



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 02:47 PM EDT

PDB ID : 4LYL  
Title : Crystal structure of uracil-DNA glycosylase from cod (*Gadus morhua*) in complex with the proteinaceous inhibitor UGI  
Authors : Assefa, N.G.; Niiranen, L.M.K.; Johnson, K.A.; Leiros, H.-K.S.; Smalas, A.O.; Willassen, N.P.; Moe, E.  
Deposited on : 2013-07-31  
Resolution : 1.93 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

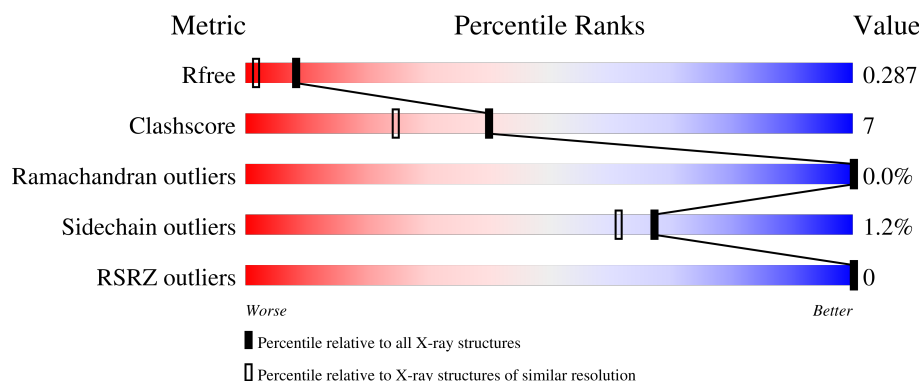
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.93 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))
$R_{free}$	164625	1306 (1.94-1.94)
Clashscore	180529	1400 (1.94-1.94)
Ramachandran outliers	177936	1387 (1.94-1.94)
Sidechain outliers	177891	1387 (1.94-1.94)
RSRZ outliers	164620	1306 (1.94-1.94)

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  $\geq 3$ , 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	223	
1	C	223	
1	E	223	
1	G	223	
1	I	223	

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Mol	Chain	Length	Quality of chain
1	K	223	 86% 14%
1	M	223	 85% 15%
1	O	223	 90% 10%
2	B	84	 85% 13% •
2	D	84	 80% 18% •
2	F	84	 87% 11% •
2	H	84	 77% 19% ••
2	J	84	 71% 26% •
2	L	84	 75% 23% •
2	N	84	 80% 18% •
2	P	84	 81% 17% •

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21002 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 Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	1	0
			1792	1152	320	312	8			
1	C	223	Total	C	N	O	S	0	0	0
			1787	1148	320	312	7			
1	E	223	Total	C	N	O	S	0	0	0
			1787	1148	320	312	7			
1	G	223	Total	C	N	O	S	0	1	0
			1793	1152	321	313	7			
1	I	223	Total	C	N	O	S	0	3	0
			1805	1163	323	312	7			
1	K	223	Total	C	N	O	S	0	0	0
			1787	1148	320	312	7			
1	M	223	Total	C	N	O	S	0	0	0
			1787	1148	320	312	7			
1	O	223	Total	C	N	O	S	0	0	0
			1787	1148	320	312	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	MET	-	expression tag	UNP Q9I983
A	83	GLU	-	expression tag	UNP Q9I983
A	84	PHE	-	expression tag	UNP Q9I983
C	82	MET	-	expression tag	UNP Q9I983
C	83	GLU	-	expression tag	UNP Q9I983
C	84	PHE	-	expression tag	UNP Q9I983
E	82	MET	-	expression tag	UNP Q9I983
E	83	GLU	-	expression tag	UNP Q9I983
E	84	PHE	-	expression tag	UNP Q9I983
G	82	MET	-	expression tag	UNP Q9I983
G	83	GLU	-	expression tag	UNP Q9I983
G	84	PHE	-	expression tag	UNP Q9I983
I	82	MET	-	expression tag	UNP Q9I983

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Chain	Residue	Modelled	Actual	Comment	Reference
I	83	GLU	-	expression tag	UNP Q9I983
I	84	PHE	-	expression tag	UNP Q9I983
K	82	MET	-	expression tag	UNP Q9I983
K	83	GLU	-	expression tag	UNP Q9I983
K	84	PHE	-	expression tag	UNP Q9I983
M	82	MET	-	expression tag	UNP Q9I983
M	83	GLU	-	expression tag	UNP Q9I983
M	84	PHE	-	expression tag	UNP Q9I983
O	82	MET	-	expression tag	UNP Q9I983
O	83	GLU	-	expression tag	UNP Q9I983
O	84	PHE	-	expression tag	UNP Q9I983

- Molecule 2 is a protein called Uracil-DNA glycosylase inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	S	0	1	0
			653	410	99	141	3			
2	D	82	Total	C	N	O	S	0	0	0
			647	406	99	139	3			
2	F	82	Total	C	N	O	S	0	1	0
			653	410	99	141	3			
2	H	82	Total	C	N	O	S	0	0	0
			647	406	99	139	3			
2	J	82	Total	C	N	O	S	0	1	0
			653	410	99	141	3			
2	L	82	Total	C	N	O	S	0	0	0
			647	406	99	139	3			
2	N	82	Total	C	N	O	S	0	0	0
			647	406	99	139	3			
2	P	82	Total	C	N	O	S	0	0	0
			647	406	99	139	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	50	Total	O	0	0
			50	50		
3	C	167	Total	O	0	0
			167	167		
3	D	54	Total	O	0	0
			54	54		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	143	Total 143	O 143	0	0
3	F	48	Total 48	O 48	0	0
3	G	129	Total 129	O 129	0	0
3	H	43	Total 43	O 43	0	0
3	I	153	Total 153	O 153	0	0
3	J	37	Total 37	O 37	0	0
3	K	143	Total 143	O 143	0	0
3	L	43	Total 43	O 43	0	0
3	M	117	Total 117	O 117	0	0
3	N	30	Total 30	O 30	0	0
3	O	146	Total 146	O 146	0	0
3	P	28	Total 28	O 28	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.

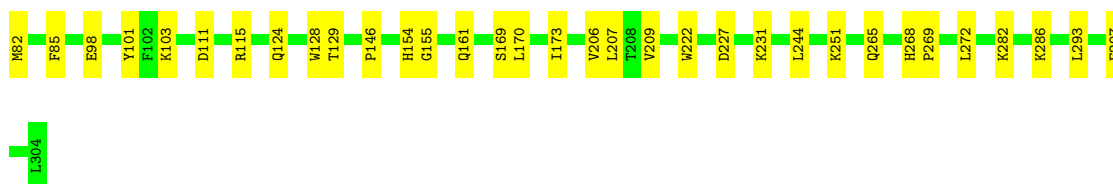
- Molecule 1: Uracil-DNA glycosylase

Chain A: 




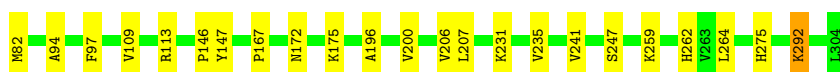
- Molecule 1: Uracil-DNA glycosylase

Chain C: 




- Molecule 1: Uracil-DNA glycosylase

Chain E: 



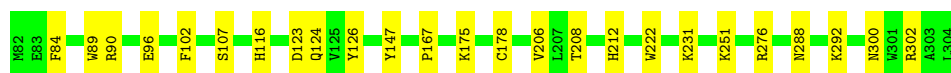
- Molecule 1: Uracil-DNA glycosylase

Chain G: 

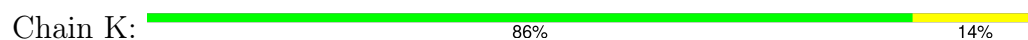


- Molecule 1: Uracil-DNA glycosylase

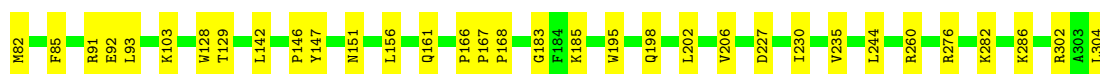
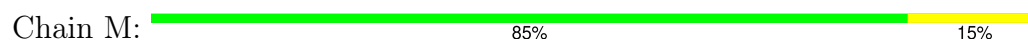
Chain I: 



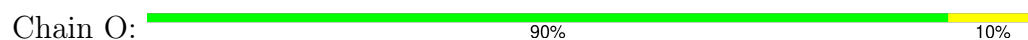
- Molecule 1: Uracil-DNA glycosylase



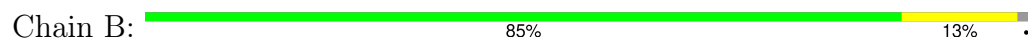
- Molecule 1: Uracil-DNA glycosylase



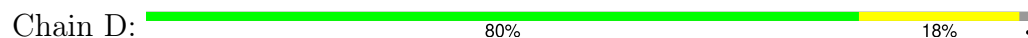
- Molecule 1: Uracil-DNA glycosylase



- Molecule 2: Uracil-DNA glycosylase inhibitor



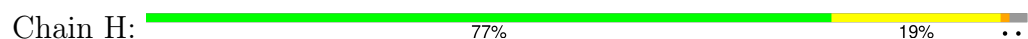
- Molecule 2: Uracil-DNA glycosylase inhibitor



- Molecule 2: Uracil-DNA glycosylase inhibitor



- Molecule 2: Uracil-DNA glycosylase inhibitor







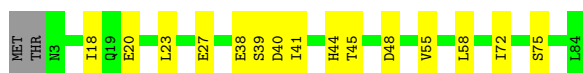
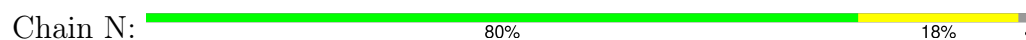
- Molecule 2: Uracil-DNA glycosylase inhibitor



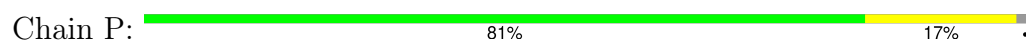
- Molecule 2: Uracil-DNA glycosylase inhibitor



- Molecule 2: Uracil-DNA glycosylase inhibitor



- Molecule 2: Uracil-DNA glycosylase inhibitor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.21Å 86.92Å 175.37Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	29.48 – 1.93 29.48 – 1.94	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.48-1.93) 89.8 (29.48-1.94)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.237 , 0.283 0.240 , 0.287	Depositor DCC
$R_{free}$ test set	10000 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 21.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.199 for h,-k,-l	Xtriage
Reported twinning fraction	0.763 for H, K, L 0.237 for -h,-k,l	Depositor
Outliers	1 of 199006 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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 33.86 % 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 7.4766e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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	0.64	0/1852	0.86	3/2513 (0.1%)
1	C	0.65	0/1844	0.84	1/2503 (0.0%)
1	E	0.58	0/1844	0.84	1/2503 (0.0%)
1	G	0.58	0/1853	0.81	1/2515 (0.0%)
1	I	0.61	0/1871	0.81	0/2536
1	K	0.64	0/1844	0.82	1/2503 (0.0%)
1	M	0.59	0/1844	0.81	1/2503 (0.0%)
1	O	0.63	0/1844	0.84	1/2503 (0.0%)
2	B	0.55	0/664	0.84	0/899
2	D	0.58	0/655	0.83	0/887
2	F	0.51	0/664	0.81	1/899 (0.1%)
2	H	0.52	0/655	0.90	0/887
2	J	0.47	0/664	0.79	0/899
2	L	0.47	0/655	0.81	0/887
2	N	0.46	0/655	0.72	0/887
2	P	0.52	0/655	0.81	0/887
All	All	0.59	0/20063	0.82	10/27211 (0.0%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	191	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	227	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	227	ASP	CB-CG-OD1	5.74	123.47	118.30
2	F	74	ASP	CB-CG-OD1	5.69	123.42	118.30
1	O	191	ASP	CB-CG-OD1	5.51	123.26	118.30
1	K	174	TYR	CB-CG-CD1	5.28	124.17	121.00
1	E	207	LEU	CB-CG-CD1	5.23	119.89	111.00
1	M	227	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	123	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	182	ASP	CB-CG-OD1	5.01	122.81	118.30

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	1792	0	1757	14	0
1	C	1787	0	1748	23	0
1	E	1787	0	1748	17	0
1	G	1793	0	1756	27	0
1	I	1805	0	1787	21	0
1	K	1787	0	1748	22	0
1	M	1787	0	1748	27	0
1	O	1787	0	1748	14	0
2	B	653	0	646	13	0
2	D	647	0	640	11	0
2	F	653	0	646	6	0
2	H	647	0	640	13	0
2	J	653	0	646	15	0
2	L	647	0	640	19	0
2	N	647	0	640	8	0
2	P	647	0	640	14	0
3	A	152	0	0	4	0
3	B	50	0	0	5	0
3	C	167	0	0	6	0
3	D	54	0	0	6	0
3	E	143	0	0	6	0
3	F	48	0	0	4	0
3	G	129	0	0	12	0
3	H	43	0	0	5	0
3	I	153	0	0	6	0
3	J	37	0	0	4	0
3	K	143	0	0	9	0
3	L	43	0	0	6	0
3	M	117	0	0	10	0
3	N	30	0	0	4	0
3	O	146	0	0	9	0
3	P	28	0	0	1	0
All	All	21002	0	19178	252	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 7.

All (252) 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:K:161:GLN:HA	3:K:429:HOH:O	1.39	1.23
1:O:192:LEU:HD22	3:O:461:HOH:O	1.50	1.12
2:N:20:GLU:HB3	3:N:108:HOH:O	1.53	1.06
2:D:57:LEU:HG	3:D:122:HOH:O	1.56	1.05
1:K:302:ARG:HG3	3:K:532:HOH:O	1.64	0.98
2:D:59:THR:HG23	3:D:122:HOH:O	1.62	0.98
1:I:251[B]:LYS:HE3	1:I:251[B]:LYS:HA	1.49	0.92
1:I:251[B]:LYS:HA	1:I:251[B]:LYS:CE	2.00	0.92
1:M:183:GLY:HA2	3:M:417:HOH:O	1.72	0.89
2:D:35:ASN:ND2	3:D:123:HOH:O	2.05	0.89
2:F:34:GLY:HA2	3:F:131:HOH:O	1.72	0.87
2:F:84:LEU:HD23	3:F:106:HOH:O	1.74	0.86
1:G:248:TYR:CG	3:G:471:HOH:O	2.28	0.86
1:M:167:PRO:HB3	3:N:108:HOH:O	1.77	0.85
1:E:82:MET:HB2	3:E:450:HOH:O	1.78	0.83
1:G:248:TYR:CD2	3:G:471:HOH:O	2.32	0.82
1:G:208:THR:HG22	3:G:442:HOH:O	1.78	0.82
1:E:264:LEU:HG	3:E:424:HOH:O	1.79	0.81
2:D:17:VAL:HG13	3:D:133:HOH:O	1.81	0.81
2:L:71:VAL:HG12	3:L:102:HOH:O	1.80	0.79
3:A:456:HOH:O	1:K:107:SER:HB2	1.84	0.77
1:M:167:PRO:CB	3:N:108:HOH:O	2.32	0.77
1:I:231[A]:LYS:HE3	3:I:421:HOH:O	1.84	0.77
1:E:109:VAL:HG13	3:E:449:HOH:O	1.85	0.76
2:B:60:SER:OG	2:B:66:LYS:HG2	1.88	0.74
2:P:60:SER:OG	2:P:66:LYS:HG3	1.87	0.73
2:H:82:LYS:HB2	3:H:126:HOH:O	1.88	0.73
1:M:93:LEU:HG	3:M:413:HOH:O	1.87	0.73
1:C:161:GLN:CD	3:C:473:HOH:O	2.28	0.72
2:D:59:THR:CG2	3:D:122:HOH:O	2.27	0.72
1:G:144:GLN:HG2	3:G:471:HOH:O	1.90	0.72
1:G:248:TYR:HB2	3:H:117:HOH:O	1.92	0.69
1:K:184:PHE:HA	1:K:302:ARG:HG2	1.74	0.69
1:K:133:ASP:OD2	3:K:498:HOH:O	2.11	0.69
2:L:60:SER:OG	2:L:66:LYS:HG2	1.93	0.69
1:E:231:LYS:HD3	3:E:409:HOH:O	1.94	0.68
1:C:231:LYS:HD3	3:C:438:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:96:GLU:HB3	3:I:425:HOH:O	1.93	0.67
2:P:28:GLU:HA	2:P:31:GLU:OE2	1.94	0.67
1:M:91:ARG:NH1	3:M:490:HOH:O	2.29	0.66
1:K:247:SER:OG	2:L:28:GLU:HG3	1.95	0.66
1:O:195:TRP:CE2	3:O:461:HOH:O	2.49	0.66
2:L:80:LYS:HE2	3:L:119:HOH:O	1.96	0.65
2:P:60:SER:CB	2:P:66:LYS:HG3	2.26	0.65
2:B:60:SER:OG	2:B:66:LYS:CG	2.44	0.65
2:P:60:SER:OG	2:P:66:LYS:CG	2.44	0.65
2:L:82:LYS:HD2	3:L:120:HOH:O	1.95	0.65
1:O:184:PHE:HA	1:O:302:ARG:HG2	1.79	0.65
2:J:78:GLU:HB3	3:J:112:HOH:O	1.98	0.64
2:J:73:GLN:HB2	2:J:79:ASN:OD1	1.96	0.64
1:M:103:LYS:HE2	3:M:430:HOH:O	1.96	0.63
3:K:485:HOH:O	2:L:4:LEU:HD11	1.97	0.63
1:M:91:ARG:CZ	1:M:92:GLU:OE2	2.47	0.62
1:K:193:SER:O	1:K:197:LYS:HG3	2.00	0.61
2:L:73:GLN:N	3:L:102:HOH:O	2.33	0.61
1:E:147:TYR:CZ	1:E:167:PRO:HG2	2.35	0.61
1:I:251[B]:LYS:HA	1:I:251[B]:LYS:HE2	1.82	0.61
1:I:288:ASN:O	1:I:292[B]:LYS:HG2	2.01	0.60
1:M:147:TYR:HE1	3:N:108:HOH:O	1.83	0.60
2:H:33:ILE:HA	2:H:81:ILE:HD13	1.84	0.59
1:M:91:ARG:NH1	1:M:92:GLU:OE2	2.35	0.59
1:K:154:HIS:HB3	1:K:161:GLN:OE1	2.03	0.59
1:K:179:THR:HG23	3:K:433:HOH:O	2.01	0.59
1:G:259:LYS:HB3	2:L:15:GLN:OE1	2.03	0.58
2:N:18:ILE:HD13	2:N:44:HIS:HB3	1.84	0.58
2:D:47:TYR:OH	2:D:52:ASP:HA	2.04	0.58
1:G:292:LYS:HA	3:G:487:HOH:O	2.02	0.58
1:G:120:PRO:HD2	3:G:442:HOH:O	2.04	0.57
1:E:292:LYS:HA	3:E:468:HOH:O	2.05	0.57
1:O:235:VAL:O	1:O:260:ARG:NH2	2.27	0.57
1:E:146:PRO:HD3	1:E:206:VAL:O	2.04	0.57
1:M:198:GLN:HA	3:M:450:HOH:O	2.06	0.56
1:M:142:LEU:HD12	1:M:244:LEU:HD22	1.88	0.56
2:D:18:ILE:HD13	2:D:44:HIS:HB3	1.86	0.56
1:I:175:LYS:HG3	3:I:486:HOH:O	2.05	0.56
2:N:41:ILE:HG21	2:N:58:LEU:HD23	1.87	0.56
2:B:66:LYS:CD	3:B:124:HOH:O	2.54	0.55
2:N:55:VAL:HG13	2:N:72:ILE:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:92:GLU:HB2	3:M:413:HOH:O	2.06	0.55
2:B:66:LYS:HD2	3:B:124:HOH:O	2.06	0.55
1:C:154:HIS:HB3	1:C:161:GLN:HG2	1.89	0.54
1:C:293:LEU:HB2	3:C:432:HOH:O	2.07	0.54
1:I:102:PHE:CD1	3:I:425:HOH:O	2.53	0.54
2:J:4:LEU:HA	2:J:7:ILE:HD12	1.90	0.54
2:B:11:GLU:OE1	2:B:82:LYS:NZ	2.30	0.54
1:G:196:ALA:HA	1:G:200:VAL:O	2.08	0.54
1:K:172:ASN:OD1	1:K:175:LYS:HD3	2.07	0.54
2:P:60:SER:HB3	2:P:66:LYS:HG3	1.89	0.53
1:I:276:ARG:NH2	2:J:31:GLU:OE1	2.34	0.53
1:C:268:HIS:CG	1:C:269:PRO:HD2	2.42	0.53
1:M:302:ARG:NH1	3:M:435:HOH:O	2.41	0.53
1:C:251:LYS:HG3	3:C:450:HOH:O	2.08	0.53
1:C:98:GLU:HA	1:C:103:LYS:HE3	1.90	0.52
2:L:78:GLU:OE1	2:L:78:GLU:HA	2.09	0.52
1:C:272:LEU:CD1	2:D:32:VAL:HG11	2.40	0.52
1:G:127:SER:HA	1:G:130:GLU:OE1	2.10	0.52
1:A:175:LYS:HD2	3:A:458:HOH:O	2.10	0.52
1:E:247:SER:N	2:F:28:GLU:OE2	2.38	0.52
1:O:302:ARG:HG3	3:O:462:HOH:O	2.08	0.51
1:G:218:LYS:NZ	2:H:62:ALA:O	2.43	0.51
1:K:231:LYS:O	1:K:235:VAL:HG23	2.10	0.51
2:L:60:SER:O	2:L:65:TYR:HA	2.10	0.51
1:O:138:LYS:HE2	1:O:296:THR:HG23	1.92	0.51
2:J:52:ASP:OD2	2:J:75:SER:OG	2.28	0.51
1:A:184:PHE:HA	1:A:302:ARG:HG2	1.93	0.51
1:I:212:HIS:HB3	3:I:460:HOH:O	2.10	0.51
1:O:195:TRP:CD2	3:O:461:HOH:O	2.63	0.51
1:I:251[B]:LYS:CE	1:I:251[B]:LYS:CA	2.74	0.51
1:M:128:TRP:CZ3	1:M:129:THR:HG22	2.45	0.50
2:J:23:LEU:HD11	2:J:40:ASP:HB3	1.94	0.50
1:K:247:SER:OG	2:L:28:GLU:CG	2.59	0.50
1:M:146:PRO:HD3	1:M:206:VAL:O	2.12	0.50
1:K:207:LEU:HD12	1:K:222:TRP:CZ3	2.46	0.50
1:E:241:VAL:HG22	1:E:262:HIS:HB2	1.94	0.50
2:L:4:LEU:HA	2:L:7:ILE:HD12	1.93	0.50
1:G:207:LEU:HD12	1:G:222:TRP:CZ3	2.47	0.49
1:C:297:GLU:HG2	3:C:416:HOH:O	2.11	0.49
1:O:144:GLN:HB3	3:O:454:HOH:O	2.12	0.49
1:G:125:VAL:HG22	3:G:442:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:70:LEU:HD23	2:J:70:LEU:C	2.33	0.49
1:M:235:VAL:O	1:M:260:ARG:NH2	2.46	0.49
1:K:90:ARG:CZ	3:K:428:HOH:O	2.61	0.49
1:M:156:LEU:HD22	1:M:202:LEU:HB2	1.94	0.49
2:L:73:GLN:HB2	3:L:102:HOH:O	2.13	0.49
1:G:120:PRO:CD	3:G:442:HOH:O	2.59	0.48
2:H:81:ILE:HB	3:H:129:HOH:O	2.12	0.48
1:K:302:ARG:NH2	3:K:444:HOH:O	2.46	0.48
3:O:483:HOH:O	2:P:32:VAL:HG21	2.13	0.48
1:A:207:LEU:HB2	1:A:222:TRP:CD2	2.49	0.48
1:I:276:ARG:HD2	2:J:32:VAL:HG22	1.95	0.48
2:P:65:TYR:O	2:P:67:PRO:HD3	2.14	0.48
1:G:124:GLN:O	1:G:127:SER:OG	2.32	0.48
2:P:15:GLN:O	2:P:15:GLN:HG2	2.14	0.47
1:C:111:ASP:O	1:C:115:ARG:HG3	2.15	0.47
2:J:11:GLU:HA	2:J:11:GLU:OE1	2.14	0.47
1:C:282:LYS:O	1:C:286:LYS:HG3	2.14	0.47
1:E:231:LYS:O	1:E:235:VAL:HG23	2.13	0.47
2:J:14:LYS:NZ	2:J:48:ASP:OD2	2.39	0.47
2:H:9:GLU:OE1	2:H:15:GLN:NE2	2.39	0.47
2:P:4:LEU:HB2	2:P:18:ILE:CD1	2.44	0.47
2:D:58:LEU:C	3:D:122:HOH:O	2.53	0.47
1:G:147:TYR:CZ	1:G:167:PRO:HG2	2.49	0.47
2:H:30:GLU:O	2:H:31:GLU:C	2.52	0.47
1:A:259:LYS:HD3	3:A:503:HOH:O	2.15	0.47
1:C:146:PRO:HD3	1:C:206:VAL:O	2.15	0.47
1:G:206:VAL:HA	1:G:222:TRP:HB3	1.97	0.47
1:E:259:LYS:HE3	3:J:118:HOH:O	2.14	0.47
1:K:230:ILE:HD12	1:K:252:LYS:HE3	1.96	0.47
1:C:169:SER:HB3	1:C:269:PRO:HG2	1.96	0.47
1:K:84:PHE:CD2	1:K:123:ASP:HA	2.49	0.47
1:K:268:HIS:CG	1:K:269:PRO:HD2	2.49	0.46
2:B:66:LYS:HE3	3:B:124:HOH:O	2.15	0.46
1:O:297:GLU:CD	1:O:298:PRO:HD2	2.36	0.46
2:H:80:LYS:HA	3:H:121:HOH:O	2.15	0.46
1:A:243:LEU:HD22	1:A:283:HIS:HB3	1.98	0.46
1:E:94:ALA:HA	1:E:97:PHE:CE2	2.50	0.46
1:K:196:ALA:HA	1:K:200:VAL:O	2.15	0.46
1:M:142:LEU:HD21	1:M:230:ILE:HD11	1.98	0.46
2:H:23:LEU:HD11	2:H:40:ASP:HB3	1.97	0.46
1:O:111:ASP:O	1:O:114:SER:OG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:MET:HG2	1:C:85:PHE:HB3	1.97	0.46
1:G:154:HIS:HB3	1:G:161:GLN:HG3	1.97	0.46
2:B:12:THR:HA	3:B:114:HOH:O	2.15	0.46
2:H:44:HIS:HB2	2:H:57:LEU:O	2.16	0.46
2:F:3:ASN:ND2	3:F:142:HOH:O	2.48	0.45
1:G:231:LYS:HG2	3:G:408:HOH:O	2.15	0.45
1:G:297:GLU:HA	1:G:298:PRO:HD2	1.69	0.45
1:I:147:TYR:CZ	1:I:167:PRO:HG2	2.51	0.45
1:C:98:GLU:O	1:C:103:LYS:NZ	2.34	0.45
1:M:276:ARG:NH2	3:M:477:HOH:O	2.39	0.45
2:P:50:SER:O	3:P:104:HOH:O	2.21	0.45
1:A:159:SER:HB2	1:A:192:LEU:HB2	1.99	0.45
1:C:170:LEU:HA	1:C:173:ILE:HD12	1.99	0.45
1:I:206:VAL:HA	1:I:222:TRP:HB3	1.97	0.45
1:O:304:LEU:HD21	3:O:461:HOH:O	2.16	0.45
1:M:151:ASN:ND2	3:M:467:HOH:O	2.50	0.45
1:K:136:ASP:HB3	3:K:410:HOH:O	2.17	0.45
1:C:98:GLU:HA	1:C:103:LYS:CE	2.46	0.45
2:F:45:THR:OG1	2:F:56:MET:HG2	2.17	0.45
1:G:99:LYS:CD	3:G:467:HOH:O	2.64	0.45
1:I:123:ASP:OD1	1:I:124:GLN:HG3	2.17	0.45
2:J:63:PRO:HD2	2:J:64[B]:GLU:OE1	2.16	0.45
3:G:506:HOH:O	1:I:178:CYS:HB3	2.17	0.44
1:M:195:TRP:NE1	1:M:304:LEU:HD21	2.32	0.44
1:A:124:GLN:O	1:A:155:GLY:HA3	2.18	0.44
1:A:176:GLU:HA	1:A:176:GLU:OE1	2.18	0.44
2:B:27[A]:GLU:CD	2:B:27[A]:GLU:H	2.21	0.44
1:E:196:ALA:HA	1:E:200:VAL:O	2.18	0.44
1:G:140:VAL:HG22	1:G:201:LEU:HB3	1.99	0.44
2:N:23:LEU:HD11	2:N:40:ASP:HB3	2.00	0.44
1:A:89:TRP:CE3	1:A:134:ILE:HD12	2.53	0.44
1:I:89:TRP:O	1:I:90:ARG:C	2.56	0.44
1:A:225:PHE:O	1:A:228:ALA:HB3	2.18	0.44
2:H:82:LYS:HD2	2:H:84:LEU:CD2	2.48	0.44
1:E:172:ASN:OD1	1:E:175:LYS:HD3	2.18	0.43
2:L:58:LEU:N	2:L:58:LEU:HD12	2.33	0.43
2:B:60:SER:OG	2:B:66:LYS:HG3	2.17	0.43
1:I:300:ASN:OD1	1:I:302:ARG:HB3	2.18	0.43
2:N:27:GLU:CD	2:N:27:GLU:H	2.20	0.43
1:A:220:ARG:NH2	3:A:456:HOH:O	2.51	0.43
1:G:184:PHE:C	1:G:184:PHE:CD1	2.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:LEU:HD12	1:C:222:TRP:CZ3	2.54	0.43
1:M:195:TRP:CD1	1:M:304:LEU:HD21	2.53	0.43
1:K:292:LYS:NZ	3:K:486:HOH:O	2.33	0.43
1:O:226:THR:OG1	1:O:252:LYS:NZ	2.44	0.43
2:H:29:VAL:HG11	2:H:37:PRO:HG3	2.01	0.43
2:B:60:SER:HB3	2:B:66:LYS:CE	2.49	0.43
1:E:259:LYS:HG3	2:J:15:GLN:HB3	2.00	0.43
2:F:9:GLU:HA	2:F:14:LYS:O	2.19	0.43
1:I:116:HIS:HB3	3:I:416:HOH:O	2.17	0.43
1:M:166:PRO:HA	1:M:167:PRO:HD3	1.93	0.42
2:P:4:LEU:HB2	2:P:18:ILE:HD11	2.01	0.42
1:E:275:HIS:HB2	3:F:109:HOH:O	2.19	0.42
1:I:84:PHE:O	1:I:126:TYR:HB2	2.20	0.42
2:J:73:GLN:HA	2:J:78:GLU:O	2.19	0.42
2:H:82:LYS:CB	3:H:126:HOH:O	2.57	0.42
2:L:60:SER:OG	2:L:66:LYS:CG	2.65	0.42
1:G:177:LEU:HD21	1:G:284:PHE:CG	2.54	0.42
2:H:11:GLU:HB3	2:H:82:LYS:HE3	2.00	0.42
2:J:36:LYS:CE	3:J:120:HOH:O	2.67	0.42
2:B:60:SER:HB3	2:B:66:LYS:HE3	2.00	0.42
1:E:113:ARG:HD2	3:E:476:HOH:O	2.19	0.42
1:C:244:LEU:HB2	1:C:265:GLN:HG2	2.02	0.42
1:I:208:THR:OG1	1:I:222:TRP:NE1	2.47	0.42
1:M:82:MET:HG3	1:M:85:PHE:HB3	2.01	0.42
1:C:124:GLN:O	1:C:155:GLY:HA3	2.20	0.42
2:L:60:SER:HG	2:L:66:LYS:H	1.68	0.42
1:M:103:LYS:CE	3:M:430:HOH:O	2.61	0.42
1:G:225:PHE:O	1:G:229:VAL:HG23	2.20	0.41
1:O:273:SER:HB3	3:O:483:HOH:O	2.19	0.41
1:C:272:LEU:HD11	2:D:32:VAL:HG11	2.01	0.41
2:L:72:ILE:C	3:L:102:HOH:O	2.58	0.41
2:B:7:ILE:HG23	3:B:103:HOH:O	2.18	0.41
1:C:128:TRP:CZ3	1:C:129:THR:HG22	2.56	0.41
1:C:209:VAL:HG23	3:C:412:HOH:O	2.19	0.41
2:D:60:SER:O	2:D:65:TYR:HA	2.20	0.41
2:P:60:SER:OG	2:P:66:LYS:HG2	2.19	0.41
1:A:192:LEU:HA	1:A:304:LEU:CD2	2.51	0.41
1:A:211:ALA:HB1	1:A:212:HIS:CD2	2.56	0.41
2:L:42:LEU:HD23	2:L:42:LEU:HA	1.93	0.41
2:L:62:ALA:HB1	2:L:63:PRO:HA	2.03	0.41
1:G:132:CYS:HB2	3:G:434:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:168:PRO:HG2	2:N:45:THR:CG2	2.50	0.41
1:O:196:ALA:HA	1:O:200:VAL:O	2.20	0.41
3:O:483:HOH:O	2:P:32:VAL:CG2	2.67	0.41
2:B:30:GLU:OE2	2:B:36:LYS:HB2	2.22	0.40
1:A:277:GLY:HA2	2:P:76:ASN:OD1	2.20	0.40
1:K:147:TYR:CZ	1:K:167:PRO:HG2	2.56	0.40
2:N:48:ASP:C	2:N:48:ASP:OD1	2.59	0.40
1:G:304:LEU:HA	1:G:304:LEU:HD23	1.91	0.40
2:J:36:LYS:NZ	3:J:120:HOH:O	2.46	0.40
1:M:282:LYS:O	1:M:286:LYS:HG3	2.21	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	222/223 (100%)	211 (95%)	11 (5%)	0	100	100
1	C	221/223 (99%)	212 (96%)	9 (4%)	0	100	100
1	E	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
1	G	222/223 (100%)	212 (96%)	10 (4%)	0	100	100
1	I	224/223 (100%)	217 (97%)	7 (3%)	0	100	100
1	K	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
1	M	221/223 (99%)	212 (96%)	9 (4%)	0	100	100
1	O	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
2	B	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
2	D	80/84 (95%)	79 (99%)	1 (1%)	0	100	100
2	F	81/84 (96%)	81 (100%)	0	0	100	100
2	H	80/84 (95%)	75 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	81/84 (96%)	77 (95%)	3 (4%)	1 (1%)	11	3
2	L	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
2	N	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
2	P	80/84 (95%)	76 (95%)	4 (5%)	0	100	100
All	All	2416/2456 (98%)	2325 (96%)	90 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	30	GLU

### 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	191/190 (100%)	190 (100%)	1 (0%)	86	86
1	C	190/190 (100%)	189 (100%)	1 (0%)	86	86
1	E	190/190 (100%)	189 (100%)	1 (0%)	86	86
1	G	191/190 (100%)	190 (100%)	1 (0%)	86	86
1	I	193/190 (102%)	192 (100%)	1 (0%)	86	86
1	K	190/190 (100%)	188 (99%)	2 (1%)	70	64
1	M	190/190 (100%)	188 (99%)	2 (1%)	70	64
1	O	190/190 (100%)	188 (99%)	2 (1%)	70	64
2	B	77/78 (99%)	75 (97%)	2 (3%)	41	28
2	D	76/78 (97%)	73 (96%)	3 (4%)	27	14
2	F	77/78 (99%)	77 (100%)	0	100	100
2	H	76/78 (97%)	75 (99%)	1 (1%)	65	58
2	J	77/78 (99%)	75 (97%)	2 (3%)	41	28
2	L	76/78 (97%)	74 (97%)	2 (3%)	41	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	76/78 (97%)	73 (96%)	3 (4%)	27	14
2	P	76/78 (97%)	74 (97%)	2 (3%)	41	28
All	All	2136/2144 (100%)	2110 (99%)	26 (1%)	67	61

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	MET
2	B	70	LEU
2	B	75	SER
1	C	101	TYR
2	D	70	LEU
2	D	72	ILE
2	D	75	SER
1	E	292	LYS
1	G	127	SER
2	H	9	GLU
1	I	107	SER
2	J	5	SER
2	J	29	VAL
1	K	82	MET
1	K	166	PRO
2	L	3	ASN
2	L	5	SER
1	M	161	GLN
1	M	185	LYS
2	N	38	GLU
2	N	39	SER
2	N	75	SER
1	O	131	MET
1	O	160	VAL
2	P	64	GLU
2	P	82	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	151	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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	223/223 (100%)	-0.89	0 100 100	13, 21, 32, 49	1 (0%)
1	C	223/223 (100%)	-0.94	0 100 100	12, 20, 31, 42	0
1	E	223/223 (100%)	-0.91	0 100 100	14, 23, 36, 67	0
1	G	223/223 (100%)	-0.87	0 100 100	12, 23, 38, 52	1 (0%)
1	I	223/223 (100%)	-0.93	0 100 100	12, 21, 31, 42	3 (1%)
1	K	223/223 (100%)	-0.89	0 100 100	13, 21, 30, 40	0
1	M	223/223 (100%)	-0.83	0 100 100	14, 23, 35, 66	0
1	O	223/223 (100%)	-0.94	0 100 100	15, 21, 31, 51	0
2	B	82/84 (97%)	-0.89	0 100 100	16, 24, 36, 41	1 (1%)
2	D	82/84 (97%)	-0.81	0 100 100	14, 27, 40, 56	0
2	F	82/84 (97%)	-0.77	0 100 100	15, 30, 43, 54	1 (1%)
2	H	82/84 (97%)	-0.85	0 100 100	15, 28, 40, 50	0
2	J	82/84 (97%)	-0.69	0 100 100	20, 32, 47, 52	1 (1%)
2	L	82/84 (97%)	-0.73	0 100 100	18, 32, 45, 54	0
2	N	82/84 (97%)	-0.60	0 100 100	20, 34, 48, 58	0
2	P	82/84 (97%)	-0.81	0 100 100	18, 30, 42, 50	0
All	All	2440/2456 (99%)	-0.87	0 100 100	12, 23, 40, 67	8 (0%)

There are no RSRZ outliers to report.

### 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 [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.