



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:58 am GMT

PDB ID : 3CP8  
Title : Crystal structure of GidA from Chlorobium tepidum  
Authors : Meyer, S.; Scrima, A.; Versees, W.; Wittinghofer, A.  
Deposited on : 2008-03-31  
Resolution : 3.20 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

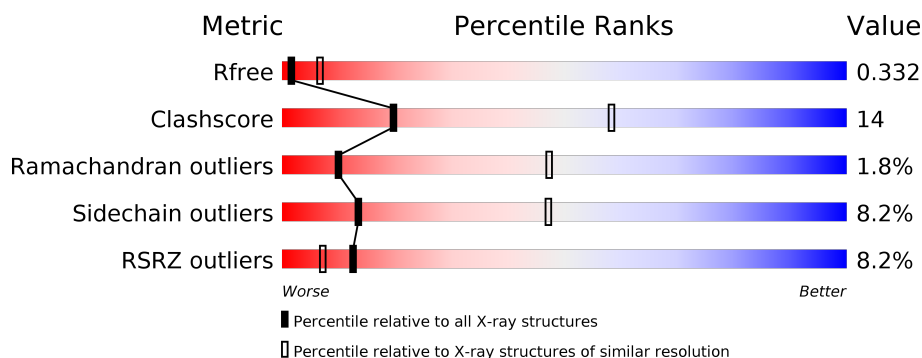
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	641	<div> <div>8%</div> <div> <div>67%</div> <div>25%</div> <div>5%</div> </div> </div>
1	B	641	<div> <div>7%</div> <div> <div>68%</div> <div>25%</div> <div>5%</div> </div> </div>
1	C	641	<div> <div>10%</div> <div> <div>67%</div> <div>25%</div> <div>5%</div> </div> </div>
1	D	641	<div> <div>6%</div> <div> <div>60%</div> <div>23%</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18567 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 tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	611	Total	C	N	O	S	0	0	0
			4704	2945	839	896	24			
1	B	611	Total	C	N	O	S	0	0	0
			4704	2945	839	896	24			
1	C	611	Total	C	N	O	S	0	0	0
			4704	2945	839	896	24			
1	D	552	Total	C	N	O	S	0	0	0
			4243	2658	752	810	23			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q8KA85
A	-18	GLY	-	EXPRESSION TAG	UNP Q8KA85
A	-17	SER	-	EXPRESSION TAG	UNP Q8KA85
A	-16	SER	-	EXPRESSION TAG	UNP Q8KA85
A	-15	HIS	-	EXPRESSION TAG	UNP Q8KA85
A	-14	HIS	-	EXPRESSION TAG	UNP Q8KA85
A	-13	HIS	-	EXPRESSION TAG	UNP Q8KA85
A	-12	HIS	-	EXPRESSION TAG	UNP Q8KA85
A	-11	HIS	-	EXPRESSION TAG	UNP Q8KA85
A	-10	HIS	-	EXPRESSION TAG	UNP Q8KA85
A	-9	SER	-	EXPRESSION TAG	UNP Q8KA85
A	-8	SER	-	EXPRESSION TAG	UNP Q8KA85
A	-7	GLY	-	EXPRESSION TAG	UNP Q8KA85
A	-6	LEU	-	EXPRESSION TAG	UNP Q8KA85
A	-5	VAL	-	EXPRESSION TAG	UNP Q8KA85
A	-4	PRO	-	EXPRESSION TAG	UNP Q8KA85
A	-3	ARG	-	EXPRESSION TAG	UNP Q8KA85
A	-2	GLY	-	EXPRESSION TAG	UNP Q8KA85
A	-1	SER	-	EXPRESSION TAG	UNP Q8KA85
A	0	HIS	-	EXPRESSION TAG	UNP Q8KA85

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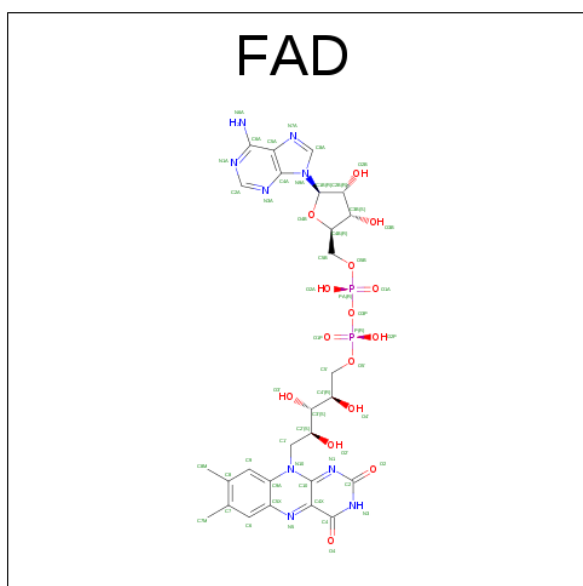
Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	EXPRESSION TAG	UNP Q8KA85
B	-18	GLY	-	EXPRESSION TAG	UNP Q8KA85
B	-17	SER	-	EXPRESSION TAG	UNP Q8KA85
B	-16	SER	-	EXPRESSION TAG	UNP Q8KA85
B	-15	HIS	-	EXPRESSION TAG	UNP Q8KA85
B	-14	HIS	-	EXPRESSION TAG	UNP Q8KA85
B	-13	HIS	-	EXPRESSION TAG	UNP Q8KA85
B	-12	HIS	-	EXPRESSION TAG	UNP Q8KA85
B	-11	HIS	-	EXPRESSION TAG	UNP Q8KA85
B	-10	HIS	-	EXPRESSION TAG	UNP Q8KA85
B	-9	SER	-	EXPRESSION TAG	UNP Q8KA85
B	-8	SER	-	EXPRESSION TAG	UNP Q8KA85
B	-7	GLY	-	EXPRESSION TAG	UNP Q8KA85
B	-6	LEU	-	EXPRESSION TAG	UNP Q8KA85
B	-5	VAL	-	EXPRESSION TAG	UNP Q8KA85
B	-4	PRO	-	EXPRESSION TAG	UNP Q8KA85
B	-3	ARG	-	EXPRESSION TAG	UNP Q8KA85
B	-2	GLY	-	EXPRESSION TAG	UNP Q8KA85
B	-1	SER	-	EXPRESSION TAG	UNP Q8KA85
B	0	HIS	-	EXPRESSION TAG	UNP Q8KA85
C	-19	MET	-	EXPRESSION TAG	UNP Q8KA85
C	-18	GLY	-	EXPRESSION TAG	UNP Q8KA85
C	-17	SER	-	EXPRESSION TAG	UNP Q8KA85
C	-16	SER	-	EXPRESSION TAG	UNP Q8KA85
C	-15	HIS	-	EXPRESSION TAG	UNP Q8KA85
C	-14	HIS	-	EXPRESSION TAG	UNP Q8KA85
C	-13	HIS	-	EXPRESSION TAG	UNP Q8KA85
C	-12	HIS	-	EXPRESSION TAG	UNP Q8KA85
C	-11	HIS	-	EXPRESSION TAG	UNP Q8KA85
C	-10	HIS	-	EXPRESSION TAG	UNP Q8KA85
C	-9	SER	-	EXPRESSION TAG	UNP Q8KA85
C	-8	SER	-	EXPRESSION TAG	UNP Q8KA85
C	-7	GLY	-	EXPRESSION TAG	UNP Q8KA85
C	-6	LEU	-	EXPRESSION TAG	UNP Q8KA85
C	-5	VAL	-	EXPRESSION TAG	UNP Q8KA85
C	-4	PRO	-	EXPRESSION TAG	UNP Q8KA85
C	-3	ARG	-	EXPRESSION TAG	UNP Q8KA85
C	-2	GLY	-	EXPRESSION TAG	UNP Q8KA85
C	-1	SER	-	EXPRESSION TAG	UNP Q8KA85
C	0	HIS	-	EXPRESSION TAG	UNP Q8KA85
D	-19	MET	-	EXPRESSION TAG	UNP Q8KA85
D	-18	GLY	-	EXPRESSION TAG	UNP Q8KA85

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-17	SER	-	EXPRESSION TAG	UNP Q8KA85
D	-16	SER	-	EXPRESSION TAG	UNP Q8KA85
D	-15	HIS	-	EXPRESSION TAG	UNP Q8KA85
D	-14	HIS	-	EXPRESSION TAG	UNP Q8KA85
D	-13	HIS	-	EXPRESSION TAG	UNP Q8KA85
D	-12	HIS	-	EXPRESSION TAG	UNP Q8KA85
D	-11	HIS	-	EXPRESSION TAG	UNP Q8KA85
D	-10	HIS	-	EXPRESSION TAG	UNP Q8KA85
D	-9	SER	-	EXPRESSION TAG	UNP Q8KA85
D	-8	SER	-	EXPRESSION TAG	UNP Q8KA85
D	-7	GLY	-	EXPRESSION TAG	UNP Q8KA85
D	-6	LEU	-	EXPRESSION TAG	UNP Q8KA85
D	-5	VAL	-	EXPRESSION TAG	UNP Q8KA85
D	-4	PRO	-	EXPRESSION TAG	UNP Q8KA85
D	-3	ARG	-	EXPRESSION TAG	UNP Q8KA85
D	-2	GLY	-	EXPRESSION TAG	UNP Q8KA85
D	-1	SER	-	EXPRESSION TAG	UNP Q8KA85
D	0	HIS	-	EXPRESSION TAG	UNP Q8KA85

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



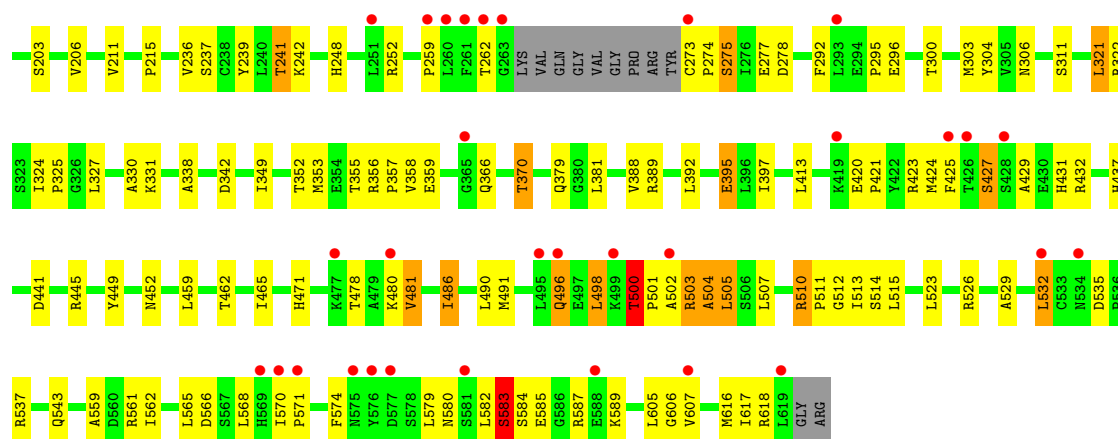
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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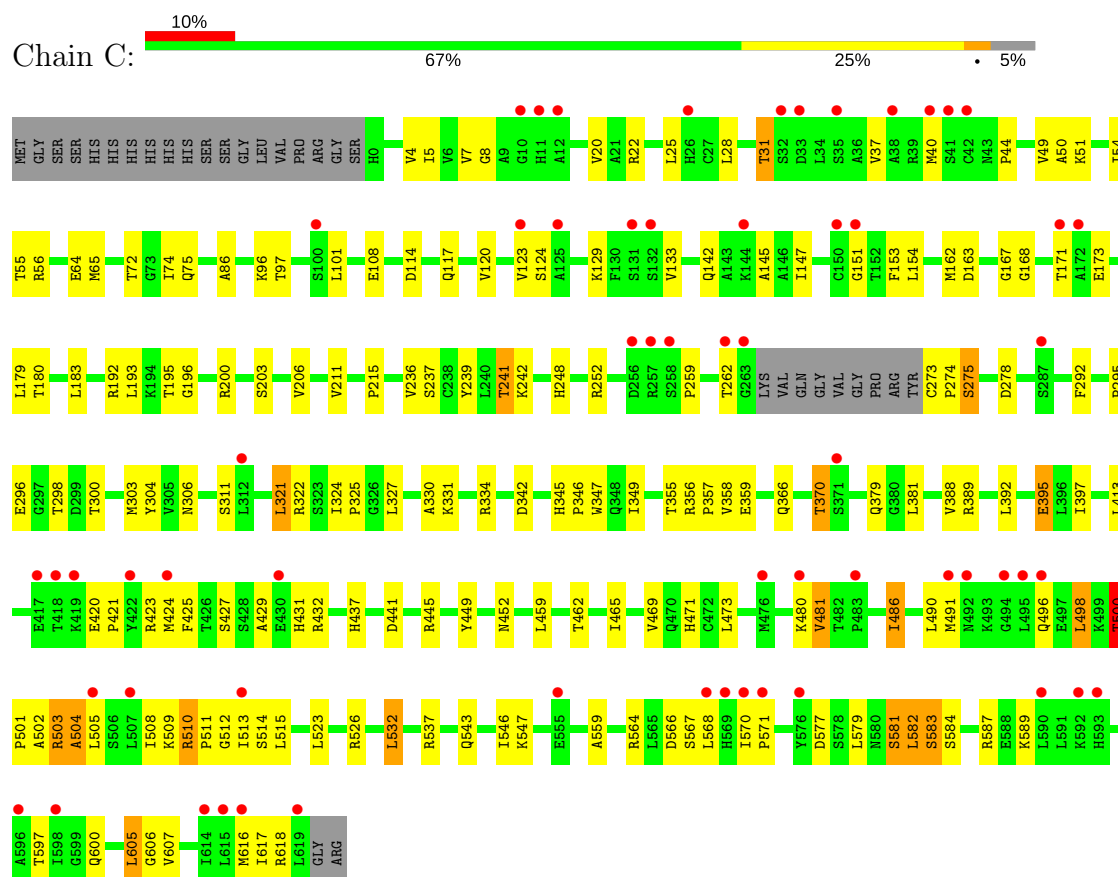
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

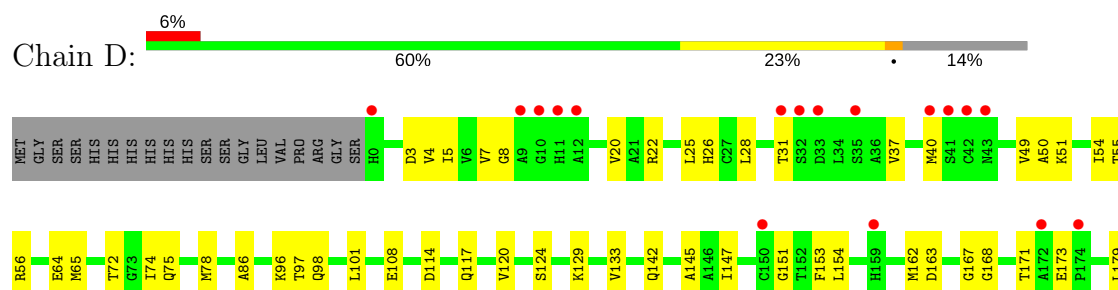




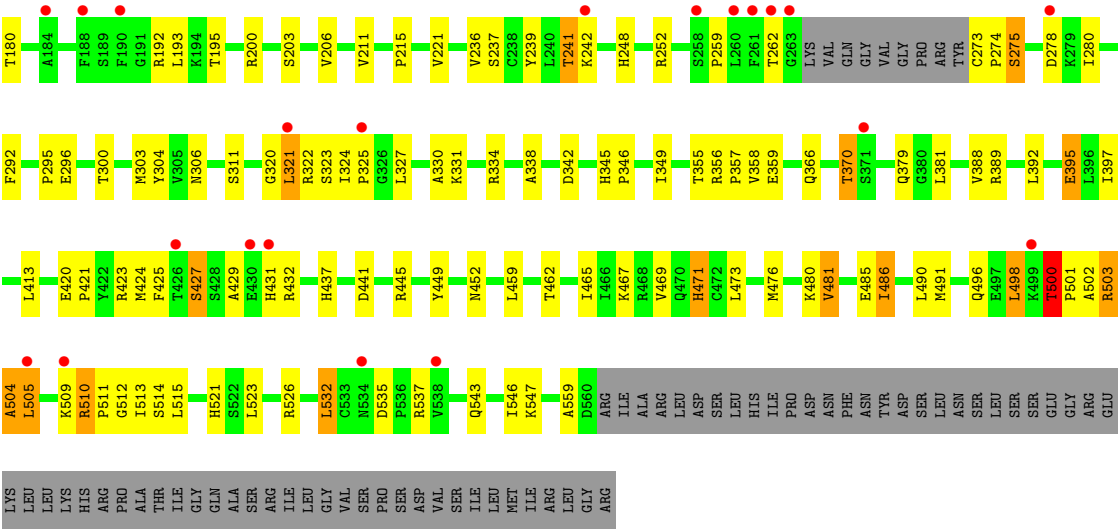
- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA



- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.50Å 71.84Å 171.93Å 90.00° 91.82° 90.00°	Depositor
Resolution (Å)	44.85 – 3.20 44.85 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.85-3.20) 99.3 (44.85-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.254 , 0.278 0.325 , 0.332	Depositor DCC
$R_{free}$ test set	2467 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	98.4	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	18567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD

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	0.45	0/4785	0.57	0/6468
1	B	0.43	0/4785	0.56	0/6468
1	C	0.40	0/4785	0.56	0/6468
1	D	0.40	0/4317	0.55	0/5836
All	All	0.42	0/18672	0.56	0/25240

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	A	0	1
1	B	0	2
1	C	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	582	LEU	Peptide
1	B	582	LEU	Peptide
1	B	583	SER	Peptide
1	C	582	LEU	Peptide
1	C	583	SER	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	4704	0	4748	143	0
1	B	4704	0	4748	139	0
1	C	4704	0	4748	133	0
1	D	4243	0	4269	129	0
2	A	53	0	31	10	0
2	B	53	0	31	12	0
2	C	53	0	31	13	0
2	D	53	0	31	9	0
All	All	18567	0	18637	530	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 14.

All (530) 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:B:500:THR:HB	1:B:501:PRO:CD	1.73	1.18
1:C:500:THR:HB	1:C:501:PRO:CD	1.73	1.18
1:A:500:THR:HB	1:A:501:PRO:CD	1.73	1.16
1:D:500:THR:HB	1:D:501:PRO:CD	1.70	1.16
1:C:370:THR:HG21	1:C:379:GLN:HE22	1.10	1.15
1:A:498:LEU:HD21	1:A:502:ALA:HB3	1.24	1.12
1:B:498:LEU:HD21	1:B:502:ALA:HB3	1.26	1.12
1:D:498:LEU:HD21	1:D:502:ALA:HB3	1.23	1.12
1:B:370:THR:HG21	1:B:379:GLN:HE22	1.15	1.11
1:A:195:THR:CB	2:A:622:FAD:HM83	1.80	1.10
1:A:500:THR:CB	1:A:501:PRO:HD3	1.83	1.09
1:C:498:LEU:HD21	1:C:502:ALA:HB3	1.34	1.09
1:D:498:LEU:HD21	1:D:502:ALA:CB	1.83	1.09
1:B:500:THR:CB	1:B:501:PRO:HD3	1.83	1.09
1:C:500:THR:CB	1:C:501:PRO:HD3	1.82	1.08
1:D:500:THR:CB	1:D:501:PRO:HD3	1.82	1.08
1:D:370:THR:HG21	1:D:379:GLN:HE22	1.12	1.08
1:C:195:THR:CB	2:C:622:FAD:HM83	1.84	1.07
1:A:195:THR:HB	2:A:622:FAD:C8M	1.83	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HD13	1:D:500:THR:CG2	1.85	1.07
1:C:583:SER:HB3	1:C:587:ARG:HB2	1.31	1.06
1:A:498:LEU:HD21	1:A:502:ALA:CB	1.86	1.06
1:D:195:THR:HB	2:D:622:FAD:HM83	1.08	1.06
1:B:498:LEU:HD21	1:B:502:ALA:CB	1.86	1.05
1:A:583:SER:HB3	1:A:587:ARG:HB2	1.37	1.05
1:A:370:THR:HG21	1:A:379:GLN:HE22	1.18	1.04
1:A:583:SER:CB	1:A:587:ARG:HB2	1.88	1.03
1:B:195:THR:HB	2:B:622:FAD:HM83	1.03	1.02
1:B:121:ILE:CD1	1:D:500:THR:CG2	2.38	1.02
1:B:195:THR:CB	2:B:622:FAD:HM83	1.91	0.99
1:C:501:PRO:O	1:C:503:ARG:HG3	1.61	0.98
1:C:195:THR:HB	2:C:622:FAD:HM83	0.99	0.98
1:B:121:ILE:CD1	1:D:500:THR:HG22	1.95	0.97
1:A:532:LEU:H	1:A:532:LEU:HD23	1.30	0.96
1:C:532:LEU:H	1:C:532:LEU:HD23	1.32	0.95
1:D:532:LEU:H	1:D:532:LEU:HD23	1.30	0.94
1:D:195:THR:CB	2:D:622:FAD:HM83	1.96	0.94
1:B:532:LEU:HD23	1:B:532:LEU:H	1.31	0.94
1:D:153:PHE:HE2	2:D:622:FAD:H3B	1.35	0.91
1:B:153:PHE:HE2	2:B:622:FAD:H3B	1.34	0.91
1:B:121:ILE:HD13	1:D:500:THR:HG21	1.52	0.91
1:A:153:PHE:HE2	2:A:622:FAD:H3B	1.36	0.90
1:C:195:THR:HB	2:C:622:FAD:C8M	1.96	0.90
1:C:500:THR:HB	1:C:501:PRO:HD3	0.91	0.89
1:B:121:ILE:HD13	1:D:500:THR:HG22	1.53	0.89
1:A:500:THR:HB	1:A:501:PRO:HD3	0.91	0.88
1:B:195:THR:HB	2:B:622:FAD:C8M	1.99	0.88
1:C:153:PHE:HE2	2:C:622:FAD:H3B	1.38	0.88
1:B:583:SER:HB2	1:B:584:SER:O	1.74	0.87
1:A:195:THR:HB	2:A:622:FAD:HM83	0.90	0.86
1:B:500:THR:HB	1:B:501:PRO:HD3	0.91	0.85
1:D:500:THR:HB	1:D:501:PRO:HD3	0.88	0.85
1:A:153:PHE:CE2	2:A:622:FAD:H3B	2.11	0.84
1:D:195:THR:HB	2:D:622:FAD:C8M	2.04	0.81
1:D:153:PHE:CE2	2:D:622:FAD:H3B	2.15	0.81
1:A:583:SER:HB2	1:A:587:ARG:CB	2.11	0.81
1:A:420:GLU:HG3	1:A:421:PRO:HD2	1.64	0.80
1:B:153:PHE:CE2	2:B:622:FAD:H3B	2.16	0.80
1:A:211:VAL:HG11	1:A:239:TYR:HB3	1.64	0.79
1:B:583:SER:HB3	1:B:587:ARG:HB2	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HD21	1:A:532:LEU:HD12	1.66	0.78
1:D:211:VAL:HG11	1:D:239:TYR:HB3	1.66	0.77
1:D:498:LEU:CD2	1:D:502:ALA:HB3	2.10	0.77
1:C:583:SER:HB3	1:C:587:ARG:CB	2.13	0.77
1:A:583:SER:CB	1:A:587:ARG:CB	2.62	0.77
1:B:121:ILE:HD12	1:D:500:THR:HG22	1.67	0.76
1:B:514:SER:HA	1:B:543:GLN:NE2	2.00	0.76
1:B:211:VAL:HG11	1:B:239:TYR:HB3	1.67	0.75
1:A:583:SER:HB2	1:A:587:ARG:HB2	1.66	0.75
1:B:583:SER:HB3	1:B:587:ARG:CB	2.17	0.75
1:C:420:GLU:HG3	1:C:421:PRO:HD2	1.69	0.75
1:C:153:PHE:CE2	2:C:622:FAD:H3B	2.22	0.75
1:A:480:LYS:HA	1:A:503:ARG:HB3	1.68	0.74
1:C:515:LEU:HD21	1:C:532:LEU:HD12	1.67	0.74
1:D:480:LYS:HA	1:D:503:ARG:HB3	1.69	0.74
1:B:515:LEU:HD21	1:B:532:LEU:HD12	1.69	0.74
1:A:5:ILE:HG22	1:A:28:LEU:HB3	1.70	0.74
1:C:5:ILE:HG22	1:C:28:LEU:HB3	1.69	0.74
1:B:420:GLU:HG3	1:B:421:PRO:HD2	1.70	0.73
1:A:481:VAL:HB	1:A:486:ILE:HD11	1.70	0.72
1:C:370:THR:HG21	1:C:379:GLN:NE2	1.96	0.72
1:C:211:VAL:HG11	1:C:239:TYR:HB3	1.71	0.72
1:D:515:LEU:HD21	1:D:532:LEU:HD12	1.70	0.72
1:A:498:LEU:CD2	1:A:502:ALA:HB3	2.12	0.72
1:D:420:GLU:HG3	1:D:421:PRO:HD2	1.70	0.72
1:D:481:VAL:HB	1:D:486:ILE:HD11	1.72	0.71
1:A:56:ARG:HH11	1:A:437:HIS:CD2	2.09	0.71
1:B:5:ILE:HG22	1:B:28:LEU:HB3	1.72	0.70
1:B:481:VAL:HB	1:B:486:ILE:HD11	1.72	0.70
1:A:476:MET:O	1:A:505:LEU:HB2	1.91	0.70
1:C:481:VAL:HB	1:C:486:ILE:HD11	1.73	0.70
1:B:56:ARG:HH11	1:B:437:HIS:CD2	2.10	0.69
1:A:211:VAL:CG1	1:A:239:TYR:HB3	2.23	0.69
1:C:153:PHE:HD1	1:C:168:GLY:HA3	1.57	0.69
1:B:211:VAL:CG1	1:B:239:TYR:HB3	2.22	0.69
1:B:322:ARG:NH1	1:B:330:ALA:O	2.26	0.69
1:D:211:VAL:CG1	1:D:239:TYR:HB3	2.23	0.69
1:C:583:SER:HB2	1:C:584:SER:O	1.92	0.69
1:A:153:PHE:CD1	1:A:168:GLY:HA3	2.28	0.68
1:C:56:ARG:HH11	1:C:437:HIS:CD2	2.11	0.68
1:B:535:ASP:OD1	1:B:537:ARG:HB2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ILE:HG22	1:D:28:LEU:HB3	1.74	0.68
1:D:322:ARG:NH1	1:D:330:ALA:O	2.27	0.68
1:A:441:ASP:O	1:A:445:ARG:HB2	1.93	0.68
1:D:86:ALA:HB1	1:D:432:ARG:HB3	1.75	0.68
1:C:153:PHE:CD1	1:C:168:GLY:HA3	2.29	0.67
1:C:86:ALA:HB1	1:C:432:ARG:HB3	1.75	0.67
1:B:153:PHE:HD1	1:B:168:GLY:HA3	1.60	0.67
1:B:153:PHE:CD1	1:B:168:GLY:HA3	2.29	0.66
1:B:273:CYS:N	1:B:423:ARG:HH12	1.93	0.66
1:D:153:PHE:CD1	1:D:168:GLY:HA3	2.30	0.66
1:D:56:ARG:HH11	1:D:437:HIS:CD2	2.13	0.66
1:B:498:LEU:CD2	1:B:502:ALA:HB3	2.13	0.66
1:C:273:CYS:N	1:C:423:ARG:HH12	1.94	0.66
1:C:441:ASP:O	1:C:445:ARG:HB2	1.95	0.66
1:C:514:SER:HA	1:C:543:GLN:NE2	2.11	0.66
1:A:322:ARG:NH1	1:A:330:ALA:O	2.29	0.66
1:B:441:ASP:O	1:B:445:ARG:HB2	1.95	0.66
1:B:86:ALA:HB1	1:B:432:ARG:HB3	1.77	0.65
1:B:480:LYS:HA	1:B:503:ARG:HB3	1.76	0.65
1:A:86:ALA:HB1	1:A:432:ARG:HB3	1.78	0.65
1:C:322:ARG:NH1	1:C:330:ALA:O	2.30	0.65
1:A:72:THR:HG22	1:A:72:THR:O	1.94	0.65
1:B:616:MET:C	1:B:618:ARG:H	1.99	0.65
1:A:4:VAL:HA	1:A:145:ALA:O	1.96	0.65
1:B:72:THR:HG22	1:B:72:THR:O	1.96	0.65
1:D:153:PHE:HD1	1:D:168:GLY:HA3	1.63	0.65
1:C:211:VAL:CG1	1:C:239:TYR:HB3	2.26	0.64
1:C:349:ILE:HG22	1:C:355:THR:HG22	1.80	0.64
1:C:4:VAL:HA	1:C:145:ALA:O	1.97	0.64
1:C:616:MET:C	1:C:618:ARG:H	2.00	0.64
1:D:206:VAL:HG21	1:D:303:MET:HE1	1.78	0.64
1:B:424:MET:O	1:B:427:SER:HB3	1.98	0.64
1:A:153:PHE:HD1	1:A:168:GLY:HA3	1.60	0.64
1:A:480:LYS:CA	1:A:503:ARG:HB3	2.28	0.64
1:B:589:LYS:HG3	1:B:606:GLY:HA3	1.80	0.64
1:C:481:VAL:H	1:C:503:ARG:HB3	1.62	0.64
1:D:273:CYS:N	1:D:423:ARG:HH12	1.96	0.64
1:D:349:ILE:HG22	1:D:355:THR:HG22	1.80	0.64
1:D:370:THR:HG21	1:D:379:GLN:NE2	1.98	0.64
1:D:441:ASP:O	1:D:445:ARG:HB2	1.96	0.64
1:B:56:ARG:HH11	1:B:437:HIS:HD2	1.44	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ILE:HG22	1:A:355:THR:HG22	1.80	0.63
1:A:589:LYS:HG3	1:A:606:GLY:HA3	1.81	0.63
1:D:4:VAL:HA	1:D:145:ALA:O	1.98	0.63
1:A:616:MET:C	1:A:618:ARG:H	2.01	0.63
1:B:206:VAL:HG21	1:B:303:MET:HE1	1.79	0.63
1:B:431:HIS:HE1	1:B:559:ALA:HA	1.64	0.63
1:D:498:LEU:HD21	1:D:502:ALA:HB2	1.77	0.63
1:D:480:LYS:CA	1:D:503:ARG:HB3	2.28	0.62
1:A:431:HIS:HE1	1:A:559:ALA:HA	1.63	0.62
1:B:4:VAL:HA	1:B:145:ALA:O	1.98	0.62
1:D:431:HIS:HE1	1:D:559:ALA:HA	1.64	0.62
1:A:56:ARG:HH11	1:A:437:HIS:HD2	1.46	0.62
1:A:498:LEU:HD21	1:A:502:ALA:HB2	1.81	0.62
1:C:431:HIS:HE1	1:C:559:ALA:HA	1.65	0.62
1:A:480:LYS:HA	1:A:503:ARG:CB	2.30	0.61
1:C:72:THR:O	1:C:72:THR:HG22	2.00	0.61
1:D:424:MET:O	1:D:427:SER:HB3	2.00	0.61
1:A:532:LEU:H	1:A:532:LEU:CD2	2.09	0.61
1:C:498:LEU:HD21	1:C:502:ALA:CB	2.22	0.61
1:C:589:LYS:HG3	1:C:606:GLY:HA3	1.82	0.61
1:B:50:ALA:HB3	1:B:424:MET:HB3	1.83	0.61
1:A:241:THR:HG21	1:A:325:PRO:O	2.01	0.61
1:D:72:THR:HG22	1:D:72:THR:O	2.00	0.61
1:B:22:ARG:HH12	1:B:64:GLU:HG2	1.65	0.61
1:A:206:VAL:HG21	1:A:303:MET:HE1	1.84	0.60
1:A:583:SER:HB2	1:A:587:ARG:HB3	1.84	0.60
1:B:370:THR:HG21	1:B:379:GLN:NE2	2.01	0.60
1:D:480:LYS:HA	1:D:503:ARG:CB	2.31	0.60
1:B:349:ILE:HG22	1:B:355:THR:HG22	1.82	0.60
1:B:275:SER:HB3	1:B:278:ASP:H	1.66	0.59
1:C:503:ARG:O	1:C:504:ALA:C	2.38	0.59
1:C:22:ARG:HH12	1:C:64:GLU:HG2	1.67	0.59
1:D:500:THR:CB	1:D:501:PRO:CD	2.55	0.59
1:D:490:LEU:HD21	1:D:513:ILE:HD11	1.85	0.59
1:D:50:ALA:HB3	1:D:424:MET:HB3	1.85	0.59
1:A:273:CYS:N	1:A:423:ARG:HH12	1.99	0.59
1:C:56:ARG:HH11	1:C:437:HIS:HD2	1.49	0.59
1:C:490:LEU:HD21	1:C:513:ILE:HD11	1.84	0.59
1:D:275:SER:HB3	1:D:278:ASP:H	1.67	0.59
1:D:193:LEU:HD22	1:D:421:PRO:HD3	1.84	0.59
1:A:501:PRO:O	1:A:503:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ALA:CB	1:D:424:MET:HB3	2.33	0.58
1:C:50:ALA:CB	1:C:424:MET:HB3	2.33	0.58
1:B:501:PRO:O	1:B:503:ARG:HG3	2.02	0.58
1:D:501:PRO:O	1:D:503:ARG:HG3	2.02	0.58
1:A:503:ARG:O	1:A:504:ALA:C	2.41	0.58
1:B:503:ARG:O	1:B:504:ALA:C	2.41	0.58
1:A:275:SER:HB3	1:A:278:ASP:H	1.68	0.58
1:B:167:GLY:HA2	1:B:173:GLU:O	2.03	0.58
1:B:241:THR:HG21	1:B:325:PRO:O	2.04	0.58
1:B:50:ALA:CB	1:B:424:MET:HB3	2.34	0.58
1:C:50:ALA:HB3	1:C:424:MET:HB3	1.85	0.58
1:D:389:ARG:HD2	1:D:395:GLU:O	2.04	0.58
1:D:503:ARG:O	1:D:504:ALA:C	2.42	0.58
1:A:50:ALA:CB	1:A:424:MET:HB3	2.34	0.58
1:B:193:LEU:HD22	1:B:421:PRO:HD3	1.86	0.58
1:D:509:LYS:HG3	1:D:546:ILE:HD11	1.86	0.58
1:A:75:GLN:HG3	1:A:75:GLN:O	2.04	0.57
1:A:490:LEU:HD21	1:A:513:ILE:HD11	1.87	0.57
1:B:500:THR:CB	1:B:501:PRO:CD	2.56	0.57
1:B:459:LEU:O	1:B:462:THR:HG22	2.03	0.57
1:B:480:LYS:CA	1:B:503:ARG:HB3	2.34	0.57
1:C:167:GLY:HA2	1:C:173:GLU:O	2.03	0.57
1:D:241:THR:HG21	1:D:325:PRO:O	2.05	0.57
1:A:22:ARG:HH12	1:A:64:GLU:HG2	1.68	0.57
1:A:459:LEU:O	1:A:462:THR:HG22	2.04	0.57
1:C:275:SER:HB3	1:C:278:ASP:H	1.68	0.57
1:C:583:SER:CB	1:C:587:ARG:HB2	2.21	0.57
1:A:151:GLY:HA2	1:A:366:GLN:HB3	1.87	0.56
1:D:459:LEU:O	1:D:462:THR:HG22	2.05	0.56
1:A:50:ALA:HB3	1:A:424:MET:HB3	1.86	0.56
1:B:498:LEU:HD21	1:B:502:ALA:HB2	1.79	0.56
1:C:193:LEU:HD22	1:C:421:PRO:HD3	1.87	0.56
1:C:459:LEU:O	1:C:462:THR:HG22	2.05	0.56
1:A:167:GLY:HA2	1:A:173:GLU:O	2.05	0.56
1:B:75:GLN:O	1:B:75:GLN:HG3	2.04	0.56
1:B:151:GLY:HA2	1:B:366:GLN:HB3	1.86	0.56
1:B:532:LEU:CD2	1:B:532:LEU:H	2.09	0.56
1:C:259:PRO:HD2	1:C:311:SER:HB3	1.88	0.56
1:A:424:MET:O	1:A:427:SER:HB3	2.05	0.56
1:C:241:THR:HG21	1:C:325:PRO:O	2.05	0.56
1:D:22:ARG:HH12	1:D:64:GLU:HG2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:MET:O	1:C:427:SER:HB3	2.05	0.56
1:A:206:VAL:HG21	1:A:303:MET:CE	2.36	0.56
1:D:56:ARG:HH11	1:D:437:HIS:HD2	1.52	0.56
1:C:206:VAL:HG21	1:C:303:MET:HE1	1.88	0.56
1:C:51:LYS:HA	1:C:54:ILE:HG22	1.88	0.56
1:C:51:LYS:HA	1:C:54:ILE:CG2	2.36	0.55
1:C:8:GLY:HA2	2:C:622:FAD:H1B	1.88	0.55
1:B:490:LEU:HD21	1:B:513:ILE:HD11	1.87	0.55
1:C:151:GLY:HA2	1:C:366:GLN:HB3	1.89	0.55
1:C:500:THR:CB	1:C:501:PRO:CD	2.56	0.55
1:A:193:LEU:HD22	1:A:421:PRO:HD3	1.88	0.55
1:B:449:TYR:CG	1:B:459:LEU:HD22	2.42	0.55
1:D:167:GLY:HA2	1:D:173:GLU:O	2.07	0.55
1:C:75:GLN:O	1:C:75:GLN:HG3	2.06	0.55
1:C:196:GLY:H	2:C:622:FAD:HM71	1.72	0.55
1:D:151:GLY:HA2	1:D:366:GLN:HB3	1.87	0.55
1:C:120:VAL:HG13	1:C:133:VAL:HG13	1.89	0.55
1:D:449:TYR:CG	1:D:459:LEU:HD22	2.42	0.54
1:D:75:GLN:HG3	1:D:75:GLN:O	2.06	0.54
1:A:370:THR:HG21	1:A:379:GLN:NE2	2.03	0.54
1:C:96:LYS:HE2	1:C:296:GLU:CD	2.27	0.54
1:C:449:TYR:CG	1:C:459:LEU:HD22	2.43	0.54
1:C:389:ARG:HD2	1:C:395:GLU:O	2.07	0.54
1:C:564:ARG:O	1:C:567:SER:HB3	2.07	0.54
1:C:501:PRO:O	1:C:503:ARG:CG	2.47	0.54
1:B:121:ILE:CD1	1:D:500:THR:HG21	2.24	0.54
1:D:206:VAL:HG21	1:D:303:MET:CE	2.36	0.54
1:C:236:VAL:HG11	1:C:295:PRO:HG2	1.88	0.54
1:A:389:ARG:HD2	1:A:395:GLU:O	2.08	0.53
1:A:449:TYR:CG	1:A:459:LEU:HD22	2.43	0.53
1:D:532:LEU:H	1:D:532:LEU:CD2	2.09	0.53
1:A:445:ARG:HB3	1:A:462:THR:HG21	1.91	0.53
1:C:445:ARG:HB3	1:C:462:THR:HG21	1.90	0.53
1:B:480:LYS:HA	1:B:503:ARG:CB	2.38	0.53
1:A:568:LEU:HD12	1:A:598:ILE:CD1	2.38	0.53
1:B:25:LEU:HD13	1:B:388:VAL:HG13	1.91	0.53
1:B:236:VAL:HG11	1:B:295:PRO:HG2	1.90	0.53
1:B:51:LYS:HA	1:B:54:ILE:HG22	1.91	0.53
2:C:622:FAD:H9	2:C:622:FAD:O2'	2.09	0.52
1:D:40:MET:HB2	1:D:96:LYS:HD2	1.91	0.52
1:C:206:VAL:HG21	1:C:303:MET:CE	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:LEU:HD13	1:D:388:VAL:HG13	1.91	0.52
1:D:51:LYS:HA	1:D:54:ILE:HG22	1.92	0.52
1:B:206:VAL:HG21	1:B:303:MET:CE	2.39	0.52
1:D:514:SER:HA	1:D:543:GLN:NE2	2.24	0.52
1:D:51:LYS:HA	1:D:54:ILE:CG2	2.40	0.52
1:A:120:VAL:HG13	1:A:133:VAL:HG13	1.92	0.52
1:B:445:ARG:HB3	1:B:462:THR:HG21	1.90	0.52
1:B:259:PRO:HD2	1:B:311:SER:HB3	1.91	0.52
1:C:8:GLY:HA2	2:C:622:FAD:C1B	2.40	0.52
1:D:120:VAL:HG13	1:D:133:VAL:HG13	1.92	0.51
1:A:215:PRO:HA	1:A:237:SER:HB3	1.92	0.51
1:A:322:ARG:HA	1:A:327:LEU:O	2.10	0.51
1:C:577:ASP:HA	1:C:587:ARG:HD3	1.91	0.51
1:D:445:ARG:HB3	1:D:462:THR:HG21	1.91	0.51
1:A:500:THR:CB	1:A:501:PRO:CD	2.57	0.51
1:C:514:SER:HA	1:C:543:GLN:HE21	1.74	0.51
1:D:389:ARG:CZ	1:D:397:ILE:HD11	2.40	0.51
1:A:583:SER:O	1:A:584:SER:OG	2.27	0.51
1:C:192:ARG:NH1	1:C:342:ASP:OD1	2.43	0.51
1:D:259:PRO:HD2	1:D:311:SER:HB3	1.93	0.51
1:D:476:MET:O	1:D:505:LEU:HB2	2.10	0.51
1:A:51:LYS:HA	1:A:54:ILE:HG22	1.93	0.51
1:B:389:ARG:CZ	1:B:397:ILE:HD11	2.41	0.51
1:B:431:HIS:NE2	1:B:562:ILE:HD12	2.26	0.51
1:C:509:LYS:HZ2	1:C:546:ILE:HD13	1.76	0.51
1:D:200:ARG:NH1	1:D:304:TYR:CD2	2.79	0.51
1:A:236:VAL:HG11	1:A:295:PRO:HG2	1.92	0.51
1:A:509:LYS:HG3	1:A:546:ILE:HD11	1.92	0.51
1:A:96:LYS:HE2	1:A:296:GLU:CD	2.31	0.51
1:C:331:LYS:HD3	1:D:114:ASP:OD2	2.11	0.51
1:A:389:ARG:CZ	1:A:397:ILE:HD11	2.41	0.51
1:A:570:ILE:N	1:A:571:PRO:CD	2.74	0.51
1:C:420:GLU:CG	1:C:421:PRO:HD2	2.41	0.50
1:B:74:ILE:HG23	1:B:236:VAL:HG23	1.93	0.50
1:C:347:TRP:HB3	1:C:605:LEU:HD13	1.93	0.50
1:B:120:VAL:HG12	1:B:179:LEU:HD13	1.93	0.50
1:B:215:PRO:HA	1:B:237:SER:HB3	1.94	0.50
1:C:503:ARG:O	1:C:505:LEU:N	2.45	0.50
1:D:510:ARG:H	1:D:511:PRO:CD	2.25	0.50
1:A:420:GLU:CG	1:A:421:PRO:HD2	2.38	0.50
1:B:51:LYS:HA	1:B:54:ILE:CG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:PRO:HA	1:C:237:SER:HB3	1.94	0.50
1:C:481:VAL:HG23	1:C:503:ARG:HA	1.93	0.50
1:A:569:HIS:C	1:A:571:PRO:HD2	2.31	0.50
1:C:389:ARG:CZ	1:C:397:ILE:HD11	2.42	0.50
1:A:25:LEU:HD13	1:A:388:VAL:HG13	1.93	0.50
1:A:51:LYS:HA	1:A:54:ILE:CG2	2.41	0.50
1:A:583:SER:C	1:A:584:SER:OG	2.50	0.50
1:C:25:LEU:HD13	1:C:388:VAL:HG13	1.93	0.49
1:C:40:MET:HB2	1:C:96:LYS:HD2	1.93	0.49
1:C:334:ARG:HG2	1:D:117:GLN:HB3	1.93	0.49
1:D:532:LEU:O	1:D:535:ASP:O	2.30	0.49
1:D:236:VAL:HG11	1:D:295:PRO:HG2	1.93	0.49
1:D:420:GLU:CG	1:D:421:PRO:HD2	2.42	0.49
1:B:196:GLY:O	2:B:622:FAD:HM82	2.12	0.49
1:A:200:ARG:NH1	1:A:304:TYR:CD2	2.81	0.49
1:A:321:LEU:HA	1:A:324:ILE:HD12	1.94	0.49
1:A:568:LEU:HD12	1:A:598:ILE:HD11	1.95	0.49
1:B:120:VAL:HG13	1:B:133:VAL:HG13	1.94	0.49
1:B:389:ARG:HD2	1:B:395:GLU:O	2.13	0.49
1:C:322:ARG:HA	1:C:327:LEU:O	2.11	0.49
1:C:583:SER:CB	1:C:587:ARG:CB	2.88	0.49
2:D:622:FAD:O2'	2:D:622:FAD:H9	2.12	0.48
1:A:120:VAL:HG12	1:A:179:LEU:HD13	1.94	0.48
1:A:509:LYS:HZ2	1:A:546:ILE:HD13	1.77	0.48
1:A:509:LYS:NZ	1:A:546:ILE:HD13	2.28	0.48
1:C:465:ILE:HD11	1:C:537:ARG:HB3	1.96	0.48
1:D:120:VAL:HG12	1:D:179:LEU:HD13	1.95	0.48
1:A:153:PHE:CE2	2:A:622:FAD:H51A	2.47	0.48
1:A:108:GLU:OE1	1:B:300:THR:HA	2.12	0.48
2:A:622:FAD:H9	2:A:622:FAD:O2'	2.13	0.48
1:A:465:ILE:HD11	1:A:537:ARG:HB3	1.95	0.48
1:C:509:LYS:NZ	1:C:546:ILE:HD13	2.28	0.48
1:B:153:PHE:CE2	2:B:622:FAD:C3B	2.94	0.48
1:C:300:THR:HA	1:D:108:GLU:OE1	2.14	0.48
1:D:322:ARG:HA	1:D:327:LEU:O	2.14	0.48
1:A:509:LYS:HG3	1:A:546:ILE:CD1	2.44	0.48
1:D:321:LEU:HA	1:D:324:ILE:HD12	1.96	0.48
1:A:510:ARG:H	1:A:511:PRO:CD	2.26	0.48
1:C:321:LEU:HA	1:C:324:ILE:HD12	1.96	0.48
1:B:4:VAL:HB	1:B:20:VAL:HG11	1.96	0.48
1:B:55:THR:HG23	1:B:65:MET:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:PRO:HA	1:D:237:SER:HB3	1.95	0.47
1:D:345:HIS:HA	1:D:346:PRO:HD3	1.77	0.47
1:A:153:PHE:HE2	2:A:622:FAD:H51A	1.79	0.47
1:C:200:ARG:NH1	1:C:304:TYR:CD2	2.83	0.47
1:D:96:LYS:HE2	1:D:296:GLU:CD	2.34	0.47
1:A:192:ARG:NH1	1:A:342:ASP:OD1	2.47	0.47
1:B:420:GLU:CG	1:B:421:PRO:HD2	2.43	0.47
1:C:120:VAL:HG12	1:C:179:LEU:HD13	1.97	0.47
1:C:195:THR:CB	2:C:622:FAD:C8M	2.74	0.47
1:D:509:LYS:NZ	1:D:546:ILE:HD13	2.29	0.47
2:B:622:FAD:H9	2:B:622:FAD:O2'	2.14	0.47
1:C:445:ARG:CB	1:C:462:THR:HG21	2.44	0.47
1:C:108:GLU:OE1	1:D:300:THR:HA	2.14	0.47
1:D:509:LYS:HG3	1:D:546:ILE:CD1	2.44	0.47
1:B:200:ARG:NH1	1:B:304:TYR:CD2	2.82	0.47
1:B:311:SER:OG	1:B:338:ALA:HB2	2.15	0.47
1:C:74:ILE:HG23	1:C:236:VAL:HG23	1.95	0.47
1:C:532:LEU:H	1:C:532:LEU:CD2	2.10	0.47
1:D:465:ILE:HD11	1:D:537:ARG:HB3	1.97	0.47
1:B:321:LEU:HA	1:B:324:ILE:HD12	1.96	0.46
1:B:40:MET:HB2	1:B:96:LYS:HD2	1.97	0.46
1:C:616:MET:C	1:C:618:ARG:N	2.69	0.46
1:D:4:VAL:HB	1:D:20:VAL:HG11	1.96	0.46
1:A:570:ILE:N	1:A:571:PRO:HD2	2.30	0.46
1:C:480:LYS:HA	1:C:503:ARG:HB2	1.95	0.46
1:A:72:THR:CG2	1:A:72:THR:O	2.63	0.46
1:B:241:THR:HG22	1:B:242:LYS:H	1.80	0.46
1:B:96:LYS:HE2	1:B:296:GLU:CD	2.35	0.46
1:A:259:PRO:HD2	1:A:311:SER:HB3	1.98	0.46
1:B:514:SER:HA	1:B:543:GLN:HE21	1.79	0.46
1:B:153:PHE:HD2	2:B:622:FAD:H8A	1.79	0.46
1:C:345:HIS:HA	1:C:346:PRO:HD3	1.77	0.46
1:D:292:PHE:HB2	1:D:306:ASN:HB3	1.98	0.46
1:C:4:VAL:HB	1:C:20:VAL:HG11	1.97	0.46
1:A:331:LYS:HD3	1:B:114:ASP:OD2	2.15	0.46
1:B:570:ILE:N	1:B:571:PRO:CD	2.79	0.46
1:C:462:THR:HA	1:C:465:ILE:HG22	1.98	0.46
1:C:510:ARG:H	1:C:511:PRO:CD	2.29	0.45
1:A:4:VAL:HB	1:A:20:VAL:HG11	1.97	0.45
1:B:535:ASP:C	1:B:537:ARG:N	2.69	0.45
1:C:566:ASP:O	1:C:597:THR:OG1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:THR:O	1:A:465:ILE:HG22	2.16	0.45
1:C:292:PHE:HB2	1:C:306:ASN:HB3	1.98	0.45
1:A:292:PHE:HB2	1:A:306:ASN:HB3	1.98	0.45
1:B:56:ARG:NH1	1:B:437:HIS:HD2	2.11	0.45
1:B:584:SER:HB3	1:B:585:GLU:H	1.55	0.45
1:B:292:PHE:HB2	1:B:306:ASN:HB3	1.98	0.45
1:D:462:THR:HA	1:D:465:ILE:HG22	1.99	0.45
1:A:56:ARG:NH1	1:A:437:HIS:HD2	2.14	0.45
1:B:561:ARG:HH11	1:B:561:ARG:HG3	1.81	0.45
1:B:72:THR:O	1:B:72:THR:CG2	2.64	0.45
1:C:481:VAL:H	1:C:503:ARG:CB	2.29	0.45
1:D:50:ALA:O	1:D:54:ILE:HG22	2.17	0.45
1:B:192:ARG:NH1	1:B:342:ASP:OD1	2.50	0.45
1:D:445:ARG:CB	1:D:462:THR:HG21	2.47	0.45
1:D:476:MET:SD	1:D:505:LEU:HD12	2.57	0.45
1:A:74:ILE:CG2	1:A:236:VAL:HB	2.47	0.45
1:A:50:ALA:O	1:A:54:ILE:HG22	2.17	0.45
1:A:153:PHE:CE2	2:A:622:FAD:C3B	2.93	0.44
1:A:479:ALA:HB3	1:A:505:LEU:HG	1.98	0.44
1:C:56:ARG:NH1	1:C:437:HIS:HD2	2.15	0.44
1:A:586:GLY:O	1:A:589:LYS:N	2.50	0.44
1:A:114:ASP:OD2	1:B:331:LYS:HD3	2.17	0.44
1:D:74:ILE:HG23	1:D:236:VAL:HG23	1.99	0.44
1:A:616:MET:C	1:A:618:ARG:N	2.70	0.44
1:D:192:ARG:NH1	1:D:342:ASP:OD1	2.50	0.44
1:A:248:HIS:O	1:A:252:ARG:HG3	2.18	0.44
1:A:195:THR:CB	2:A:622:FAD:C8M	2.64	0.44
1:A:478:THR:O	1:A:479:ALA:C	2.54	0.44
1:A:532:LEU:O	1:A:535:ASP:O	2.36	0.44
1:C:129:LYS:HG3	1:C:359:GLU:HB3	1.99	0.44
1:D:241:THR:HG22	1:D:242:LYS:H	1.83	0.44
1:C:117:GLN:HB3	1:D:334:ARG:HG2	1.99	0.44
1:B:510:ARG:H	1:B:511:PRO:CD	2.30	0.44
1:B:570:ILE:N	1:B:571:PRO:HD2	2.33	0.44
1:A:498:LEU:HD23	1:A:498:LEU:HA	1.82	0.44
1:D:129:LYS:HG3	1:D:359:GLU:HB3	1.99	0.44
1:B:248:HIS:O	1:B:252:ARG:HG3	2.18	0.44
1:B:322:ARG:HA	1:B:327:LEU:O	2.18	0.44
1:C:248:HIS:O	1:C:252:ARG:HG3	2.18	0.44
1:B:462:THR:HA	1:B:465:ILE:HG22	2.00	0.43
1:D:55:THR:HG23	1:D:65:MET:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:THR:HG22	1:A:242:LYS:H	1.83	0.43
1:B:565:LEU:HA	1:B:568:LEU:HD12	2.00	0.43
1:B:129:LYS:HG3	1:B:359:GLU:HB3	2.00	0.43
1:C:241:THR:HG22	1:C:242:LYS:H	1.83	0.43
1:C:55:THR:HG23	1:C:65:MET:HG2	1.99	0.43
1:A:445:ARG:CB	1:A:462:THR:HG21	2.49	0.43
1:B:616:MET:C	1:B:618:ARG:N	2.68	0.43
1:B:153:PHE:CE2	2:B:622:FAD:H51A	2.53	0.43
1:B:75:GLN:HB3	1:B:236:VAL:O	2.18	0.43
1:C:513:ILE:O	1:C:547:LYS:HE3	2.19	0.43
1:C:74:ILE:CG2	1:C:236:VAL:HB	2.48	0.43
1:A:597:THR:HG23	1:A:600:GLN:H	1.83	0.43
1:C:581:SER:OG	1:C:581:SER:O	2.36	0.43
1:D:485:GLU:HG2	1:D:521:HIS:O	2.18	0.43
1:B:462:THR:O	1:B:465:ILE:HG22	2.19	0.43
1:B:503:ARG:O	1:B:505:LEU:N	2.51	0.43
1:B:121:ILE:HD12	1:D:500:THR:CG2	2.27	0.43
1:C:196:GLY:O	2:C:622:FAD:HM82	2.18	0.43
1:A:356:ARG:HB2	1:A:357:PRO:HD3	2.00	0.43
1:A:462:THR:HA	1:A:465:ILE:HG22	2.00	0.43
1:A:476:MET:SD	1:A:505:LEU:HD12	2.59	0.43
1:D:509:LYS:HZ2	1:D:546:ILE:HD13	1.84	0.43
1:D:3:ASP:OD2	1:D:26:HIS:N	2.52	0.43
1:A:40:MET:HB2	1:A:96:LYS:HD2	2.00	0.42
1:A:481:VAL:H	1:A:503:ARG:HB3	1.84	0.42
1:C:50:ALA:O	1:C:54:ILE:HG22	2.19	0.42
1:B:273:CYS:N	1:B:423:ARG:NH1	2.65	0.42
1:B:445:ARG:CB	1:B:462:THR:HG21	2.48	0.42
1:B:465:ILE:HD11	1:B:537:ARG:HB3	2.01	0.42
1:C:273:CYS:N	1:C:423:ARG:NH1	2.65	0.42
1:C:75:GLN:HB3	1:C:236:VAL:O	2.19	0.42
1:D:469:VAL:O	1:D:473:LEU:HG	2.19	0.42
1:C:40:MET:CE	1:C:44:PRO:HA	2.48	0.42
1:C:462:THR:O	1:C:465:ILE:HG22	2.19	0.42
1:D:56:ARG:NH1	1:D:437:HIS:HD2	2.15	0.42
1:B:504:ALA:O	1:B:505:LEU:C	2.58	0.42
1:D:153:PHE:CE2	2:D:622:FAD:C3B	2.95	0.42
1:A:485:GLU:HG2	1:A:521:HIS:O	2.19	0.42
1:A:568:LEU:HB2	1:A:598:ILE:HG12	2.02	0.42
1:C:153:PHE:HE2	2:C:622:FAD:C3B	2.21	0.42
1:A:579:LEU:HD13	1:A:582:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLN:HB3	1:A:236:VAL:O	2.20	0.42
1:B:352:THR:O	1:B:353:MET:HB2	2.19	0.42
1:A:110:GLU:HA	1:A:111:PRO:HD3	1.89	0.42
1:C:236:VAL:CG1	1:C:295:PRO:HG2	2.50	0.42
1:C:509:LYS:HG3	1:C:546:ILE:HD11	2.02	0.42
1:C:597:THR:HG23	1:C:600:GLN:H	1.85	0.42
1:D:75:GLN:HB3	1:D:236:VAL:O	2.19	0.42
1:D:78:MET:HE2	1:D:221:VAL:HG21	2.02	0.42
1:B:110:GLU:HA	1:B:111:PRO:HD3	1.91	0.41
1:C:72:THR:O	1:C:72:THR:CG2	2.67	0.41
1:D:248:HIS:O	1:D:252:ARG:HG3	2.20	0.41
1:D:480:LYS:CB	1:D:503:ARG:HB3	2.50	0.41
1:A:311:SER:OG	1:A:338:ALA:HB2	2.19	0.41
1:A:503:ARG:O	1:A:505:LEU:N	2.53	0.41
1:D:498:LEU:HD11	1:D:502:ALA:HB3	2.02	0.41
1:D:72:THR:HG23	1:D:98:GLN:HB3	2.02	0.41
1:A:56:ARG:NH1	1:A:437:HIS:CD2	2.85	0.41
1:B:356:ARG:HB2	1:B:357:PRO:HD3	2.00	0.41
1:A:55:THR:HG23	1:A:65:MET:HG2	2.03	0.41
1:D:248:HIS:CD2	1:D:280:ILE:HG12	2.55	0.41
1:D:510:ARG:HA	1:D:547:LYS:HG2	2.03	0.41
1:A:345:HIS:HA	1:A:346:PRO:HD3	1.79	0.41
1:A:469:VAL:O	1:A:473:LEU:HG	2.21	0.41
1:A:563:ALA:O	1:A:567:SER:HB2	2.21	0.41
1:D:510:ARG:H	1:D:511:PRO:HD3	1.84	0.41
1:A:96:LYS:HE2	1:A:296:GLU:OE1	2.20	0.41
1:A:480:LYS:CB	1:A:503:ARG:HB3	2.51	0.41
1:B:480:LYS:CB	1:B:503:ARG:HB3	2.51	0.41
1:B:583:SER:HB3	1:B:587:ARG:HB3	1.99	0.41
1:C:469:VAL:O	1:C:473:LEU:HG	2.20	0.41
1:C:96:LYS:HE2	1:C:296:GLU:OE1	2.19	0.41
1:B:236:VAL:CG1	1:B:295:PRO:HG2	2.51	0.41
1:B:504:ALA:O	1:B:507:LEU:N	2.49	0.41
1:B:529:ALA:HB1	1:B:532:LEU:CD2	2.51	0.41
1:D:467:LYS:O	1:D:471:HIS:HB2	2.20	0.41
1:B:496:GLN:HB2	1:B:496:GLN:HE21	1.63	0.41
1:C:570:ILE:N	1:C:571:PRO:HD2	2.36	0.41
1:C:114:ASP:OD2	1:D:331:LYS:HD3	2.21	0.41
1:A:546:ILE:HG13	1:A:547:LYS:N	2.35	0.41
1:B:498:LEU:HD23	1:B:498:LEU:HA	1.83	0.41
1:B:8:GLY:HA2	2:B:622:FAD:H1B	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:HB2	1:C:357:PRO:HD3	2.03	0.41
1:D:311:SER:OG	1:D:338:ALA:HB2	2.21	0.41
1:D:481:VAL:H	1:D:503:ARG:HB3	1.85	0.41
1:A:445:ARG:HG3	1:A:454:VAL:HG11	2.04	0.40
1:B:40:MET:CE	1:B:44:PRO:HA	2.51	0.40
1:B:498:LEU:HD11	1:B:502:ALA:HB3	2.02	0.40
1:C:31:THR:HA	2:C:622:FAD:N3A	2.36	0.40
1:D:8:GLY:HA2	2:D:622:FAD:H1B	2.03	0.40
1:B:153:PHE:HE2	2:B:622:FAD:H51A	1.85	0.40
1:D:320:GLY:O	1:D:323:SER:OG	2.31	0.40
1:D:356:ARG:HB2	1:D:357:PRO:HD3	2.03	0.40
1:A:504:ALA:O	1:A:507:LEU:N	2.50	0.40
1:A:510:ARG:H	1:A:511:PRO:HD3	1.85	0.40
1:A:558:VAL:HG12	1:A:562:ILE:HD13	2.03	0.40
1:B:535:ASP:C	1:B:537:ARG:H	2.24	0.40
1:D:498:LEU:HA	1:D:498:LEU:HD23	1.84	0.40
1:D:153:PHE:CE2	2:D:622:FAD:H51A	2.56	0.40
1:A:334:ARG:HG2	1:B:117:GLN:HB3	2.03	0.40
1:C:123:VAL:HG12	1:C:183:LEU:CD1	2.52	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	607/641 (95%)	545 (90%)	50 (8%)	12 (2%)	9	44
1	B	607/641 (95%)	552 (91%)	43 (7%)	12 (2%)	9	44
1	C	607/641 (95%)	553 (91%)	44 (7%)	10 (2%)	11	50
1	D	548/641 (86%)	505 (92%)	34 (6%)	9 (2%)	11	50
All	All	2369/2564 (92%)	2155 (91%)	171 (7%)	43 (2%)	10	47

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	THR
1	B	500	THR
1	C	500	THR
1	C	504	ALA
1	D	500	THR
1	A	585	GLU
1	A	586	GLY
1	A	617	ILE
1	B	617	ILE
1	C	617	ILE
1	A	49	VAL
1	A	274	PRO
1	A	429	ALA
1	A	505	LEU
1	A	510	ARG
1	B	274	PRO
1	B	429	ALA
1	B	505	LEU
1	B	510	ARG
1	C	429	ALA
1	C	510	ARG
1	C	568	LEU
1	D	274	PRO
1	D	429	ALA
1	D	505	LEU
1	D	510	ARG
1	A	427	SER
1	A	504	ALA
1	B	49	VAL
1	B	504	ALA
1	C	274	PRO
1	D	427	SER
1	B	580	ASN
1	D	49	VAL
1	D	504	ALA
1	A	512	GLY
1	B	427	SER
1	B	512	GLY
1	B	583	SER
1	C	49	VAL
1	C	512	GLY
1	D	512	GLY

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Mol	Chain	Res	Type
1	C	508	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 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	515/539 (96%)	472 (92%)	43 (8%)	13	46
1	B	515/539 (96%)	473 (92%)	42 (8%)	13	47
1	C	515/539 (96%)	472 (92%)	43 (8%)	13	46
1	D	462/539 (86%)	425 (92%)	37 (8%)	14	49
All	All	2007/2156 (93%)	1842 (92%)	165 (8%)	13	47

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	31	THR
1	A	37	VAL
1	A	97	THR
1	A	124	SER
1	A	142	GLN
1	A	147	ILE
1	A	154	LEU
1	A	162	MET
1	A	163	ASP
1	A	171	THR
1	A	180	THR
1	A	203	SER
1	A	241	THR
1	A	262	THR
1	A	275	SER
1	A	298	THR
1	A	321	LEU
1	A	358	VAL
1	A	370	THR

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Mol	Chain	Res	Type
1	A	381	LEU
1	A	392	LEU
1	A	395	GLU
1	A	413	LEU
1	A	425	PHE
1	A	452	ASN
1	A	471	HIS
1	A	481	VAL
1	A	486	ILE
1	A	491	MET
1	A	496	GLN
1	A	498	LEU
1	A	500	THR
1	A	503	ARG
1	A	523	LEU
1	A	526	ARG
1	A	532	LEU
1	A	561	ARG
1	A	567	SER
1	A	569	HIS
1	A	584	SER
1	A	605	LEU
1	A	607	VAL
1	B	7	VAL
1	B	37	VAL
1	B	97	THR
1	B	124	SER
1	B	142	GLN
1	B	147	ILE
1	B	154	LEU
1	B	162	MET
1	B	163	ASP
1	B	171	THR
1	B	180	THR
1	B	203	SER
1	B	241	THR
1	B	262	THR
1	B	275	SER
1	B	277	GLU
1	B	321	LEU
1	B	358	VAL
1	B	370	THR

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Mol	Chain	Res	Type
1	B	381	LEU
1	B	392	LEU
1	B	395	GLU
1	B	413	LEU
1	B	425	PHE
1	B	452	ASN
1	B	471	HIS
1	B	478	THR
1	B	481	VAL
1	B	486	ILE
1	B	491	MET
1	B	496	GLN
1	B	498	LEU
1	B	500	THR
1	B	503	ARG
1	B	523	LEU
1	B	526	ARG
1	B	532	LEU
1	B	566	ASP
1	B	574	PHE
1	B	579	LEU
1	B	605	LEU
1	B	607	VAL
1	C	7	VAL
1	C	31	THR
1	C	37	VAL
1	C	97	THR
1	C	101	LEU
1	C	124	SER
1	C	142	GLN
1	C	147	ILE
1	C	154	LEU
1	C	162	MET
1	C	163	ASP
1	C	171	THR
1	C	180	THR
1	C	203	SER
1	C	241	THR
1	C	262	THR
1	C	275	SER
1	C	298	THR
1	C	321	LEU

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Mol	Chain	Res	Type
1	C	358	VAL
1	C	370	THR
1	C	381	LEU
1	C	392	LEU
1	C	395	GLU
1	C	413	LEU
1	C	425	PHE
1	C	452	ASN
1	C	471	HIS
1	C	481	VAL
1	C	486	ILE
1	C	491	MET
1	C	496	GLN
1	C	498	LEU
1	C	500	THR
1	C	503	ARG
1	C	523	LEU
1	C	526	ARG
1	C	532	LEU
1	C	579	LEU
1	C	581	SER
1	C	582	LEU
1	C	605	LEU
1	C	607	VAL
1	D	7	VAL
1	D	31	THR
1	D	37	VAL
1	D	97	THR
1	D	101	LEU
1	D	124	SER
1	D	142	GLN
1	D	147	ILE
1	D	154	LEU
1	D	162	MET
1	D	163	ASP
1	D	171	THR
1	D	180	THR
1	D	203	SER
1	D	241	THR
1	D	262	THR
1	D	275	SER
1	D	321	LEU

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Mol	Chain	Res	Type
1	D	358	VAL
1	D	370	THR
1	D	381	LEU
1	D	392	LEU
1	D	395	GLU
1	D	413	LEU
1	D	425	PHE
1	D	452	ASN
1	D	471	HIS
1	D	481	VAL
1	D	486	ILE
1	D	491	MET
1	D	496	GLN
1	D	498	LEU
1	D	500	THR
1	D	503	ARG
1	D	523	LEU
1	D	526	ARG
1	D	532	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	A	142	GLN
1	A	431	HIS
1	A	437	HIS
1	B	26	HIS
1	B	142	GLN
1	B	437	HIS
1	B	543	GLN
1	C	11	HIS
1	C	26	HIS
1	C	142	GLN
1	C	431	HIS
1	C	437	HIS
1	C	543	GLN
1	D	11	HIS
1	D	26	HIS
1	D	142	GLN
1	D	431	HIS
1	D	437	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	A	622	-	51,58,58	1.42	7 (13%)	54,89,89	2.11	11 (20%)
2	FAD	B	622	-	51,58,58	1.45	7 (13%)	54,89,89	2.16	11 (20%)
2	FAD	C	622	-	51,58,58	1.46	7 (13%)	54,89,89	2.09	12 (22%)
2	FAD	D	622	-	51,58,58	1.48	7 (13%)	54,89,89	2.06	11 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	622	-	-	0/28/50/50	0/6/6/6
2	FAD	B	622	-	-	0/28/50/50	0/6/6/6
2	FAD	C	622	-	-	0/28/50/50	0/6/6/6
2	FAD	D	622	-	-	0/28/50/50	0/6/6/6



All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	622	FAD	C5'-C4'	2.04	1.54	1.51
2	D	622	FAD	C5'-C4'	2.31	1.55	1.51
2	B	622	FAD	C5'-C4'	2.46	1.55	1.51
2	C	622	FAD	C5'-C4'	2.51	1.55	1.51
2	D	622	FAD	C4-N3	2.82	1.38	1.33
2	B	622	FAD	C2A-N1A	2.82	1.39	1.33
2	A	622	FAD	C4-N3	2.83	1.38	1.33
2	C	622	FAD	C2A-N1A	2.84	1.39	1.33
2	C	622	FAD	C4-N3	2.85	1.38	1.33
2	A	622	FAD	C2A-N1A	2.86	1.39	1.33
2	B	622	FAD	C4-N3	2.92	1.38	1.33
2	D	622	FAD	C2A-N1A	3.05	1.39	1.33
2	A	622	FAD	C4X-N5	3.14	1.37	1.33
2	C	622	FAD	C4X-N5	3.21	1.38	1.33
2	D	622	FAD	C4X-N5	3.23	1.38	1.33
2	B	622	FAD	C4X-N5	3.28	1.38	1.33
2	B	622	FAD	C1'-N10	3.82	1.52	1.48
2	D	622	FAD	C1'-N10	3.87	1.52	1.48
2	A	622	FAD	C1'-N10	3.91	1.52	1.48
2	C	622	FAD	C1'-N10	4.04	1.52	1.48
2	A	622	FAD	C10-N1	4.14	1.39	1.33
2	C	622	FAD	C10-N1	4.21	1.39	1.33
2	A	622	FAD	C2A-N3A	4.22	1.39	1.32
2	B	622	FAD	C10-N1	4.24	1.39	1.33
2	D	622	FAD	C10-N1	4.27	1.39	1.33
2	B	622	FAD	C2A-N3A	4.31	1.39	1.32
2	C	622	FAD	C2A-N3A	4.44	1.39	1.32
2	D	622	FAD	C2A-N3A	4.69	1.40	1.32

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	622	FAD	N3A-C2A-N1A	-9.68	120.43	128.86
2	A	622	FAD	N3A-C2A-N1A	-9.27	120.78	128.86
2	D	622	FAD	N3A-C2A-N1A	-9.10	120.94	128.86
2	C	622	FAD	N3A-C2A-N1A	-8.79	121.20	128.86
2	A	622	FAD	C1'-N10-C9A	-4.02	114.66	118.35
2	D	622	FAD	C1'-N10-C9A	-3.91	114.76	118.35
2	C	622	FAD	C1'-N10-C9A	-3.89	114.78	118.35
2	B	622	FAD	C1'-N10-C9A	-3.78	114.88	118.35
2	B	622	FAD	C4X-C4-N3	-2.61	119.77	123.48
2	D	622	FAD	O5B-C5B-C4B	-2.59	99.81	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	622	FAD	C4X-C4-N3	-2.56	119.84	123.48
2	C	622	FAD	C4X-C4-N3	-2.55	119.86	123.48
2	D	622	FAD	C1'-N10-C10	-2.51	115.92	118.50
2	B	622	FAD	C1'-N10-C10	-2.51	115.93	118.50
2	D	622	FAD	C4X-C4-N3	-2.46	119.99	123.48
2	C	622	FAD	O5B-C5B-C4B	-2.39	100.53	109.00
2	C	622	FAD	C8M-C8-C9	-2.31	114.56	120.34
2	C	622	FAD	C1'-N10-C10	-2.26	116.18	118.50
2	A	622	FAD	C1'-N10-C10	-2.21	116.23	118.50
2	B	622	FAD	C8M-C8-C9	-2.20	114.83	120.34
2	A	622	FAD	C8M-C8-C9	-2.14	114.97	120.34
2	D	622	FAD	C8M-C8-C9	-2.05	115.20	120.34
2	A	622	FAD	O5B-C5B-C4B	-2.04	101.78	109.00
2	D	622	FAD	O4B-C4B-C3B	2.01	109.15	105.17
2	C	622	FAD	C4B-O4B-C1B	2.02	111.92	109.77
2	A	622	FAD	C4'-C3'-C2'	2.03	117.78	113.41
2	C	622	FAD	C6-C5X-C9A	2.05	121.66	119.00
2	D	622	FAD	C6-C5X-C9A	2.05	121.67	119.00
2	B	622	FAD	C4'-C3'-C2'	2.11	117.96	113.41
2	C	622	FAD	C4'-C3'-C2'	2.14	118.02	113.41
2	B	622	FAD	C4B-O4B-C1B	2.14	112.05	109.77
2	A	622	FAD	C6-C5X-C9A	2.15	121.79	119.00
2	B	622	FAD	C6-C5X-C9A	2.20	121.85	119.00
2	C	622	FAD	C4X-N5-C5X	2.25	119.14	116.76
2	A	622	FAD	C4X-N5-C5X	2.29	119.18	116.76
2	B	622	FAD	C4X-N5-C5X	2.37	119.27	116.76
2	D	622	FAD	C4X-N5-C5X	2.52	119.42	116.76
2	D	622	FAD	C4-N3-C2	5.15	119.66	115.16
2	A	622	FAD	C4-N3-C2	5.20	119.70	115.16
2	C	622	FAD	C4-N3-C2	5.26	119.76	115.16
2	B	622	FAD	C4-N3-C2	5.27	119.77	115.16
2	D	622	FAD	C5X-C9A-N10	6.24	122.29	117.66
2	C	622	FAD	C5X-C9A-N10	6.45	122.44	117.66
2	B	622	FAD	C5X-C9A-N10	6.51	122.49	117.66
2	A	622	FAD	C5X-C9A-N10	6.57	122.53	117.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	622	FAD	10	0
2	B	622	FAD	12	0
2	C	622	FAD	13	0
2	D	622	FAD	9	0

## 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	611/641 (95%)	0.71	53 (8%) 11 6	123, 126, 129, 133	0
1	B	611/641 (95%)	0.59	44 (7%) 16 10	123, 126, 129, 134	0
1	C	611/641 (95%)	0.70	61 (9%) 8 5	117, 126, 129, 133	0
1	D	552/641 (86%)	0.62	38 (6%) 18 10	123, 126, 129, 134	0
All	All	2385/2564 (93%)	0.66	196 (8%) 12 7	117, 126, 129, 134	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	GLY	7.3
1	A	581	SER	6.1
1	B	570	ILE	5.4
1	D	426	THR	4.8
1	D	263	GLY	4.8
1	A	580	ASN	4.6
1	D	262	THR	4.6
1	C	619	LEU	4.5
1	A	617	ILE	4.4
1	A	570	ILE	4.4
1	B	571	PRO	4.3
1	D	431	HIS	4.2
1	D	10	GLY	4.2
1	C	41	SER	4.1
1	C	26	HIS	4.0
1	B	496	GLN	4.0
1	C	507	LEU	3.8
1	A	431	HIS	3.8
1	D	0	HIS	3.7
1	D	261	PHE	3.7
1	B	262	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	172	ALA	3.5
1	A	41	SER	3.5
1	A	571	PRO	3.5
1	C	570	ILE	3.5
1	A	578	SER	3.4
1	C	576	TYR	3.4
1	C	131	SER	3.4
1	D	42	CYS	3.4
1	B	35	SER	3.3
1	C	593	HIS	3.3
1	C	569	HIS	3.3
1	C	123	VAL	3.3
1	A	40	MET	3.3
1	A	10	GLY	3.3
1	A	583	SER	3.3
1	C	11	HIS	3.3
1	D	190	PHE	3.2
1	B	499	LYS	3.2
1	B	261	PHE	3.2
1	D	538	VAL	3.2
1	A	579	LEU	3.2
1	D	430	GLU	3.2
1	D	11	HIS	3.2
1	C	418	THR	3.2
1	A	618	ARG	3.2
1	C	476	MET	3.1
1	A	11	HIS	3.1
1	C	33	ASP	3.1
1	A	582	LEU	3.1
1	A	573	ASN	3.1
1	C	263	GLY	3.1
1	C	262	THR	3.1
1	A	39	ARG	3.1
1	D	159	HIS	3.0
1	A	150	CYS	3.0
1	D	43	ASN	3.0
1	A	598	ILE	3.0
1	C	505	LEU	3.0
1	B	577	ASP	3.0
1	B	588	GLU	3.0
1	A	42	CYS	3.0
1	A	584	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	426	THR	2.9
1	C	144	LYS	2.9
1	D	33	ASP	2.8
1	C	590	LEU	2.8
1	B	575	ASN	2.8
1	B	581	SER	2.8
1	D	32	SER	2.8
1	D	258	SER	2.8
1	D	499	LYS	2.8
1	B	40	MET	2.8
1	C	483	PRO	2.8
1	A	151	GLY	2.8
1	A	588	GLU	2.7
1	C	513	ILE	2.7
1	C	256	ASP	2.7
1	A	43	ASN	2.7
1	C	417	GLU	2.7
1	A	577	ASP	2.7
1	D	184	ALA	2.7
1	A	397	ILE	2.7
1	D	41	SER	2.6
1	C	42	CYS	2.6
1	C	492	ASN	2.6
1	C	10	GLY	2.6
1	B	569	HIS	2.6
1	B	532	LEU	2.6
1	C	568	LEU	2.6
1	B	251	LEU	2.6
1	A	606	GLY	2.6
1	A	38	ALA	2.6
1	C	494	GLY	2.6
1	C	422	TYR	2.6
1	D	150	CYS	2.6
1	B	11	HIS	2.6
1	A	35	SER	2.5
1	D	40	MET	2.5
1	D	509	LYS	2.5
1	B	502	ALA	2.5
1	C	258	SER	2.5
1	C	495	LEU	2.5
1	A	587	ARG	2.5
1	C	257	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	424	MET	2.5
1	C	571	PRO	2.5
1	A	505	LEU	2.5
1	C	596	ALA	2.5
1	B	41	SER	2.5
1	B	428	SER	2.5
1	C	312	LEU	2.4
1	A	149	ALA	2.4
1	B	10	GLY	2.4
1	D	174	PRO	2.4
1	C	12	ALA	2.4
1	A	576	TYR	2.4
1	B	419	LYS	2.4
1	B	477	LYS	2.4
1	C	614	ILE	2.4
1	B	495	LEU	2.4
1	C	419	LYS	2.4
1	D	371	SER	2.4
1	C	38	ALA	2.4
1	D	172	ALA	2.4
1	A	572	ASP	2.4
1	B	39	ARG	2.4
1	D	260	LEU	2.4
1	B	425	PHE	2.4
1	D	242	LYS	2.3
1	C	496	GLN	2.3
1	D	325	PRO	2.3
1	C	480	LYS	2.3
1	A	596	ALA	2.3
1	C	150	CYS	2.3
1	C	35	SER	2.3
1	C	616	MET	2.3
1	A	146	ALA	2.3
1	D	35	SER	2.3
1	B	50	ALA	2.3
1	A	513	ILE	2.3
1	A	589	LYS	2.3
1	D	534	ASN	2.2
1	A	125	ALA	2.2
1	C	491	MET	2.2
1	B	534	ASN	2.2
1	A	595	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	150	CYS	2.2
1	B	607	VAL	2.2
1	B	260	LEU	2.2
1	B	619	LEU	2.2
1	C	32	SER	2.2
1	C	615	LEU	2.2
1	A	392	LEU	2.2
1	A	371	SER	2.2
1	C	40	MET	2.2
1	B	0	HIS	2.2
1	C	287	SER	2.1
1	B	293	LEU	2.1
1	B	273	CYS	2.1
1	A	172	ALA	2.1
1	B	38	ALA	2.1
1	B	480	LYS	2.1
1	C	592	LYS	2.1
1	A	374	GLU	2.1
1	A	575	ASN	2.1
1	C	151	GLY	2.1
1	B	32	SER	2.1
1	A	45	ALA	2.1
1	A	502	ALA	2.1
1	D	9	ALA	2.1
1	D	12	ALA	2.1
1	A	379	GLN	2.1
1	D	188	PHE	2.1
1	C	430	GLU	2.1
1	A	47	GLY	2.1
1	D	505	LEU	2.1
1	D	31	THR	2.1
1	A	33	ASP	2.1
1	B	365	GLY	2.1
1	B	42	CYS	2.1
1	B	43	ASN	2.1
1	C	125	ALA	2.1
1	C	598	ILE	2.1
1	D	278	ASP	2.1
1	C	132	SER	2.0
1	A	14	CYS	2.0
1	B	259	PRO	2.0
1	C	171	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	555	GLU	2.0
1	B	576	TYR	2.0
1	D	321	LEU	2.0
1	C	100	SER	2.0
1	C	371	SER	2.0
1	A	9	ALA	2.0
1	A	585	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FAD	D	622	53/53	0.89	0.35	-0.31	81,87,251,251	0
2	FAD	C	622	53/53	0.91	0.33	-0.31	81,86,251,251	0
2	FAD	B	622	53/53	0.90	0.32	-0.49	81,86,251,251	0
2	FAD	A	622	53/53	0.92	0.32	-0.96	82,86,251,251	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.