



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 09:57 AM EDT

PDB ID : 6EWN
Title : HspA from *Thermosynechococcus vulcanus* in the presence of 2M urea with initial stages of denaturation
Authors : Adir, N.; Ghosh, S.; Salama, F.; Dines, M.
Deposited on : 2017-11-06
Resolution : 2.29 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

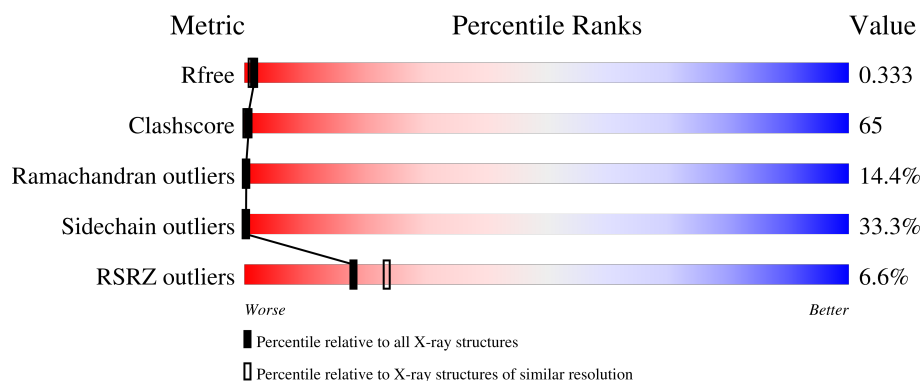
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	99	
1	B	99	

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	URE	A	201	-	X	-	-
2	URE	A	202	-	X	X	-
2	URE	A	203	-	X	X	-
2	URE	A	204	-	X	-	-
2	URE	A	205	-	X	-	-
2	URE	A	206	-	X	-	-
2	URE	A	207	-	X	-	-
2	URE	A	211	-	X	X	-
2	URE	A	212	-	X	-	-
2	URE	A	213	-	X	-	-
2	URE	A	214	-	X	-	-
2	URE	A	215	-	X	-	-
2	URE	B	202	-	-	X	-
2	URE	B	204	-	-	X	-
2	URE	B	205	-	X	-	-
2	URE	B	206	-	X	-	-
2	URE	B	207	-	X	-	-
2	URE	B	208	-	X	-	-
2	URE	B	209	-	X	-	-
2	URE	B	210	-	X	-	-
2	URE	B	211	-	-	X	-
2	URE	B	212	-	X	-	-
2	URE	B	213	-	X	-	-
2	URE	B	214	-	X	-	-
2	URE	B	215	-	X	-	-
2	URE	B	216	-	X	-	-
2	URE	B	218	-	X	X	-
2	URE	B	219	-	X	-	-
2	URE	B	221	-	X	-	-
2	URE	B	222	-	X	-	-
2	URE	B	223	-	-	X	-
2	URE	B	224	-	X	-	-
2	URE	B	225	-	X	-	-
2	URE	B	227	-	X	-	-

2 Entry composition [i](#)

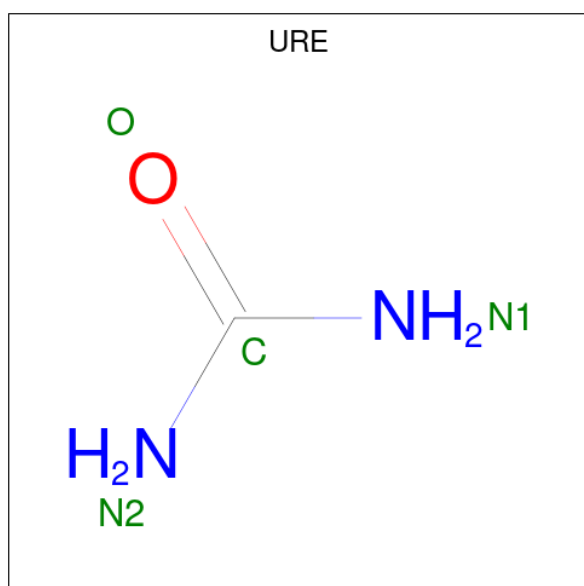
There are 3 unique types of molecules in this entry. The entry contains 1858 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HspA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	99	Total	C	N	O	S	0	4	0
			804	511	133	156	4			
1	B	99	Total	C	N	O	S	0	0	0
			780	493	129	156	2			

- Molecule 2 is UREA (three-letter code: URE) (formula: CH₄N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			4	1	2	1		
2	A	1	Total	C	N	O	0	0
			4	1	2	1		
2	A	1	Total	C	N	O	0	0
			4	1	2	1		
2	A	1	Total	C	N	O	0	0
			4	1	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	A	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0
2	B	1	Total 4	C 1	N 2	O 1	0	0

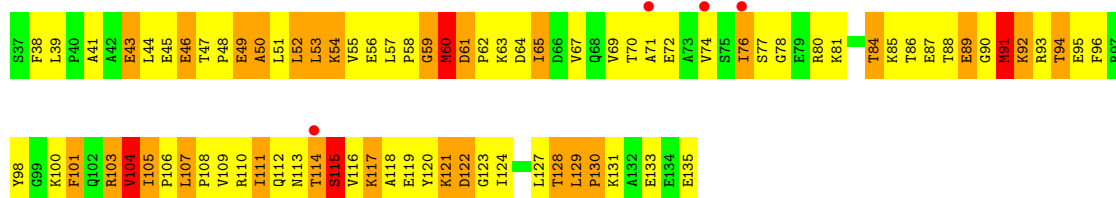
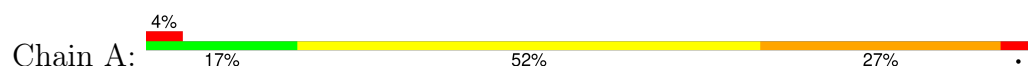
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total 45	O 45	0	0
3	B	53	Total 53	O 53	0	0

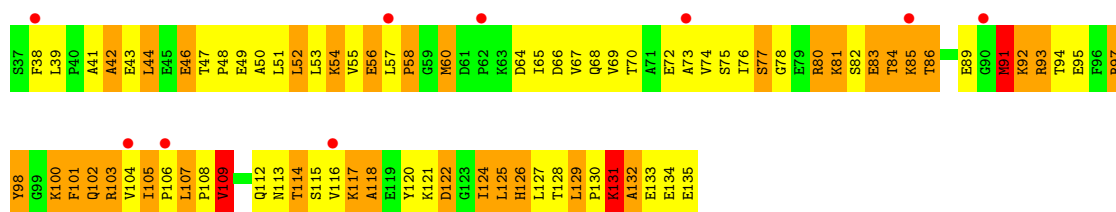
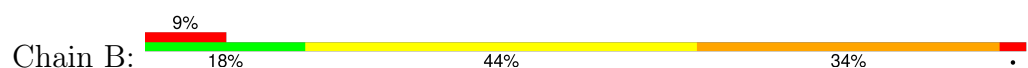
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: HspA



• Molecule 1: HspA



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	88.65Å 88.65Å 114.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.03 – 2.29 42.23 – 2.29	Depositor EDS
% Data completeness (in resolution range)	100.0 (70.03-2.29) 99.6 (42.23-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.58 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.280 , 0.342 0.297 , 0.333	Depositor DCC
R_{free} test set	1011 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	9.5	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 114.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.166 for -h,k,-l	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	1858	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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, 0.333 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: URE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.03	4/828 (0.5%)	1.07	8/1114 (0.7%)
1	B	1.12	8/792 (1.0%)	1.04	5/1069 (0.5%)
All	All	1.07	12/1620 (0.7%)	1.06	13/2183 (0.6%)

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	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	133	GLU	C-O	-10.45	1.03	1.23
1	A	91[A]	MET	CA-C	10.21	1.79	1.52
1	A	91[B]	MET	CA-C	10.21	1.79	1.52
1	B	131	LYS	C-O	-9.96	1.04	1.23
1	B	132	ALA	C-O	-9.20	1.05	1.23
1	A	60[A]	MET	N-CA	8.20	1.62	1.46
1	A	60[B]	MET	N-CA	8.20	1.62	1.46
1	B	133	GLU	CD-OE1	-8.15	1.16	1.25
1	B	131	LYS	CB-CG	-6.86	1.34	1.52
1	B	133	GLU	CD-OE2	-6.76	1.18	1.25
1	B	91	MET	CG-SD	-6.41	1.64	1.81
1	B	91	MET	C-O	-6.34	1.11	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91[A]	MET	CA-C-N	-8.13	99.31	117.20
1	A	91[B]	MET	CA-C-N	-8.13	99.31	117.20
1	B	131	LYS	CG-CD-CE	6.95	132.74	111.90
1	B	131	LYS	C-N-CA	6.74	138.54	121.70
1	A	90	GLY	C-N-CA	6.19	137.17	121.70
1	B	91	MET	CA-CB-CG	6.05	123.59	113.30
1	B	91	MET	CB-CG-SD	5.80	129.80	112.40
1	A	60[A]	MET	CA-C-O	5.53	131.72	120.10
1	A	60[B]	MET	CA-C-O	5.53	131.72	120.10
1	A	60[A]	MET	CA-C-N	-5.23	105.70	117.20
1	A	60[B]	MET	CA-C-N	-5.23	105.70	117.20
1	B	66	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	103	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91[A]	MET	Mainchain
1	A	91[B]	MET	Mainchain

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	804	0	839	120	2
1	B	780	0	794	104	2
2	A	64	0	64	9	0
2	B	112	0	112	16	0
3	A	45	0	0	8	0
3	B	53	0	0	10	0
All	All	1858	0	1809	233	2

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 65.

All (233) 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:131:LYS:NZ	2:B:202:URE:O	1.63	1.30
1:A:44:LEU:N	3:A:301:HOH:O	1.87	1.05
1:B:83:GLU:OE2	1:B:85:LYS:NZ	1.96	0.98
2:B:223:URE:N2	3:B:301:HOH:O	1.97	0.97
1:B:131:LYS:NZ	1:B:132:ALA:O	1.97	0.96
2:B:205:URE:N1	3:B:302:HOH:O	1.99	0.91
1:B:131:LYS:HZ3	2:B:202:URE:C	1.84	0.89
1:A:96:PHE:O	2:A:202:URE:N1	2.07	0.88
2:A:207:URE:O	3:A:302:HOH:O	1.94	0.86
1:A:91[A]:MET:CA	1:A:92:LYS:N	2.40	0.85
1:A:59:GLY:O	1:A:60[B]:MET:CG	2.26	0.84
1:A:59:GLY:O	1:A:60[B]:MET:HG3	1.79	0.83
1:A:91[B]:MET:CA	1:A:92:LYS:N	2.42	0.82
1:B:53:LEU:O	1:B:126:HIS:HB2	1.80	0.81
1:B:47:THR:OG1	1:B:50:ALA:O	1.97	0.81
2:B:227:URE:N2	3:B:304:HOH:O	2.13	0.81
1:B:76:ILE:O	1:B:103:ARG:N	2.13	0.80
2:A:209:URE:O	2:A:211:URE:N2	2.16	0.79
1:B:42:ALA:O	3:B:303:HOH:O	2.01	0.78
1:B:95:GLU:O	1:B:97:ARG:NH2	2.18	0.77
1:A:94:THR:O	1:A:96:PHE:N	2.18	0.76
1:B:91:MET:O	1:B:93:ARG:N	2.19	0.75
1:B:74:VAL:O	1:B:104:VAL:HA	1.87	0.75
1:B:42:ALA:HA	1:B:54:LYS:O	1.87	0.74
1:B:46:GLU:HA	1:B:51:LEU:HG	1.68	0.74
1:A:77:SER:HA	1:A:101:PHE:O	1.89	0.72
1:B:108:PRO:O	1:B:109:VAL:HG13	1.90	0.71
1:A:59:GLY:C	1:A:60[A]:MET:HG2	2.11	0.71
1:B:52:LEU:O	1:B:53:LEU:HD12	1.91	0.71
1:B:53:LEU:HD21	1:B:105:ILE:HG21	1.74	0.70
2:B:211:URE:N2	3:B:305:HOH:O	2.17	0.70
1:A:57:LEU:HD21	1:A:101:PHE:CE1	2.26	0.70
1:A:60[A]:MET:HB3	1:A:64:ASP:HB3	1.74	0.70
1:A:86:THR:O	1:A:89:GLU:HG2	1.92	0.69
1:A:51:LEU:HB2	1:A:129:LEU:O	1.92	0.69
1:A:122:ASP:OD2	3:A:303:HOH:O	2.10	0.68
1:A:59:GLY:C	1:A:60[B]:MET:HG3	2.13	0.67
1:A:44:LEU:HD22	1:A:105:ILE:HG21	1.76	0.67
1:B:41:ALA:O	1:B:54:LYS:O	2.13	0.67
1:B:73:ALA:HA	1:B:105:ILE:O	1.94	0.67
1:B:48:PRO:O	1:B:131:LYS:HD3	1.94	0.66
1:A:49:GLU:N	1:A:49:GLU:OE1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:210:URE:N2	3:A:307:HOH:O	2.29	0.65
1:A:112:GLN:O	1:A:116:VAL:HG23	1.97	0.64
1:A:117:LYS:HE2	1:A:117:LYS:HA	1.79	0.64
1:B:46:GLU:OE1	2:B:218:URE:N2	2.31	0.64
1:A:59:GLY:O	1:A:60[A]:MET:HG2	1.97	0.64
1:B:77:SER:HB3	1:B:101:PHE:O	1.98	0.63
1:B:81:LYS:HE2	1:B:82:SER:H	1.62	0.63
1:A:39:LEU:HD13	1:A:56:GLU:HB3	1.80	0.63
1:B:107:LEU:H	1:B:107:LEU:HD12	1.62	0.63
1:A:114:THR:OG1	1:A:115:SER:N	2.31	0.63
1:B:72:GLU:O	1:B:107:LEU:HD12	1.99	0.63
1:B:56:GLU:C	1:B:57:LEU:HD22	2.21	0.61
1:B:52:LEU:HA	1:B:127:LEU:O	2.00	0.61
2:B:212:URE:O	2:B:218:URE:N2	2.32	0.61
1:A:60[B]:MET:HB3	1:A:64:ASP:CB	2.31	0.61
2:B:217:URE:N1	3:B:307:HOH:O	2.29	0.61
1:B:76:ILE:HB	1:B:103:ARG:HB2	1.81	0.61
1:A:128:THR:O	1:A:130:PRO:HD3	2.01	0.60
1:A:114:THR:O	1:A:116:VAL:N	2.34	0.60
1:A:45:GLU:O	1:A:46:GLU:HB2	2.02	0.60
1:B:80:ARG:HG2	1:B:81:LYS:H	1.67	0.59
1:A:46:GLU:OE2	1:A:131:LYS:NZ	2.27	0.59
1:A:60[B]:MET:HB3	1:A:64:ASP:HB3	1.85	0.59
1:A:107:LEU:HD23	1:A:108:PRO:HD2	1.84	0.58
1:A:53:LEU:HD11	1:A:105:ILE:HD12	1.85	0.58
1:A:60[A]:MET:HB3	1:A:64:ASP:CB	2.33	0.58
1:B:92:LYS:N	3:B:309:HOH:O	2.35	0.58
1:A:53:LEU:HD23	1:A:54:LYS:O	2.03	0.57
1:A:49:GLU:O	1:A:50:ALA:HB2	2.04	0.57
1:A:106:PRO:HD3	2:A:215:URE:C	2.35	0.56
1:A:118:ALA:O	1:A:119:GLU:HG2	2.05	0.56
1:B:85:LYS:O	1:B:86:THR:C	2.43	0.56
1:A:44:LEU:HD12	1:A:52:LEU:O	2.06	0.55
1:A:69:VAL:HG21	1:A:111:ILE:HD13	1.88	0.55
1:A:67:VAL:O	2:A:203:URE:O	2.23	0.55
1:B:56:GLU:HG3	1:B:58:PRO:HD3	1.87	0.55
1:A:57:LEU:CD2	1:A:101:PHE:CE1	2.90	0.55
1:A:78:GLY:O	1:A:100:LYS:HA	2.07	0.55
1:A:55:VAL:HG12	1:A:57:LEU:HG	1.88	0.54
1:A:76:ILE:HB	1:A:103:ARG:HB3	1.88	0.54
1:A:121:LYS:HB2	3:A:319:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:C	1:B:98:TYR:CD1	2.81	0.54
1:A:41:ALA:HB3	1:A:56:GLU:HB2	1.89	0.54
1:B:116:VAL:HG13	1:B:128:THR:O	2.07	0.54
1:B:104:VAL:O	1:B:105:ILE:HG22	2.08	0.54
1:B:49:GLU:O	1:B:50:ALA:HB2	2.08	0.54
1:A:51:LEU:HD13	1:A:107:LEU:HD21	1.90	0.53
1:A:67:VAL:O	2:A:203:URE:C	2.56	0.53
1:B:60:MET:CA	1:B:80:ARG:HG3	2.39	0.53
1:A:43:GLU:OE1	1:A:45:GLU:OE2	2.26	0.53
1:A:53:LEU:HD23	1:A:54:LYS:N	2.23	0.53
1:B:46:GLU:HG3	1:B:46:GLU:O	2.08	0.53
1:B:83:GLU:O	1:B:85:LYS:N	2.35	0.53
1:A:59:GLY:C	1:A:60[B]:MET:CG	2.76	0.53
1:A:112:GLN:OE1	1:A:112:GLN:HA	2.09	0.53
1:A:62:PRO:HA	1:A:65:ILE:HD11	1.90	0.53
1:B:76:ILE:N	1:B:103:ARG:O	2.36	0.53
1:B:60:MET:HA	1:B:80:ARG:HG3	1.90	0.52
1:A:58:PRO:O	1:A:60[B]:MET:HG3	2.09	0.52
1:A:61:ASP:O	1:A:65:ILE:HD13	2.09	0.52
1:A:91[B]:MET:HB2	1:A:94:THR:OG1	2.10	0.52
1:A:51:LEU:HD13	1:A:107:LEU:CD2	2.39	0.52
1:A:59:GLY:O	1:A:60[B]:MET:HG2	2.06	0.52
1:A:113:ASN:OD1	3:A:304:HOH:O	2.19	0.52
1:B:97:ARG:H	1:B:97:ARG:HE	1.56	0.52
1:B:41:ALA:O	1:B:43:GLU:HG3	2.10	0.52
1:A:80:ARG:HH21	1:A:98:TYR:HD2	1.59	0.51
1:B:68:GLN:O	1:B:75:SER:HB2	2.10	0.51
2:B:223:URE:C	3:B:301:HOH:O	2.50	0.51
1:A:57:LEU:CD2	1:A:101:PHE:CZ	2.93	0.51
1:B:51:LEU:O	1:B:129:LEU:O	2.28	0.51
1:A:121:LYS:NZ	3:A:310:HOH:O	2.42	0.51
1:B:46:GLU:O	1:B:46:GLU:CG	2.58	0.51
1:A:122:ASP:O	1:A:124:ILE:HD12	2.10	0.51
1:A:60[A]:MET:CB	1:A:64:ASP:HB2	2.41	0.51
1:A:60[B]:MET:CE	1:A:80:ARG:HB2	2.41	0.51
1:A:120:TYR:CD1	1:A:124:ILE:O	2.63	0.51
1:A:58:PRO:HA	1:A:123:GLY:O	2.11	0.50
1:B:41:ALA:O	1:B:43:GLU:N	2.36	0.50
1:B:38:PHE:HD1	1:B:103:ARG:HE	1.60	0.50
1:B:127:LEU:HG	1:B:129:LEU:HD23	1.92	0.50
1:B:116:VAL:HG11	1:B:127:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60[A]:MET:CB	1:A:64:ASP:CB	2.89	0.50
1:B:78:GLY:O	1:B:100:LYS:CG	2.60	0.50
1:B:76:ILE:HD12	1:B:103:ARG:C	2.33	0.50
1:B:49:GLU:HA	1:B:131:LYS:HD3	1.94	0.49
1:B:44:LEU:HA	1:B:53:LEU:HA	1.95	0.49
1:B:86:THR:HB	1:B:89:GLU:HG2	1.93	0.49
1:A:60[A]:MET:HE2	1:A:65:ILE:HG22	1.95	0.49
1:B:78:GLY:O	1:B:100:LYS:HG3	2.11	0.49
1:A:74:VAL:O	1:A:104:VAL:HA	2.11	0.49
1:A:100:LYS:CG	1:A:101:PHE:N	2.75	0.49
1:A:60[B]:MET:HB3	1:A:64:ASP:HB2	1.95	0.49
1:B:65:ILE:HD11	1:B:120:TYR:HE2	1.78	0.49
1:A:63:LYS:HB3	2:A:211:URE:N2	2.28	0.49
1:A:100:LYS:HG2	1:A:101:PHE:N	2.27	0.48
1:A:104:VAL:O	1:A:105:ILE:HB	2.12	0.48
1:A:69:VAL:HG11	1:A:111:ILE:CD1	2.43	0.48
1:B:57:LEU:HD23	1:B:125:LEU:HD23	1.95	0.48
1:B:134:GLU:HG2	2:B:202:URE:O	2.14	0.48
1:B:57:LEU:HB2	1:B:125:LEU:HD23	1.95	0.48
1:A:69:VAL:HG11	1:A:111:ILE:HG12	1.94	0.48
1:B:42:ALA:CA	1:B:54:LYS:O	2.59	0.48
1:A:43:GLU:O	1:A:53:LEU:HG	2.14	0.47
1:A:55:VAL:CG1	1:A:57:LEU:HG	2.43	0.47
1:A:57:LEU:HD22	1:A:60[A]:MET:HE2	1.95	0.47
1:A:52:LEU:HG	1:A:128:THR:CG2	2.45	0.47
1:A:116:VAL:HG13	1:A:129:LEU:HA	1.96	0.47
1:B:39:LEU:HG	1:B:103:ARG:HH12	1.79	0.47
1:B:92:LYS:NZ	1:B:93:ARG:HB3	2.28	0.47
1:A:43:GLU:HA	3:A:301:HOH:O	2.14	0.47
1:B:97:ARG:HE	1:B:97:ARG:N	2.12	0.47
1:A:46:GLU:HG3	1:A:51:LEU:CD2	2.45	0.47
1:B:102:GLN:HE22	1:B:104:VAL:CG1	2.28	0.47
1:B:98:TYR:CD1	1:B:98:TYR:N	2.83	0.47
1:B:60:MET:CB	1:B:80:ARG:HG3	2.45	0.47
1:A:44:LEU:HD13	1:A:53:LEU:HD12	1.97	0.46
1:A:60[A]:MET:HE3	1:A:64:ASP:O	2.16	0.46
1:A:60[B]:MET:HE2	1:A:80:ARG:HB2	1.96	0.46
1:A:98:TYR:HD2	2:A:202:URE:N1	2.13	0.46
1:A:49:GLU:N	1:A:49:GLU:CD	2.69	0.46
1:B:80:ARG:HG2	1:B:81:LYS:N	2.30	0.46
1:B:83:GLU:C	1:B:85:LYS:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ARG:HH21	2:B:204:URE:HN22	1.63	0.46
1:B:55:VAL:HG13	1:B:57:LEU:CD2	2.45	0.46
1:A:52:LEU:HG	1:A:128:THR:HG23	1.97	0.46
1:A:52:LEU:CG	1:A:128:THR:HG23	2.46	0.46
1:A:86:THR:C	1:A:88:THR:H	2.19	0.46
2:B:211:URE:C	3:B:305:HOH:O	2.62	0.46
1:A:52:LEU:O	1:A:53:LEU:HB2	2.16	0.45
1:B:113:ASN:H	1:B:113:ASN:ND2	2.14	0.45
1:A:104:VAL:O	1:A:105:ILE:CB	2.65	0.45
1:B:57:LEU:O	1:B:120:TYR:OH	2.15	0.45
1:B:121:LYS:O	1:B:122:ASP:CB	2.65	0.45
1:B:77:SER:HB3	1:B:102:GLN:HA	1.98	0.45
1:A:46:GLU:HG3	1:A:51:LEU:HD23	1.99	0.44
1:B:86:THR:HG22	1:B:89:GLU:H	1.83	0.44
1:A:50:ALA:HA	1:A:130:PRO:HA	1.99	0.44
1:B:42:ALA:HB3	2:B:203:URE:N2	2.33	0.44
1:B:76:ILE:HD12	1:B:103:ARG:O	2.17	0.44
1:B:64:ASP:OD2	1:B:80:ARG:O	2.35	0.44
1:B:132:ALA:O	2:B:202:URE:O	2.35	0.44
1:B:83:GLU:OE2	1:B:85:LYS:CE	2.66	0.44
1:B:38:PHE:HD1	1:B:103:ARG:NE	2.16	0.43
1:A:71:ALA:HB2	1:B:135:GLU:HG3	1.99	0.43
1:B:112:GLN:HG3	1:B:114:THR:HG23	1.99	0.43
1:B:105:ILE:O	1:B:105:ILE:HG13	2.18	0.43
1:B:69:VAL:HB	1:B:113:ASN:OD1	2.19	0.43
1:A:55:VAL:CG1	1:A:76:ILE:HD11	2.48	0.43
1:B:117:LYS:O	1:B:118:ALA:HB2	2.19	0.42
1:A:53:LEU:CD1	1:A:105:ILE:HD12	2.48	0.42
1:A:86:THR:O	1:A:88:THR:N	2.53	0.42
1:A:91[A]:MET:HB2	1:A:94:THR:OG1	2.20	0.42
1:A:53:LEU:HD23	1:A:54:LYS:C	2.39	0.42
1:A:71:ALA:CB	1:B:135:GLU:HA	2.49	0.41
1:B:83:GLU:N	3:B:312:HOH:O	2.37	0.41
1:B:101:PHE:HD2	1:B:103:ARG:CG	2.33	0.41
1:B:121:LYS:O	1:B:124:ILE:CD1	2.68	0.41
1:A:45:GLU:O	1:A:46:GLU:CB	2.68	0.41
1:B:94:THR:HG21	1:B:97:ARG:CG	2.49	0.41
1:B:77:SER:HA	1:B:101:PHE:O	2.20	0.41
1:B:55:VAL:HG13	1:B:57:LEU:HD21	2.01	0.41
1:B:56:GLU:O	1:B:57:LEU:HD22	2.20	0.41
1:A:48:PRO:C	1:A:49:GLU:OE1	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:GLU:CD	1:A:46:GLU:O	2.58	0.41
1:B:57:LEU:CG	1:B:125:LEU:HD23	2.51	0.41
1:A:107:LEU:HD13	1:A:111:ILE:CG2	2.50	0.41
1:B:60:MET:SD	1:B:65:ILE:HD13	2.60	0.41
1:B:93:ARG:HE	2:B:204:URE:HN12	1.68	0.41
1:A:55:VAL:HG11	1:A:76:ILE:HD11	2.01	0.41
1:B:38:PHE:HB3	1:B:103:ARG:HH21	1.85	0.41
1:A:43:GLU:HG3	1:A:54:LYS:HG2	2.03	0.41
1:B:82:SER:HB3	1:B:84:THR:HG23	2.02	0.41
1:B:92:LYS:HG3	1:B:93:ARG:N	2.36	0.41
1:B:38:PHE:O	1:B:39:LEU:C	2.59	0.40
1:B:107:LEU:C	1:B:109:VAL:H	2.25	0.40
1:B:121:LYS:O	1:B:122:ASP:HB2	2.21	0.40
1:B:80:ARG:CG	1:B:81:LYS:H	2.30	0.40
1:A:51:LEU:O	1:A:129:LEU:O	2.40	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLU:OE2	1:B:84:THR:OG1[6_555]	1.67	0.53
1:A:133:GLU:O	1:B:86:THR:OG1[6_555]	2.14	0.06

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	101/99 (102%)	64 (63%)	18 (18%)	19 (19%)	0	0
1	B	97/99 (98%)	69 (71%)	17 (18%)	11 (11%)	0	0
All	All	198/198 (100%)	133 (67%)	35 (18%)	30 (15%)	0	0

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	GLU
1	A	61	ASP
1	A	85[A]	LYS
1	A	85[B]	LYS
1	A	89	GLU
1	A	92	LYS
1	A	95	GLU
1	A	115	SER
1	B	92	LYS
1	A	53	LEU
1	A	59	GLY
1	A	72	GLU
1	A	105	ILE
1	A	114	THR
1	B	84	THR
1	B	122	ASP
1	A	60[A]	MET
1	A	60[B]	MET
1	A	87	GLU
1	A	130	PRO
1	B	42	ALA
1	B	83	GLU
1	B	109	VAL
1	B	118	ALA
1	B	130	PRO
1	A	50	ALA
1	B	86	THR
1	B	106	PRO
1	A	104	VAL
1	B	58	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	91/87 (105%)	63 (69%)	28 (31%)	0	0
1	B	87/87 (100%)	56 (64%)	31 (36%)	0	0
All	All	178/174 (102%)	119 (67%)	59 (33%)	0	0

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	PHE
1	A	43	GLU
1	A	47	THR
1	A	49	GLU
1	A	52	LEU
1	A	54	LYS
1	A	60[A]	MET
1	A	60[B]	MET
1	A	65	ILE
1	A	70	THR
1	A	76	ILE
1	A	81	LYS
1	A	84	THR
1	A	93	ARG
1	A	94	THR
1	A	101	PHE
1	A	104	VAL
1	A	107	LEU
1	A	109	VAL
1	A	110	ARG
1	A	111	ILE
1	A	115	SER
1	A	117	LYS
1	A	121	LYS
1	A	122	ASP
1	A	127	LEU
1	A	128	THR
1	A	129	LEU
1	B	44	LEU
1	B	46	GLU
1	B	52	LEU
1	B	54	LYS

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Mol	Chain	Res	Type
1	B	56	GLU
1	B	60	MET
1	B	67	VAL
1	B	70	THR
1	B	77	SER
1	B	80	ARG
1	B	81	LYS
1	B	85	LYS
1	B	91	MET
1	B	93	ARG
1	B	97	ARG
1	B	98	TYR
1	B	100	LYS
1	B	101	PHE
1	B	102	GLN
1	B	103	ARG
1	B	105	ILE
1	B	107	LEU
1	B	109	VAL
1	B	114	THR
1	B	115	SER
1	B	117	LYS
1	B	124	ILE
1	B	125	LEU
1	B	126	HIS
1	B	129	LEU
1	B	131	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

44 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	URE	A	213	-	3,3,3	3.35	3 (100%)	3,3,3	1.11	0
2	URE	B	210	-	3,3,3	3.55	3 (100%)	3,3,3	0.64	0
2	URE	B	223	-	3,3,3	4.05	2 (66%)	3,3,3	1.07	0
2	URE	A	204	-	3,3,3	3.20	3 (100%)	3,3,3	0.72	0
2	URE	B	221	-	3,3,3	3.78	3 (100%)	3,3,3	1.39	0
2	URE	B	211	-	3,3,3	3.50	2 (66%)	3,3,3	0.77	0
2	URE	A	203	-	3,3,3	3.70	3 (100%)	3,3,3	2.19	2 (66%)
2	URE	B	225	-	3,3,3	3.81	3 (100%)	3,3,3	1.82	1 (33%)
2	URE	B	227	-	3,3,3	3.75	3 (100%)	3,3,3	1.31	0
2	URE	B	214	-	3,3,3	3.64	3 (100%)	3,3,3	1.78	1 (33%)
2	URE	B	228	-	3,3,3	3.85	2 (66%)	3,3,3	1.23	0
2	URE	B	218	-	3,3,3	3.90	3 (100%)	3,3,3	1.53	1 (33%)
2	URE	B	226	-	3,3,3	3.72	2 (66%)	3,3,3	1.24	0
2	URE	A	209	-	3,3,3	3.48	2 (66%)	3,3,3	0.97	0
2	URE	B	204	-	3,3,3	3.77	2 (66%)	3,3,3	0.95	0
2	URE	B	206	-	3,3,3	3.35	3 (100%)	3,3,3	1.22	0
2	URE	B	219	-	3,3,3	3.74	3 (100%)	3,3,3	1.74	2 (66%)
2	URE	B	209	-	3,3,3	3.52	3 (100%)	3,3,3	1.06	0
2	URE	A	211	-	3,3,3	3.46	3 (100%)	3,3,3	1.94	1 (33%)
2	URE	B	207	-	3,3,3	3.20	3 (100%)	3,3,3	1.36	0
2	URE	B	205	-	3,3,3	3.90	3 (100%)	3,3,3	1.66	1 (33%)
2	URE	B	217	-	3,3,3	3.78	2 (66%)	3,3,3	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	URE	A	208	-	3,3,3	3.89	2 (66%)	3,3,3	1.30	0
2	URE	A	212	-	3,3,3	3.66	3 (100%)	3,3,3	1.09	0
2	URE	B	202	-	3,3,3	3.71	2 (66%)	3,3,3	0.36	0
2	URE	A	205	-	3,3,3	4.02	3 (100%)	3,3,3	3.09	2 (66%)
2	URE	B	215	-	3,3,3	3.38	3 (100%)	3,3,3	1.31	0
2	URE	B	212	-	3,3,3	3.45	3 (100%)	3,3,3	1.00	0
2	URE	A	206	-	3,3,3	3.43	3 (100%)	3,3,3	1.95	2 (66%)
2	URE	B	224	-	3,3,3	3.61	3 (100%)	3,3,3	1.64	1 (33%)
2	URE	A	216	-	3,3,3	0.62	0	3,3,3	0.06	0
2	URE	A	214	-	3,3,3	3.34	3 (100%)	3,3,3	0.87	0
2	URE	A	201	-	3,3,3	3.68	3 (100%)	3,3,3	0.43	0
2	URE	B	222	-	3,3,3	3.73	3 (100%)	3,3,3	1.42	1 (33%)
2	URE	A	207	-	3,3,3	3.67	3 (100%)	3,3,3	1.13	0
2	URE	B	208	-	3,3,3	3.52	3 (100%)	3,3,3	0.50	0
2	URE	A	215	-	3,3,3	3.05	2 (66%)	3,3,3	5.46	3 (100%)
2	URE	B	213	-	3,3,3	3.91	3 (100%)	3,3,3	1.96	1 (33%)
2	URE	B	220	-	3,3,3	3.55	2 (66%)	3,3,3	1.29	0
2	URE	B	216	-	3,3,3	3.71	3 (100%)	3,3,3	1.48	1 (33%)
2	URE	A	202	-	3,3,3	3.35	3 (100%)	3,3,3	0.60	0
2	URE	B	201	-	3,3,3	3.70	2 (66%)	3,3,3	0.71	0
2	URE	B	203	-	3,3,3	3.59	2 (66%)	3,3,3	0.42	0
2	URE	A	210	-	3,3,3	3.36	2 (66%)	3,3,3	1.32	0

All (115) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	223	URE	C-N2	4.89	1.47	1.34
2	B	218	URE	C-N1	4.81	1.47	1.34
2	A	205	URE	C-N1	4.76	1.47	1.34
2	B	205	URE	C-N1	4.72	1.46	1.34
2	B	223	URE	C-N1	4.70	1.46	1.34
2	B	219	URE	C-N1	4.67	1.46	1.34
2	B	201	URE	C-N2	4.66	1.46	1.34
2	B	220	URE	C-N2	4.66	1.46	1.34
2	A	203	URE	C-N1	4.65	1.46	1.34
2	A	208	URE	C-N2	4.64	1.46	1.34
2	B	216	URE	C-N1	4.64	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	213	URE	C-N1	4.60	1.46	1.34
2	B	202	URE	C-N1	4.60	1.46	1.34
2	B	228	URE	C-N2	4.58	1.46	1.34
2	B	226	URE	C-N1	4.56	1.46	1.34
2	B	227	URE	C-N1	4.55	1.46	1.34
2	B	221	URE	C-N2	4.55	1.46	1.34
2	B	217	URE	C-N2	4.51	1.46	1.34
2	B	225	URE	C-N1	4.51	1.46	1.34
2	B	214	URE	C-N2	4.49	1.46	1.34
2	B	210	URE	C-N2	4.48	1.46	1.34
2	A	201	URE	C-N1	4.47	1.46	1.34
2	A	208	URE	C-N1	4.46	1.46	1.34
2	B	213	URE	C-N2	4.46	1.46	1.34
2	B	222	URE	C-N1	4.45	1.46	1.34
2	B	224	URE	C-N2	4.43	1.46	1.34
2	B	228	URE	C-N1	4.41	1.46	1.34
2	B	204	URE	C-N1	4.40	1.46	1.34
2	B	217	URE	C-N1	4.39	1.46	1.34
2	B	204	URE	C-N2	4.39	1.46	1.34
2	A	207	URE	C-N2	4.37	1.46	1.34
2	A	209	URE	C-N2	4.30	1.45	1.34
2	B	209	URE	C-N2	4.29	1.45	1.34
2	B	203	URE	C-N2	4.26	1.45	1.34
2	B	221	URE	C-N1	4.25	1.45	1.34
2	B	218	URE	C-N2	4.24	1.45	1.34
2	A	205	URE	C-N2	4.24	1.45	1.34
2	B	202	URE	C-N2	4.24	1.45	1.34
2	B	203	URE	C-N1	4.21	1.45	1.34
2	B	206	URE	C-N2	4.20	1.45	1.34
2	A	213	URE	C-N1	4.19	1.45	1.34
2	A	215	URE	O-C	-4.16	1.11	1.26
2	A	212	URE	C-N1	4.15	1.45	1.34
2	A	212	URE	C-N2	4.15	1.45	1.34
2	B	225	URE	C-N2	4.14	1.45	1.34
2	B	211	URE	C-N2	4.14	1.45	1.34
2	B	222	URE	C-N2	4.14	1.45	1.34
2	A	210	URE	C-N2	4.13	1.45	1.34
2	B	227	URE	C-N2	4.12	1.45	1.34
2	B	226	URE	C-N2	4.10	1.45	1.34
2	B	208	URE	C-N2	4.09	1.45	1.34
2	A	214	URE	C-N1	4.07	1.45	1.34
2	A	201	URE	C-N2	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	URE	C-N1	4.04	1.45	1.34
2	A	207	URE	C-N1	4.01	1.45	1.34
2	B	208	URE	C-N1	3.99	1.45	1.34
2	B	205	URE	C-N2	3.98	1.44	1.34
2	B	212	URE	C-N2	3.98	1.44	1.34
2	B	211	URE	C-N1	3.97	1.44	1.34
2	A	211	URE	C-N1	3.96	1.44	1.34
2	A	202	URE	C-N2	3.94	1.44	1.34
2	B	219	URE	C-N2	3.91	1.44	1.34
2	A	206	URE	C-N1	3.91	1.44	1.34
2	A	209	URE	C-N1	3.89	1.44	1.34
2	A	204	URE	C-N1	3.86	1.44	1.34
2	B	216	URE	C-N2	3.83	1.44	1.34
2	A	210	URE	C-N1	3.79	1.44	1.34
2	B	212	URE	C-N1	3.79	1.44	1.34
2	B	215	URE	C-N1	3.79	1.44	1.34
2	A	203	URE	C-N2	3.78	1.44	1.34
2	B	214	URE	C-N1	3.78	1.44	1.34
2	B	209	URE	C-N1	3.73	1.44	1.34
2	A	211	URE	C-N2	3.72	1.44	1.34
2	B	224	URE	C-N1	3.66	1.44	1.34
2	B	207	URE	C-N1	3.61	1.44	1.34
2	B	210	URE	C-N1	3.60	1.43	1.34
2	A	206	URE	C-N2	3.59	1.43	1.34
2	B	220	URE	C-N1	3.53	1.43	1.34
2	A	214	URE	C-N2	3.52	1.43	1.34
2	B	207	URE	C-N2	3.52	1.43	1.34
2	B	215	URE	C-N2	3.34	1.43	1.34
2	A	204	URE	C-N2	3.33	1.43	1.34
2	A	202	URE	C-N1	3.29	1.43	1.34
2	A	215	URE	C-N1	3.24	1.42	1.34
2	B	206	URE	C-N1	3.11	1.42	1.34
2	A	213	URE	C-N2	3.06	1.42	1.34
2	B	215	URE	O-C	-2.97	1.15	1.26
2	A	205	URE	O-C	-2.79	1.16	1.26
2	B	205	URE	O-C	-2.74	1.16	1.26
2	A	202	URE	O-C	-2.71	1.16	1.26
2	A	206	URE	O-C	-2.68	1.16	1.26
2	A	213	URE	O-C	-2.59	1.17	1.26
2	B	206	URE	O-C	-2.54	1.17	1.26
2	A	211	URE	O-C	-2.52	1.17	1.26
2	B	224	URE	O-C	-2.48	1.17	1.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	225	URE	O-C	-2.48	1.17	1.26
2	A	212	URE	O-C	-2.39	1.17	1.26
2	B	212	URE	O-C	-2.35	1.17	1.26
2	B	214	URE	O-C	-2.31	1.18	1.26
2	A	207	URE	O-C	-2.30	1.18	1.26
2	A	203	URE	O-C	-2.30	1.18	1.26
2	B	207	URE	O-C	-2.28	1.18	1.26
2	B	216	URE	O-C	-2.27	1.18	1.26
2	B	209	URE	O-C	-2.20	1.18	1.26
2	B	210	URE	O-C	-2.20	1.18	1.26
2	B	213	URE	O-C	-2.19	1.18	1.26
2	B	219	URE	O-C	-2.17	1.18	1.26
2	B	222	URE	O-C	-2.17	1.18	1.26
2	A	204	URE	O-C	-2.16	1.18	1.26
2	A	214	URE	O-C	-2.14	1.18	1.26
2	B	227	URE	O-C	-2.12	1.18	1.26
2	B	218	URE	O-C	-2.12	1.18	1.26
2	B	208	URE	O-C	-2.11	1.18	1.26
2	B	221	URE	O-C	-2.04	1.18	1.26
2	A	201	URE	O-C	-2.03	1.19	1.26

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	215	URE	O-C-N2	-7.16	105.36	121.04
2	A	215	URE	N2-C-N1	5.60	127.90	117.77
2	A	205	URE	N2-C-N1	4.63	126.14	117.77
2	A	203	URE	N2-C-N1	3.07	123.32	117.77
2	B	213	URE	N2-C-N1	2.89	122.99	117.77
2	A	211	URE	N2-C-N1	2.76	122.76	117.77
2	B	225	URE	N2-C-N1	2.74	122.72	117.77
2	A	215	URE	O-C-N1	2.59	126.71	121.04
2	B	214	URE	N2-C-N1	2.59	122.45	117.77
2	A	206	URE	N2-C-N1	2.52	122.33	117.77
2	B	205	URE	N2-C-N1	2.46	122.22	117.77
2	B	218	URE	N2-C-N1	2.28	121.90	117.77
2	A	206	URE	O-C-N2	-2.24	116.14	121.04
2	B	219	URE	N2-C-N1	2.21	121.76	117.77
2	A	203	URE	O-C-N2	-2.20	116.22	121.04
2	B	224	URE	N2-C-N1	2.13	121.63	117.77
2	B	222	URE	N2-C-N1	2.12	121.60	117.77
2	A	205	URE	O-C-N2	-2.09	116.47	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	219	URE	O-C-N2	-2.03	116.61	121.04
2	B	216	URE	N2-C-N1	2.00	121.39	117.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	223	URE	2	0
2	B	211	URE	2	0
2	A	203	URE	2	0
2	B	227	URE	1	0
2	B	218	URE	2	0
2	A	209	URE	1	0
2	B	204	URE	2	0
2	A	211	URE	2	0
2	B	205	URE	1	0
2	B	217	URE	1	0
2	B	202	URE	4	0
2	B	212	URE	1	0
2	A	207	URE	1	0
2	A	215	URE	1	0
2	A	202	URE	2	0
2	B	203	URE	1	0
2	A	210	URE	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	99/99 (100%)	0.38	4 (4%) 38 45	5, 15, 24, 30	0
1	B	99/99 (100%)	0.62	9 (9%) 9 12	6, 17, 27, 31	0
All	All	198/198 (100%)	0.50	13 (6%) 18 23	5, 16, 26, 31	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	LYS	4.8
1	B	62	PRO	3.1
1	B	104	VAL	2.9
1	B	90	GLY	2.9
1	B	57	LEU	2.8
1	B	106	PRO	2.7
1	B	38	PHE	2.5
1	B	73	ALA	2.4
1	A	76	ILE	2.3
1	B	116	VAL	2.2
1	A	74	VAL	2.1
1	A	71	ALA	2.1
1	A	114	THR	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 monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å ²)	Q<0.9
2	URE	B	220	4/4	0.74	0.19	11,14,28,28	0
2	URE	B	228	4/4	0.77	0.14	23,25,29,31	0
2	URE	B	226	4/4	0.78	0.16	7,12,17,17	0
2	URE	A	216	4/4	0.79	0.27	15,19,24,27	0
2	URE	A	214	4/4	0.84	0.19	7,11,11,34	0
2	URE	B	224	4/4	0.85	0.16	6,9,23,27	0
2	URE	B	208	4/4	0.88	0.14	11,18,24,31	0
2	URE	B	209	4/4	0.88	0.17	18,19,25,28	0
2	URE	B	222	4/4	0.90	0.13	2,7,15,19	0
2	URE	B	221	4/4	0.90	0.11	10,14,21,32	0
2	URE	A	208	4/4	0.91	0.09	2,5,10,22	0
2	URE	A	209	4/4	0.91	0.12	6,7,7,13	0
2	URE	B	201	4/4	0.92	0.19	4,10,18,18	0
2	URE	B	211	4/4	0.92	0.14	4,5,6,17	0
2	URE	B	215	4/4	0.92	0.14	1,2,12,17	0
2	URE	B	217	4/4	0.92	0.12	9,20,23,33	0
2	URE	A	206	4/4	0.92	0.15	2,3,3,10	0
2	URE	B	204	4/4	0.93	0.12	5,7,8,21	0
2	URE	B	223	4/4	0.93	0.12	18,21,29,41	0
2	URE	A	211	4/4	0.93	0.11	3,5,14,16	0
2	URE	A	207	4/4	0.93	0.15	6,7,11,15	0
2	URE	B	227	4/4	0.93	0.10	7,9,10,18	0
2	URE	B	203	4/4	0.93	0.11	7,12,12,14	0
2	URE	B	202	4/4	0.94	0.16	3,5,5,16	0
2	URE	B	219	4/4	0.94	0.23	10,14,28,29	0
2	URE	B	225	4/4	0.94	0.16	25,26,28,33	0
2	URE	B	206	4/4	0.94	0.16	0,3,4,11	0
2	URE	B	213	4/4	0.94	0.13	5,7,13,22	0
2	URE	A	213	4/4	0.94	0.12	2,3,8,11	0
2	URE	B	216	4/4	0.95	0.10	11,12,19,21	0
2	URE	B	210	4/4	0.95	0.12	2,8,14,20	0
2	URE	B	207	4/4	0.95	0.13	2,2,6,29	0
2	URE	B	212	4/4	0.95	0.12	5,6,13,15	0
2	URE	A	204	4/4	0.95	0.11	3,4,8,11	0
2	URE	A	212	4/4	0.95	0.15	5,9,11,39	0
2	URE	A	210	4/4	0.96	0.08	0,2,15,22	0
2	URE	A	215	4/4	0.96	0.10	15,24,24,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	URE	A	202	4/4	0.96	0.14	2,5,6,18	0
2	URE	B	218	4/4	0.96	0.16	2,3,6,7	0
2	URE	A	205	4/4	0.96	0.13	1,1,2,2	0
2	URE	A	203	4/4	0.96	0.13	1,1,2,3	0
2	URE	B	214	4/4	0.96	0.13	4,7,11,14	0
2	URE	B	205	4/4	0.97	0.10	2,3,4,5	0
2	URE	A	201	4/4	0.97	0.09	2,3,5,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.