



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:01 PM UTC

PDB ID : 5GNW / pdb_00005gnw
Title : Crystal structure of Uracil DNA glycosylase-Uracil complex from *Bradyrhizobium diazoefficiens*.
Authors : Patil, V.V.; Chembazhi, U.V.; Varshney, U.; Woo, E.
Deposited on : 2016-07-25
Resolution : 2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

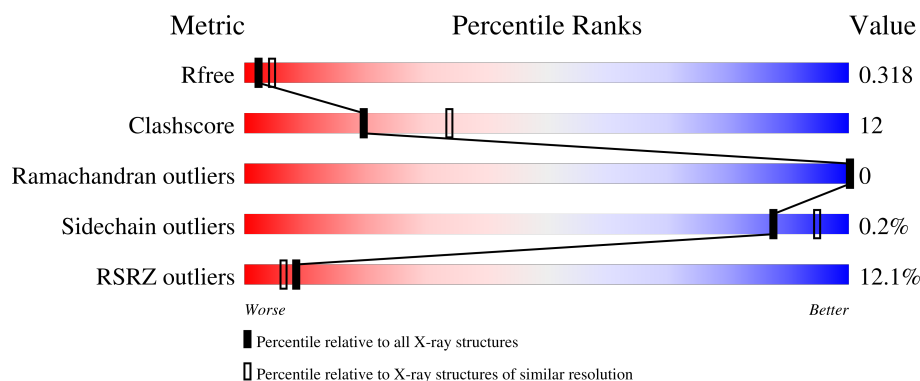
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	272	10% 85% 15%
1	B	272	11% 84% 14% .
1	C	272	16% 73% 26% .
1	D	272	8% 77% 20% .
1	E	272	5% 78% 21% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	272	
1	G	272	
1	H	272	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	URA	A	301	-	X	-	-
2	URA	B	301	-	X	-	-
2	URA	C	301	-	X	-	-
2	URA	D	301	-	X	-	-
2	URA	E	301	-	X	-	-
2	URA	F	301	-	X	-	-
2	URA	G	301	-	X	-	-
2	URA	H	301	-	X	-	-

2 Entry composition

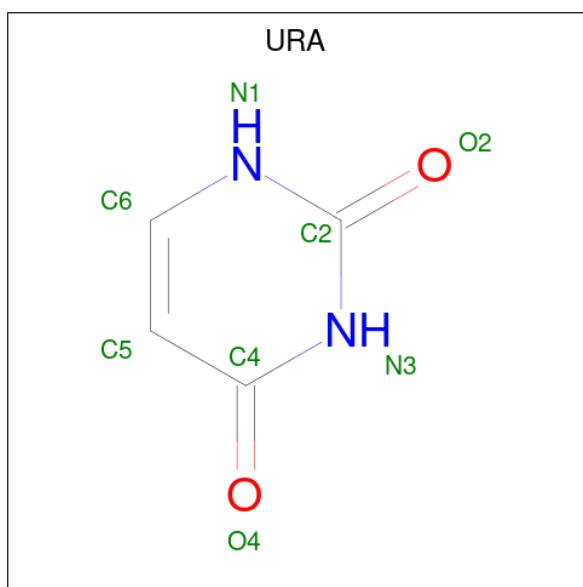
There are 2 unique types of molecules in this entry. The entry contains 32863 atoms, of which 16007 are hydrogens and 0 are deuteriums.

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 Blr0248 protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	C	272	Total	C	H	N	O	S	Se	0	0	0
			4082	1344	1983	368	381	1	5			
1	D	272	Total	C	H	N	O	S	Se	0	0	0
			4103	1344	2004	368	381	1	5			
1	E	272	Total	C	H	N	O	S	Se	0	0	0
			4117	1344	2018	368	381	1	5			
1	F	272	Total	C	H	N	O	S	Se	0	0	0
			4110	1344	2011	368	381	1	5			
1	A	272	Total	C	H	N	O	S	Se	0	0	0
			4124	1344	2025	368	381	1	5			
1	B	272	Total	C	H	N	O	S	Se	0	0	0
			4073	1344	1974	368	381	1	5			
1	G	272	Total	C	H	N	O	S	Se	0	0	0
			4084	1344	1985	368	381	1	5			
1	H	272	Total	C	H	N	O	S	Se	0	0	0
			4074	1344	1975	368	381	1	5			

- Molecule 2 is URACIL (CCD ID: URA) (formula: C₄H₄N₂O₂).

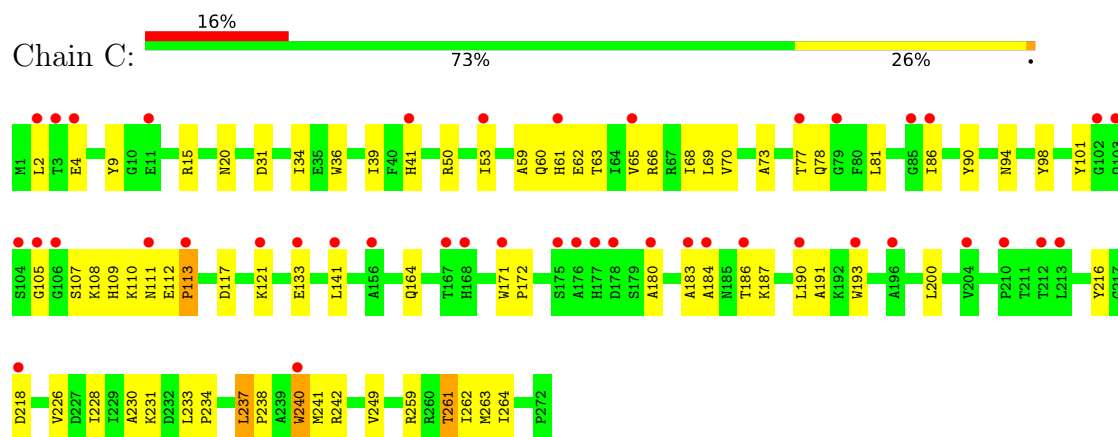


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	H	N	O	0	0
			12	4	4	2	2		
2	D	1	Total	C	H	N	O	0	0
			12	4	4	2	2		
2	E	1	Total	C	H	N	O	0	0
			12	4	4	2	2		
2	F	1	Total	C	H	N	O	0	0
			12	4	4	2	2		
2	A	1	Total	C	H	N	O	0	0
			12	4	4	2	2		
2	B	1	Total	C	H	N	O	0	0
			12	4	4	2	2		
2	G	1	Total	C	H	N	O	0	0
			12	4	4	2	2		
2	H	1	Total	C	H	N	O	0	0
			12	4	4	2	2		

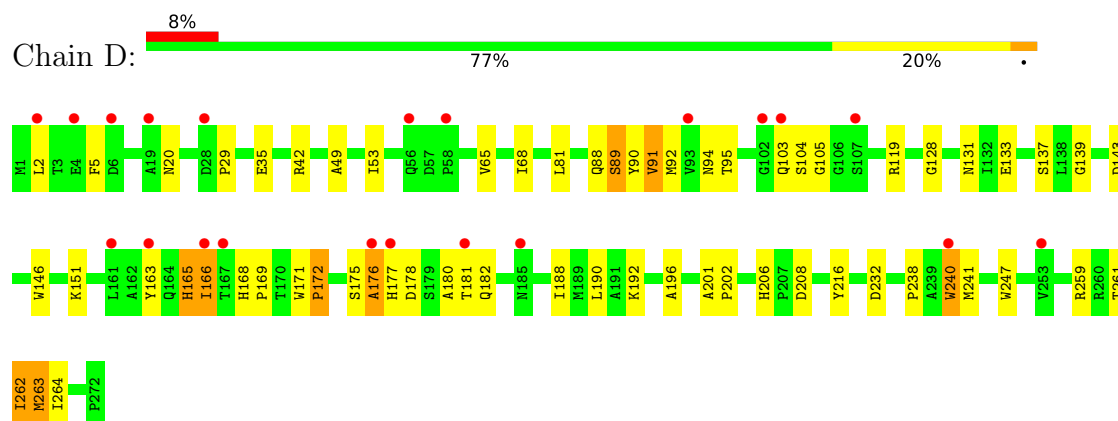
3 Residue-property plots [i](#)

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.

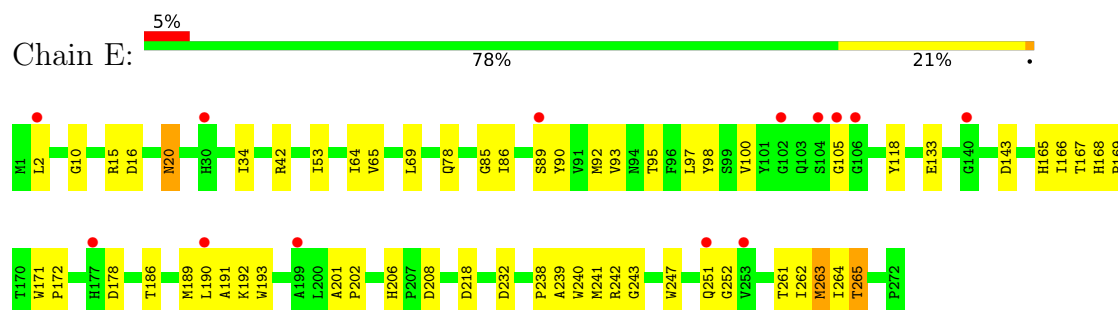
• Molecule 1: Blr0248 protein



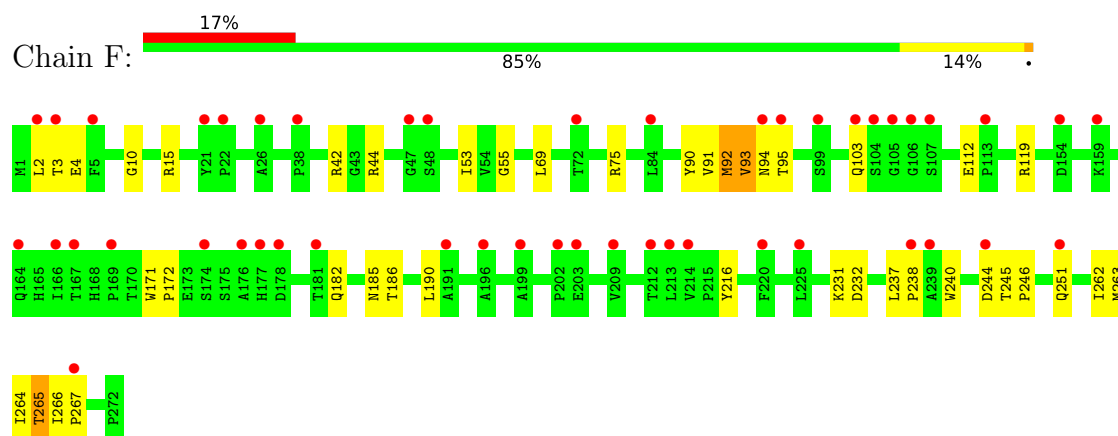
• Molecule 1: Blr0248 protein



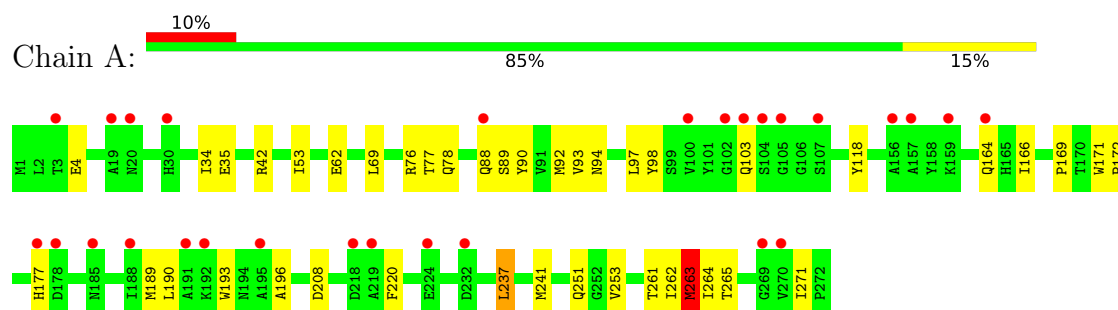
• Molecule 1: Blr0248 protein



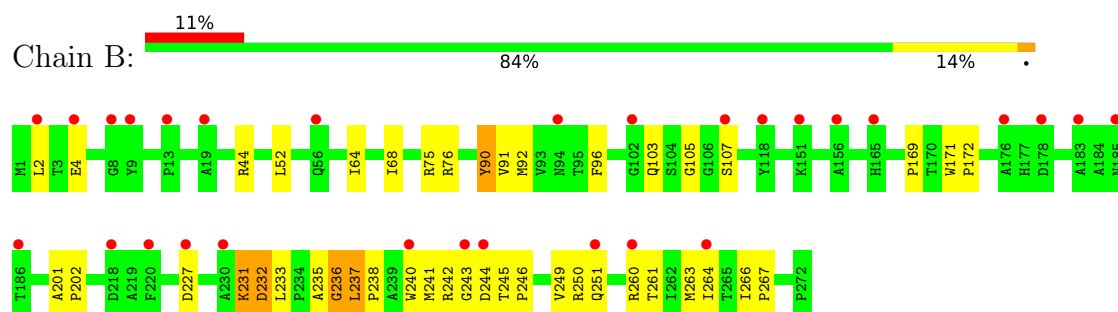
- Molecule 1: Blr0248 protein



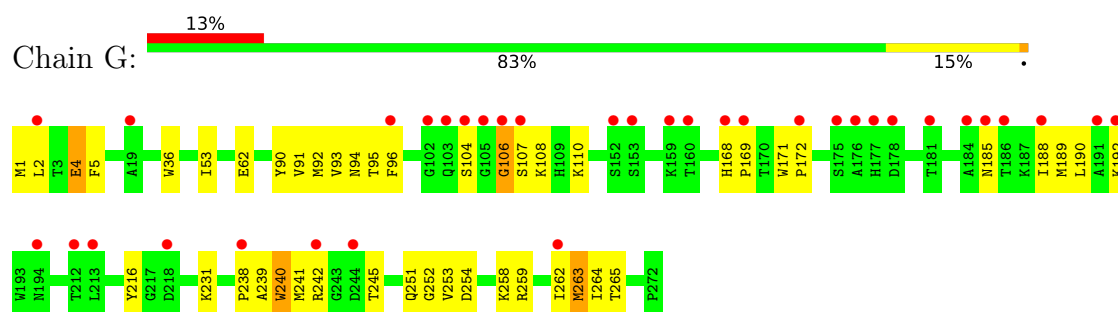
- Molecule 1: Blr0248 protein



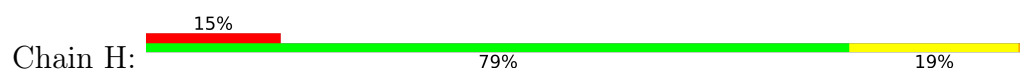
- Molecule 1: Blr0248 protein

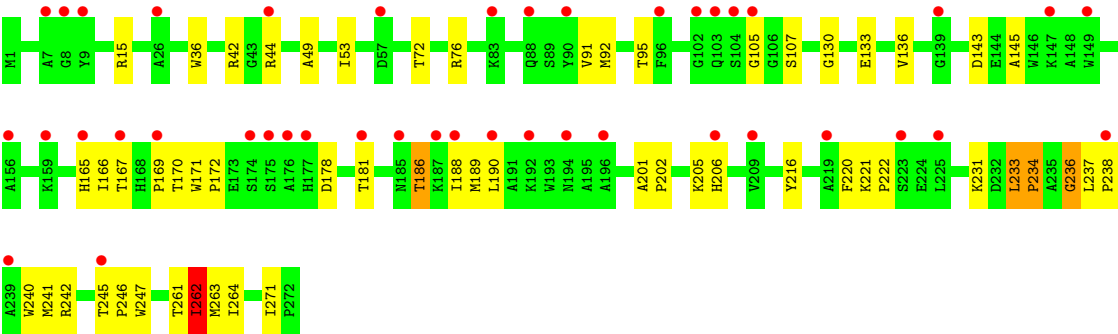


- Molecule 1: Blr0248 protein



- Molecule 1: Blr0248 protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	209.54Å 89.63Å 143.78Å 90.00° 96.20° 90.00°	Depositor
Resolution (Å)	29.62 – 2.87 29.62 – 2.87	Depositor EDS
% Data completeness (in resolution range)	83.2 (29.62-2.87) 83.1 (29.62-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.85Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.251 , 0.302 0.274 , 0.318	Depositor DCC
R_{free} test set	2000 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.899	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	32863	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.52 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.5452e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.75	9/2155 (0.4%)	0.79	3/2932 (0.1%)
1	B	0.78	11/2155 (0.5%)	0.80	4/2932 (0.1%)
1	C	0.78	7/2155 (0.3%)	0.83	3/2932 (0.1%)
1	D	1.04	11/2155 (0.5%)	0.90	7/2932 (0.2%)
1	E	0.87	12/2155 (0.6%)	0.78	1/2932 (0.0%)
1	F	0.72	8/2155 (0.4%)	0.84	5/2932 (0.2%)
1	G	1.00	13/2155 (0.6%)	0.83	3/2932 (0.1%)
1	H	0.96	12/2155 (0.6%)	0.89	10/2932 (0.3%)
All	All	0.87	83/17240 (0.5%)	0.83	36/23456 (0.2%)

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	PRO	N-CD	-22.11	1.16	1.47
1	D	172	PRO	N-CD	-11.28	1.31	1.47
1	B	264	ILE	C-O	-8.93	1.14	1.24
1	C	112	GLU	C-N	8.79	1.40	1.33
1	H	264	ILE	C-O	-8.78	1.14	1.24
1	E	262	ILE	C-O	-8.20	1.15	1.24
1	D	262	ILE	C-O	-7.90	1.16	1.24
1	G	245	THR	C-O	-7.79	1.14	1.24
1	H	262	ILE	C-O	-7.31	1.16	1.24
1	B	232	ASP	C-O	-6.97	1.14	1.23
1	E	166	ILE	C-O	-6.93	1.15	1.23
1	C	264	ILE	C-O	-6.91	1.16	1.24
1	H	247	TRP	C-O	-6.85	1.16	1.24
1	H	236	GLY	C-O	-6.79	1.14	1.23
1	G	245	THR	CA-C	-6.59	1.43	1.52
1	G	4	GLU	C-O	-6.58	1.15	1.23
1	D	166	ILE	C-O	-6.53	1.17	1.24
1	E	20	ASN	C-O	-6.37	1.16	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	264	ILE	C-O	-6.35	1.16	1.24
1	A	93	VAL	C-O	-6.34	1.17	1.24
1	B	261	THR	C-O	-6.34	1.16	1.24
1	F	92	MSE	CA-C	-6.17	1.44	1.52
1	F	237	LEU	CA-C	-6.17	1.46	1.53
1	H	261	THR	C-O	-6.14	1.16	1.24
1	D	168	HIS	C-O	-6.14	1.16	1.24
1	B	235	ALA	CA-C	-6.14	1.44	1.52
1	E	93	VAL	C-O	-6.11	1.17	1.23
1	A	262	ILE	C-O	-5.96	1.18	1.24
1	B	231	LYS	CA-C	-5.86	1.44	1.52
1	E	193	TRP	C-O	-5.80	1.17	1.24
1	D	180	ALA	CA-C	-5.80	1.46	1.52
1	D	89	SER	C-O	-5.79	1.17	1.23
1	H	264	ILE	CA-C	-5.78	1.45	1.52
1	D	263	MSE	CA-C	-5.75	1.45	1.52
1	F	93	VAL	C-O	-5.74	1.17	1.24
1	C	94	ASN	C-O	-5.72	1.16	1.23
1	G	95	THR	C-O	-5.70	1.17	1.24
1	G	264	ILE	C-O	-5.70	1.17	1.24
1	F	245	THR	C-N	5.66	1.41	1.33
1	H	245	THR	C-N	5.64	1.40	1.33
1	E	265	THR	C-O	-5.62	1.17	1.24
1	C	90	TYR	C-O	-5.60	1.17	1.23
1	B	237	LEU	CA-C	-5.59	1.45	1.52
1	A	261	THR	C-O	-5.58	1.16	1.23
1	G	240	TRP	CA-C	-5.58	1.45	1.52
1	D	165	HIS	C-O	-5.57	1.17	1.23
1	E	192	LYS	CA-C	-5.55	1.45	1.52
1	H	231	LYS	CA-C	-5.54	1.44	1.52
1	H	246	PRO	C-O	-5.53	1.17	1.23
1	F	262	ILE	C-O	-5.52	1.18	1.24
1	H	231	LYS	C-O	-5.49	1.17	1.24
1	C	237	LEU	CA-C	-5.49	1.47	1.53
1	E	243	GLY	C-O	-5.47	1.17	1.23
1	B	90	TYR	C-O	-5.42	1.16	1.23
1	A	264	ILE	C-O	-5.41	1.17	1.24
1	B	246	PRO	N-CD	5.40	1.55	1.47
1	F	246	PRO	N-CD	5.39	1.55	1.47
1	A	4	GLU	C-O	-5.39	1.16	1.23
1	F	90	TYR	C-O	-5.37	1.17	1.23
1	B	267	PRO	N-CD	5.37	1.55	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	95	THR	CB-CG2	-5.37	1.34	1.52
1	A	4	GLU	CA-C	-5.37	1.45	1.53
1	H	233	LEU	C-N	5.35	1.40	1.33
1	F	267	PRO	N-CD	5.33	1.55	1.47
1	A	94	ASN	C-O	-5.33	1.17	1.23
1	G	94	ASN	C-O	-5.32	1.16	1.23
1	G	265	THR	C-O	-5.31	1.18	1.23
1	B	236	GLY	C-O	-5.30	1.16	1.24
1	C	261	THR	C-O	-5.21	1.17	1.23
1	D	168	HIS	CA-C	-5.18	1.47	1.52
1	E	95	THR	CB-CG2	-5.17	1.35	1.52
1	B	96	PHE	C-O	-5.17	1.17	1.24
1	C	113	PRO	N-CD	5.16	1.54	1.47
1	E	191	ALA	C-O	-5.16	1.18	1.24
1	G	94	ASN	CA-C	-5.15	1.46	1.53
1	G	91	VAL	C-O	-5.15	1.19	1.24
1	G	93	VAL	C-O	-5.14	1.18	1.24
1	D	261	THR	C-O	-5.13	1.17	1.23
1	H	222	PRO	N-CD	5.12	1.54	1.47
1	E	192	LYS	C-O	-5.09	1.17	1.24
1	G	90	TYR	C-O	-5.07	1.17	1.23
1	A	189	MSE	CA-C	-5.07	1.46	1.52
1	A	265	THR	C-O	-5.01	1.18	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	240	TRP	N-CA-C	-8.64	102.87	113.50
1	D	103	GLN	N-CA-C	-8.34	102.66	113.17
1	D	104	SER	N-CA-C	-7.40	102.22	111.11
1	H	233	LEU	CA-C-N	-7.06	113.44	120.21
1	H	233	LEU	C-N-CA	-7.06	113.44	120.21
1	F	245	THR	CA-C-N	-6.79	112.97	119.89
1	F	245	THR	C-N-CA	-6.79	112.97	119.89
1	G	106	GLY	N-CA-C	-6.61	106.66	115.32
1	C	112	GLU	CA-C-N	-6.42	113.28	121.04
1	C	112	GLU	C-N-CA	-6.42	113.28	121.04
1	D	176	ALA	N-CA-C	6.14	118.51	109.24
1	D	105	GLY	N-CA-C	6.07	122.32	112.61
1	H	246	PRO	CA-N-CD	-6.00	103.60	112.00
1	F	265	THR	N-CA-C	5.77	117.81	108.34
1	D	169	PRO	N-CD-CG	5.65	111.67	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	186	THR	N-CA-C	-5.59	104.68	112.45
1	H	221	LYS	CA-C-N	-5.56	113.94	119.56
1	H	221	LYS	C-N-CA	-5.56	113.94	119.56
1	B	245	THR	CA-C-N	-5.49	112.98	119.84
1	B	245	THR	C-N-CA	-5.49	112.98	119.84
1	F	266	ILE	CA-C-N	-5.48	112.99	119.84
1	F	266	ILE	C-N-CA	-5.48	112.99	119.84
1	B	266	ILE	CA-C-N	-5.48	112.99	119.84
1	B	266	ILE	C-N-CA	-5.48	112.99	119.84
1	A	263	MSE	N-CA-C	5.41	117.72	108.90
1	D	240	TRP	N-CA-C	-5.33	106.63	113.23
1	H	234	PRO	CA-N-CD	-5.31	104.56	112.00
1	E	263	MSE	N-CA-C	5.29	117.14	108.52
1	D	172	PRO	N-CD-CG	5.29	111.13	103.20
1	G	263	MSE	N-CA-CB	-5.28	102.27	110.57
1	A	237	LEU	CA-C-N	-5.17	115.27	120.85
1	A	237	LEU	C-N-CA	-5.17	115.27	120.85
1	H	245	THR	CA-C-N	-5.17	114.66	120.14
1	H	245	THR	C-N-CA	-5.17	114.66	120.14
1	C	240	TRP	N-CA-C	-5.14	106.95	113.18
1	H	264	ILE	N-CA-C	-5.09	101.15	108.53

There are no chirality outliers.

There are no planarity outliers.

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	2099	2025	2072	39	0
1	B	2099	1974	2072	44	0
1	C	2099	1983	2072	77	0
1	D	2099	2004	2072	72	0
1	E	2099	2018	2072	42	0
1	F	2099	2011	2072	48	0
1	G	2099	1985	2072	49	0
1	H	2099	1975	2072	59	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	8	4	3	2	0
2	B	8	4	3	0	0
2	C	8	4	3	0	0
2	D	8	4	3	0	0
2	E	8	4	3	0	0
2	F	8	4	3	1	0
2	G	8	4	3	1	0
2	H	8	4	3	0	0
All	All	16856	16007	16600	385	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (385) 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:H:53:ILE:HB	1:H:92:MSE:HG2	1.23	1.10
1:C:61:HIS:O	1:C:70:VAL:CG2	2.06	1.02
1:D:53:ILE:HB	1:D:92:MSE:HG2	1.41	1.01
1:A:53:ILE:HB	1:A:92:MSE:HG2	1.44	0.97
1:G:53:ILE:HB	1:G:92:MSE:HG2	1.42	0.97
1:G:263:MSE:SE	1:H:263:MSE:HB2	2.17	0.94
1:D:68:ILE:HD11	1:D:92:MSE:O	1.68	0.93
1:H:42:ARG:NH2	1:H:92:MSE:HE1	1.84	0.92
1:C:238:PRO:HG2	1:C:241:MSE:HG3	1.50	0.91
1:D:42:ARG:CZ	1:D:92:MSE:HE1	2.01	0.91
1:E:167:THR:HB	1:E:189:MSE:HG3	1.53	0.89
1:F:75:ARG:NH2	1:F:244:ASP:HB3	1.88	0.88
1:A:263:MSE:SE	1:B:263:MSE:HG3	2.25	0.86
1:C:249:VAL:CG2	1:C:263:MSE:HE2	2.05	0.86
1:E:263:MSE:SE	1:F:263:MSE:HG3	2.25	0.86
1:G:2:LEU:HD11	1:G:4:GLU:HG2	1.55	0.85
1:D:176:ALA:O	1:D:182:GLN:NE2	2.10	0.83
1:C:238:PRO:HB2	1:C:240:TRP:CD1	2.14	0.83
1:D:146:TRP:CD1	1:D:163:TYR:CD1	2.66	0.83
1:G:2:LEU:CD1	1:G:4:GLU:HG2	2.10	0.82
1:H:240:TRP:CH2	1:H:241:MSE:HE3	2.17	0.79
1:F:2:LEU:HD13	1:F:3:THR:N	1.96	0.79
1:D:178:ASP:OD1	1:D:181:THR:OG1	2.01	0.78
1:D:238:PRO:HB2	1:D:240:TRP:CD1	2.18	0.78
1:H:240:TRP:CZ3	1:H:241:MSE:HG3	2.19	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ASN:OD1	1:H:205:LYS:NZ	2.18	0.77
1:C:15:ARG:HG3	1:D:5:PHE:CZ	2.21	0.76
1:C:61:HIS:O	1:C:70:VAL:HG21	1.85	0.75
1:C:61:HIS:O	1:C:70:VAL:HG23	1.85	0.75
1:C:230:ALA:HB2	1:C:242:ARG:NH2	2.01	0.75
1:E:252:GLY:C	1:B:263:MSE:HE1	2.12	0.74
1:E:186:THR:O	1:E:190:LEU:HG	1.87	0.74
1:H:42:ARG:CZ	1:H:92:MSE:HE1	2.17	0.74
1:B:44:ARG:NH1	1:B:232:ASP:OD1	2.21	0.74
1:B:90:TYR:OH	1:B:232:ASP:OD2	2.04	0.73
1:E:242:ARG:HG3	1:E:242:ARG:O	1.88	0.73
1:H:42:ARG:HH21	1:H:92:MSE:HE1	1.53	0.73
1:G:2:LEU:HD11	1:G:4:GLU:CG	2.18	0.72
1:D:171:TRP:CD1	1:D:175:SER:HG	2.07	0.72
1:D:90:TYR:CE1	1:D:92:MSE:HE2	2.24	0.72
1:D:166:ILE:HD11	1:D:196:ALA:CB	2.21	0.71
1:F:238:PRO:HB2	1:F:240:TRP:CD1	2.26	0.71
1:E:42:ARG:NH2	1:E:78:GLN:OE1	2.25	0.70
1:B:44:ARG:NH2	1:B:232:ASP:OD1	2.25	0.70
1:E:241:MSE:HE3	1:E:247:TRP:CH2	2.26	0.70
1:A:263:MSE:SE	1:B:263:MSE:CG	2.90	0.70
1:G:168:HIS:O	1:G:189:MSE:HE1	1.92	0.69
1:D:143:ASP:HA	1:D:163:TYR:OH	1.92	0.69
1:F:2:LEU:HD22	1:F:3:THR:H	1.58	0.69
1:H:53:ILE:CB	1:H:92:MSE:HG2	2.14	0.69
1:F:91:VAL:HG12	1:F:92:MSE:N	2.08	0.68
1:G:96:PHE:CE2	1:G:106:GLY:HA3	2.29	0.68
1:E:65:VAL:HG22	1:E:241:MSE:HE2	1.75	0.67
1:D:166:ILE:HD11	1:D:196:ALA:HB2	1.76	0.67
1:H:105:GLY:C	1:H:107:SER:H	2.03	0.67
1:D:238:PRO:CG	1:D:240:TRP:NE1	2.57	0.67
1:H:240:TRP:HH2	1:H:241:MSE:HE3	1.59	0.67
1:D:42:ARG:NH2	1:D:92:MSE:HE1	2.09	0.67
1:F:2:LEU:O	1:F:3:THR:HG23	1.94	0.67
1:C:249:VAL:HG23	1:C:263:MSE:HE2	1.76	0.67
1:D:139:GLY:O	1:D:165:HIS:HE1	1.78	0.67
1:F:2:LEU:HD13	1:F:2:LEU:C	2.19	0.66
1:D:89:SER:OG	1:D:208:ASP:OD1	2.09	0.66
1:H:44:ARG:N	1:H:91:VAL:HG22	2.10	0.66
1:C:238:PRO:HB2	1:C:240:TRP:NE1	2.11	0.66
1:E:178:ASP:HA	1:B:103:GLN:HE21	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:107:SER:HA	1:G:110:LYS:HE2	1.78	0.65
1:H:44:ARG:O	1:H:91:VAL:HG21	1.96	0.65
1:G:253:VAL:HG13	1:G:254:ASP:N	2.10	0.65
1:B:238:PRO:HG3	1:B:240:TRP:NE1	2.11	0.65
1:F:75:ARG:CZ	1:F:244:ASP:HB3	2.25	0.65
1:B:250:ARG:O	1:B:251:GLN:NE2	2.30	0.65
1:C:105:GLY:O	1:C:141:LEU:HD11	1.96	0.65
1:D:139:GLY:O	1:D:165:HIS:CE1	2.50	0.64
1:G:36:TRP:CH2	1:G:262:ILE:HD12	2.32	0.64
1:H:44:ARG:H	1:H:91:VAL:HG22	1.62	0.64
1:C:9:TYR:HE1	1:C:41:HIS:ND1	1.94	0.64
1:C:230:ALA:HB2	1:C:242:ARG:HH21	1.63	0.64
1:B:105:GLY:C	1:B:107:SER:H	2.04	0.63
1:D:171:TRP:NE1	1:D:175:SER:OG	2.32	0.63
1:C:233:LEU:HD22	1:C:242:ARG:HD3	1.80	0.63
1:D:190:LEU:HD13	1:D:216:TYR:HB3	1.80	0.63
1:E:2:LEU:HD12	1:E:2:LEU:O	1.99	0.63
1:E:252:GLY:CA	1:B:263:MSE:HE1	2.29	0.62
1:A:77:THR:HG21	1:A:92:MSE:HE2	1.80	0.62
1:G:104:SER:HB2	1:G:108:LYS:HE2	1.81	0.62
1:D:143:ASP:HB2	1:D:165:HIS:ND1	2.14	0.62
1:D:171:TRP:N	1:D:172:PRO:CD	2.63	0.62
1:G:188:ILE:O	1:G:192:LYS:HG3	2.00	0.62
1:F:92:MSE:O	1:F:93:VAL:HG23	2.00	0.62
1:F:112:GLU:OE1	1:F:112:GLU:N	2.32	0.62
1:B:238:PRO:CG	1:B:240:TRP:NE1	2.63	0.62
1:F:2:LEU:O	1:F:3:THR:CG2	2.48	0.61
1:B:2:LEU:HD12	1:B:2:LEU:C	2.25	0.61
1:D:176:ALA:HB3	1:D:182:GLN:HG2	1.82	0.61
1:G:2:LEU:CD1	1:G:4:GLU:CG	2.77	0.61
1:H:188:ILE:O	1:H:188:ILE:HG22	2.01	0.61
1:C:238:PRO:O	1:C:241:MSE:HB2	2.00	0.61
1:D:133:GLU:OE2	1:D:206:HIS:ND1	2.33	0.61
1:G:239:ALA:HA	1:G:242:ARG:NH1	2.16	0.61
1:H:170:THR:HG22	1:H:170:THR:O	2.01	0.61
1:C:15:ARG:HG3	1:D:5:PHE:HZ	1.66	0.60
1:E:42:ARG:NH1	1:E:69:LEU:O	2.34	0.60
1:B:238:PRO:HD2	1:B:241:MSE:SE	2.50	0.60
1:F:238:PRO:HB2	1:F:240:TRP:NE1	2.16	0.60
1:H:72:THR:O	1:H:76:ARG:HG3	2.01	0.60
1:C:237:LEU:HG	1:C:241:MSE:SE	2.51	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:VAL:HG12	1:F:92:MSE:H	1.64	0.60
1:F:251:GLN:OE1	1:F:263:MSE:SE	2.70	0.60
1:C:190:LEU:HD13	1:C:216:TYR:HB3	1.83	0.60
1:E:53:ILE:HG13	1:E:92:MSE:HE2	1.84	0.60
1:H:171:TRP:N	1:H:172:PRO:CD	2.64	0.60
1:G:36:TRP:CZ3	1:G:262:ILE:HD12	2.37	0.60
1:C:4:GLU:CD	1:C:231:LYS:HB2	2.28	0.59
1:D:238:PRO:HG3	1:D:240:TRP:NE1	2.17	0.59
1:D:238:PRO:HG3	1:D:240:TRP:HE1	1.68	0.59
1:G:172:PRO:HD3	1:G:189:MSE:HE3	1.84	0.59
1:E:90:TYR:OH	1:E:232:ASP:OD2	2.20	0.59
1:A:271:ILE:HD12	1:B:260:ARG:HG2	1.82	0.59
1:H:36:TRP:CH2	1:H:262:ILE:HG13	2.38	0.59
1:C:249:VAL:CG2	1:C:263:MSE:CE	2.80	0.59
1:B:238:PRO:HG3	1:B:240:TRP:HE1	1.67	0.59
1:D:49:ALA:HB1	1:D:91:VAL:HG23	1.84	0.59
1:A:53:ILE:HG13	1:A:92:MSE:HE2	1.84	0.59
1:D:29:PRO:O	1:D:259:ARG:NH2	2.36	0.58
1:G:263:MSE:SE	1:H:263:MSE:CB	2.97	0.58
1:H:44:ARG:O	1:H:91:VAL:CG2	2.52	0.58
1:C:9:TYR:HE1	1:C:41:HIS:HD1	1.49	0.58
1:D:53:ILE:CB	1:D:92:MSE:HG2	2.26	0.58
1:A:42:ARG:NH2	1:A:69:LEU:O	2.36	0.58
1:G:5:PHE:CE1	1:H:15:ARG:HG3	2.38	0.58
1:C:101:TYR:CZ	1:C:259:ARG:HD2	2.38	0.58
1:E:263:MSE:SE	1:F:263:MSE:CG	3.01	0.58
1:F:190:LEU:HD22	1:F:216:TYR:CG	2.39	0.58
1:G:168:HIS:CD2	1:G:169:PRO:HD2	2.38	0.58
1:F:182:GLN:O	1:F:186:THR:OG1	2.21	0.57
1:G:96:PHE:CZ	1:G:106:GLY:HA3	2.39	0.57
1:H:49:ALA:HB2	1:H:91:VAL:HG23	1.87	0.57
1:F:265:THR:CB	1:A:253:VAL:HG21	2.34	0.57
1:C:238:PRO:CB	1:C:240:TRP:NE1	2.67	0.57
1:C:65:VAL:HG13	1:C:233:LEU:HG	1.87	0.56
1:C:187:LYS:HD2	1:C:190:LEU:HB2	1.87	0.56
1:D:238:PRO:HD2	1:D:241:MSE:SE	2.54	0.56
1:E:2:LEU:HD12	1:E:2:LEU:C	2.30	0.56
1:F:75:ARG:CZ	1:F:244:ASP:CB	2.83	0.56
1:G:252:GLY:O	1:G:258:LYS:HE3	2.05	0.56
1:H:234:PRO:HD2	1:H:237:LEU:CD1	2.35	0.56
1:G:168:HIS:O	1:G:189:MSE:CE	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ILE:CD1	1:D:92:MSE:O	2.50	0.56
1:A:35:GLU:O	1:B:240:TRP:NE1	2.33	0.56
1:B:68:ILE:HD11	1:B:92:MSE:C	2.31	0.56
1:H:186:THR:HG23	1:H:189:MSE:HE2	1.88	0.55
1:H:234:PRO:HD2	1:H:237:LEU:HD11	1.88	0.55
1:E:263:MSE:SE	1:F:263:MSE:HA	2.56	0.55
1:A:77:THR:CG2	1:A:92:MSE:HE2	2.35	0.55
1:B:4:GLU:CD	1:B:231:LYS:HB2	2.32	0.55
1:C:105:GLY:O	1:C:141:LEU:CD1	2.55	0.55
1:G:5:PHE:CZ	1:H:15:ARG:HG3	2.41	0.55
1:G:172:PRO:HD3	1:G:189:MSE:CE	2.37	0.55
1:H:238:PRO:HB2	1:H:240:TRP:CD1	2.42	0.55
1:E:178:ASP:HA	1:B:103:GLN:NE2	2.21	0.55
1:A:76:ARG:NH1	1:A:169:PRO:O	2.40	0.55
1:H:172:PRO:CD	1:H:189:MSE:SE	3.05	0.55
1:E:238:PRO:O	1:E:241:MSE:HB2	2.07	0.55
1:G:253:VAL:CG1	1:G:254:ASP:N	2.70	0.55
1:F:2:LEU:C	1:F:3:THR:HG23	2.31	0.54
1:F:265:THR:OG1	1:A:253:VAL:HG21	2.08	0.54
1:B:249:VAL:HG22	1:B:251:GLN:HE21	1.71	0.54
1:G:62:GLU:CD	2:G:301:URA:H5	2.15	0.54
1:A:62:GLU:CD	2:A:301:URA:H5	2.15	0.54
1:G:107:SER:HA	1:G:110:LYS:CE	2.37	0.54
1:E:252:GLY:C	1:B:263:MSE:CE	2.81	0.54
1:A:89:SER:OG	1:A:208:ASP:OD1	2.15	0.54
1:C:107:SER:O	1:C:110:LYS:HG2	2.08	0.54
1:C:186:THR:HG22	1:C:218:ASP:O	2.08	0.54
1:C:2:LEU:CD1	1:D:20:ASN:CG	2.81	0.54
1:D:178:ASP:O	1:D:182:GLN:HG3	2.07	0.54
1:H:42:ARG:NH2	1:H:92:MSE:CE	2.67	0.54
1:F:4:GLU:OE2	1:F:231:LYS:HE2	2.08	0.53
1:G:238:PRO:HB2	1:G:240:TRP:CD1	2.43	0.53
1:H:49:ALA:CB	1:H:91:VAL:HG23	2.39	0.53
1:H:172:PRO:CG	1:H:189:MSE:SE	3.06	0.53
1:D:90:TYR:OH	1:D:232:ASP:OD2	2.18	0.53
1:C:20:ASN:CG	1:D:2:LEU:HD12	2.33	0.53
1:F:91:VAL:O	1:F:92:MSE:HG2	2.09	0.53
1:F:103:GLN:HG3	1:A:177:HIS:ND1	2.24	0.53
1:F:171:TRP:CZ3	1:F:185:ASN:HB3	2.43	0.53
1:C:183:ALA:O	1:C:186:THR:OG1	2.23	0.53
1:E:64:ILE:HG22	1:E:241:MSE:HE1	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:GLU:OE1	1:C:231:LYS:HB2	2.09	0.53
1:G:53:ILE:HG13	1:G:92:MSE:HE2	1.90	0.53
1:F:103:GLN:O	1:F:103:GLN:HG2	2.08	0.52
1:E:242:ARG:O	1:E:242:ARG:CG	2.55	0.52
1:F:265:THR:HB	1:A:253:VAL:HG21	1.91	0.52
1:C:20:ASN:ND2	1:D:2:LEU:HD12	2.24	0.52
1:E:190:LEU:HD12	1:E:218:ASP:O	2.10	0.52
1:C:9:TYR:CE1	1:C:41:HIS:ND1	2.77	0.52
1:C:180:ALA:O	1:C:184:ALA:N	2.40	0.52
1:A:237:LEU:HD13	1:A:241:MSE:SE	2.60	0.52
1:A:271:ILE:HD12	1:B:260:ARG:CG	2.40	0.51
1:G:168:HIS:CG	1:G:169:PRO:HD2	2.45	0.51
1:D:146:TRP:CD1	1:D:163:TYR:CE1	2.99	0.51
1:B:44:ARG:CZ	1:B:232:ASP:OD1	2.57	0.51
1:A:42:ARG:NH1	1:A:78:GLN:OE1	2.43	0.51
1:D:49:ALA:CB	1:D:91:VAL:CG2	2.89	0.51
1:E:190:LEU:HD12	1:E:218:ASP:C	2.36	0.51
1:C:263:MSE:HA	1:D:263:MSE:SE	2.60	0.51
1:D:68:ILE:HD11	1:D:92:MSE:C	2.36	0.51
1:H:42:ARG:NE	1:H:92:MSE:HE1	2.25	0.50
1:H:76:ARG:NH1	1:H:169:PRO:O	2.43	0.50
1:B:233:LEU:HD23	1:B:237:LEU:HD12	1.91	0.50
1:D:166:ILE:CD1	1:D:196:ALA:HB2	2.40	0.50
1:B:4:GLU:OE2	1:B:231:LYS:HB2	2.12	0.50
1:G:36:TRP:CH2	1:G:262:ILE:CD1	2.94	0.50
1:E:261:THR:HA	1:F:264:ILE:O	2.12	0.50
1:F:91:VAL:C	1:F:92:MSE:CG	2.85	0.50
1:A:77:THR:HG21	1:A:92:MSE:CE	2.42	0.50
1:H:233:LEU:HD22	1:H:242:ARG:HD3	1.94	0.50
1:G:238:PRO:HD2	1:G:241:MSE:SE	2.61	0.50
1:F:75:ARG:NH2	1:F:244:ASP:CB	2.69	0.49
1:D:206:HIS:NE2	1:H:130:GLY:O	2.35	0.49
1:H:172:PRO:HD3	1:H:189:MSE:SE	2.63	0.49
1:E:97:LEU:HD11	1:E:118:TYR:CE2	2.47	0.49
1:F:238:PRO:CB	1:F:240:TRP:NE1	2.75	0.49
1:E:86:ILE:HG23	1:E:89:SER:O	2.12	0.49
1:H:133:GLU:CD	1:H:205:LYS:H	2.19	0.49
1:B:105:GLY:C	1:B:107:SER:N	2.70	0.49
1:H:136:VAL:CG1	1:H:166:ILE:HG12	2.43	0.49
1:E:86:ILE:CG2	1:E:89:SER:O	2.60	0.49
1:B:52:LEU:HD13	1:B:91:VAL:HG13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:TRP:CZ3	1:B:241:MSE:HG2	2.48	0.49
1:F:10:GLY:O	1:F:15:ARG:NH1	2.46	0.48
1:G:1:MSE:N	1:G:2:LEU:CA	2.76	0.48
1:C:187:LYS:HD3	1:C:218:ASP:HA	1.95	0.48
1:C:240:TRP:NE1	1:D:35:GLU:O	2.43	0.48
1:D:139:GLY:C	1:D:165:HIS:HE1	2.21	0.48
1:F:2:LEU:HD22	1:F:3:THR:N	2.27	0.48
1:C:187:LYS:HE2	1:C:191:ALA:HB2	1.94	0.48
1:H:42:ARG:CZ	1:H:92:MSE:CE	2.89	0.48
1:A:190:LEU:O	1:A:193:TRP:HB2	2.13	0.48
1:C:228:ILE:O	1:C:242:ARG:HD2	2.14	0.48
1:F:44:ARG:NH2	1:F:232:ASP:OD1	2.45	0.47
1:H:36:TRP:CZ2	1:H:262:ILE:HG13	2.49	0.47
1:A:237:LEU:HD22	1:A:241:MSE:SE	2.65	0.47
1:H:95:THR:HG23	1:H:145:ALA:HB2	1.96	0.47
1:D:90:TYR:CD1	1:D:92:MSE:HE2	2.48	0.47
1:B:76:ARG:NH1	1:B:169:PRO:O	2.47	0.47
1:H:238:PRO:HG3	1:H:240:TRP:CE2	2.49	0.47
1:E:168:HIS:CG	1:E:169:PRO:HD2	2.50	0.47
1:D:188:ILE:HG22	1:D:192:LYS:HE3	1.97	0.47
1:E:133:GLU:OE2	1:E:206:HIS:ND1	2.43	0.47
1:E:90:TYR:CD1	1:E:90:TYR:C	2.92	0.47
1:A:263:MSE:SE	1:B:263:MSE:CB	3.12	0.47
1:C:261:THR:CG2	1:D:263:MSE:HE3	2.45	0.47
1:H:178:ASP:OD1	1:H:181:THR:OG1	2.31	0.47
1:G:263:MSE:SE	1:H:263:MSE:SE	3.34	0.46
1:D:65:VAL:HG22	1:D:241:MSE:HE2	1.96	0.46
1:H:167:THR:OG1	1:H:189:MSE:HG3	2.16	0.46
1:H:238:PRO:HG3	1:H:240:TRP:CZ2	2.50	0.46
1:A:77:THR:CG2	1:A:92:MSE:CE	2.92	0.46
1:A:263:MSE:SE	1:B:263:MSE:HB2	2.66	0.46
1:C:81:LEU:HD22	1:C:86:ILE:HD11	1.97	0.46
1:E:238:PRO:HB2	1:E:240:TRP:CD1	2.51	0.46
1:B:236:GLY:O	1:B:237:LEU:C	2.58	0.46
1:H:143:ASP:HB2	1:H:165:HIS:HD2	1.81	0.46
1:B:64:ILE:HG22	1:B:241:MSE:HE1	1.98	0.46
1:B:227:ASP:OD1	1:B:243:GLY:O	2.33	0.45
1:C:68:ILE:O	1:C:69:LEU:HB2	2.17	0.45
1:C:73:ALA:O	1:C:77:THR:HG23	2.16	0.45
1:F:55:GLY:HA3	1:F:94:ASN:OD1	2.16	0.45
1:C:234:PRO:HG2	1:C:237:LEU:HD22	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:VAL:HG21	1:C:263:MSE:CE	2.46	0.45
1:E:251:GLN:OE1	1:B:251:GLN:HB3	2.17	0.45
1:C:249:VAL:HG21	1:C:263:MSE:HE2	1.95	0.45
1:F:2:LEU:C	1:F:2:LEU:CD1	2.90	0.45
1:C:4:GLU:OE2	1:C:231:LYS:HE3	2.16	0.45
1:C:110:LYS:HG3	1:C:111:ASN:OD1	2.17	0.45
1:E:16:ASP:O	1:E:20:ASN:HB2	2.16	0.45
1:E:171:TRP:N	1:E:172:PRO:CD	2.80	0.45
1:C:20:ASN:OD1	1:D:2:LEU:CD1	2.65	0.45
1:A:164:GLN:HG2	1:A:196:ALA:HB1	1.98	0.45
1:G:171:TRP:HZ3	1:G:185:ASN:O	1.99	0.45
1:G:252:GLY:HA3	1:G:258:LYS:HG2	1.99	0.45
1:D:146:TRP:CD1	1:D:163:TYR:CG	3.04	0.44
1:A:69:LEU:HD13	1:A:92:MSE:SE	2.67	0.44
1:C:50:ARG:HB3	1:C:133:GLU:OE2	2.17	0.44
1:G:4:GLU:OE1	1:G:231:LYS:HE3	2.18	0.44
1:G:251:GLN:HB2	1:G:263:MSE:HG3	2.00	0.44
1:C:9:TYR:CE1	1:C:41:HIS:CE1	3.06	0.44
1:D:128:GLY:O	1:H:206:HIS:NE2	2.50	0.44
1:G:171:TRP:N	1:G:172:PRO:CD	2.80	0.44
1:G:190:LEU:HD13	1:G:216:TYR:HB3	2.00	0.44
1:D:166:ILE:CD1	1:D:196:ALA:CB	2.95	0.44
1:G:4:GLU:OE1	1:G:231:LYS:CE	2.66	0.44
1:G:263:MSE:SE	1:H:263:MSE:CG	3.15	0.44
1:H:190:LEU:HD13	1:H:216:TYR:HB3	1.99	0.44
1:F:94:ASN:ND2	2:F:301:URA:N3	2.65	0.44
1:H:76:ARG:HD3	1:H:220:PHE:CZ	2.53	0.44
1:C:164:GLN:HB2	1:C:200:LEU:HD11	2.00	0.44
1:F:91:VAL:CG1	1:F:92:MSE:N	2.80	0.44
1:A:190:LEU:O	1:A:193:TRP:N	2.50	0.44
1:C:107:SER:C	1:C:109:HIS:N	2.75	0.44
1:F:171:TRP:N	1:F:172:PRO:CD	2.81	0.44
1:A:190:LEU:HD21	1:A:220:PHE:CZ	2.54	0.43
1:C:190:LEU:O	1:C:193:TRP:HB2	2.17	0.43
1:E:239:ALA:HA	1:E:242:ARG:NH1	2.34	0.43
1:C:34:ILE:HA	1:C:98:TYR:CD1	2.54	0.43
1:D:238:PRO:HG2	1:D:241:MSE:HG3	1.99	0.43
1:E:34:ILE:HA	1:E:98:TYR:CD1	2.54	0.43
1:F:95:THR:HG23	1:F:119:ARG:NH1	2.32	0.43
1:G:188:ILE:O	1:G:192:LYS:CG	2.64	0.43
1:H:201:ALA:N	1:H:202:PRO:HD2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:103:GLN:NE2	1:A:177:HIS:O	2.51	0.43
1:D:171:TRP:NE1	1:D:175:SER:HG	2.07	0.43
1:F:42:ARG:NH2	1:F:92:MSE:HE1	2.33	0.43
1:G:251:GLN:CB	1:G:263:MSE:HG3	2.48	0.43
1:C:230:ALA:CB	1:C:242:ARG:NH2	2.77	0.43
1:E:85:GLY:O	1:E:208:ASP:N	2.51	0.43
1:H:171:TRP:N	1:H:172:PRO:HD2	2.33	0.43
1:C:59:ALA:N	1:C:62:GLU:OE1	2.48	0.43
1:C:78:GLN:HB3	1:C:226:VAL:HB	2.00	0.43
1:C:4:GLU:HG3	1:C:230:ALA:HB3	2.01	0.43
1:C:171:TRP:N	1:C:172:PRO:CD	2.82	0.43
1:A:69:LEU:N	2:A:301:URA:O4	2.43	0.43
1:B:75:ARG:NH2	1:B:244:ASP:HB3	2.34	0.43
1:H:240:TRP:CE3	1:H:241:MSE:HG3	2.53	0.43
1:D:49:ALA:CB	1:D:91:VAL:HG23	2.48	0.43
1:D:262:ILE:HD13	1:D:262:ILE:HG21	1.84	0.43
1:B:171:TRP:N	1:B:172:PRO:CD	2.82	0.43
1:H:238:PRO:CG	1:H:240:TRP:CE2	3.01	0.43
1:D:201:ALA:N	1:D:202:PRO:HD2	2.34	0.42
1:G:253:VAL:CG1	1:G:254:ASP:H	2.32	0.42
1:C:60:GLN:HG2	1:C:61:HIS:N	2.35	0.42
1:D:165:HIS:O	1:D:166:ILE:HD13	2.19	0.42
1:D:177:HIS:ND1	1:D:178:ASP:N	2.66	0.42
1:A:34:ILE:HA	1:A:98:TYR:CD1	2.55	0.42
1:G:263:MSE:HE3	1:G:263:MSE:HB3	1.89	0.42
1:D:137:SER:HB3	1:D:163:TYR:CE1	2.54	0.42
1:A:164:GLN:HG3	1:A:166:ILE:HG23	2.01	0.42
1:A:171:TRP:N	1:A:172:PRO:CD	2.83	0.42
1:G:242:ARG:O	1:G:242:ARG:HG3	2.20	0.42
1:C:262:ILE:HG21	1:C:262:ILE:HD13	1.86	0.42
1:E:100:VAL:HG13	1:E:105:GLY:HA3	2.01	0.42
1:F:53:ILE:O	1:F:92:MSE:HA	2.19	0.42
1:H:236:GLY:O	1:H:237:LEU:C	2.62	0.42
1:F:251:GLN:OE1	1:A:251:GLN:HG3	2.19	0.42
1:B:103:GLN:HG2	1:B:103:GLN:O	2.19	0.42
1:C:20:ASN:OD1	1:D:2:LEU:HD12	2.20	0.42
1:C:39:ILE:HG23	1:C:66:ARG:C	2.45	0.42
1:C:39:ILE:HG23	1:C:66:ARG:O	2.20	0.42
1:G:259:ARG:HD3	1:H:271:ILE:HD13	2.02	0.42
1:C:31:ASP:OD2	1:C:109:HIS:NE2	2.49	0.41
1:C:183:ALA:C	1:C:186:THR:HG1	2.26	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:168:HIS:O	1:G:169:PRO:C	2.63	0.41
1:H:172:PRO:HG2	1:H:189:MSE:SE	2.70	0.41
1:D:53:ILE:HD11	1:D:81:LEU:HD21	2.01	0.41
1:E:143:ASP:HB2	1:E:165:HIS:CD2	2.55	0.41
1:E:201:ALA:N	1:E:202:PRO:CD	2.84	0.41
1:B:2:LEU:C	1:B:2:LEU:CD1	2.91	0.41
1:C:15:ARG:HG3	1:D:5:PHE:CE1	2.56	0.41
1:C:108:LYS:HB2	1:C:109:HIS:CD2	2.56	0.41
1:C:36:TRP:HB3	1:C:63:THR:HG23	2.03	0.41
1:C:53:ILE:HD11	1:C:81:LEU:HD21	2.03	0.41
1:C:113:PRO:O	1:C:117:ASP:OD2	2.39	0.41
1:E:10:GLY:O	1:E:15:ARG:NH1	2.50	0.41
1:F:42:ARG:NE	1:F:69:LEU:O	2.53	0.41
1:B:201:ALA:N	1:B:202:PRO:HD2	2.36	0.41
1:D:94:ASN:O	1:D:95:THR:C	2.62	0.41
1:D:151:LYS:HG2	1:D:151:LYS:O	2.21	0.41
1:A:97:LEU:HD21	1:A:118:TYR:CE2	2.56	0.41
1:A:103:GLN:N	1:A:103:GLN:OE1	2.54	0.41
1:C:117:ASP:O	1:C:121:LYS:HG3	2.20	0.41
1:D:241:MSE:HA	1:D:247:TRP:NE1	2.36	0.41
1:C:39:ILE:HG12	1:C:62:GLU:O	2.21	0.40
1:F:2:LEU:C	1:F:3:THR:CG2	2.94	0.40
1:D:95:THR:CG2	1:D:119:ARG:NH1	2.84	0.40
1:D:264:ILE:HD13	1:D:264:ILE:HG21	1.86	0.40
1:A:88:GLN:HA	1:A:90:TYR:CE2	2.57	0.40
1:A:237:LEU:HB3	1:A:241:MSE:SE	2.71	0.40
1:C:263:MSE:HB2	1:D:263:MSE:SE	2.71	0.40
1:D:88:GLN:O	1:D:90:TYR:N	2.51	0.40
1:B:233:LEU:HD23	1:B:237:LEU:CD1	2.51	0.40
1:C:242:ARG:HG3	1:C:242:ARG:O	2.22	0.40
1:B:75:ARG:NE	1:B:227:ASP:OD1	2.53	0.40
1:B:227:ASP:HB3	1:B:242:ARG:O	2.22	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	270/272 (99%)	256 (95%)	14 (5%)	0	100	100
1	B	270/272 (99%)	254 (94%)	16 (6%)	0	100	100
1	C	270/272 (99%)	254 (94%)	16 (6%)	0	100	100
1	D	270/272 (99%)	257 (95%)	13 (5%)	0	100	100
1	E	270/272 (99%)	257 (95%)	13 (5%)	0	100	100
1	F	270/272 (99%)	254 (94%)	16 (6%)	0	100	100
1	G	270/272 (99%)	254 (94%)	16 (6%)	0	100	100
1	H	270/272 (99%)	250 (93%)	20 (7%)	0	100	100
All	All	2160/2176 (99%)	2036 (94%)	124 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	213/208 (102%)	212 (100%)	1 (0%)	81	90
1	B	213/208 (102%)	213 (100%)	0	100	100
1	C	213/208 (102%)	213 (100%)	0	100	100
1	D	213/208 (102%)	212 (100%)	1 (0%)	81	90
1	E	213/208 (102%)	212 (100%)	1 (0%)	81	90
1	F	213/208 (102%)	213 (100%)	0	100	100
1	G	213/208 (102%)	213 (100%)	0	100	100
1	H	213/208 (102%)	212 (100%)	1 (0%)	81	90
All	All	1704/1664 (102%)	1700 (100%)	4 (0%)	87	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	91	VAL
1	E	265	THR
1	A	263	MSE
1	H	262	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	165	HIS
1	D	251	GLN
1	E	30	HIS
1	E	88	GLN
1	E	165	HIS
1	F	56	GLN
1	F	131	ASN
1	A	185	ASN
1	B	20	ASN
1	B	185	ASN
1	G	164	GLN
1	G	185	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	URA	G	301	-	8,8,8	1.73	2 (25%)	10,10,10	3.19	6 (60%)
2	URA	H	301	-	8,8,8	1.73	2 (25%)	10,10,10	3.18	6 (60%)
2	URA	B	301	-	8,8,8	1.72	2 (25%)	10,10,10	3.20	6 (60%)
2	URA	F	301	-	8,8,8	1.74	2 (25%)	10,10,10	3.18	6 (60%)
2	URA	E	301	-	8,8,8	1.73	2 (25%)	10,10,10	3.17	6 (60%)
2	URA	C	301	-	8,8,8	1.73	2 (25%)	10,10,10	3.18	6 (60%)
2	URA	D	301	-	8,8,8	1.71	2 (25%)	10,10,10	3.19	6 (60%)
2	URA	A	301	-	8,8,8	1.72	2 (25%)	10,10,10	3.18	6 (60%)

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	URA	G	301	-	-	-	0/1/1/1
2	URA	H	301	-	-	-	0/1/1/1
2	URA	B	301	-	-	-	0/1/1/1
2	URA	F	301	-	-	-	0/1/1/1
2	URA	E	301	-	-	-	0/1/1/1
2	URA	C	301	-	-	-	0/1/1/1
2	URA	D	301	-	-	-	0/1/1/1
2	URA	A	301	-	-	-	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	URA	C4-N3	-2.65	1.34	1.38
2	B	301	URA	C4-N3	-2.62	1.34	1.38
2	H	301	URA	C4-N3	-2.61	1.34	1.38
2	C	301	URA	C4-N3	-2.61	1.34	1.38
2	A	301	URA	C4-N3	-2.60	1.34	1.38
2	D	301	URA	C4-N3	-2.60	1.34	1.38
2	F	301	URA	C4-N3	-2.58	1.34	1.38
2	G	301	URA	C4-N3	-2.55	1.34	1.38
2	F	301	URA	C5-C4	-2.12	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	301	URA	C5-C4	-2.12	1.39	1.43
2	H	301	URA	C5-C4	-2.11	1.39	1.43
2	E	301	URA	C5-C4	-2.07	1.39	1.43
2	A	301	URA	C5-C4	-2.07	1.39	1.43
2	B	301	URA	C5-C4	-2.07	1.39	1.43
2	C	301	URA	C5-C4	-2.07	1.39	1.43
2	D	301	URA	C5-C4	-2.06	1.39	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	URA	N1-C2-N3	5.69	121.17	115.17
2	B	301	URA	N1-C2-N3	5.68	121.16	115.17
2	C	301	URA	N1-C2-N3	5.67	121.15	115.17
2	D	301	URA	N1-C2-N3	5.66	121.14	115.17
2	F	301	URA	N1-C2-N3	5.66	121.14	115.17
2	A	301	URA	N1-C2-N3	5.66	121.14	115.17
2	H	301	URA	N1-C2-N3	5.65	121.13	115.17
2	E	301	URA	N1-C2-N3	5.62	121.10	115.17
2	G	301	URA	C4-N3-C2	-5.18	120.53	125.55
2	B	301	URA	C4-N3-C2	-5.16	120.55	125.55
2	H	301	URA	C4-N3-C2	-5.13	120.58	125.55
2	D	301	URA	C4-N3-C2	-5.12	120.58	125.55
2	C	301	URA	C4-N3-C2	-5.12	120.59	125.55
2	F	301	URA	C4-N3-C2	-5.11	120.60	125.55
2	A	301	URA	C4-N3-C2	-5.10	120.61	125.55
2	E	301	URA	C4-N3-C2	-5.08	120.62	125.55
2	B	301	URA	C5-C4-N3	3.33	119.46	114.80
2	D	301	URA	C5-C4-N3	3.32	119.44	114.80
2	H	301	URA	C5-C4-N3	3.32	119.44	114.80
2	A	301	URA	C5-C4-N3	3.31	119.44	114.80
2	G	301	URA	C5-C4-N3	3.31	119.44	114.80
2	F	301	URA	C5-C4-N3	3.30	119.42	114.80
2	E	301	URA	C5-C4-N3	3.30	119.42	114.80
2	D	301	URA	O2-C2-N1	-3.29	119.39	122.79
2	A	301	URA	O2-C2-N1	-3.28	119.41	122.79
2	C	301	URA	C5-C4-N3	3.28	119.39	114.80
2	E	301	URA	O2-C2-N1	-3.28	119.41	122.79
2	B	301	URA	O2-C2-N1	-3.26	119.43	122.79
2	H	301	URA	O2-C2-N1	-3.24	119.45	122.79
2	G	301	URA	O2-C2-N1	-3.24	119.45	122.79
2	C	301	URA	O2-C2-N1	-3.23	119.45	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	URA	O2-C2-N1	-3.23	119.46	122.79
2	B	301	URA	C6-N1-C2	-3.01	120.56	122.40
2	D	301	URA	C6-N1-C2	-3.00	120.56	122.40
2	C	301	URA	C6-N1-C2	-2.94	120.60	122.40
2	A	301	URA	C6-N1-C2	-2.94	120.60	122.40
2	F	301	URA	C6-N1-C2	-2.93	120.60	122.40
2	G	301	URA	C6-N1-C2	-2.92	120.61	122.40
2	H	301	URA	C6-N1-C2	-2.88	120.63	122.40
2	E	301	URA	C6-N1-C2	-2.88	120.63	122.40
2	E	301	URA	O4-C4-C5	-2.86	120.23	125.16
2	A	301	URA	O4-C4-C5	-2.86	120.24	125.16
2	B	301	URA	O4-C4-C5	-2.83	120.28	125.16
2	D	301	URA	O4-C4-C5	-2.83	120.28	125.16
2	F	301	URA	O4-C4-C5	-2.83	120.28	125.16
2	C	301	URA	O4-C4-C5	-2.82	120.30	125.16
2	G	301	URA	O4-C4-C5	-2.81	120.31	125.16
2	H	301	URA	O4-C4-C5	-2.81	120.32	125.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	301	URA	1	0
2	F	301	URA	1	0
2	A	301	URA	2	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, 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	267/272 (98%)	0.97	28 (10%) 11 9	12, 27, 56, 80	0
1	B	267/272 (98%)	0.89	29 (10%) 10 8	11, 24, 43, 71	0
1	C	267/272 (98%)	1.25	43 (16%) 4 4	12, 28, 49, 73	0
1	D	267/272 (98%)	0.75	21 (7%) 18 14	8, 19, 38, 78	0
1	E	267/272 (98%)	0.63	13 (4%) 35 27	4, 16, 35, 65	0
1	F	267/272 (98%)	1.16	47 (17%) 4 3	9, 30, 50, 80	0
1	G	267/272 (98%)	0.99	35 (13%) 7 5	10, 26, 55, 79	0
1	H	267/272 (98%)	1.02	42 (15%) 5 4	14, 29, 46, 93	0
All	All	2136/2176 (98%)	0.96	258 (12%) 8 6	4, 25, 47, 93	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	LEU	6.9
1	B	102	GLY	6.6
1	F	3	THR	5.7
1	B	2	LEU	5.6
1	H	188	ILE	5.4
1	B	156	ALA	5.1
1	C	61	HIS	4.9
1	D	103	GLN	4.6
1	G	106	GLY	4.6
1	E	251	GLN	4.6
1	F	103	GLN	4.6
1	E	177	HIS	4.5
1	G	177	HIS	4.4
1	F	177	HIS	4.4
1	C	65	VAL	4.3
1	A	192	LYS	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	184	ALA	4.3
1	E	104	SER	4.2
1	A	104	SER	4.1
1	G	169	PRO	4.0
1	D	102	GLY	4.0
1	G	185	ASN	4.0
1	F	104	SER	3.9
1	E	102	GLY	3.8
1	A	177	HIS	3.8
1	B	19	ALA	3.8
1	H	176	ALA	3.7
1	F	212	THR	3.7
1	F	251	GLN	3.7
1	F	169	PRO	3.6
1	C	212	THR	3.6
1	H	102	GLY	3.6
1	F	174	SER	3.6
1	A	19	ALA	3.6
1	C	113	PRO	3.6
1	C	183	ALA	3.5
1	F	106	GLY	3.5
1	G	107	SER	3.5
1	H	90	TYR	3.5
1	F	2	LEU	3.4
1	C	133	GLU	3.4
1	A	218	ASP	3.4
1	F	164	GLN	3.4
1	G	105	GLY	3.4
1	D	240	TRP	3.3
1	G	104	SER	3.3
1	H	181	THR	3.3
1	G	238	PRO	3.2
1	G	103	GLN	3.2
1	H	103	GLN	3.2
1	F	178	ASP	3.2
1	G	184	ALA	3.2
1	H	219	ALA	3.2
1	E	106	GLY	3.2
1	A	105	GLY	3.2
1	H	88	GLN	3.1
1	A	191	ALA	3.1
1	G	102	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	30	HIS	3.1
1	A	178	ASP	3.1
1	H	147	LYS	3.1
1	C	177	HIS	3.1
1	C	3	THR	3.0
1	F	107	SER	3.0
1	B	8	GLY	3.0
1	H	139	GLY	3.0
1	G	19	ALA	3.0
1	F	176	ALA	3.0
1	E	140	GLY	3.0
1	B	240	TRP	2.9
1	B	56	GLN	2.9
1	C	218	ASP	2.9
1	H	174	SER	2.9
1	C	121	LYS	2.9
1	C	186	THR	2.9
1	H	187	LYS	2.9
1	A	102	GLY	2.9
1	H	177	HIS	2.8
1	B	185	ASN	2.8
1	G	2	LEU	2.8
1	G	186	THR	2.8
1	E	2	LEU	2.8
1	H	206	HIS	2.8
1	A	20	ASN	2.8
1	C	178	ASP	2.8
1	B	218	ASP	2.8
1	A	3	THR	2.8
1	C	111	ASN	2.8
1	F	95	THR	2.8
1	A	232	ASP	2.8
1	B	107	SER	2.8
1	D	4	GLU	2.7
1	D	161	LEU	2.7
1	C	4	GLU	2.7
1	C	196	ALA	2.7
1	G	218	ASP	2.7
1	H	223	SER	2.7
1	C	240	TRP	2.7
1	B	251	GLN	2.7
1	C	213	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	77	THR	2.7
1	F	47	GLY	2.7
1	F	267	PRO	2.7
1	F	99	SER	2.7
1	H	104	SER	2.7
1	D	167	THR	2.6
1	D	181	THR	2.6
1	B	227	ASP	2.6
1	D	176	ALA	2.6
1	C	103	GLN	2.6
1	C	168	HIS	2.6
1	B	13	PRO	2.6
1	D	56	GLN	2.6
1	F	94	ASN	2.6
1	H	156	ALA	2.6
1	H	239	ALA	2.6
1	H	238	PRO	2.6
1	G	191	ALA	2.6
1	C	175	SER	2.5
1	H	169	PRO	2.5
1	E	253	VAL	2.5
1	F	199	ALA	2.5
1	C	86	ILE	2.5
1	F	21	TYR	2.5
1	H	44	ARG	2.5
1	G	172	PRO	2.5
1	H	105	GLY	2.5
1	C	193	TRP	2.5
1	C	156	ALA	2.5
1	F	167	THR	2.5
1	B	230	ALA	2.5
1	F	159	LYS	2.5
1	F	238	PRO	2.5
1	C	106	GLY	2.5
1	G	96	PHE	2.5
1	F	181	THR	2.5
1	G	244	ASP	2.4
1	A	156	ALA	2.4
1	G	159	LYS	2.4
1	H	192	LYS	2.4
1	D	166	ILE	2.4
1	G	188	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	104	SER	2.4
1	A	164	GLN	2.4
1	G	194	ASN	2.4
1	G	262	ILE	2.4
1	C	85	GLY	2.4
1	E	105	GLY	2.4
1	F	105	GLY	2.4
1	G	178	ASP	2.4
1	E	199	ALA	2.4
1	G	176	ALA	2.4
1	G	212	THR	2.4
1	C	210	PRO	2.4
1	F	214	VAL	2.4
1	D	28	ASP	2.4
1	C	11	GLU	2.4
1	A	107	SER	2.4
1	A	270	VAL	2.3
1	B	183	ALA	2.3
1	A	88	GLN	2.3
1	D	107	SER	2.3
1	G	153	SER	2.3
1	H	175	SER	2.3
1	C	167	THR	2.3
1	G	213	LEU	2.3
1	G	242	ARG	2.3
1	C	79	GLY	2.3
1	H	194	ASN	2.3
1	B	4	GLU	2.3
1	B	244	ASP	2.3
1	H	26	ALA	2.3
1	C	141	LEU	2.3
1	G	168	HIS	2.3
1	B	260	ARG	2.3
1	C	105	GLY	2.3
1	B	94	ASN	2.3
1	F	26	ALA	2.3
1	F	84	LEU	2.3
1	E	89	SER	2.3
1	H	149	TRP	2.3
1	H	159	LYS	2.3
1	A	100	VAL	2.3
1	C	102	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	269	GLY	2.3
1	B	264	ILE	2.3
1	H	245	THR	2.3
1	F	220	PHE	2.2
1	A	103	GLN	2.2
1	B	178	ASP	2.2
1	C	41	HIS	2.2
1	B	186	THR	2.2
1	F	209	VAL	2.2
1	A	219	ALA	2.2
1	C	190	LEU	2.2
1	A	159	LYS	2.2
1	C	171	TRP	2.2
1	F	72	THR	2.2
1	F	113	PRO	2.2
1	H	96	PHE	2.2
1	C	176	ALA	2.2
1	F	166	ILE	2.2
1	H	165	HIS	2.2
1	F	244	ASP	2.2
1	H	57	ASP	2.2
1	H	209	VAL	2.2
1	F	48	SER	2.2
1	B	151	LYS	2.2
1	F	213	LEU	2.2
1	F	225	LEU	2.2
1	H	225	LEU	2.2
1	F	191	ALA	2.2
1	H	196	ALA	2.2
1	A	185	ASN	2.2
1	F	154	ASP	2.2
1	B	243	GLY	2.2
1	H	83	LYS	2.2
1	F	239	ALA	2.2
1	A	157	ALA	2.2
1	A	188	ILE	2.1
1	E	30	HIS	2.1
1	H	185	ASN	2.1
1	H	8	GLY	2.1
1	B	118	TYR	2.1
1	C	204	VAL	2.1
1	G	192	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	180	ALA	2.1
1	F	196	ALA	2.1
1	B	9	TYR	2.1
1	B	176	ALA	2.1
1	H	9	TYR	2.1
1	C	53	ILE	2.1
1	F	203	GLU	2.1
1	G	152	SER	2.1
1	D	185	ASN	2.1
1	F	22	PRO	2.1
1	B	220	PHE	2.1
1	D	163	TYR	2.1
1	A	224	GLU	2.1
1	G	175	SER	2.1
1	D	177	HIS	2.1
1	B	165	HIS	2.1
1	D	58	PRO	2.1
1	D	2	LEU	2.1
1	E	190	LEU	2.1
1	G	160	THR	2.1
1	H	7	ALA	2.1
1	F	38	PRO	2.0
1	H	167	THR	2.0
1	D	93	VAL	2.0
1	D	253	VAL	2.0
1	F	202	PRO	2.0
1	H	190	LEU	2.0
1	F	5	PHE	2.0
1	D	19	ALA	2.0
1	A	195	ALA	2.0
1	G	181	THR	2.0
1	D	6	ASP	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	URA	B	301	8/8	0.84	0.14	12,17,21,25	0
2	URA	F	301	8/8	0.88	0.13	20,26,32,36	0
2	URA	A	301	8/8	0.88	0.14	18,22,29,30	0
2	URA	D	301	8/8	0.88	0.17	8,11,18,22	0
2	URA	E	301	8/8	0.91	0.12	7,13,20,22	0
2	URA	C	301	8/8	0.93	0.13	11,16,24,25	0
2	URA	G	301	8/8	0.93	0.12	9,14,18,19	0
2	URA	H	301	8/8	0.95	0.09	12,21,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.