYS:HD3	1:D:12:LYS:N	2.26	0.46
1:D:188:TRP:C	1:D:190:PRO:HD2	2.41	0.46
1:E:30:GLN:HG3	1:E:40:LEU:CD1	2.45	0.46
1:C:20:ARG:NH1	1:C:91:ASN:OD1	2.44	0.46
1:F:127:LYS:NZ	3:F:538:HOH:O	2.47	0.46
1:E:70:VAL:HA	1:E:110:ARG:O	2.15	0.46
1:F:146:HIS:ND1	1:F:198:GLU:OE1	2.47	0.46
1:E:79:MET:HE3	1:E:92:LEU:HD21	1.98	0.46
1:F:1:MET:HE2	1:F:67:GLY:HA3	1.97	0.46
1:F:158:PHE:N	1:F:159:PRO:CD	2.79	0.46
1:F:193:VAL:C	1:F:196:PRO:HD2	2.41	0.46
1:D:254:ASN:H	1:D:257:LYS:NZ	2.13	0.46
1:C:316:LYS:O	1:C:320:LYS:HG3	2.15	0.46
1:C:129:MET:O	1:C:133:VAL:HG23	2.16	0.46
1:D:203:ILE:O	1:D:207:ILE:HG13	2.15	0.46
1:E:4:ASP:OD2	1:E:290:THR:HB	2.15	0.46
1:F:31:HIS:CD2	1:F:31:HIS:N	2.83	0.46
1:B:207:ILE:HG23	1:B:258:TYR:CD2	2.51	0.46
1:E:63:MET:HE1	1:E:111:PHE:CE1	2.51	0.46
1:F:191:TRP:HA	1:F:195:MET:HG3	1.98	0.46
1:F:186:LYS:O	1:F:189:LEU:HG	2.16	0.46
1:A:8:HIS:HD2	1:A:75:THR:O	2.00	0.45
1:C:114:LEU:HA	1:C:140:GLY:O	2.16	0.45
1:D:20:ARG:NH1	1:D:91:ASN:OD1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:LEU:HD11	1:E:272:LEU:HB3	1.97	0.45
1:E:4:ASP:CG	1:E:290:THR:HB	2.42	0.45
1:B:332:ARG:CD	1:B:332:ARG:H	2.30	0.45
1:D:195:MET:HE3	1:E:235:ARG:NH2	2.24	0.45
1:D:207:ILE:HG23	1:D:258:TYR:CD2	2.52	0.45
1:E:258:TYR:O	1:E:261:SER:HB2	2.17	0.45
1:A:213:GLU:HB3	1:A:214:LYS:HZ1	1.82	0.45
1:A:2:LYS:HB3	1:A:321:ALA:HB2	1.99	0.44
1:D:70:VAL:HA	1:D:110:ARG:O	2.17	0.44
1:D:224:HIS:HD2	3:D:503:HOH:O	2.00	0.44
1:E:51:GLU:HA	1:E:54:TRP:CE2	2.51	0.44
1:A:70:VAL:HA	1:A:110:ARG:O	2.17	0.44
1:C:33:SER:OG	1:C:34:LYS:N	2.50	0.44
1:E:290:THR:CG2	1:E:292:TYR:H	2.16	0.44
1:B:281:ILE:HG22	1:B:285:LYS:HB2	1.99	0.44
1:D:98:ASN:OD1	1:D:131:ARG:NH2	2.26	0.44
1:A:213:GLU:HB3	1:A:214:LYS:NZ	2.32	0.44
1:D:2:LYS:HB2	1:D:321:ALA:HB2	1.99	0.44
1:A:253:MET:HA	1:A:257:LYS:HZ2	1.82	0.44
1:B:195:MET:CE	1:B:224:HIS:NE2	2.80	0.44
1:A:4:ASP:CG	1:A:290:THR:HB	2.42	0.44
1:A:219:LYS:HE2	1:A:219:LYS:HB3	1.90	0.44
1:B:193:VAL:C	1:B:196:PRO:HD2	2.41	0.44
1:F:76:VAL:HA	1:F:77:PRO:HD3	1.85	0.44
1:F:193:VAL:O	1:F:196:PRO:HD2	2.18	0.44
1:A:242:MET:HE2	1:A:242:MET:HA	2.00	0.44
1:B:12:LYS:HE3	1:B:12:LYS:N	2.25	0.44
1:B:206:MET:CE	1:B:211:VAL:HG11	2.45	0.44
1:D:129:MET:HE1	1:D:164:ALA:HB2	1.99	0.44
1:E:254:ASN:HB3	1:E:257:LYS:HE3	1.99	0.44
1:F:12:LYS:HG2	1:F:13:GLU:H	1.82	0.44
1:A:63:MET:HE2	1:A:71:GLN:CD	2.43	0.44
1:D:224:HIS:HE1	3:D:591:HOH:O	2.00	0.44
1:A:62:GLU:O	1:A:66:LYS:HG2	2.18	0.43
1:A:134:LYS:HA	1:A:134:LYS:HD3	1.85	0.43
1:F:224:HIS:CE1	3:F:554:HOH:O	2.70	0.43
1:C:265:ASP:OD1	1:C:265:ASP:C	2.62	0.43
1:E:121:ALA:O	1:E:122:PRO:C	2.59	0.43
1:C:176:TRP:CG	1:C:177:ASP:N	2.85	0.43
1:F:332:ARG:H	1:F:332:ARG:NE	2.16	0.43
1:A:193:VAL:O	1:A:196:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:128:GLU:OE1	1:E:128:GLU:HA	2.18	0.43
1:D:152:LEU:HB3	1:D:206:MET:HG3	2.00	0.43
1:E:290:THR:CG2	1:E:292:TYR:N	2.79	0.43
1:B:186:LYS:HD2	1:B:187:TYR:CD1	2.54	0.43
1:C:195:MET:N	1:C:196:PRO:CD	2.82	0.43
1:D:42:ASP:HB2	3:D:526:HOH:O	2.18	0.43
1:E:310:GLU:HB2	3:E:551:HOH:O	2.19	0.43
1:B:1:MET:SD	1:B:2:LYS:HG2	2.58	0.42
1:D:276:LEU:HD22	1:E:276:LEU:HD22	2.00	0.42
1:C:59:ARG:HB3	1:C:63:MET:CE	2.49	0.42
1:D:145:THR:CG2	1:D:175:PRO:HA	2.49	0.42
1:B:5:ILE:HG13	1:B:5:ILE:O	2.18	0.42
1:F:8:HIS:CD2	1:F:294:PHE:HE1	2.36	0.42
1:B:294:PHE:HB3	1:B:295:PRO:HD2	2.01	0.42
1:D:254:ASN:HB3	1:D:257:LYS:HE3	2.02	0.42
1:E:32:HIS:CE1	1:E:38:LYS:HG3	2.54	0.42
1:E:60:ILE:HA	1:E:63:MET:HE3	2.02	0.42
1:F:1:MET:H2	1:F:288:LEU:CD2	2.32	0.42
1:B:254:ASN:H	1:B:257:LYS:HZ3	1.66	0.42
1:B:155:GLN:O	1:B:158:PHE:HB2	2.19	0.42
1:E:281:ILE:HG22	1:E:285:LYS:HB2	2.01	0.42
1:F:44:LYS:O	1:F:45:VAL:O	2.38	0.42
1:A:30:GLN:CD	1:A:40:LEU:HD21	2.45	0.42
1:B:76:VAL:HG12	1:B:78:VAL:HG12	2.02	0.42
1:F:128:GLU:OE1	1:F:128:GLU:HA	2.20	0.42
1:B:275:LYS:HE2	1:B:310:GLU:HB3	2.02	0.42
1:A:102:SER:CB	1:B:102:SER:HB3	2.50	0.41
1:B:32:HIS:CE1	1:B:36:GLU:HB2	2.55	0.41
1:D:142:GLN:HA	1:D:172:PHE:O	2.20	0.41
1:D:328:LEU:HD23	1:D:328:LEU:HA	1.90	0.41
1:F:84:ALA:O	1:F:85:LYS:C	2.61	0.41
1:A:147:VAL:O	1:A:148:ASN:HB2	2.19	0.41
1:B:287:ILE:HG23	1:B:324:ALA:HB2	2.00	0.41
1:D:4:ASP:OD1	1:D:289:GLY:HA2	2.19	0.41
1:D:253:MET:CG	1:D:257:LYS:HD2	2.47	0.41
1:A:1:MET:O	1:A:2:LYS:HG2	2.20	0.41
1:A:15:PRO:HG2	1:A:20:ARG:NH2	2.34	0.41
1:A:93:CYS:SG	1:A:116:THR:HG23	2.61	0.41
1:A:189:LEU:N	1:A:190:PRO:CD	2.83	0.41
1:C:265:ASP:HA	1:C:287:ILE:O	2.20	0.41
1:F:1:MET:H2	1:F:288:LEU:HD21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:59:ARG:C	1:F:63:MET:HE3	2.46	0.41
1:A:276:LEU:HD22	1:F:276:LEU:HD22	2.01	0.41
1:E:193:VAL:C	1:E:196:PRO:HD2	2.45	0.41
1:F:298:GLU:OE1	1:F:301:PRO:HA	2.20	0.41
1:A:276:LEU:HD22	1:F:276:LEU:CD2	2.51	0.41
1:C:306:GLU:OE2	1:C:320:LYS:NZ	2.51	0.41
1:B:55:ASP:HA	1:B:56:PRO:HD3	1.95	0.41
1:C:56:PRO:HG3	1:C:103:THR:HG23	2.02	0.41
1:E:55:ASP:HA	1:E:56:PRO:HD2	1.89	0.41
1:F:189:LEU:O	1:F:190:PRO:C	2.60	0.41
1:A:29:LEU:HD13	1:A:39:LEU:CD2	2.50	0.41
1:C:260:GLY:O	1:C:285:LYS:NZ	2.54	0.41
1:C:290:THR:O	1:C:290:THR:HG22	2.20	0.41
1:D:296:LEU:CD1	1:E:235:ARG:NH2	2.84	0.41
1:E:40:LEU:HD12	1:E:40:LEU:N	2.36	0.41
1:E:155:GLN:O	1:E:158:PHE:HB2	2.21	0.41
1:F:66:LYS:HD3	1:F:66:LYS:HA	1.73	0.41
1:F:100:LEU:HD12	1:F:100:LEU:HA	1.94	0.41
1:A:265:ASP:OD1	1:A:265:ASP:C	2.64	0.41
1:F:180:MET:HE1	1:F:191:TRP:CZ3	2.56	0.41
1:A:254:ASN:N	1:A:257:LYS:HZ2	2.13	0.40
1:D:66:LYS:HD3	1:D:66:LYS:HA	1.93	0.40
1:F:176:TRP:O	1:F:177:ASP:HB2	2.16	0.40
1:A:224:HIS:HD2	3:A:563:HOH:O	2.04	0.40
1:B:304:LEU:O	1:B:308:MET:HG2	2.21	0.40
1:C:2:LYS:CB	1:C:321:ALA:HB2	2.51	0.40
1:C:63:MET:HB3	1:C:68:VAL:HB	2.04	0.40
1:A:50:ARG:CD	3:A:572:HOH:O	2.68	0.40
1:A:51:GLU:HA	1:A:54:TRP:CE2	2.55	0.40
1:E:66:LYS:HD2	1:E:300:GLU:OE2	2.21	0.40
1:F:13:GLU:HG2	1:F:14:TRP:N	2.36	0.40

There are no symmetry-related clashes.

## 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	330/332 (99%)	312 (94%)	15 (4%)	3 (1%)	14	22
1	B	330/332 (99%)	316 (96%)	11 (3%)	3 (1%)	14	22
1	C	330/332 (99%)	309 (94%)	20 (6%)	1 (0%)	36	50
1	D	330/332 (99%)	318 (96%)	11 (3%)	1 (0%)	36	50
1	E	330/332 (99%)	312 (94%)	17 (5%)	1 (0%)	36	50
1	F	330/332 (99%)	305 (92%)	19 (6%)	6 (2%)	6	9
All	All	1980/1992 (99%)	1872 (94%)	93 (5%)	15 (1%)	16	25

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	44	LYS
1	D	42	ASP
1	F	45	VAL
1	B	34	LYS
1	F	42	ASP
1	F	250	ASP
1	A	42	ASP
1	A	187	TYR
1	B	2	LYS
1	B	269	HIS
1	F	47	ARG
1	F	309	GLU
1	F	43	GLY
1	A	2	LYS
1	E	187	TYR

### 5.3.2 Protein sidechains [i](#)

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	285/285 (100%)	260 (91%)	25 (9%)	9	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	285/285 (100%)	261 (92%)	24 (8%)	10	17
1	C	285/285 (100%)	265 (93%)	20 (7%)	14	24
1	D	285/285 (100%)	268 (94%)	17 (6%)	17	31
1	E	285/285 (100%)	261 (92%)	24 (8%)	10	17
1	F	285/285 (100%)	260 (91%)	25 (9%)	9	15
All	All	1710/1710 (100%)	1575 (92%)	135 (8%)	11	19

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	27	VAL
1	A	40	LEU
1	A	44	LYS
1	A	60	ILE
1	A	61	ARG
1	A	70	VAL
1	A	105	VAL
1	A	116	THR
1	A	123	GLU
1	A	130	GLU
1	A	152	LEU
1	A	166	ARG
1	A	168	LYS
1	A	178	MET
1	A	214	LYS
1	A	219	LYS
1	A	249	GLN
1	A	256	LYS
1	A	261	SER
1	A	296	LEU
1	A	309	GLU
1	A	313	GLU
1	A	314	GLU
1	A	332	ARG
1	B	1	MET
1	B	2	LYS
1	B	12	LYS
1	B	27	VAL
1	B	34	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	42	ASP
1	B	57	GLU
1	B	70	VAL
1	B	81	SER
1	B	100	LEU
1	B	102	SER
1	B	109	ARG
1	B	123	GLU
1	B	127	LYS
1	B	149	GLU
1	B	152	LEU
1	B	178	MET
1	B	186	LYS
1	B	285	LYS
1	B	296	LEU
1	B	303	LYS
1	B	314	GLU
1	B	319	LEU
1	B	332	ARG
1	C	1	MET
1	C	9	ILE
1	C	12	LYS
1	C	27	VAL
1	C	30	GLN
1	C	70	VAL
1	C	81	SER
1	C	94	GLN
1	C	130	GLU
1	C	131	ARG
1	C	152	LEU
1	C	178	MET
1	C	214	LYS
1	C	249	GLN
1	C	256	LYS
1	C	296	LEU
1	C	299	LEU
1	C	313	GLU
1	C	319	LEU
1	C	332	ARG
1	D	12	LYS
1	D	27	VAL
1	D	33	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	60	ILE
1	D	70	VAL
1	D	123	GLU
1	D	127	LYS
1	D	131	ARG
1	D	151	ASP
1	D	152	LEU
1	D	155	GLN
1	D	253	MET
1	D	255	PRO
1	D	296	LEU
1	D	299	LEU
1	D	314	GLU
1	D	332	ARG
1	E	1	MET
1	E	12	LYS
1	E	13	GLU
1	E	27	VAL
1	E	36	GLU
1	E	40	LEU
1	E	60	ILE
1	E	69	THR
1	E	70	VAL
1	E	87	GLU
1	E	100	LEU
1	E	105	VAL
1	E	123	GLU
1	E	127	LYS
1	E	130	GLU
1	E	152	LEU
1	E	177	ASP
1	E	178	MET
1	E	253	MET
1	E	290	THR
1	E	296	LEU
1	E	299	LEU
1	E	309	GLU
1	E	332	ARG
1	F	1	MET
1	F	2	LYS
1	F	13	GLU
1	F	27	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	F	31	HIS
1	F	34	LYS
1	F	40	LEU
1	F	60	ILE
1	F	70	VAL
1	F	100	LEU
1	F	134	LYS
1	F	143	ILE
1	F	149	GLU
1	F	152	LEU
1	F	160	VAL
1	F	214	LYS
1	F	217	LYS
1	F	249	GLN
1	F	256	LYS
1	F	290	THR
1	F	296	LEU
1	F	300	GLU
1	F	303	LYS
1	F	318	LYS
1	F	332	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	94	GLN
1	B	30	GLN
1	B	32	HIS
1	B	142	GLN
1	B	148	ASN
1	B	155	GLN
1	B	251	ASN
1	C	32	HIS
1	D	8	HIS
1	D	224	HIS
1	D	238	HIS
1	D	251	ASN
1	D	269	HIS
1	E	32	HIS
1	E	146	HIS
1	E	317	ASN
1	F	31	HIS

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Mol	Chain	Res	Type
1	F	91	ASN
1	F	148	ASN
1	F	153	ASN
1	F	224	HIS
1	F	249	GLN

### 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 6 ligands modelled in this entry, 6 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	332/332 (100%)	0.10	6 (1%) 67 63	12, 23, 46, 61	0
1	B	332/332 (100%)	-0.05	5 (1%) 72 68	9, 21, 40, 68	0
1	C	332/332 (100%)	0.04	7 (2%) 63 59	12, 23, 47, 88	0
1	D	332/332 (100%)	-0.06	3 (0%) 81 78	12, 22, 43, 63	0
1	E	332/332 (100%)	0.18	8 (2%) 59 55	14, 27, 51, 75	0
1	F	332/332 (100%)	0.42	20 (6%) 27 24	14, 32, 65, 96	0
All	All	1992/1992 (100%)	0.10	49 (2%) 58 54	9, 24, 51, 96	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	5.9
1	F	1	MET	5.8
1	C	1	MET	5.4
1	A	176	TRP	5.3
1	B	1	MET	5.2
1	A	32	HIS	4.7
1	A	1	MET	4.5
1	F	35	GLY	4.1
1	A	313	GLU	3.5
1	A	42	ASP	3.5
1	E	1	MET	3.4
1	B	33	SER	3.3
1	E	43	GLY	3.2
1	F	45	VAL	3.2
1	F	32	HIS	3.2
1	C	43	GLY	3.1
1	F	33	SER	3.1
1	E	299	LEU	2.9
1	C	299	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	177	ASP	2.7
1	E	317	ASN	2.7
1	E	332	ARG	2.6
1	F	43	GLY	2.6
1	F	54	TRP	2.5
1	F	34	LYS	2.5
1	C	32	HIS	2.5
1	F	40	LEU	2.5
1	F	332	ARG	2.4
1	B	332	ARG	2.4
1	E	34	LYS	2.4
1	F	42	ASP	2.4
1	E	32	HIS	2.3
1	F	249	GLN	2.3
1	B	34	LYS	2.2
1	F	133	VAL	2.2
1	C	45	VAL	2.2
1	B	32	HIS	2.2
1	C	42	ASP	2.1
1	F	46	PHE	2.1
1	F	25	GLY	2.1
1	F	19	LYS	2.1
1	F	298	GLU	2.1
1	E	46	PHE	2.1
1	F	176	TRP	2.1
1	F	44	LYS	2.0
1	C	313	GLU	2.0
1	D	42	ASP	2.0
1	F	299	LEU	2.0
1	A	149	GLU	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ZN	A	401	1/1	0.99	0.02	21,21,21,21	0
2	ZN	B	401	1/1	0.99	0.03	21,21,21,21	0
2	ZN	C	401	1/1	0.99	0.02	23,23,23,23	0
2	ZN	D	401	1/1	0.99	0.03	27,27,27,27	0
2	ZN	E	401	1/1	0.99	0.02	27,27,27,27	0
2	ZN	F	401	1/1	0.99	0.03	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.