



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:51 AM GMT

PDB ID : 3CES
Title : Crystal Structure of E.coli MnmG (GidA), a Highly-Conserved tRNA Modifying Enzyme
Authors : Shi, R.; Matte, A.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2008-02-29
Resolution : 2.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

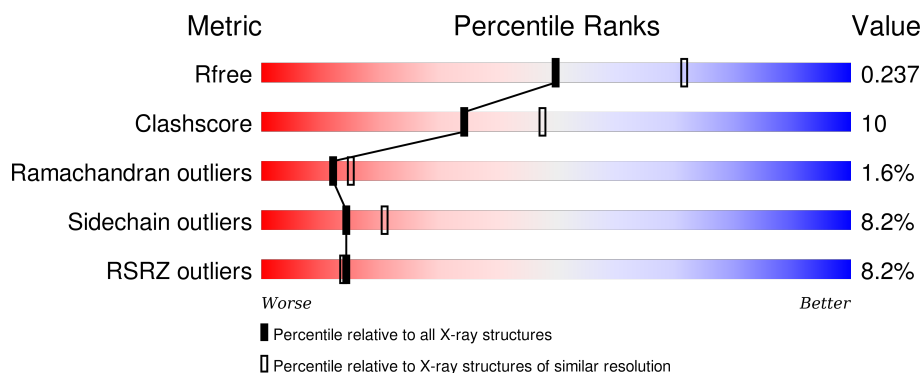
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	651	<div> <div>62%</div> <div>15%</div> <div>•</div> <div>18%</div> </div>
1	B	651	<div>7%</div> <div>62%</div> <div>15%</div> <div>•</div> <div>20%</div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15980 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	531	Total	C	N	O	S	0	1	0
			4098	2562	739	778	19			
1	B	519	Total	C	N	O	S	0	1	0
			3895	2447	696	735	17			
1	C	516	Total	C	N	O	S	0	0	0
			3884	2433	699	734	18			
1	D	507	Total	C	N	O	S	0	1	0
			3771	2370	678	705	18			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP P0A6U3
A	-20	GLY	-	EXPRESSION TAG	UNP P0A6U3
A	-19	SER	-	EXPRESSION TAG	UNP P0A6U3
A	-18	SER	-	EXPRESSION TAG	UNP P0A6U3
A	-17	HIS	-	EXPRESSION TAG	UNP P0A6U3
A	-16	HIS	-	EXPRESSION TAG	UNP P0A6U3
A	-15	HIS	-	EXPRESSION TAG	UNP P0A6U3
A	-14	HIS	-	EXPRESSION TAG	UNP P0A6U3
A	-13	HIS	-	EXPRESSION TAG	UNP P0A6U3
A	-12	HIS	-	EXPRESSION TAG	UNP P0A6U3
A	-11	HIS	-	EXPRESSION TAG	UNP P0A6U3
A	-10	HIS	-	EXPRESSION TAG	UNP P0A6U3
A	-9	SER	-	EXPRESSION TAG	UNP P0A6U3
A	-8	SER	-	EXPRESSION TAG	UNP P0A6U3
A	-7	GLY	-	EXPRESSION TAG	UNP P0A6U3
A	-6	LEU	-	EXPRESSION TAG	UNP P0A6U3
A	-5	VAL	-	EXPRESSION TAG	UNP P0A6U3
A	-4	PRO	-	EXPRESSION TAG	UNP P0A6U3
A	-3	ARG	-	EXPRESSION TAG	UNP P0A6U3
A	-2	GLY	-	EXPRESSION TAG	UNP P0A6U3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP P0A6U3
A	0	HIS	-	EXPRESSION TAG	UNP P0A6U3
B	-21	MET	-	EXPRESSION TAG	UNP P0A6U3
B	-20	GLY	-	EXPRESSION TAG	UNP P0A6U3
B	-19	SER	-	EXPRESSION TAG	UNP P0A6U3
B	-18	SER	-	EXPRESSION TAG	UNP P0A6U3
B	-17	HIS	-	EXPRESSION TAG	UNP P0A6U3
B	-16	HIS	-	EXPRESSION TAG	UNP P0A6U3
B	-15	HIS	-	EXPRESSION TAG	UNP P0A6U3
B	-14	HIS	-	EXPRESSION TAG	UNP P0A6U3
B	-13	HIS	-	EXPRESSION TAG	UNP P0A6U3
B	-12	HIS	-	EXPRESSION TAG	UNP P0A6U3
B	-11	HIS	-	EXPRESSION TAG	UNP P0A6U3
B	-10	HIS	-	EXPRESSION TAG	UNP P0A6U3
B	-9	SER	-	EXPRESSION TAG	UNP P0A6U3
B	-8	SER	-	EXPRESSION TAG	UNP P0A6U3
B	-7	GLY	-	EXPRESSION TAG	UNP P0A6U3
B	-6	LEU	-	EXPRESSION TAG	UNP P0A6U3
B	-5	VAL	-	EXPRESSION TAG	UNP P0A6U3
B	-4	PRO	-	EXPRESSION TAG	UNP P0A6U3
B	-3	ARG	-	EXPRESSION TAG	UNP P0A6U3
B	-2	GLY	-	EXPRESSION TAG	UNP P0A6U3
B	-1	SER	-	EXPRESSION TAG	UNP P0A6U3
B	0	HIS	-	EXPRESSION TAG	UNP P0A6U3
C	-21	MET	-	EXPRESSION TAG	UNP P0A6U3
C	-20	GLY	-	EXPRESSION TAG	UNP P0A6U3
C	-19	SER	-	EXPRESSION TAG	UNP P0A6U3
C	-18	SER	-	EXPRESSION TAG	UNP P0A6U3
C	-17	HIS	-	EXPRESSION TAG	UNP P0A6U3
C	-16	HIS	-	EXPRESSION TAG	UNP P0A6U3
C	-15	HIS	-	EXPRESSION TAG	UNP P0A6U3
C	-14	HIS	-	EXPRESSION TAG	UNP P0A6U3
C	-13	HIS	-	EXPRESSION TAG	UNP P0A6U3
C	-12	HIS	-	EXPRESSION TAG	UNP P0A6U3
C	-11	HIS	-	EXPRESSION TAG	UNP P0A6U3
C	-10	HIS	-	EXPRESSION TAG	UNP P0A6U3
C	-9	SER	-	EXPRESSION TAG	UNP P0A6U3
C	-8	SER	-	EXPRESSION TAG	UNP P0A6U3
C	-7	GLY	-	EXPRESSION TAG	UNP P0A6U3
C	-6	LEU	-	EXPRESSION TAG	UNP P0A6U3
C	-5	VAL	-	EXPRESSION TAG	UNP P0A6U3
C	-4	PRO	-	EXPRESSION TAG	UNP P0A6U3

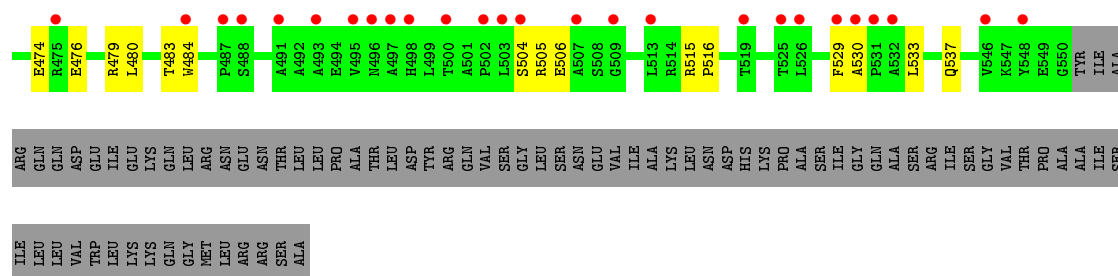
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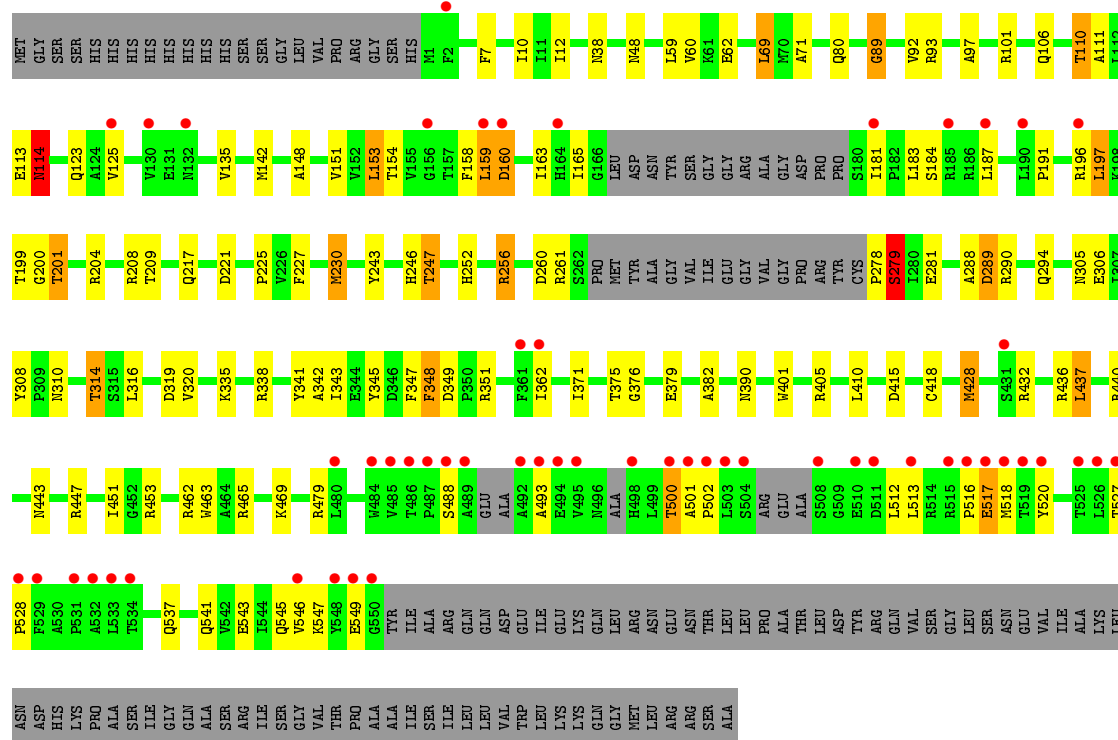
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ARG	-	EXPRESSION TAG	UNP P0A6U3
C	-2	GLY	-	EXPRESSION TAG	UNP P0A6U3
C	-1	SER	-	EXPRESSION TAG	UNP P0A6U3
C	0	HIS	-	EXPRESSION TAG	UNP P0A6U3
D	-21	MET	-	EXPRESSION TAG	UNP P0A6U3
D	-20	GLY	-	EXPRESSION TAG	UNP P0A6U3
D	-19	SER	-	EXPRESSION TAG	UNP P0A6U3
D	-18	SER	-	EXPRESSION TAG	UNP P0A6U3
D	-17	HIS	-	EXPRESSION TAG	UNP P0A6U3
D	-16	HIS	-	EXPRESSION TAG	UNP P0A6U3
D	-15	HIS	-	EXPRESSION TAG	UNP P0A6U3
D	-14	HIS	-	EXPRESSION TAG	UNP P0A6U3
D	-13	HIS	-	EXPRESSION TAG	UNP P0A6U3
D	-12	HIS	-	EXPRESSION TAG	UNP P0A6U3
D	-11	HIS	-	EXPRESSION TAG	UNP P0A6U3
D	-10	HIS	-	EXPRESSION TAG	UNP P0A6U3
D	-9	SER	-	EXPRESSION TAG	UNP P0A6U3
D	-8	SER	-	EXPRESSION TAG	UNP P0A6U3
D	-7	GLY	-	EXPRESSION TAG	UNP P0A6U3
D	-6	LEU	-	EXPRESSION TAG	UNP P0A6U3
D	-5	VAL	-	EXPRESSION TAG	UNP P0A6U3
D	-4	PRO	-	EXPRESSION TAG	UNP P0A6U3
D	-3	ARG	-	EXPRESSION TAG	UNP P0A6U3
D	-2	GLY	-	EXPRESSION TAG	UNP P0A6U3
D	-1	SER	-	EXPRESSION TAG	UNP P0A6U3
D	0	HIS	-	EXPRESSION TAG	UNP P0A6U3

- Molecule 2 is water.

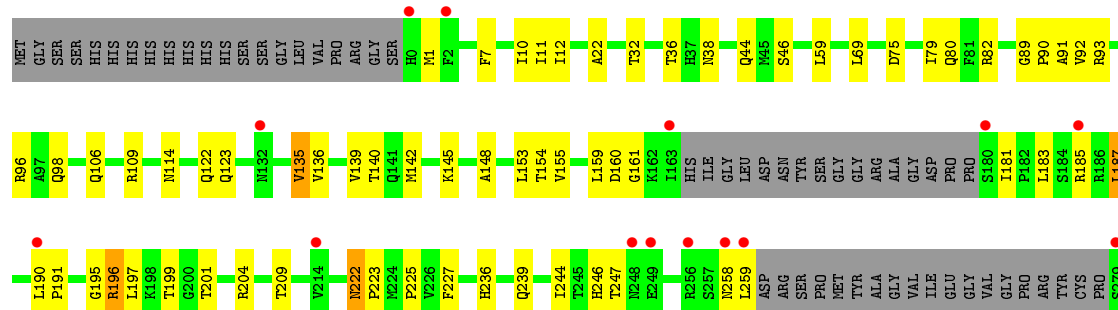
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	147	Total O 147 147	0	0
2	B	114	Total O 114 114	0	0
2	C	41	Total O 41 41	0	0
2	D	30	Total O 30 30	0	0

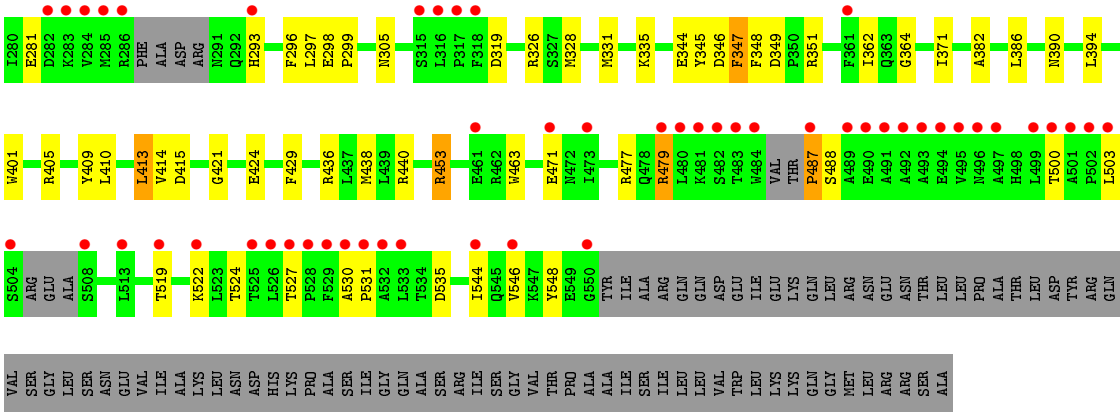


- Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme gidA



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.90Å 144.33Å 147.75Å 90.00° 106.63° 90.00°	Depositor
Resolution (Å)	141.42 – 2.41 47.75 – 2.41	Depositor EDS
% Data completeness (in resolution range)	97.4 (141.42-2.41) 97.4 (47.75-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.201 , 0.238 0.201 , 0.237	Depositor DCC
R_{free} test set	6511 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.7	EDS
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 129227 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15980	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.78	2/4174 (0.0%)	0.87	13/5651 (0.2%)
1	B	0.68	0/3970	0.85	14/5391 (0.3%)
1	C	0.54	1/3949 (0.0%)	0.85	10/5354 (0.2%)
1	D	0.47	0/3843	0.84	6/5213 (0.1%)
All	All	0.63	3/15936 (0.0%)	0.85	43/21609 (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	1	1
1	C	0	2
1	D	0	3
All	All	1	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	0	HIS	C-N	14.28	1.66	1.34
1	C	500	THR	C-N	-6.51	1.19	1.34
1	A	506	GLU	CB-CG	-5.92	1.40	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	487	PRO	O-C-N	-35.11	66.53	122.70
1	C	500	THR	O-C-N	-32.11	71.33	122.70
1	D	487	PRO	CA-C-N	15.40	151.09	117.20
1	A	447	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	C	500	THR	CA-C-N	-8.81	97.82	117.20
1	B	338	ARG	NE-CZ-NH1	8.75	124.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	PHE	C-N-CA	8.60	143.21	121.70
1	A	0	HIS	O-C-N	-8.43	109.22	122.70
1	C	256	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	A	447	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	A	101	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	447	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	447	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	101	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	459	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	338	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	A	338	ARG	CG-CD-NE	6.43	125.31	111.80
1	C	101	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	347	PHE	CA-C-N	6.29	131.04	117.20
1	C	101	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	C	256	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	B	338	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	113	GLU	C-N-CA	6.08	136.90	121.70
1	D	347	PHE	C-N-CA	5.96	136.61	121.70
1	B	347	PHE	O-C-N	-5.95	113.18	122.70
1	B	436	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	206	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	197	LEU	CA-CB-CG	5.63	128.25	115.30
1	B	82	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	487	PRO	C-N-CA	5.54	135.54	121.70
1	C	113	GLU	N-CA-C	5.49	125.83	111.00
1	D	413	LEU	CA-CB-CG	5.44	127.81	115.30
1	B	347	PHE	N-CA-C	-5.41	96.38	111.00
1	B	69	LEU	CA-CB-CG	5.39	127.69	115.30
1	D	347	PHE	N-CA-C	-5.38	96.48	111.00
1	B	204	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	B	413	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	82	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	485	VAL	CB-CA-C	-5.20	101.52	111.40
1	A	204	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	0	HIS	CA-C-N	-5.16	105.84	117.20
1	C	347	PHE	C-N-CA	5.14	134.55	121.70
1	A	59	LEU	CB-CG-CD1	5.08	119.63	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	348	PHE	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	89	GLY	Peptide
1	C	500	THR	Mainchain
1	C	89	GLY	Peptide
1	D	487	PRO	Mainchain,Peptide
1	D	89	GLY	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	4098	0	4061	95	0
1	B	3895	0	3741	71	0
1	C	3884	0	3757	78	0
1	D	3771	0	3604	73	0
2	A	147	0	0	5	0
2	B	114	0	0	2	0
2	C	41	0	0	2	0
2	D	30	0	0	2	0
All	All	15980	0	15163	309	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 (309) 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:230:MET:HE2	1:C:230:MET:HA	1.25	1.12
1:D:154:THR:HG21	2:D:647:HOH:O	1.51	1.10
1:B:49:PRO:HB3	1:B:101:ARG:NH1	1.67	1.09
1:C:288:ALA:O	1:C:289:ASP:HB2	1.52	1.03
1:D:90:PRO:HB2	1:D:440:ARG:HD2	1.39	1.02
1:B:49:PRO:HB3	1:B:101:ARG:HH12	1.31	0.93
1:A:247:THR:HG23	1:A:252:HIS:NE2	1.88	0.89
1:C:106:GLN:O	1:C:110:THR:HB	1.73	0.88
1:D:154:THR:CG2	2:D:647:HOH:O	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:O	1:A:289:ASP:HB2	1.77	0.85
1:A:247:THR:CG2	1:A:252:HIS:NE2	2.40	0.83
1:A:96:ARG:HH12	1:A:98:GLN:HE21	1.25	0.83
1:C:230:MET:CE	1:C:465:ARG:HG2	2.09	0.83
1:A:209:THR:HG21	1:A:335:LYS:HG3	1.60	0.82
1:C:436:ARG:O	1:C:437:LEU:HB3	1.79	0.82
1:B:90:PRO:HB2	1:B:440:ARG:HD2	1.61	0.82
1:A:96:ARG:HH12	1:A:98:GLN:NE2	1.77	0.81
1:D:390:ASN:HD21	1:D:401:TRP:H	1.30	0.80
1:C:230:MET:HE2	1:C:230:MET:CA	2.11	0.80
1:B:154:THR:HG21	2:B:663:HOH:O	1.82	0.79
1:C:247:THR:CG2	1:C:252:HIS:NE2	2.45	0.79
1:C:278:PRO:O	1:C:279:SER:HB3	1.82	0.78
1:B:390:ASN:HD21	1:B:401:TRP:H	1.30	0.78
1:B:49:PRO:CB	1:B:101:ARG:HH12	1.97	0.77
1:A:142:MET:CE	1:B:339:PRO:HG3	2.15	0.77
1:C:89:GLY:HA2	1:C:93:ARG:HH21	1.50	0.77
1:A:191:PRO:HG2	1:A:361:PHE:CE2	2.20	0.77
1:B:106:GLN:O	1:B:110:THR:HB	1.84	0.77
1:A:306:GLU:OE1	1:A:338:ARG:NH1	2.19	0.76
1:C:382:ALA:HB1	1:C:410:LEU:HD13	1.67	0.75
1:C:230:MET:HE1	1:C:465:ARG:HG2	1.65	0.75
1:A:440:ARG:HH21	1:A:541:GLN:HE22	1.34	0.75
1:A:210:ILE:HG23	1:A:331:MET:CE	2.16	0.75
1:C:247:THR:HG23	1:C:252:HIS:NE2	2.01	0.75
1:A:142:MET:HE1	1:B:339:PRO:HG3	1.69	0.74
1:A:123:GLN:CD	1:A:142:MET:HE2	2.08	0.74
1:D:453:ARG:HG3	1:D:463:TRP:CE3	2.22	0.74
1:B:154:THR:CG2	2:B:663:HOH:O	2.35	0.74
1:D:530:ALA:HB3	1:D:531:PRO:HD3	1.68	0.74
1:C:123:GLN:HG3	1:C:142:MET:HE2	1.68	0.74
1:A:155:VAL:HG23	1:A:370:GLN:HG2	1.70	0.73
1:A:390:ASN:HD21	1:A:401:TRP:H	1.36	0.73
1:A:338:ARG:HH11	1:A:338:ARG:HG3	1.53	0.73
1:A:348:PHE:HD2	1:A:371:ILE:CD1	2.02	0.73
1:A:436:ARG:O	1:A:437:LEU:HB3	1.90	0.72
1:B:314:THR:HG22	1:B:316:LEU:HD12	1.72	0.72
1:A:91:ALA:HB2	1:A:437:LEU:HA	1.72	0.71
1:A:210:ILE:HG23	1:A:331:MET:HE2	1.70	0.71
1:D:351:ARG:HD2	1:D:421:GLY:HA3	1.73	0.71
1:D:185:ARG:HH11	1:D:185:ARG:HG2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD13	1:A:370:GLN:HE21	1.56	0.70
1:B:123:GLN:HE21	1:B:140:THR:HB	1.57	0.70
1:A:440:ARG:HH21	1:A:541:GLN:NE2	1.89	0.69
1:C:338:ARG:HG3	1:C:338:ARG:HH11	1.56	0.69
1:D:297:LEU:HD11	1:D:331[B]:MET:CE	2.22	0.69
1:D:349:ASP:OD1	1:D:351:ARG:HD3	1.93	0.68
1:B:101:ARG:HH11	1:B:101:ARG:CG	2.05	0.67
1:C:440:ARG:HH21	1:C:541:GLN:HE22	1.42	0.67
1:B:102:VAL:O	1:B:106:GLN:HG2	1.95	0.67
1:B:191:PRO:HG2	1:B:361:PHE:CE2	2.30	0.67
1:B:314:THR:CG2	1:B:316:LEU:HD12	2.25	0.66
1:A:306:GLU:CD	1:A:338:ARG:HH12	1.98	0.66
1:A:154:THR:CG2	2:A:646:HOH:O	2.44	0.66
1:B:154:THR:HG22	1:B:155:VAL:HG12	1.78	0.65
1:D:96:ARG:HH12	1:D:98:GLN:NE2	1.95	0.65
1:C:469:LYS:HE3	1:C:537:GLN:HB3	1.79	0.65
1:D:297:LEU:HD11	1:D:331[B]:MET:HE3	1.78	0.64
1:A:288:ALA:O	1:A:289:ASP:CB	2.45	0.64
1:D:351:ARG:HD2	1:D:421:GLY:CA	2.28	0.64
1:B:436:ARG:O	1:B:438:MET:N	2.28	0.63
1:A:438:MET:O	1:A:447:ARG:HD2	1.99	0.63
1:B:390:ASN:ND2	1:B:401:TRP:H	1.96	0.63
1:C:390:ASN:HD21	1:C:401:TRP:H	1.48	0.62
1:D:453:ARG:HG3	1:D:463:TRP:CD2	2.33	0.62
1:D:181:ILE:HG22	1:D:183:LEU:H	1.64	0.62
1:A:10:ILE:HG13	1:A:148:ALA:HB2	1.79	0.62
1:A:390:ASN:ND2	1:A:401:TRP:H	1.98	0.62
1:D:477:ARG:HH21	1:D:546:VAL:HA	1.64	0.62
1:D:123:GLN:HE22	1:D:142:MET:H	1.47	0.62
1:C:230:MET:HE3	1:C:465:ARG:HG2	1.80	0.62
1:A:157:THR:CG2	1:A:181:ILE:HD13	2.29	0.62
1:C:348:PHE:HD2	1:C:371:ILE:HD11	1.65	0.61
1:A:114:ASN:ND2	1:B:305:ASN:HD21	1.98	0.61
1:C:405:ARG:HD2	1:C:415:ASP:OD2	2.00	0.61
1:D:181:ILE:H	1:D:181:ILE:HD12	1.65	0.61
1:A:154:THR:HG21	2:A:646:HOH:O	2.00	0.61
1:B:101:ARG:HH11	1:B:101:ARG:HG3	1.66	0.61
1:A:314:THR:HG21	1:A:316:LEU:HD12	1.83	0.61
1:A:196:ARG:HD3	1:A:346:ASP:OD2	2.00	0.61
1:A:314:THR:HB	1:A:316:LEU:H	1.64	0.60
1:D:225:PRO:O	1:D:236:HIS:HE1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:GLU:OE1	1:C:338:ARG:NH1	2.35	0.60
1:C:187:LEU:HD23	1:C:348:PHE:CE2	2.37	0.60
1:A:281:GLU:OE1	1:A:314:THR:CG2	2.50	0.60
1:D:222:ASN:HD22	1:D:223:PRO:HA	1.67	0.59
1:D:347:PHE:HB2	1:D:371:ILE:O	2.02	0.59
1:C:390:ASN:ND2	1:C:401:TRP:H	2.00	0.59
1:C:512:LEU:O	1:C:518:MET:HG2	2.03	0.59
1:A:157:THR:HG22	1:A:181:ILE:HD13	1.84	0.58
1:C:479:ARG:O	1:C:479:ARG:HD2	2.04	0.58
1:A:305:ASN:HD21	1:B:114:ASN:ND2	2.01	0.58
1:A:142:MET:HE3	1:B:339:PRO:HG3	1.86	0.58
1:B:297:LEU:HD11	1:B:331:MET:HE3	1.85	0.57
1:B:476:GLU:HG2	1:B:533:LEU:HD22	1.87	0.56
1:A:389:LEU:HD13	1:A:457:LEU:HD11	1.87	0.56
1:C:288:ALA:O	1:C:289:ASP:CB	2.32	0.56
1:D:246:HIS:O	1:D:328:MET:HG2	2.05	0.56
1:B:372:ASN:HD22	1:B:383:GLN:NE2	2.03	0.56
1:A:12:ILE:O	1:A:154:THR:HB	2.06	0.56
1:A:127:ASP:OD2	1:A:186:ARG:NH1	2.38	0.56
1:D:123:GLN:NE2	1:D:142:MET:H	2.02	0.56
1:C:543:GLU:O	1:C:547:LYS:HG2	2.06	0.56
1:C:306:GLU:CD	1:C:338:ARG:HH12	2.09	0.56
1:C:135:VAL:HG13	1:C:362:ILE:HG21	1.88	0.56
1:B:49:PRO:HB3	1:B:101:ARG:HH11	1.63	0.55
1:A:142:MET:HE1	1:B:339:PRO:CG	2.36	0.55
1:A:338:ARG:CG	1:A:338:ARG:HH11	2.14	0.55
1:A:89:GLY:HA2	1:A:93:ARG:HH21	1.72	0.55
1:B:38:ASN:ND2	1:B:40:ASP:H	2.04	0.55
1:A:348:PHE:HD2	1:A:371:ILE:HD11	1.72	0.55
1:D:209:THR:HG21	1:D:335:LYS:HD2	1.89	0.55
1:D:544:ILE:O	1:D:548:TYR:HD1	1.90	0.55
1:A:222:ASN:HD22	1:A:223:PRO:HA	1.72	0.55
1:C:48:ASN:HB3	1:C:308:TYR:CE2	2.41	0.55
1:D:96:ARG:HH12	1:D:98:GLN:HE21	1.55	0.54
1:C:348:PHE:CD2	1:C:371:ILE:HD11	2.43	0.54
1:A:281:GLU:OE1	1:A:314:THR:HG23	2.08	0.54
1:B:474:GLU:HA	1:B:474:GLU:OE1	2.06	0.54
1:B:194:VAL:HG22	1:B:348:PHE:CE1	2.43	0.54
1:A:405:ARG:HD2	1:A:415:ASP:OD2	2.07	0.54
1:D:90:PRO:HA	1:D:93:ARG:HE	1.74	0.53
1:A:282:ASP:OD2	1:A:286:ARG:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ASP:O	1:B:196:ARG:NH2	2.40	0.53
1:C:153:LEU:HD22	1:C:158:PHE:CZ	2.44	0.53
1:D:382:ALA:HB1	1:D:410:LEU:HD13	1.88	0.53
1:D:247:THR:CG2	1:D:293:HIS:H	2.21	0.53
1:A:159:LEU:O	1:A:160:ASP:HB2	2.08	0.53
1:C:80:GLN:O	1:C:97:ALA:HA	2.08	0.53
1:B:101:ARG:CG	1:B:101:ARG:NH1	2.69	0.53
1:A:48:ASN:HB3	1:A:308:TYR:CE2	2.43	0.53
1:B:131:GLU:O	1:B:132:ASN:HB2	2.07	0.53
1:B:427:ARG:CZ	1:B:428:MET:HE2	2.38	0.53
1:D:244:ILE:HG12	1:D:296:PHE:CE1	2.44	0.53
1:A:54:ILE:HG23	1:A:429:PHE:CD2	2.43	0.52
1:D:159:LEU:O	1:D:160:ASP:HB3	2.08	0.52
2:C:668:HOH:O	1:D:305:ASN:HB2	2.09	0.52
1:B:194:VAL:HG22	1:B:348:PHE:HE1	1.73	0.52
1:D:247:THR:HG22	1:D:293:HIS:H	1.73	0.52
1:C:306:GLU:OE2	1:C:338:ARG:NH1	2.38	0.52
1:C:7:PHE:O	1:C:148:ALA:HA	2.08	0.52
1:D:80:GLN:NE2	1:D:82:ARG:HD3	2.25	0.52
1:A:127:ASP:OD1	1:A:186:ARG:NH1	2.42	0.52
1:D:159:LEU:HD22	1:D:346:ASP:O	2.09	0.52
1:B:323:GLN:O	1:B:327:SER:HB3	2.10	0.52
1:A:157:THR:CG2	1:A:181:ILE:CD1	2.88	0.52
1:B:230:MET:CE	1:B:465:ARG:HG2	2.41	0.51
1:C:123:GLN:CG	1:C:142:MET:HE2	2.37	0.51
1:A:348:PHE:CD2	1:A:371:ILE:HD11	2.44	0.51
1:C:60:VAL:HG12	1:C:71:ALA:HB2	1.92	0.51
1:D:390:ASN:ND2	1:D:401:TRP:H	2.02	0.51
1:B:12:ILE:O	1:B:154:THR:HB	2.11	0.51
1:B:427:ARG:NH2	1:B:428:MET:CE	2.73	0.51
1:C:12:ILE:O	1:C:154:THR:HB	2.11	0.51
1:B:297:LEU:HD11	1:B:331:MET:CE	2.40	0.51
1:A:80:GLN:O	1:A:97:ALA:HA	2.10	0.51
1:B:306:GLU:OE1	1:B:338:ARG:HD2	2.10	0.51
1:C:209:THR:HG21	1:C:335:LYS:HD2	1.92	0.51
1:D:123:GLN:HE21	1:D:140:THR:HB	1.77	0.50
1:A:306:GLU:CD	1:A:338:ARG:NH1	2.59	0.50
1:A:281:GLU:OE1	1:A:314:THR:HG22	2.11	0.50
1:D:197:LEU:O	1:D:344:GLU:HA	2.10	0.50
1:B:469:LYS:HE3	1:B:537:GLN:HB3	1.93	0.50
1:A:425:PRO:HD2	1:A:428:MET:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ASN:HD21	1:D:114:ASN:ND2	2.10	0.50
1:D:297:LEU:HD11	1:D:331[B]:MET:HE1	1.92	0.49
1:C:453:ARG:HG2	1:C:463:TRP:CE2	2.47	0.49
1:D:154:THR:HG22	1:D:155:VAL:HG12	1.95	0.49
1:A:127:ASP:CG	1:A:186:ARG:NH1	2.66	0.49
1:D:10:ILE:HG13	1:D:148:ALA:HB2	1.94	0.49
1:A:154:THR:HG23	2:A:646:HOH:O	2.10	0.49
1:D:161:GLY:HA2	1:D:345:TYR:HB3	1.95	0.49
1:A:315:SER:HB3	1:A:342:ALA:HB2	1.93	0.49
1:C:428:MET:O	1:C:432:ARG:HD3	2.12	0.49
1:B:62:GLU:OE2	1:B:447:ARG:NH2	2.45	0.49
1:C:201:THR:HG22	1:C:341:TYR:H	1.78	0.49
1:A:209:THR:HG21	1:A:335:LYS:CG	2.39	0.49
1:C:443:ASN:O	1:C:447:ARG:HG3	2.12	0.49
1:C:541:GLN:O	1:C:545:GLN:HG2	2.13	0.49
1:B:7:PHE:O	1:B:148:ALA:HA	2.13	0.49
1:A:114:ASN:HD21	1:B:305:ASN:HD21	1.59	0.48
1:A:45:MET:O	1:A:101:ARG:NH2	2.46	0.48
1:A:102:VAL:O	1:A:106[B]:GLN:HG2	2.13	0.48
1:B:139:VAL:HG13	1:B:145:LYS:HG2	1.94	0.48
1:A:372:ASN:HD22	1:A:383:GLN:NE2	2.12	0.48
1:A:443:ASN:OD1	1:A:447:ARG:HD3	2.13	0.48
1:C:545:GLN:O	1:C:549:GLU:HG3	2.13	0.48
1:D:7:PHE:O	1:D:148:ALA:HA	2.14	0.48
1:C:256:ARG:HD2	2:C:647:HOH:O	2.12	0.48
1:C:281:GLU:OE1	1:C:314:THR:CG2	2.62	0.48
1:C:230:MET:CE	1:C:230:MET:HA	2.17	0.48
1:C:513:LEU:HD23	1:C:546:VAL:HG11	1.95	0.48
1:C:200:GLY:HA2	1:C:342:ALA:HA	1.96	0.48
1:A:-3:ARG:HB3	1:A:0:HIS:HB2	1.96	0.48
1:A:349:ASP:OD1	1:A:351:ARG:HD2	2.14	0.48
1:C:527:THR:N	1:C:528:PRO:HD2	2.29	0.47
1:C:10:ILE:HB	1:C:151:VAL:HG22	1.96	0.47
1:B:129:ILE:HG22	1:B:136:VAL:HG12	1.96	0.47
1:A:38:ASN:ND2	1:A:40:ASP:H	2.12	0.47
1:A:157:THR:HG23	1:A:181:ILE:CD1	2.44	0.47
1:C:181:ILE:HG22	1:C:183:LEU:H	1.79	0.47
1:C:306:GLU:CD	1:C:338:ARG:NH1	2.68	0.47
1:B:349:ASP:OD1	1:B:351:ARG:HD3	2.14	0.47
1:B:181:ILE:HG22	1:B:183:LEU:H	1.78	0.47
1:A:90:PRO:HB2	1:A:440:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ARG:HH11	1:C:338:ARG:CG	2.21	0.47
1:D:477:ARG:NH2	1:D:546:VAL:HA	2.29	0.47
1:D:160:ASP:OD1	1:D:196:ARG:NH2	2.48	0.46
1:D:11:ILE:CD1	1:D:32:THR:CG2	2.94	0.46
1:C:376:GLY:HA3	1:C:379:GLU:OE1	2.15	0.46
1:A:349:ASP:OD1	1:A:351:ARG:CD	2.64	0.46
1:C:247:THR:HG21	1:C:252:HIS:NE2	2.29	0.46
1:A:155:VAL:HA	1:A:159:LEU:HD11	1.97	0.46
1:A:518:MET:O	1:A:547:LYS:NZ	2.31	0.46
1:C:221:ASP:HB2	1:C:225:PRO:HD3	1.98	0.45
1:A:247:THR:O	1:A:292:GLN:HB3	2.15	0.45
1:B:255:ILE:HG12	1:B:255:ILE:H	1.62	0.45
1:A:348:PHE:CD2	1:A:371:ILE:CD1	2.90	0.45
1:B:153:LEU:HD22	1:B:158:PHE:CZ	2.52	0.45
1:D:91:ALA:HA	1:D:440:ARG:HG2	1.98	0.45
1:A:38:ASN:C	1:A:38:ASN:HD22	2.20	0.45
1:C:160:ASP:HB3	1:C:345:TYR:HA	1.97	0.45
1:B:479:ARG:O	1:B:479:ARG:HD2	2.16	0.45
1:D:259:LEU:HD11	1:D:281:GLU:HB2	1.98	0.45
1:D:106:GLN:NE2	1:D:109:ARG:HH21	2.14	0.45
1:D:106:GLN:HE22	1:D:109:ARG:HH21	1.65	0.45
1:A:256:ARG:HD2	2:A:695:HOH:O	2.16	0.45
1:B:405:ARG:HD2	1:B:415:ASP:OD2	2.17	0.45
1:B:80:GLN:O	1:B:97:ALA:HA	2.17	0.45
1:C:516:PRO:O	1:C:517:GLU:HB3	2.17	0.44
1:D:12:ILE:O	1:D:154:THR:HB	2.17	0.44
1:D:409:TYR:CE2	1:D:429:PHE:CE1	3.05	0.44
1:A:210:ILE:HG23	1:A:331:MET:HE1	1.96	0.44
1:B:326:ARG:HA	1:B:331:MET:O	2.18	0.44
1:C:217:GLN:HG2	1:C:243:TYR:CE1	2.52	0.44
1:D:364:GLY:HA2	1:D:394:LEU:HD13	1.99	0.44
1:C:349:ASP:OD1	1:C:351:ARG:HD2	2.18	0.44
1:B:280:ILE:HB	1:B:312:ILE:HA	1.98	0.44
1:D:185:ARG:NH1	1:D:185:ARG:HG2	2.28	0.44
1:C:135:VAL:HG13	1:C:362:ILE:CG2	2.48	0.44
1:C:89:GLY:HA2	1:C:93:ARG:NH2	2.27	0.43
1:C:230:MET:SD	1:C:462:ARG:HA	2.58	0.43
1:C:12:ILE:HG21	1:C:125:VAL:HG11	2.00	0.43
1:A:155:VAL:HG23	1:A:370:GLN:CG	2.45	0.43
1:C:261:ARG:NH2	1:C:319:ASP:OD2	2.52	0.43
1:D:139:VAL:HG13	1:D:145:LYS:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:MET:HG3	2:A:721:HOH:O	2.18	0.43
1:B:247:THR:HG22	1:B:293:HIS:H	1.84	0.43
1:C:440:ARG:NH2	1:C:541:GLN:HE22	2.13	0.43
1:D:424:GLU:OE1	1:D:436:ARG:NH2	2.47	0.43
1:B:23:MET:SD	1:B:112:LEU:HD23	2.59	0.43
1:C:316:LEU:HD13	1:C:320:VAL:HG11	2.01	0.43
1:C:348:PHE:HD2	1:C:371:ILE:CD1	2.31	0.43
1:B:483:THR:O	1:B:529:PHE:HE1	2.02	0.43
1:D:142:MET:HE2	1:D:142:MET:HB2	1.85	0.43
1:B:158:PHE:HE1	1:B:371:ILE:HD12	1.84	0.43
1:A:321:GLN:O	1:A:325:VAL:HG23	2.19	0.43
1:D:195:GLY:N	1:D:347:PHE:O	2.50	0.42
1:A:199:THR:CG2	1:A:200:GLY:N	2.82	0.42
1:C:281:GLU:OE1	1:C:314:THR:HG22	2.19	0.42
1:D:11:ILE:HD13	1:D:22:ALA:HA	2.01	0.42
1:D:298:GLU:HA	1:D:299:PRO:HD3	1.89	0.42
1:A:247:THR:HG21	1:A:252:HIS:NE2	2.33	0.42
1:D:196:ARG:HD3	1:D:344:GLU:HG2	2.01	0.42
1:B:10:ILE:HG13	1:B:148:ALA:HB2	2.02	0.42
1:C:187:LEU:HD23	1:C:348:PHE:HE2	1.84	0.42
1:C:246:HIS:CD2	1:C:294:GLN:HG2	2.55	0.42
1:B:91:ALA:HA	1:B:440:ARG:HG2	2.02	0.42
1:A:90:PRO:HB2	1:A:440:ARG:CD	2.50	0.42
1:B:427:ARG:NH2	1:B:428:MET:HE2	2.35	0.41
1:A:310:ASN:HD22	1:A:311:GLY:N	2.18	0.41
1:A:101:ARG:HG3	1:A:300:GLU:O	2.20	0.41
1:D:424:GLU:CD	1:D:436:ARG:HH22	2.23	0.41
1:B:476:GLU:O	1:B:480:LEU:HB2	2.19	0.41
1:D:79:ILE:O	1:D:239:GLN:HA	2.20	0.41
1:A:74:ILE:CD1	1:A:99:ALA:HB2	2.51	0.41
1:D:479:ARG:HB3	1:D:479:ARG:NH1	2.36	0.41
1:D:187:LEU:HD12	1:D:190:LEU:HD12	2.02	0.41
1:D:90:PRO:HB2	1:D:440:ARG:CD	2.28	0.41
1:D:75:ASP:O	1:D:236:HIS:HD2	2.04	0.41
1:B:160:ASP:HB3	1:B:196:ARG:HH21	1.85	0.41
1:C:208:ARG:HD2	1:C:305:ASN:HD22	1.86	0.41
1:D:36:THR:O	1:D:122:GLN:HA	2.20	0.41
1:B:298:GLU:HA	1:B:299:PRO:HD3	1.93	0.41
1:D:135:VAL:HG13	1:D:362:ILE:HG21	2.02	0.41
1:A:96:ARG:NH1	1:A:98:GLN:NE2	2.58	0.41
1:B:197:LEU:O	1:B:344:GLU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:PRO:HB2	1:B:440:ARG:CD	2.42	0.40
1:B:281:GLU:HB3	1:B:316:LEU:HD11	2.03	0.40
1:C:62:GLU:OE2	1:C:447:ARG:NH2	2.55	0.40
1:A:41:THR:O	1:A:44:GLN:HB2	2.21	0.40
1:C:114:ASN:HA	1:C:114:ASN:HD22	1.57	0.40
1:D:386:LEU:CD2	1:D:414:VAL:HG21	2.51	0.40
1:D:405:ARG:NH1	1:D:415:ASP:OD2	2.47	0.40
1:A:440:ARG:NH2	1:A:541:GLN:NE2	2.66	0.40
1:A:12:ILE:HG21	1:A:125:VAL:HG11	2.04	0.40
1:C:69:LEU:HD11	1:C:111:ALA:HB3	2.03	0.40
1:B:515:ARG:HA	1:B:516:PRO:HD3	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	526/651 (81%)	507 (96%)	14 (3%)	5 (1%)	19	27
1	B	514/651 (79%)	476 (93%)	33 (6%)	5 (1%)	19	27
1	C	504/651 (77%)	461 (92%)	28 (6%)	15 (3%)	5	4
1	D	496/651 (76%)	466 (94%)	22 (4%)	8 (2%)	12	15
All	All	2040/2604 (78%)	1910 (94%)	97 (5%)	33 (2%)	12	15

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	ASP
1	B	348	PHE
1	B	437	LEU
1	B	504	SER

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Mol	Chain	Res	Type
1	C	279	SER
1	C	348	PHE
1	C	493	ALA
1	C	501	ALA
1	D	488	SER
1	D	503	LEU
1	A	199	THR
1	A	289	ASP
1	C	114	ASN
1	C	160	ASP
1	C	289	ASP
1	C	488	SER
1	C	520	TYR
1	D	535	ASP
1	B	505	ARG
1	D	348	PHE
1	D	500	THR
1	A	-3	ARG
1	A	181	ILE
1	B	530	ALA
1	C	159	LEU
1	D	191	PRO
1	D	519	THR
1	C	437	LEU
1	C	517	GLU
1	C	502	PRO
1	C	165	ILE
1	C	191	PRO
1	D	527	THR

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	429/535 (80%)	389 (91%)	40 (9%)	11	16
1	B	383/535 (72%)	349 (91%)	34 (9%)	12	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	389/535 (73%)	361 (93%)	28 (7%)	18	27
1	D	365/535 (68%)	339 (93%)	26 (7%)	18	28
All	All	1566/2140 (73%)	1438 (92%)	128 (8%)	14	21

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	LEU
1	A	38	ASN
1	A	59	LEU
1	A	69	LEU
1	A	92	VAL
1	A	135	VAL
1	A	136	VAL
1	A	153	LEU
1	A	154	THR
1	A	155	VAL
1	A	157	THR
1	A	187	LEU
1	A	196	ARG
1	A	201	THR
1	A	204	ARG
1	A	222	ASN
1	A	227	PHE
1	A	247	THR
1	A	260	ASP
1	A	262	SER
1	A	279	SER
1	A	289	ASP
1	A	310	ASN
1	A	314	THR
1	A	319	ASP
1	A	335	LYS
1	A	343	ILE
1	A	351	ARG
1	A	371	ILE
1	A	410	LEU
1	A	428	MET
1	A	431	SER
1	A	440	ARG
1	A	461	GLU

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Mol	Chain	Res	Type
1	A	468	GLU
1	A	482	SER
1	A	485	VAL
1	A	499	LEU
1	A	500	THR
1	A	525	THR
1	B	1	MET
1	B	38	ASN
1	B	46	SER
1	B	59	LEU
1	B	69	LEU
1	B	101	ARG
1	B	110	THR
1	B	135	VAL
1	B	136	VAL
1	B	149	LYS
1	B	154	THR
1	B	160	ASP
1	B	187	LEU
1	B	196	ARG
1	B	197	LEU
1	B	199	THR
1	B	201	THR
1	B	204	ARG
1	B	222	ASN
1	B	227	PHE
1	B	247	THR
1	B	255	ILE
1	B	258	ASN
1	B	259	LEU
1	B	310	ASN
1	B	314	THR
1	B	337	VAL
1	B	343	ILE
1	B	348	PHE
1	B	351	ARG
1	B	389	LEU
1	B	413	LEU
1	B	484	TRP
1	B	506	GLU
1	C	38	ASN
1	C	59	LEU

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Mol	Chain	Res	Type
1	C	69	LEU
1	C	92	VAL
1	C	110	THR
1	C	114	ASN
1	C	153	LEU
1	C	159	LEU
1	C	163	ILE
1	C	184	SER
1	C	196	ARG
1	C	197	LEU
1	C	199	THR
1	C	201	THR
1	C	204	ARG
1	C	227	PHE
1	C	230	MET
1	C	247	THR
1	C	260	ASP
1	C	279	SER
1	C	290	ARG
1	C	310	ASN
1	C	314	THR
1	C	343	ILE
1	C	375	THR
1	C	418	CYS
1	C	428	MET
1	C	451	ILE
1	D	1	MET
1	D	38	ASN
1	D	44	GLN
1	D	46	SER
1	D	59	LEU
1	D	69	LEU
1	D	92	VAL
1	D	135	VAL
1	D	136	VAL
1	D	153	LEU
1	D	187	LEU
1	D	196	ARG
1	D	199	THR
1	D	201	THR
1	D	204	ARG
1	D	222	ASN

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Mol	Chain	Res	Type
1	D	227	PHE
1	D	258	ASN
1	D	319	ASP
1	D	413	LEU
1	D	438	MET
1	D	453	ARG
1	D	471	GLU
1	D	479	ARG
1	D	522	LYS
1	D	524	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	31	GLN
1	A	38	ASN
1	A	98	GLN
1	A	114	ASN
1	A	117	ASN
1	A	217	GLN
1	A	222	ASN
1	A	294	GLN
1	A	310	ASN
1	A	363	GLN
1	A	370	GLN
1	A	383	GLN
1	A	390	ASN
1	A	498	HIS
1	A	541	GLN
1	B	30	GLN
1	B	38	ASN
1	B	114	ASN
1	B	123	GLN
1	B	252	HIS
1	B	294	GLN
1	B	310	ASN
1	B	323	GLN
1	B	383	GLN
1	B	390	ASN
1	C	38	ASN
1	C	80	GLN

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Mol	Chain	Res	Type
1	C	114	ASN
1	C	123	GLN
1	C	217	GLN
1	C	219	HIS
1	C	222	ASN
1	C	291	ASN
1	C	294	GLN
1	C	310	ASN
1	C	390	ASN
1	C	541	GLN
1	D	30	GLN
1	D	38	ASN
1	D	80	GLN
1	D	98	GLN
1	D	106	GLN
1	D	114	ASN
1	D	123	GLN
1	D	222	ASN
1	D	236	HIS
1	D	258	ASN
1	D	310	ASN
1	D	363	GLN
1	D	390	ASN
1	D	541	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 carbohydrates 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	531/651 (81%)	0.07	4 (0%) 87 87	20, 34, 63, 86	0
1	B	519/651 (79%)	0.43	43 (8%) 14 13	23, 38, 125, 136	0
1	C	516/651 (79%)	0.71	56 (10%) 7 7	36, 58, 105, 148	4 (0%)
1	D	507/651 (77%)	0.75	66 (13%) 5 4	40, 61, 128, 160	1 (0%)
All	All	2073/2604 (79%)	0.49	169 (8%) 14 14	20, 49, 114, 160	5 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	504	SER	28.3
1	C	503	LEU	22.1
1	C	502	PRO	15.0
1	D	259	LEU	8.7
1	D	526	LEU	7.6
1	B	507	ALA	7.3
1	B	530	ALA	6.8
1	D	532	ALA	6.7
1	D	487	PRO	6.6
1	D	482	SER	6.3
1	D	493	ALA	6.2
1	D	530	ALA	6.1
1	D	286	ARG	6.1
1	C	130	VAL	6.0
1	C	485	VAL	6.0
1	D	525	THR	5.9
1	B	502	PRO	5.9
1	C	486	THR	5.7
1	D	529	PHE	5.6
1	B	491	ALA	5.6
1	C	526	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	529	PHE	5.4
1	C	492	ALA	5.3
1	C	156	GLY	5.3
1	D	550	GLY	5.3
1	D	484	TRP	5.2
1	C	513	LEU	5.1
1	C	550	GLY	5.0
1	B	493	ALA	5.0
1	D	483	THR	5.0
1	B	513	LEU	5.0
1	D	527	THR	5.0
1	A	-8	SER	5.0
1	D	531	PRO	4.9
1	C	531	PRO	4.8
1	D	285	MET	4.6
1	C	487	PRO	4.6
1	C	501	ALA	4.5
1	D	479	ARG	4.4
1	D	500	THR	4.4
1	B	531	PRO	4.3
1	B	280	ILE	4.3
1	C	489	ALA	4.3
1	D	501	ALA	4.3
1	D	528	PRO	4.3
1	A	164	HIS	4.2
1	D	491	ALA	4.2
1	B	526	LEU	4.2
1	D	497	ALA	4.1
1	D	519	THR	4.0
1	D	502	PRO	4.0
1	B	165	ILE	3.9
1	B	488	SER	3.9
1	C	187	LEU	3.8
1	C	528	PRO	3.7
1	B	164	HIS	3.7
1	C	548	TYR	3.7
1	C	516	PRO	3.6
1	D	480	LEU	3.6
1	B	279	SER	3.5
1	B	525	THR	3.5
1	C	529	PHE	3.5
1	D	490	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	495	VAL	3.5
1	B	504	SER	3.5
1	C	500	THR	3.5
1	D	180	SER	3.4
1	D	249	GLU	3.4
1	D	284	VAL	3.4
1	C	525	THR	3.4
1	C	527	THR	3.3
1	C	431	SER	3.3
1	C	488	SER	3.3
1	C	2	PHE	3.2
1	C	515	ARG	3.2
1	C	159	LEU	3.2
1	C	494	GLU	3.2
1	D	315	SER	3.2
1	C	532	ALA	3.1
1	B	500	THR	3.1
1	C	160	ASP	3.1
1	B	315	SER	3.1
1	B	546	VAL	3.1
1	B	254	VAL	3.0
1	D	214	VAL	3.0
1	C	484	TRP	3.0
1	C	546	VAL	3.0
1	D	282	ASP	2.9
1	B	497	ALA	2.9
1	B	180	SER	2.9
1	D	258	ASN	2.9
1	C	518	MET	2.9
1	D	544	ILE	2.9
1	C	495	VAL	2.8
1	B	292	GLN	2.8
1	B	484	TRP	2.8
1	D	492	ALA	2.8
1	C	520	TYR	2.8
1	D	293	HIS	2.8
1	D	522	LYS	2.8
1	B	496	ASN	2.8
1	C	533	LEU	2.8
1	C	508	SER	2.7
1	D	489	ALA	2.7
1	B	519	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	473	ILE	2.7
1	B	475	ARG	2.7
1	B	281	GLU	2.7
1	C	498	HIS	2.7
1	D	546	VAL	2.7
1	D	316	LEU	2.6
1	B	314	THR	2.6
1	D	283	LYS	2.6
1	D	494	GLU	2.6
1	B	487	PRO	2.6
1	D	132	ASN	2.6
1	D	495	VAL	2.5
1	C	362	ILE	2.5
1	C	185	ARG	2.5
1	D	2	PHE	2.5
1	D	361	PHE	2.5
1	D	471	GLU	2.5
1	B	503	LEU	2.5
1	B	258	ASN	2.5
1	C	480	LEU	2.4
1	D	317	PRO	2.4
1	D	513	LEU	2.4
1	C	549	GLU	2.4
1	C	517	GLU	2.4
1	D	318	PHE	2.4
1	A	434	GLU	2.4
1	B	286	ARG	2.3
1	C	164	HIS	2.3
1	D	185	ARG	2.3
1	D	481	LYS	2.3
1	B	548	TYR	2.3
1	D	503	LEU	2.3
1	B	498	HIS	2.3
1	C	125	VAL	2.3
1	B	166	GLY	2.3
1	C	196	ARG	2.3
1	C	361	PHE	2.3
1	B	259	LEU	2.3
1	C	132	ASN	2.3
1	D	279	SER	2.2
1	B	255	ILE	2.2
1	B	532	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	163	ILE	2.2
1	C	511	ASP	2.2
1	C	190	LEU	2.2
1	C	519	THR	2.2
1	C	493	ALA	2.2
1	C	181	ILE	2.2
1	B	316	LEU	2.2
1	D	0	HIS	2.1
1	C	534	THR	2.1
1	D	504	SER	2.1
1	D	508	SER	2.1
1	D	461	GLU	2.1
1	D	248	ASN	2.1
1	A	159	LEU	2.1
1	B	509	GLY	2.1
1	D	499	LEU	2.1
1	D	533	LEU	2.1
1	D	496	ASN	2.0
1	B	163	ILE	2.0
1	D	190	LEU	2.0
1	C	510	GLU	2.0
1	D	256	ARG	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.