



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 06:18 AM GMT

PDB ID : 4O8R
Title : Crystal structure of orotidine 5'-monophosphate decarboxylase from methanobacterium thermoautotrophicum complexed with 5,6-dihydrouridine 5'-monophosphate
Authors : Fedorov, A.A.; Fedorov, E.V.; Chan, K.K.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2013-12-29
Resolution : 2.29 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

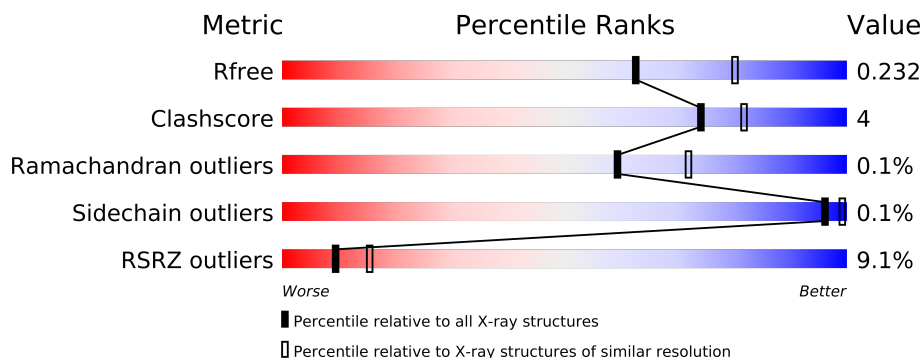
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	228	
1	B	228	
1	C	228	
1	D	228	
1	E	228	
1	F	228	
1	G	228	
1	H	228	
1	I	228	
1	J	228	
1	K	228	
1	L	228	
1	M	228	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21847 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Orotidine 5'-phosphate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	2	0
			1693	1063	299	319	12			
1	B	219	Total	C	N	O	S	0	2	0
			1683	1058	295	318	12			
1	C	225	Total	C	N	O	S	0	1	0
			1726	1083	306	324	13			
1	D	216	Total	C	N	O	S	0	2	0
			1659	1044	292	311	12			
1	E	217	Total	C	N	O	S	0	1	0
			1657	1043	289	313	12			
1	F	215	Total	C	N	O	S	0	1	0
			1641	1033	287	309	12			
1	G	213	Total	C	N	O	S	0	1	0
			1624	1021	284	307	12			
1	H	215	Total	C	N	O	S	0	1	0
			1639	1032	286	309	12			
1	I	197	Total	C	N	O	S	0	0	0
			1505	951	262	282	10			
1	J	218	Total	C	N	O	S	0	0	0
			1653	1039	289	313	12			
1	K	216	Total	C	N	O	S	0	0	0
			1638	1029	287	311	11			
1	L	213	Total	C	N	O	S	0	0	0
			1613	1013	283	306	11			
1	M	218	Total	C	N	O	S	0	1	0
			1664	1048	290	314	12			

There are 13 discrepancies between the modelled and reference sequences:

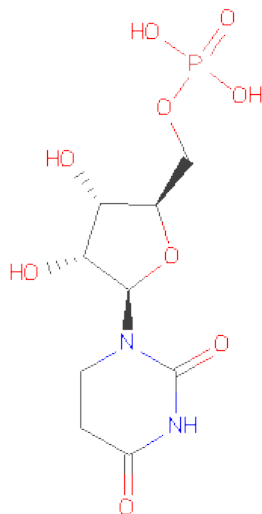
Chain	Residue	Modelled	Actual	Comment	Reference
A	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
B	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
C	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232

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Chain	Residue	Modelled	Actual	Comment	Reference
D	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
E	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
F	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
G	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
H	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
I	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
J	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
K	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
L	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232
M	101	PRO	ARG	ENGINEERED MUTATION	UNP O26232

- Molecule 2 is 5,6-DIHYDROURIDINE-5'-MONOPHOSPHATE (three-letter code: H2U) (formula: C₉H₁₅N₂O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	E	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	F	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	G	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	H	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	J	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	K	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	L	1	Total	C	N	O	P	0	0
			21	9	2	9	1		
2	M	1	Total	C	N	O	P	0	0
			21	9	2	9	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O	0	0
			36	36		
4	B	22	Total	O	0	0
			22	22		
4	C	34	Total	O	0	0
			34	34		
4	D	19	Total	O	0	0
			19	19		
4	E	7	Total	O	0	0
			7	7		
4	F	11	Total	O	0	0
			11	11		
4	G	6	Total	O	0	0
			6	6		
4	H	6	Total	O	0	0
			6	6		
4	I	11	Total	O	0	0
			11	11		
4	J	20	Total	O	0	0
			20	20		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	4	Total 4	O 4	0	0
4	M	23	Total 23	O 23	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Orotidine 5'-phosphate decarboxylase

Chain A: 



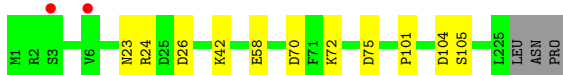
- Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain B: 



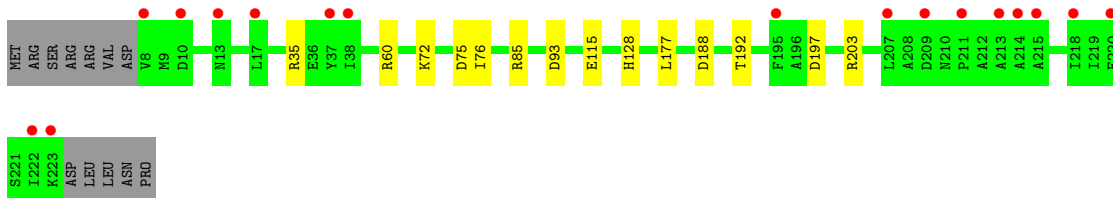
- Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain C: 



- Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain D: 



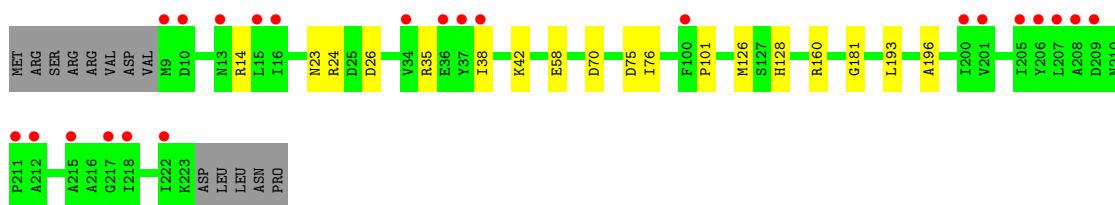
- Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain E: 



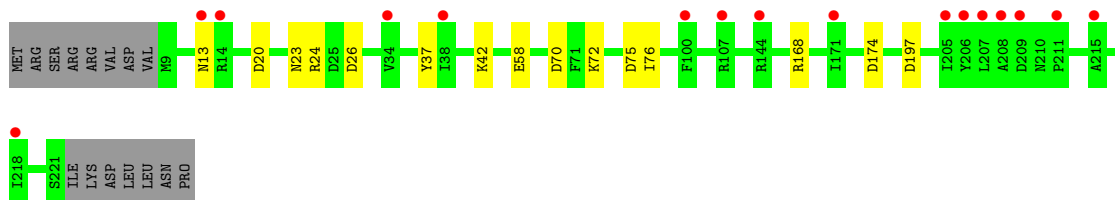
- Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain F: 



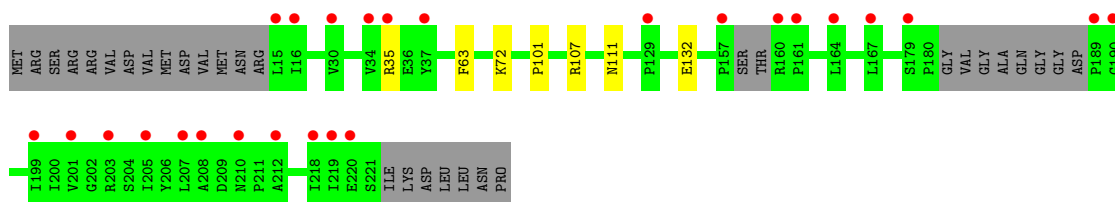
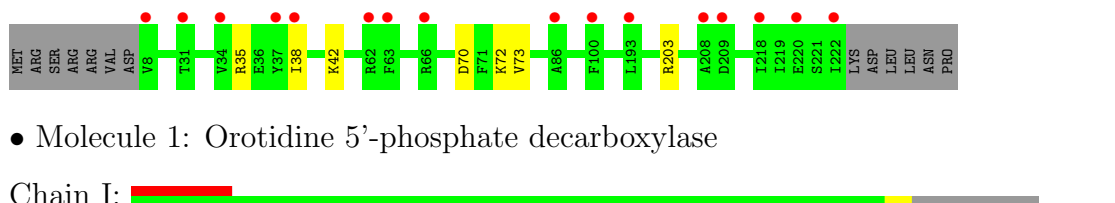
- Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain G:



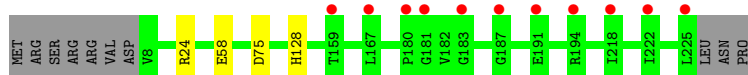
- Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain H:



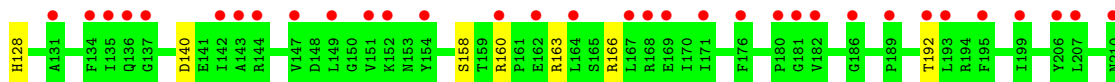
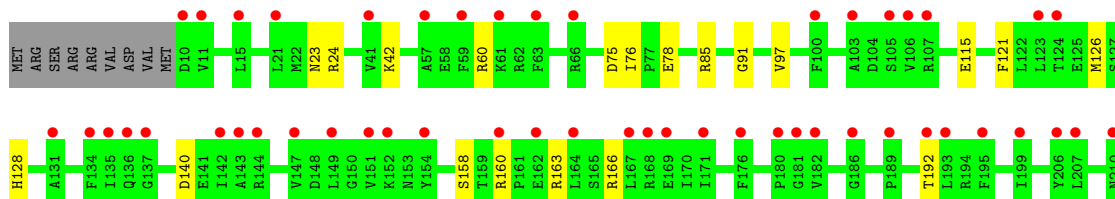
- Molecule 1: Orotidine 5'-phosphate decarboxylase

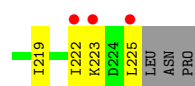
Chain J:



- Molecule 1: Orotidine 5'-phosphate decarboxylase

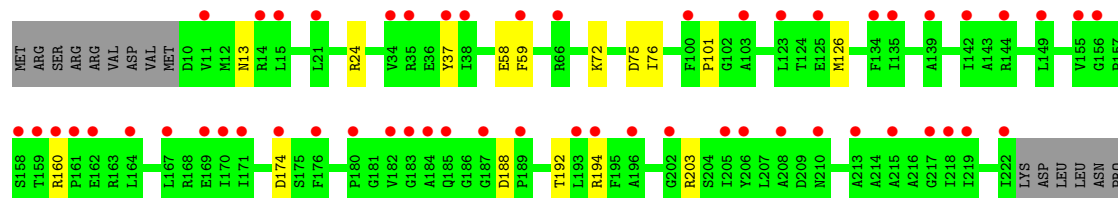
Chain K:





- Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain L:



- Molecule 1: Orotidine 5'-phosphate decarboxylase

Chain M:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.90Å 101.80Å 192.84Å 90.00° 91.59° 90.00°	Depositor
Resolution (Å)	48.19 – 2.29 48.19 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.19-2.29) 99.4 (48.19-2.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.203 , 0.231 0.205 , 0.232	Depositor DCC
R_{free} test set	3832 reflections (3.01%)	DCC
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	EDS
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 127529 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21847	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, CL

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	0.24	0/1717	0.43	0/2316
1	B	0.23	0/1707	0.41	0/2303
1	C	0.24	0/1750	0.43	0/2359
1	D	0.23	0/1683	0.41	0/2270
1	E	0.22	0/1681	0.39	0/2268
1	F	0.22	0/1665	0.40	0/2246
1	G	0.22	0/1648	0.39	0/2224
1	H	0.21	0/1663	0.39	0/2245
1	I	0.22	0/1526	0.39	0/2056
1	J	0.23	0/1676	0.40	0/2261
1	K	0.21	0/1661	0.38	0/2241
1	L	0.21	0/1636	0.37	0/2208
1	M	0.24	0/1688	0.42	0/2278
All	All	0.23	0/21701	0.40	0/29275

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1693	0	0	8	0
1	B	1683	0	0	5	0
1	C	1726	0	0	7	0
1	D	1659	0	0	9	0
1	E	1657	0	0	7	0
1	F	1641	0	0	12	0
1	G	1624	0	0	10	0
1	H	1639	0	0	4	0
1	I	1505	0	0	4	0
1	J	1653	0	0	3	0
1	K	1638	0	0	15	0
1	L	1613	0	0	9	0
1	M	1664	0	0	4	0
2	A	21	0	0	0	0
2	B	21	0	0	0	0
2	C	21	0	0	0	0
2	D	21	0	0	1	0
2	E	21	0	0	0	0
2	F	21	0	0	0	0
2	G	21	0	0	1	0
2	H	21	0	0	1	0
2	J	21	0	0	0	0
2	K	21	0	0	0	0
2	L	21	0	0	1	0
2	M	21	0	0	0	0
3	A	1	0	0	0	0
4	A	36	0	0	1	0
4	B	22	0	0	1	0
4	C	34	0	0	1	0
4	D	19	0	0	0	0
4	E	7	0	0	1	0
4	F	11	0	0	1	0
4	G	6	0	0	0	0
4	H	6	0	0	0	0
4	I	11	0	0	0	0
4	J	20	0	0	0	0
4	K	4	0	0	1	0
4	M	23	0	0	0	0
All	All	21847	0	0	88	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (88) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:23:ASN:ND2	1:G:26:ASP:OD2	2.28	0.67
1:K:140:ASP:OD1	1:K:163:ARG:NH2	2.30	0.64
1:K:126:MET:O	1:K:160:ARG:NH2	2.31	0.63
1:K:128:HIS:NE2	1:L:101:PRO:O	2.34	0.61
1:B:72:LYS:NZ	4:B:406:HOH:O	2.32	0.61
1:K:140:ASP:OD2	1:K:166:ARG:NE	2.34	0.60
1:B:85:ARG:NH1	1:B:115:GLU:OE2	2.35	0.59
1:L:24:ARG:NH2	1:L:58:GLU:OE2	2.35	0.59
1:M:35:ARG:NE	1:M:63:PHE:O	2.35	0.59
1:H:35:ARG:NH1	1:H:38:ILE:O	2.38	0.57
1:D:188:ASP:O	1:D:192:THR:OG1	2.23	0.57
1:I:107:ARG:NH1	1:I:111:ASN:OD1	2.38	0.57
1:D:35:ARG:O	1:D:35:ARG:NH1	2.38	0.57
1:K:42:LYS:NZ	4:K:404:HOH:O	2.38	0.56
1:F:35:ARG:NH1	1:F:35:ARG:O	2.39	0.56
1:F:35:ARG:NH1	1:F:38:ILE:O	2.38	0.56
1:M:24:ARG:NH2	1:M:58:GLU:OE2	2.39	0.56
1:G:24:ARG:NH2	1:G:58:GLU:OE2	2.40	0.55
1:D:85:ARG:NH2	1:D:115:GLU:OE1	2.40	0.55
1:L:126:MET:O	1:L:160:ARG:NH1	2.40	0.54
1:B:166:ARG:NH1	1:B:169:GLU:OE2	2.40	0.54
1:C:72:LYS:NZ	4:C:424:HOH:O	2.40	0.53
1:F:24:ARG:NH2	1:F:58:GLU:OE2	2.41	0.53
1:A:23:ASN:ND2	1:A:26:ASP:OD2	2.41	0.53
1:K:75:ASP:OD1	1:K:76:ILE:N	2.42	0.53
1:E:78:GLU:N	1:E:78:GLU:OE1	2.41	0.53
1:K:60:ARG:NH1	1:K:91:GLY:O	2.42	0.52
1:I:35:ARG:NE	1:I:63:PHE:O	2.42	0.52
1:E:85:ARG:NH1	1:E:115:GLU:OE1	2.43	0.52
1:C:101:PRO:O	1:D:128:HIS:NE2	2.43	0.52
1:A:107[A]:ARG:NH1	4:A:427:HOH:O	2.43	0.51
1:K:23:ASN:OD1	1:K:24:ARG:N	2.45	0.50
1:H:203:ARG:N	2:H:301:H2U:OP2	2.43	0.50
1:A:42:LYS:NZ	1:A:70:ASP:OD2	2.45	0.50
1:L:188:ASP:O	1:L:192:THR:OG1	2.29	0.49
1:B:24:ARG:NH2	1:B:58:GLU:OE2	2.46	0.49
1:G:13:ASN:ND2	1:G:37:TYR:O	2.46	0.49
1:C:24:ARG:NH2	1:C:58:GLU:OE2	2.46	0.48
1:A:35:ARG:NE	1:A:63:PHE:O	2.47	0.48
1:G:75:ASP:OD1	1:G:76:ILE:N	2.47	0.48
1:L:13:ASN:ND2	1:L:37:TYR:O	2.46	0.48
1:F:14:ARG:NH2	1:F:193:LEU:O	2.47	0.48
1:L:203:ARG:N	2:L:301:H2U:OP2	2.46	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:203:ARG:N	2:D:301:H2U:OP2	2.47	0.47
1:E:67:ILE:N	1:E:93:ASP:OD2	2.47	0.47
1:F:126:MET:O	1:F:160:ARG:NH1	2.48	0.47
1:G:70:ASP:OD1	1:G:72:LYS:NZ	2.47	0.47
1:G:174:ASP:N	1:G:174:ASP:OD1	2.48	0.47
1:J:24:ARG:NH2	1:J:58:GLU:OE2	2.48	0.47
1:A:60:ARG:NH2	1:A:93:ASP:OD1	2.49	0.46
1:K:78:GLU:N	1:K:78:GLU:OE1	2.48	0.46
1:K:222:ILE:O	1:K:225:LEU:N	2.49	0.45
1:F:42:LYS:NZ	1:F:70:ASP:OD2	2.49	0.45
1:C:104:ASP:OD1	1:C:105:SER:N	2.50	0.45
1:B:23:ASN:OD1	1:B:26:ASP:N	2.48	0.45
1:F:75:ASP:OD1	1:F:76:ILE:N	2.50	0.45
1:A:35:ARG:NH1	1:A:35:ARG:O	2.50	0.45
1:K:219:ILE:O	1:K:223:LYS:N	2.50	0.44
1:L:75:ASP:OD1	1:L:76:ILE:N	2.50	0.44
1:F:181:GLY:N	4:F:409:HOH:O	2.50	0.44
1:C:42:LYS:NZ	1:C:70:ASP:OD2	2.50	0.44
1:D:177:LEU:N	1:D:197:ASP:OD2	2.51	0.44
1:G:20:ASP:OD2	2:G:301:H2U:O3'	2.36	0.44
1:I:101:PRO:O	1:J:128:HIS:NE2	2.51	0.44
1:A:35:ARG:NH1	1:A:38:ILE:O	2.51	0.43
1:G:75:ASP:OD2	1:H:72:LYS:NZ	2.52	0.43
1:M:75:ASP:OD1	1:M:76:ILE:N	2.51	0.43
1:K:97:VAL:N	1:K:121:PHE:O	2.52	0.43
1:K:158:SER:OG	1:K:192:THR:OG1	2.37	0.43
1:C:23:ASN:ND2	1:C:26:ASP:OD2	2.52	0.43
1:F:23:ASN:ND2	1:F:26:ASP:OD1	2.52	0.42
1:E:158:SER:OG	1:E:192:THR:OG1	2.36	0.42
1:G:42:LYS:NZ	1:G:70:ASP:OD2	2.53	0.42
1:E:128:HIS:NE2	1:F:101:PRO:O	2.53	0.42
1:K:75:ASP:OD2	1:L:72:LYS:NZ	2.52	0.42
1:I:72:LYS:NZ	1:J:75:ASP:OD2	2.53	0.42
1:E:181:GLY:N	4:E:404:HOH:O	2.52	0.41
1:D:60:ARG:NH2	1:D:93:ASP:OD1	2.53	0.41
1:C:75:ASP:OD2	1:D:72:LYS:NZ	2.53	0.41
1:F:14:ARG:NH2	1:F:196:ALA:O	2.53	0.41
1:M:104:ASP:OD1	1:M:105:SER:N	2.54	0.41
1:A:78:GLU:N	1:A:78:GLU:OE1	2.53	0.41
1:H:42:LYS:NZ	1:H:70:ASP:OD2	2.54	0.41
1:K:85:ARG:NH2	1:K:115:GLU:OE1	2.55	0.40
1:L:174:ASP:OD2	1:L:174:ASP:N	2.54	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:101:PRO:O	1:F:128:HIS:NE2	2.54	0.40
1:G:168:ARG:NH2	1:G:197:ASP:OD2	2.54	0.40
1:D:75:ASP:OD1	1:D:76:ILE:N	2.55	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	220/228 (96%)	215 (98%)	5 (2%)	0	100	100
1	B	219/228 (96%)	213 (97%)	6 (3%)	0	100	100
1	C	224/228 (98%)	217 (97%)	7 (3%)	0	100	100
1	D	216/228 (95%)	211 (98%)	5 (2%)	0	100	100
1	E	216/228 (95%)	208 (96%)	8 (4%)	0	100	100
1	F	214/228 (94%)	205 (96%)	9 (4%)	0	100	100
1	G	212/228 (93%)	206 (97%)	6 (3%)	0	100	100
1	H	214/228 (94%)	209 (98%)	4 (2%)	1 (0%)	38	45
1	I	191/228 (84%)	186 (97%)	5 (3%)	0	100	100
1	J	216/228 (95%)	209 (97%)	7 (3%)	0	100	100
1	K	214/228 (94%)	205 (96%)	9 (4%)	0	100	100
1	L	211/228 (92%)	201 (95%)	9 (4%)	1 (0%)	38	45
1	M	217/228 (95%)	211 (97%)	6 (3%)	0	100	100
All	All	2784/2964 (94%)	2696 (97%)	86 (3%)	2 (0%)	59	72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	194	ARG
1	H	73	VAL

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	176/182 (97%)	176 (100%)	0	100	100
1	B	175/182 (96%)	175 (100%)	0	100	100
1	C	180/182 (99%)	180 (100%)	0	100	100
1	D	172/182 (94%)	172 (100%)	0	100	100
1	E	172/182 (94%)	172 (100%)	0	100	100
1	F	170/182 (93%)	170 (100%)	0	100	100
1	G	168/182 (92%)	168 (100%)	0	100	100
1	H	170/182 (93%)	170 (100%)	0	100	100
1	I	156/182 (86%)	155 (99%)	1 (1%)	92	97
1	J	172/182 (94%)	172 (100%)	0	100	100
1	K	170/182 (93%)	170 (100%)	0	100	100
1	L	167/182 (92%)	166 (99%)	1 (1%)	92	97
1	M	173/182 (95%)	172 (99%)	1 (1%)	92	97
All	All	2221/2366 (94%)	2218 (100%)	3 (0%)	96	99

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	132	GLU
1	L	59	PHE
1	M	115	GLU

Some 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 chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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	H2U	A	301	-	22,22,22	0.64	0	33,33,33	1.71	5 (15%)
2	H2U	B	301	-	22,22,22	0.67	0	33,33,33	1.71	6 (18%)
2	H2U	C	301	-	22,22,22	0.70	0	33,33,33	1.76	6 (18%)
2	H2U	D	301	-	22,22,22	0.69	0	33,33,33	1.79	5 (15%)
2	H2U	E	301	-	22,22,22	0.66	0	33,33,33	1.69	5 (15%)
2	H2U	F	301	-	22,22,22	0.65	0	33,33,33	1.69	5 (15%)
2	H2U	G	301	-	22,22,22	0.64	0	33,33,33	1.69	6 (18%)
2	H2U	H	301	-	22,22,22	0.66	0	33,33,33	1.73	5 (15%)
2	H2U	J	301	-	22,22,22	0.65	0	33,33,33	1.73	5 (15%)
2	H2U	K	301	-	22,22,22	0.62	0	33,33,33	1.68	5 (15%)
2	H2U	L	301	-	22,22,22	0.68	0	33,33,33	1.76	5 (15%)
2	H2U	M	301	-	22,22,22	0.65	0	33,33,33	1.76	5 (15%)

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	H2U	A	301	-	-	0/10/39/39	0/2/2/2
2	H2U	B	301	-	-	0/10/39/39	0/2/2/2
2	H2U	C	301	-	-	0/10/39/39	0/2/2/2
2	H2U	D	301	-	-	0/10/39/39	0/2/2/2
2	H2U	E	301	-	-	0/10/39/39	0/2/2/2
2	H2U	F	301	-	-	0/10/39/39	0/2/2/2
2	H2U	G	301	-	-	0/10/39/39	0/2/2/2
2	H2U	H	301	-	-	0/10/39/39	0/2/2/2
2	H2U	J	301	-	-	0/10/39/39	0/2/2/2
2	H2U	K	301	-	-	0/10/39/39	0/2/2/2
2	H2U	L	301	-	-	0/10/39/39	0/2/2/2
2	H2U	M	301	-	-	0/10/39/39	0/2/2/2

There are no bond length outliers.

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	H2U	N3-C2-N1	5.76	122.36	116.71
2	D	301	H2U	C4-N3-C2	-5.61	120.98	125.83
2	L	301	H2U	C4-N3-C2	-5.57	121.01	125.83
2	M	301	H2U	C4-N3-C2	-5.54	121.03	125.83
2	M	301	H2U	N3-C2-N1	5.53	122.13	116.71
2	L	301	H2U	N3-C2-N1	5.49	122.09	116.71
2	J	301	H2U	N3-C2-N1	5.48	122.08	116.71
2	H	301	H2U	C4-N3-C2	-5.47	121.09	125.83
2	D	301	H2U	N3-C2-N1	5.44	122.04	116.71
2	H	301	H2U	N3-C2-N1	5.42	122.03	116.71
2	F	301	H2U	N3-C2-N1	5.41	122.02	116.71
2	E	301	H2U	C4-N3-C2	-5.39	121.17	125.83
2	J	301	H2U	C4-N3-C2	-5.38	121.17	125.83
2	B	301	H2U	C4-N3-C2	-5.35	121.20	125.83
2	G	301	H2U	C4-N3-C2	-5.35	121.20	125.83
2	E	301	H2U	N3-C2-N1	5.31	121.92	116.71
2	K	301	H2U	N3-C2-N1	5.28	121.89	116.71
2	G	301	H2U	N3-C2-N1	5.28	121.88	116.71
2	B	301	H2U	N3-C2-N1	5.27	121.88	116.71
2	F	301	H2U	C4-N3-C2	-5.23	121.31	125.83
2	A	301	H2U	N3-C2-N1	5.18	121.79	116.71
2	C	301	H2U	C4-N3-C2	-5.10	121.41	125.83
2	K	301	H2U	C4-N3-C2	-5.04	121.47	125.83
2	A	301	H2U	C4-N3-C2	-5.01	121.49	125.83
2	A	301	H2U	C5-C4-N3	3.51	120.06	116.76
2	M	301	H2U	O2-C2-N1	-3.36	118.81	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	H2U	O2-C2-N1	-3.34	118.83	123.25
2	G	301	H2U	O2-C2-N1	-3.34	118.83	123.25
2	C	301	H2U	O2-C2-N1	-3.34	118.83	123.25
2	K	301	H2U	O2-C2-N1	-3.28	118.91	123.25
2	F	301	H2U	O2-C2-N1	-3.27	118.92	123.25
2	J	301	H2U	O2-C2-N1	-3.25	118.95	123.25
2	H	301	H2U	O2-C2-N1	-3.22	118.99	123.25
2	B	301	H2U	O2-C2-N1	-3.18	119.05	123.25
2	D	301	H2U	O2-C2-N1	-3.15	119.08	123.25
2	L	301	H2U	C1'-N1-C2	3.10	122.52	118.16
2	D	301	H2U	C1'-N1-C2	3.04	122.44	118.16
2	A	301	H2U	O2-C2-N1	-2.99	119.30	123.25
2	L	301	H2U	O2-C2-N1	-2.98	119.31	123.25
2	A	301	H2U	OP2-P-OP1	2.90	119.91	110.44
2	K	301	H2U	C5-C4-N3	2.82	119.42	116.76
2	D	301	H2U	OP2-P-OP1	2.75	119.44	110.44
2	J	301	H2U	OP2-P-OP1	2.68	119.21	110.44
2	M	301	H2U	OP2-P-OP1	2.68	119.19	110.44
2	F	301	H2U	OP2-P-OP1	2.67	119.17	110.44
2	G	301	H2U	OP2-P-OP1	2.67	119.16	110.44
2	J	301	H2U	C1'-N1-C2	2.61	121.83	118.16
2	H	301	H2U	C1'-N1-C2	2.59	121.79	118.16
2	H	301	H2U	OP2-P-OP1	2.57	118.83	110.44
2	L	301	H2U	OP2-P-OP1	2.56	118.81	110.44
2	E	301	H2U	OP2-P-OP1	2.55	118.79	110.44
2	M	301	H2U	C1'-N1-C2	2.55	121.74	118.16
2	C	301	H2U	OP2-P-OP1	2.54	118.76	110.44
2	K	301	H2U	OP2-P-OP1	2.52	118.66	110.44
2	B	301	H2U	OP2-P-OP1	2.50	118.63	110.44
2	B	301	H2U	C1'-N1-C2	2.47	121.63	118.16
2	B	301	H2U	C5-C4-N3	2.45	119.07	116.76
2	C	301	H2U	C5-C4-N3	2.30	118.92	116.76
2	F	301	H2U	C5-C4-N3	2.27	118.90	116.76
2	C	301	H2U	C1'-N1-C2	2.26	121.33	118.16
2	E	301	H2U	C5-C4-N3	2.21	118.84	116.76
2	G	301	H2U	C5-C4-N3	2.10	118.74	116.76
2	G	301	H2U	C1'-N1-C2	2.01	120.99	118.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	220/228 (96%)	0.05	2 (0%) 81 88	27, 40, 65, 108	0
1	B	219/228 (96%)	0.43	9 (4%) 35 46	28, 53, 88, 146	0
1	C	225/228 (98%)	0.11	2 (0%) 81 88	30, 46, 84, 120	0
1	D	216/228 (94%)	0.54	17 (7%) 13 19	33, 58, 116, 143	0
1	E	217/228 (95%)	0.64	20 (9%) 9 15	49, 75, 102, 136	0
1	F	215/228 (94%)	0.76	23 (10%) 6 10	43, 73, 117, 146	0
1	G	213/228 (93%)	0.64	16 (7%) 14 21	54, 77, 114, 135	0
1	H	215/228 (94%)	0.55	16 (7%) 14 21	54, 76, 119, 145	0
1	I	197/228 (86%)	0.79	26 (13%) 4 7	40, 72, 125, 141	0
1	J	218/228 (95%)	0.39	11 (5%) 28 38	34, 66, 113, 145	0
1	K	216/228 (94%)	1.18	53 (24%) 1 2	67, 97, 127, 150	0
1	L	213/228 (93%)	1.41	55 (25%) 1 2	64, 100, 136, 153	0
1	M	218/228 (95%)	0.38	6 (2%) 50 60	33, 54, 90, 115	0
All	All	2802/2964 (94%)	0.60	256 (9%) 9 15	27, 69, 119, 153	0

All (256) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	159	THR	7.8
1	L	167	LEU	7.5
1	F	215	ALA	6.8
1	F	218	ILE	6.6
1	L	142	ILE	6.5
1	I	189	PRO	6.5
1	L	161	PRO	6.3
1	F	9	MET	6.0
1	K	142	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	J	159	THR	5.6
1	I	37	TYR	5.5
1	D	209	ASP	5.3
1	I	164	LEU	5.3
1	L	222	ILE	5.3
1	L	217	GLY	4.9
1	K	137	GLY	4.9
1	L	205	ILE	4.7
1	G	211	PRO	4.7
1	F	217	GLY	4.6
1	E	167	LEU	4.6
1	L	164	LEU	4.6
1	E	224	ASP	4.6
1	I	161	PRO	4.6
1	L	213	ALA	4.6
1	L	15	LEU	4.5
1	L	196	ALA	4.5
1	L	155	VAL	4.5
1	B	8	VAL	4.4
1	K	135	ILE	4.3
1	K	167	LEU	4.3
1	G	209	ASP	4.3
1	D	207	LEU	4.3
1	K	152	LYS	4.2
1	F	15	LEU	4.2
1	K	225	LEU	4.2
1	K	171	ILE	4.2
1	E	182	VAL	4.1
1	K	124	THR	4.1
1	L	144	ARG	4.1
1	F	208	ALA	4.1
1	L	171	ILE	4.0
1	F	211	PRO	4.0
1	L	193	LEU	4.0
1	I	160	ARG	4.0
1	G	38	ILE	4.0
1	H	38	ILE	3.9
1	E	218	ILE	3.9
1	L	202	GLY	3.9
1	K	176	PHE	3.8
1	F	34	VAL	3.8
1	K	136	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	L	21	LEU	3.7
1	L	187	GLY	3.7
1	L	184	ALA	3.7
1	L	37	TYR	3.7
1	D	211	PRO	3.6
1	L	11	VAL	3.6
1	G	207	LEU	3.6
1	F	206	TYR	3.6
1	L	158	SER	3.6
1	B	34	VAL	3.6
1	L	139	ALA	3.6
1	D	195	PHE	3.6
1	K	10	ASP	3.6
1	I	199	ILE	3.5
1	L	135	ILE	3.5
1	B	222	ILE	3.5
1	K	195	PHE	3.5
1	H	209	ASP	3.5
1	A	6	VAL	3.5
1	K	143	ALA	3.5
1	K	15	LEU	3.4
1	M	189	PRO	3.4
1	K	149	LEU	3.4
1	J	180	PRO	3.4
1	H	218	ILE	3.4
1	I	205	ILE	3.4
1	J	225	LEU	3.4
1	E	223	LYS	3.3
1	L	100	PHE	3.3
1	D	222	ILE	3.3
1	K	11	VAL	3.3
1	L	125	GLU	3.3
1	F	13	ASN	3.3
1	I	212	ALA	3.2
1	L	182	VAL	3.2
1	G	205	ILE	3.2
1	G	218	ILE	3.2
1	L	176	PHE	3.2
1	K	192	THR	3.2
1	D	37	TYR	3.2
1	I	201	VAL	3.2
1	L	34	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	207	LEU	3.2
1	K	106	VAL	3.2
1	H	63	PHE	3.1
1	K	107	ARG	3.1
1	K	105	SER	3.1
1	K	169	GLU	3.1
1	K	103	ALA	3.1
1	L	38	ILE	3.1
1	K	223	LYS	3.1
1	H	208	ALA	3.1
1	D	8	VAL	3.1
1	E	210	ASN	3.0
1	K	41	VAL	3.0
1	F	38	ILE	3.0
1	L	169	GLU	3.0
1	L	134	PHE	3.0
1	I	157	PRO	3.0
1	G	215	ALA	2.9
1	I	15	LEU	2.9
1	J	191	GLU	2.9
1	C	6	VAL	2.9
1	K	144	ARG	2.9
1	L	103	ALA	2.9
1	I	167	LEU	2.9
1	J	167	LEU	2.9
1	J	218	ILE	2.9
1	D	38	ILE	2.9
1	E	13	ASN	2.9
1	I	207	LEU	2.8
1	L	218	ILE	2.8
1	K	63	PHE	2.8
1	K	182	VAL	2.8
1	G	206	TYR	2.8
1	G	144	ARG	2.8
1	I	34	VAL	2.8
1	I	218	ILE	2.8
1	E	9	MET	2.8
1	K	154	TYR	2.8
1	D	215	ALA	2.7
1	F	209	ASP	2.7
1	F	36	GLU	2.7
1	D	218	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	217	GLY	2.7
1	H	66	ARG	2.7
1	K	164	LEU	2.7
1	F	201	VAL	2.7
1	L	123	LEU	2.7
1	J	183	GLY	2.7
1	K	134	PHE	2.7
1	G	208	ALA	2.7
1	F	10	ASP	2.7
1	E	225	LEU	2.6
1	E	211	PRO	2.6
1	K	207	LEU	2.6
1	L	185	GLN	2.6
1	F	16	ILE	2.6
1	L	208	ALA	2.6
1	K	100	PHE	2.6
1	L	156	GLY	2.6
1	I	190	GLY	2.5
1	H	100[A]	PHE	2.5
1	L	35	ARG	2.5
1	I	219	ILE	2.5
1	L	206	TYR	2.5
1	L	183	GLY	2.5
1	I	203	ARG	2.5
1	G	100[A]	PHE	2.5
1	L	219	ILE	2.5
1	H	193	LEU	2.5
1	B	7	ASP	2.5
1	E	63	PHE	2.5
1	A	223	LYS	2.5
1	D	213	ALA	2.4
1	E	34	VAL	2.4
1	J	222	ILE	2.4
1	I	129	PRO	2.4
1	K	147	VAL	2.4
1	F	200	ILE	2.4
1	H	222	ILE	2.4
1	K	199	ILE	2.4
1	L	180	PRO	2.4
1	L	210	ASN	2.4
1	H	37	TYR	2.4
1	L	215	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	210	ASN	2.4
1	I	35	ARG	2.4
1	I	220	GLU	2.4
1	H	86	ALA	2.4
1	B	191	GLU	2.4
1	J	187	GLY	2.3
1	F	212	ALA	2.3
1	G	34	VAL	2.3
1	D	13	ASN	2.3
1	L	160	ARG	2.3
1	B	38	ILE	2.3
1	L	14	ARG	2.3
1	K	180	PRO	2.3
1	K	189	PRO	2.3
1	L	170	ILE	2.3
1	L	162	GLU	2.3
1	M	181	GLY	2.3
1	K	210	ASN	2.3
1	E	14	ARG	2.3
1	G	14	ARG	2.3
1	L	194	ARG	2.3
1	B	225	LEU	2.3
1	K	57	ALA	2.3
1	K	193	LEU	2.3
1	D	10	ASP	2.3
1	K	66	ARG	2.3
1	F	37	TYR	2.2
1	H	8	VAL	2.2
1	G	171	ILE	2.2
1	K	160	ARG	2.2
1	E	38	ILE	2.2
1	L	59	PHE	2.2
1	K	162	GLU	2.2
1	H	31	THR	2.2
1	K	206	TYR	2.2
1	F	205	ILE	2.2
1	K	222	ILE	2.2
1	D	223	LYS	2.2
1	E	15	LEU	2.2
1	K	21	LEU	2.2
1	I	30	VAL	2.2
1	E	222	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	176	PHE	2.2
1	K	61	LYS	2.2
1	B	15	LEU	2.2
1	B	116	MET	2.2
1	L	149	LEU	2.2
1	M	223	LYS	2.1
1	M	195	PHE	2.1
1	G	13	ASN	2.1
1	J	181	GLY	2.1
1	K	186	GLY	2.1
1	K	131	ALA	2.1
1	D	220	GLU	2.1
1	E	66	ARG	2.1
1	H	34	VAL	2.1
1	F	222	ILE	2.1
1	C	3	SER	2.1
1	K	181	GLY	2.1
1	E	212	ALA	2.1
1	I	208	ALA	2.1
1	I	179	SER	2.1
1	K	59	PHE	2.1
1	L	174	ASP	2.1
1	H	62	ARG	2.1
1	M	14	ARG	2.1
1	I	16	ILE	2.1
1	M	218	ILE	2.1
1	F	100[A]	PHE	2.1
1	G	107	ARG	2.0
1	K	151	VAL	2.0
1	L	189	PRO	2.0
1	D	214	ALA	2.0
1	H	220	GLU	2.0
1	D	17	LEU	2.0
1	K	123	LEU	2.0
1	J	194	ARG	2.0
1	K	168	ARG	2.0
1	L	66	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	H2U	D	301	21/21	0.18	0.81	55,59,71,73	0
2	H2U	C	301	21/21	0.13	0.08	35,38,45,47	0
2	H2U	A	301	21/21	0.12	0.00	32,34,36,38	0
2	H2U	M	301	21/21	0.15	-0.03	59,64,78,79	0
2	H2U	F	301	21/21	0.17	-0.06	69,74,84,87	0
2	H2U	J	301	21/21	0.15	-0.20	62,68,83,86	0
2	H2U	K	301	21/21	0.15	-0.30	78,83,91,92	0
2	H2U	L	301	21/21	0.20	-0.36	122,125,141,143	0
2	H2U	G	301	21/21	0.14	-0.45	71,74,82,84	0
2	H2U	H	301	21/21	0.12	-0.56	70,75,82,85	0
2	H2U	E	301	21/21	0.11	-0.57	62,70,73,74	0
2	H2U	B	301	21/21	0.11	-0.98	42,44,52,56	0
3	CL	A	302	1/1	0.08	-1.45	78,78,78,78	1

6.5 Other polymers ⓘ

There are no such residues in this entry.