



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 10:50 AM GMT

PDB ID : 4A97  
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) in complex with zopiclone  
Authors : Spurny, R.; Brams, M.; Ulens, C.  
Deposited on : 2011-11-24  
Resolution : 3.34 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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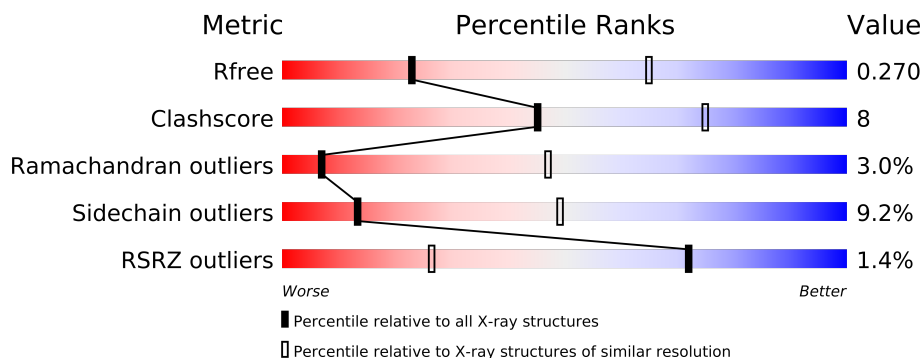
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
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 3.34 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	1421 (3.48-3.20)
Clashscore	79885	1077 (3.46-3.22)
Ramachandran outliers	78287	1053 (3.46-3.22)
Sidechain outliers	78261	1052 (3.46-3.22)
RSRZ outliers	66119	1422 (3.48-3.20)

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  $\geq 3$ , 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	307	
1	B	307	
1	C	307	
1	D	307	
1	E	307	
1	F	307	
1	G	307	
1	H	307	
1	I	307	
1	J	307	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ZPC	A	1318	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25290 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 CYS-LOOP LIGAND-GATED ION CHANNEL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	B	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	C	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	D	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	E	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	F	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	G	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	H	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	I	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			
1	J	307	Total	C	N	O	S	0	0	0
			2502	1630	416	450	6			

There are 20 discrepancies between the modelled and reference sequences:

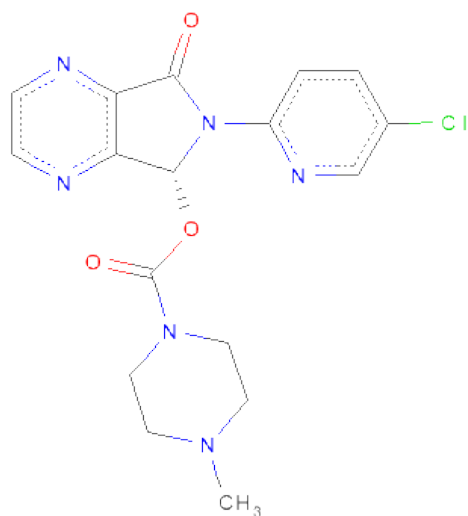
Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	INSERTION	UNP P0C7B7
A	289	ASN	MET	CONFLICT	UNP P0C7B7
B	164	GLY	-	INSERTION	UNP P0C7B7
B	289	ASN	MET	CONFLICT	UNP P0C7B7
C	164	GLY	-	INSERTION	UNP P0C7B7
C	289	ASN	MET	CONFLICT	UNP P0C7B7
D	164	GLY	-	INSERTION	UNP P0C7B7
D	289	ASN	MET	CONFLICT	UNP P0C7B7
E	164	GLY	-	INSERTION	UNP P0C7B7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	289	ASN	MET	CONFLICT	UNP P0C7B7
F	164	GLY	-	INSERTION	UNP P0C7B7
F	289	ASN	MET	CONFLICT	UNP P0C7B7
G	164	GLY	-	INSERTION	UNP P0C7B7
G	289	ASN	MET	CONFLICT	UNP P0C7B7
H	164	GLY	-	INSERTION	UNP P0C7B7
H	289	ASN	MET	CONFLICT	UNP P0C7B7
I	164	GLY	-	INSERTION	UNP P0C7B7
I	289	ASN	MET	CONFLICT	UNP P0C7B7
J	164	GLY	-	INSERTION	UNP P0C7B7
J	289	ASN	MET	CONFLICT	UNP P0C7B7

- Molecule 2 is (5R)-6-(5-CHLOROPYRIDIN-2-YL)-7-OXO-6,7-DIHYDRO-5H-PYRROLO [3,4-B]PYRAZIN-5-YL4-METHYLPIPERAZINE-1-CARBOXYLATE (three-letter code: ZPC) (formula: C<sub>17</sub>H<sub>17</sub>ClN<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	B	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	C	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	D	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	E	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		

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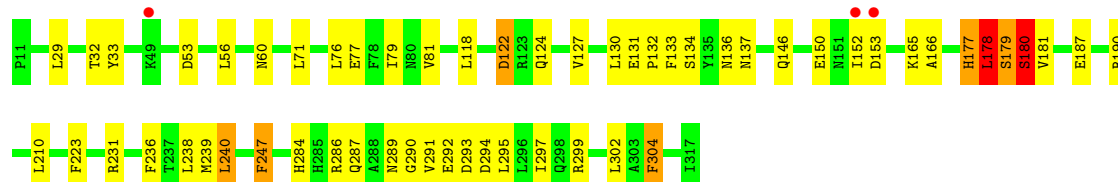
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	G	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	H	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	I	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		
2	J	1	Total	C	Cl	N	O	0	0
			27	17	1	6	3		

### 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.

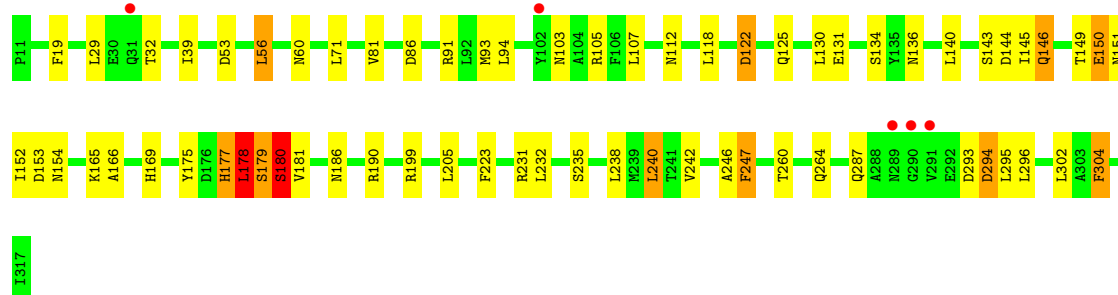
#### • Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain A: 



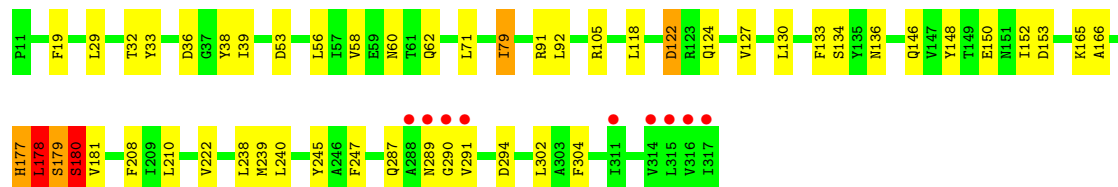
#### • Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain B: 



#### • Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

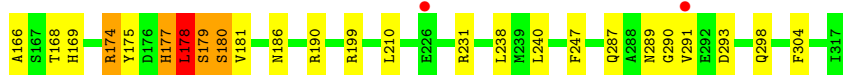
Chain C: 



#### • Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

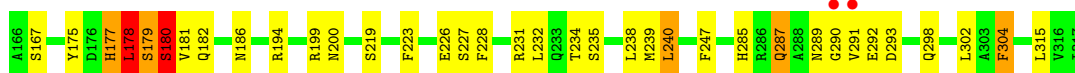
Chain D: 





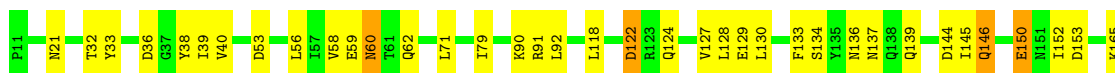
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain E:



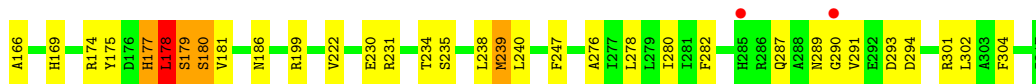
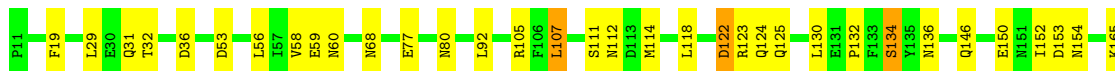
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain F:



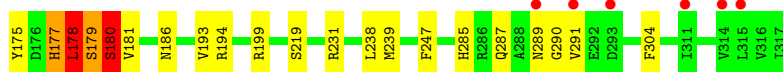
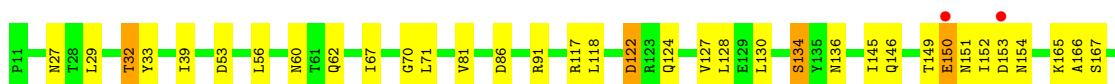
• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain G:



• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain H:

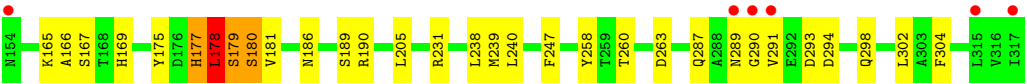


• Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain I:

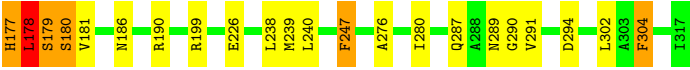






● Molecule 1: CYS-LOOP LIGAND-GATED ION CHANNEL

Chain J:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.40Å 266.83Å 110.76Å 90.00° 109.20° 90.00°	Depositor
Resolution (Å)	43.47 – 3.34 43.43 – 3.34	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.47-3.34) 99.3 (43.43-3.34)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.32Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8-1069)	Depositor
R, $R_{free}$	0.205 , 0.259 0.217 , 0.270	Depositor DCC
$R_{free}$ test set	4132 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	81.2	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 67.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 82845 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	25290	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: ZPC

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	0.57	0/2570	0.81	3/3503 (0.1%)
1	B	0.67	0/2570	0.92	2/3503 (0.1%)
1	C	0.64	0/2570	0.84	0/3503
1	D	0.67	0/2570	0.91	4/3503 (0.1%)
1	E	0.61	0/2570	0.83	4/3503 (0.1%)
1	F	0.57	0/2570	0.82	1/3503 (0.0%)
1	G	0.66	0/2570	0.90	2/3503 (0.1%)
1	H	0.60	0/2570	0.82	1/3503 (0.0%)
1	I	0.64	0/2570	0.84	1/3503 (0.0%)
1	J	0.59	0/2570	0.80	1/3503 (0.0%)
All	All	0.62	0/25700	0.85	19/35030 (0.1%)

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
1	B	0	2
1	C	0	2
1	D	0	3
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
All	All	0	21

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	LEU	CA-CB-CG	8.47	134.79	115.30
1	J	39	ILE	CB-CA-C	-7.01	97.58	111.60
1	D	199	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	A	240	LEU	CA-CB-CG	6.34	129.88	115.30
1	E	199	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	E	240	LEU	CA-CB-CG	5.91	128.90	115.30
1	F	128	LEU	CB-CG-CD1	-5.69	101.32	111.00
1	G	107	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	I	205	LEU	CA-CB-CG	-5.56	102.51	115.30
1	D	174	ARG	C-N-CA	5.53	135.53	121.70
1	G	107	LEU	CB-CG-CD1	5.52	120.38	111.00
1	A	76	LEU	CA-CB-CG	5.40	127.73	115.30
1	E	315	LEU	CA-CB-CG	5.38	127.66	115.30
1	D	117	ARG	CB-CG-CD	-5.30	97.81	111.60
1	H	117	ARG	CG-CD-NE	5.29	122.91	111.80
1	D	39	ILE	CG1-CB-CG2	-5.27	99.80	111.40
1	E	39	ILE	CB-CA-C	-5.18	101.25	111.60
1	A	210	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	205	LEU	CA-CB-CG	-5.16	103.43	115.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	HIS	Peptide
1	A	178	LEU	Peptide
1	B	177	HIS	Peptide
1	B	178	LEU	Peptide
1	C	177	HIS	Peptide
1	C	178	LEU	Peptide
1	D	174	ARG	Peptide
1	D	177	HIS	Peptide
1	D	178	LEU	Peptide
1	E	177	HIS	Peptide
1	E	178	LEU	Peptide
1	F	177	HIS	Peptide
1	F	178	LEU	Peptide
1	G	177	HIS	Peptide
1	G	178	LEU	Peptide
1	H	177	HIS	Peptide
1	H	178	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	I	177	HIS	Peptide
1	I	178	LEU	Peptide
1	J	177	HIS	Peptide
1	J	178	LEU	Peptide

## 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	2502	0	0	23	0
1	B	2502	0	0	28	0
1	C	2502	0	0	18	0
1	D	2502	0	0	23	0
1	E	2502	0	0	29	0
1	F	2502	0	0	29	0
1	G	2502	0	0	23	0
1	H	2502	0	0	20	0
1	I	2502	0	0	22	0
1	J	2502	0	0	19	0
2	A	27	0	17	5	0
2	B	27	0	17	2	0
2	C	27	0	17	4	0
2	D	27	0	17	8	0
2	E	27	0	17	3	0
2	F	27	0	17	8	0
2	G	27	0	17	5	0
2	H	27	0	17	1	0
2	I	27	0	17	6	0
2	J	27	0	17	2	0
All	All	25290	0	170	214	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 8.

All (214) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:133:PHE:O	2:J:1318:ZPC:H03A	1.56	1.05
1:H:150:GLU:OE2	2:I:1318:ZPC:H17	1.58	1.01
1:E:13:ASP:OD1	1:E:141:ARG:NH1	1.94	0.99
1:C:91:ARG:NH2	2:D:1318:ZPC:H23	1.79	0.98
1:F:133:PHE:O	2:F:1318:ZPC:H07	1.66	0.96
1:E:155:GLU:OE2	1:E:163:ARG:NH2	2.02	0.92
1:I:91:ARG:NH2	1:I:93:MET:SD	2.43	0.92
1:H:175:TYR:O	1:H:186:ASN:ND2	2.06	0.88
1:E:293:ASP:O	1:E:298:GLN:NE2	2.10	0.84
1:F:59:GLU:OE2	1:G:134:SER:OG	1.95	0.83
1:E:132:PRO:O	2:E:1318:ZPC:H01A	1.80	0.81
1:F:133:PHE:O	2:F:1318:ZPC:C07	2.28	0.81
1:A:133:PHE:O	2:A:1318:ZPC:H07	1.80	0.80
1:C:133:PHE:O	2:C:1318:ZPC:H07	1.82	0.79
1:I:293:ASP:O	1:I:298:GLN:NE2	2.16	0.78
1:F:62:GLN:NE2	1:G:68:ASN:OD1	2.19	0.76
1:F:177:HIS:O	1:F:179:SER:N	2.20	0.75
1:B:122:ASP:N	1:B:122:ASP:OD1	2.22	0.72
1:I:77:GLU:OE1	2:I:1318:ZPC:H01	1.91	0.71
1:C:122:ASP:N	1:C:122:ASP:OD1	2.22	0.71
1:B:175:TYR:O	1:B:186:ASN:ND2	2.25	0.69
1:B:149:THR:O	1:B:151:ASN:N	2.26	0.69
1:F:133:PHE:CD1	2:F:1318:ZPC:H07A	2.29	0.68
1:A:289:ASN:OD1	1:A:290:GLY:N	2.26	0.68
1:F:150:GLU:OE2	2:G:1318:ZPC:H17	1.94	0.68
1:E:177:HIS:O	1:E:179:SER:N	2.27	0.68
1:F:150:GLU:OE2	2:G:1318:ZPC:C17	2.42	0.67
1:J:177:HIS:O	1:J:179:SER:N	2.27	0.67
1:I:260:THR:N	1:I:263:ASP:OD2	2.27	0.67
1:G:289:ASN:OD1	1:G:290:GLY:N	2.28	0.67
1:D:175:TYR:O	1:D:186:ASN:ND2	2.28	0.66
1:I:179:SER:O	1:I:181:VAL:N	2.29	0.65
1:B:103:ASN:ND2	2:C:1318:ZPC:H06A	2.11	0.65
1:D:179:SER:O	1:D:181:VAL:N	2.30	0.65
1:D:144:ASP:OD1	1:D:146:GLN:NE2	2.29	0.65
1:A:179:SER:O	1:A:181:VAL:N	2.30	0.65
1:D:80:ASN:ND2	1:D:111:SER:O	2.29	0.65
1:H:179:SER:O	1:H:181:VAL:N	2.31	0.64
1:E:289:ASN:OD1	1:E:290:GLY:N	2.30	0.63
1:C:179:SER:O	1:C:181:VAL:N	2.32	0.63
1:F:175:TYR:CE2	2:F:1318:ZPC:H04A	2.35	0.62
1:F:293:ASP:O	1:F:298:GLN:NE2	2.33	0.62
1:D:122:ASP:N	1:D:122:ASP:OD1	2.33	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:143:SER:OG	1:B:144:ASP:N	2.33	0.61
1:D:177:HIS:O	1:D:179:SER:N	2.33	0.61
1:G:179:SER:O	1:G:181:VAL:N	2.34	0.61
1:A:122:ASP:OD1	1:A:122:ASP:N	2.34	0.61
1:F:122:ASP:OD1	1:F:122:ASP:N	2.32	0.61
1:D:133:PHE:O	2:D:1318:ZPC:H07	2.01	0.60
1:C:177:HIS:O	1:C:179:SER:N	2.35	0.60
1:E:175:TYR:O	1:E:186:ASN:ND2	2.35	0.60
1:H:177:HIS:O	1:H:179:SER:N	2.35	0.60
1:J:43:TRP:O	1:J:100:VAL:N	2.34	0.60
1:I:175:TYR:O	1:I:186:ASN:ND2	2.36	0.59
1:B:179:SER:O	1:B:181:VAL:N	2.36	0.59
1:E:179:SER:O	1:E:182:GLN:N	2.36	0.59
1:F:79:ILE:O	1:J:105:ARG:NH1	2.35	0.59
1:A:177:HIS:O	1:A:179:SER:N	2.36	0.59
1:G:122:ASP:N	1:G:122:ASP:OD1	2.37	0.58
1:F:179:SER:O	1:F:181:VAL:N	2.37	0.58
1:H:150:GLU:OE2	2:I:1318:ZPC:C17	2.45	0.58
1:B:19:PHE:CE2	2:C:1318:ZPC:C15	2.87	0.57
1:I:27:ASN:N	1:I:32:THR:O	2.37	0.57
1:D:79:ILE:N	1:D:129:GLU:O	2.37	0.57
1:F:33:TYR:OH	1:F:127:VAL:N	2.37	0.57
1:A:289:ASN:OD1	1:A:292:GLU:N	2.38	0.57
1:F:136:ASN:ND2	1:F:139:GLN:OE1	2.38	0.57
1:E:33:TYR:OH	1:E:127:VAL:N	2.38	0.56
1:E:82:VAL:N	1:E:109:SER:O	2.39	0.56
1:A:131:GLU:OE1	1:A:190:ARG:NH2	2.39	0.56
1:E:227:SER:OG	1:E:228:PHE:N	2.39	0.56
1:G:31:GLN:OE1	1:G:114:MET:N	2.39	0.56
1:F:144:ASP:OD2	1:F:146:GLN:NE2	2.39	0.56
1:H:33:TYR:OH	1:H:127:VAL:N	2.39	0.55
1:I:150:GLU:OE2	2:J:1318:ZPC:H17	2.06	0.55
1:C:19:PHE:CE1	1:C:148:TYR:CD2	2.95	0.55
1:B:150:GLU:OE1	2:C:1318:ZPC:H17	2.06	0.55
1:B:177:HIS:O	1:B:179:SER:N	2.40	0.55
1:F:91:ARG:NH2	2:G:1318:ZPC:H23	2.22	0.55
1:G:175:TYR:O	1:G:186:ASN:ND2	2.40	0.55
1:A:133:PHE:CD1	2:A:1318:ZPC:H07A	2.42	0.54
1:D:289:ASN:OD1	1:D:290:GLY:N	2.40	0.54
1:C:105:ARG:NH1	1:D:79:ILE:O	2.40	0.54
1:H:122:ASP:N	1:H:122:ASP:OD1	2.40	0.54
1:E:133:PHE:O	2:E:1318:ZPC:N02	2.40	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:175:TYR:O	1:J:186:ASN:ND2	2.40	0.54
1:D:293:ASP:O	1:D:298:GLN:NE2	2.41	0.54
1:E:232:LEU:O	1:E:235:SER:OG	2.26	0.54
1:H:122:ASP:OD2	1:H:199:ARG:NH2	2.41	0.53
1:F:133:PHE:O	2:F:1318:ZPC:N02	2.42	0.53
1:B:144:ASP:OD1	1:B:146:GLN:NE2	2.42	0.53
1:C:36:ASP:OD2	1:C:105:ARG:NH2	2.41	0.53
1:I:177:HIS:O	1:I:179:SER:N	2.42	0.53
1:I:133:PHE:CE1	2:I:1318:ZPC:H07A	2.44	0.52
1:G:177:HIS:O	1:G:179:SER:N	2.42	0.52
1:A:295:LEU:O	1:A:299:ARG:NE	2.42	0.52
1:E:33:TYR:OH	1:E:127:VAL:O	2.27	0.52
1:G:58:VAL:O	1:G:92:LEU:N	2.42	0.52
1:I:289:ASN:OD1	1:I:290:GLY:N	2.43	0.51
1:E:285:HIS:O	1:E:287:GLN:NE2	2.43	0.51
2:F:1318:ZPC:H23	1:J:91:ARG:NH2	2.25	0.51
1:B:91:ARG:NH2	1:B:93:MET:SD	2.83	0.51
1:E:179:SER:OG	1:E:180:SER:N	2.44	0.51
1:D:133:PHE:CE1	2:D:1318:ZPC:H07A	2.46	0.51
1:F:79:ILE:N	1:F:129:GLU:O	2.44	0.51
1:B:131:GLU:OE2	2:B:1318:ZPC:H01B	2.10	0.51
1:I:133:PHE:O	2:I:1318:ZPC:H03A	2.11	0.51
1:A:150:GLU:OE2	2:B:1318:ZPC:H17	2.10	0.50
1:H:62:GLN:NE2	1:I:68:ASN:OD1	2.43	0.50
1:I:131:GLU:OE1	1:I:190:ARG:NH2	2.44	0.50
1:D:33:TYR:OH	1:D:127:VAL:N	2.44	0.50
1:C:208:PHE:O	1:C:245:TYR:OH	2.29	0.50
1:J:149:THR:O	1:J:151:ASN:N	2.44	0.50
1:G:132:PRO:O	2:G:1318:ZPC:H01A	2.11	0.50
1:D:131:GLU:OE1	1:D:190:ARG:NE	2.45	0.50
1:J:155:GLU:OE2	1:J:163:ARG:NH1	2.44	0.50
1:G:235:SER:O	1:G:239:MET:N	2.45	0.50
1:F:133:PHE:CE1	2:F:1318:ZPC:H07A	2.46	0.50
2:A:1318:ZPC:H06	1:E:38:TYR:CE2	2.47	0.49
1:B:122:ASP:OD2	1:B:199:ARG:NH2	2.45	0.49
1:D:133:PHE:O	2:D:1318:ZPC:C07	2.61	0.49
1:B:131:GLU:OE1	1:B:190:ARG:NH2	2.46	0.49
1:F:284:HIS:CE1	1:J:226:GLU:OE2	2.65	0.49
1:C:38:TYR:CE2	2:D:1318:ZPC:H06	2.48	0.49
1:D:149:THR:O	1:D:151:ASN:N	2.45	0.49
1:G:276:ALA:O	1:G:280:ILE:N	2.45	0.49
1:E:179:SER:O	1:E:181:VAL:N	2.45	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:284:HIS:CE1	1:E:226:GLU:OE2	2.67	0.48
1:B:131:GLU:OE1	1:B:190:ARG:NE	2.46	0.48
1:E:79:ILE:N	1:E:129:GLU:O	2.46	0.48
1:H:67:ILE:O	1:H:70:GLY:N	2.47	0.48
1:G:112:ASN:ND2	1:G:125:GLN:O	2.46	0.48
1:A:223:PHE:CE2	1:A:304:PHE:CE1	3.02	0.48
1:G:122:ASP:OD2	1:G:199:ARG:NH2	2.47	0.47
1:H:91:ARG:NH2	2:I:1318:ZPC:H23	2.28	0.47
1:B:293:ASP:O	1:B:295:LEU:N	2.47	0.47
1:A:79:ILE:O	1:E:105:ARG:NH1	2.47	0.47
1:G:230:GLU:O	1:G:234:THR:OG1	2.33	0.47
1:C:62:GLN:NE2	1:D:68:ASN:OD1	2.48	0.47
1:A:137:ASN:N	1:A:187:GLU:O	2.47	0.47
1:C:289:ASN:OD1	1:C:290:GLY:N	2.48	0.47
1:I:149:THR:O	1:I:151:ASN:N	2.47	0.47
1:G:278:LEU:O	1:G:282:PHE:N	2.48	0.47
1:D:93:MET:N	1:D:101:ILE:O	2.48	0.47
1:J:289:ASN:OD1	1:J:290:GLY:N	2.48	0.47
1:E:167:SER:N	1:E:194:ARG:O	2.48	0.47
1:A:81:VAL:O	1:E:105:ARG:NH2	2.48	0.46
1:I:33:TYR:OH	1:I:127:VAL:N	2.48	0.46
1:B:86:ASP:N	1:B:107:LEU:O	2.49	0.46
1:I:143:SER:OG	1:I:144:ASP:N	2.49	0.45
1:D:133:PHE:CD1	2:D:1318:ZPC:H07A	2.51	0.45
1:H:179:SER:OG	1:H:180:SER:N	2.49	0.45
1:D:112:ASN:ND2	1:D:125:GLN:O	2.49	0.45
1:B:260:THR:O	1:B:264:GLN:NE2	2.49	0.45
1:E:304:PHE:C	1:E:304:PHE:CD1	2.90	0.45
1:C:33:TYR:OH	1:C:127:VAL:N	2.50	0.45
1:I:50:THR:OG1	1:I:54:LYS:O	2.34	0.45
1:J:82:VAL:N	1:J:109:SER:O	2.49	0.45
1:J:276:ALA:O	1:J:280:ILE:N	2.50	0.45
1:C:179:SER:OG	1:C:180:SER:N	2.50	0.44
1:F:38:TYR:OH	1:G:77:GLU:OE1	2.35	0.44
1:B:136:ASN:O	1:B:140:LEU:N	2.49	0.44
1:A:132:PRO:O	2:A:1318:ZPC:H01A	2.17	0.44
1:J:179:SER:O	1:J:181:VAL:N	2.50	0.44
1:I:80:ASN:OD1	1:I:129:GLU:N	2.50	0.44
1:B:242:VAL:O	1:B:246:ALA:N	2.49	0.44
1:A:77:GLU:OE1	2:A:1318:ZPC:H01	2.17	0.44
1:G:301:ARG:NH1	1:H:285:HIS:CE1	2.85	0.44
1:E:289:ASN:OD1	1:E:292:GLU:N	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:112:ASN:ND2	1:J:125:GLN:O	2.51	0.44
1:F:137:ASN:N	1:F:187:GLU:O	2.50	0.43
1:A:236:PHE:CD2	1:E:234:THR:CG2	3.01	0.43
1:H:167:SER:N	1:H:194:ARG:O	2.52	0.43
1:H:128:LEU:O	1:H:193:VAL:N	2.52	0.43
1:J:122:ASP:OD2	1:J:199:ARG:NE	2.51	0.43
1:C:38:TYR:OH	1:D:77:GLU:OE1	2.37	0.43
1:I:247:PHE:CD2	1:J:247:PHE:CE2	3.07	0.43
1:D:38:TYR:CE2	2:E:1318:ZPC:H06A	2.54	0.43
1:C:58:VAL:O	1:C:92:LEU:N	2.52	0.43
1:B:232:LEU:O	1:B:235:SER:OG	2.35	0.43
1:A:177:HIS:CE1	1:E:148:TYR:CD1	3.06	0.43
1:H:86:ASP:OD1	1:I:84:SER:OG	2.37	0.43
1:C:150:GLU:OE1	2:D:1318:ZPC:H17	2.19	0.43
1:H:289:ASN:OD1	1:H:290:GLY:N	2.52	0.43
2:G:1318:ZPC:N22	2:G:1318:ZPC:C08	2.83	0.42
1:A:293:ASP:O	1:A:295:LEU:N	2.52	0.42
1:J:304:PHE:C	1:J:304:PHE:CD1	2.92	0.42
1:E:223:PHE:CE2	1:E:304:PHE:CE1	3.07	0.42
1:H:149:THR:O	1:H:151:ASN:N	2.52	0.42
1:F:289:ASN:OD1	1:F:290:GLY:N	2.53	0.42
1:B:112:ASN:ND2	1:B:125:GLN:O	2.53	0.42
1:B:179:SER:OG	1:B:180:SER:N	2.52	0.42
1:G:19:PHE:CE2	2:H:1318:ZPC:C15	3.03	0.41
1:F:247:PHE:CE2	1:J:247:PHE:CD2	3.08	0.41
1:B:223:PHE:CE2	1:B:304:PHE:CE1	3.09	0.41
1:I:122:ASP:OD1	1:I:122:ASP:N	2.53	0.41
1:F:21:ASN:N	1:F:36:ASP:O	2.53	0.41
1:A:33:TYR:OH	1:A:127:VAL:N	2.53	0.41
1:G:58:VAL:N	1:G:92:LEU:O	2.52	0.41
1:E:80:ASN:ND2	1:E:127:VAL:O	2.54	0.41
1:H:27:ASN:N	1:H:32:THR:O	2.54	0.41
1:F:58:VAL:O	1:F:92:LEU:N	2.54	0.41
1:F:133:PHE:CD1	2:F:1318:ZPC:H01	2.55	0.41
1:G:80:ASN:ND2	1:G:111:SER:O	2.54	0.41
1:B:294:ASP:O	1:B:296:LEU:N	2.54	0.41
1:F:60:ASN:OD1	1:F:90:LYS:N	2.54	0.41
1:A:247:PHE:CG	1:B:247:PHE:CE2	3.08	0.41
1:B:105:ARG:NH1	1:C:79:ILE:O	2.54	0.40
1:J:131:GLU:OE1	1:J:190:ARG:NH2	2.54	0.40
1:B:56:LEU:N	1:B:94:LEU:O	2.54	0.40
1:G:59:GLU:OE2	1:H:134:SER:OG	2.39	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:133:PHE:O	2:D:1318:ZPC:N02	2.55	0.40
1:A:179:SER:OG	1:A:180:SER:N	2.54	0.40
1:G:36:ASP:OD2	1:G:105:ARG:NH2	2.54	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	305/307 (99%)	278 (91%)	18 (6%)	9 (3%)	7	47
1	B	305/307 (99%)	274 (90%)	21 (7%)	10 (3%)	6	44
1	C	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	7	47
1	D	305/307 (99%)	274 (90%)	22 (7%)	9 (3%)	7	47
1	E	305/307 (99%)	275 (90%)	21 (7%)	9 (3%)	7	47
1	F	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	7	47
1	G	305/307 (99%)	278 (91%)	17 (6%)	10 (3%)	6	44
1	H	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	7	47
1	I	305/307 (99%)	276 (90%)	20 (7%)	9 (3%)	7	47
1	J	305/307 (99%)	271 (89%)	25 (8%)	9 (3%)	7	47
All	All	3050/3070 (99%)	2754 (90%)	204 (7%)	92 (3%)	7	47

All (92) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	178	LEU
1	A	179	SER
1	A	180	SER
1	B	60	ASN
1	B	166	ALA
1	B	178	LEU

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Mol	Chain	Res	Type
1	B	179	SER
1	B	180	SER
1	C	166	ALA
1	C	178	LEU
1	C	179	SER
1	C	180	SER
1	D	60	ASN
1	D	166	ALA
1	D	178	LEU
1	D	179	SER
1	D	180	SER
1	E	60	ASN
1	E	178	LEU
1	E	179	SER
1	E	180	SER
1	F	60	ASN
1	F	178	LEU
1	F	179	SER
1	F	180	SER
1	G	60	ASN
1	G	166	ALA
1	G	178	LEU
1	G	179	SER
1	G	180	SER
1	H	60	ASN
1	H	166	ALA
1	H	178	LEU
1	H	179	SER
1	H	180	SER
1	I	60	ASN
1	I	166	ALA
1	I	178	LEU
1	I	179	SER
1	I	180	SER
1	J	60	ASN
1	J	178	LEU
1	J	179	SER
1	J	180	SER
1	A	53	ASP
1	B	53	ASP
1	B	152	ILE
1	C	53	ASP

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Mol	Chain	Res	Type
1	C	152	ILE
1	D	152	ILE
1	E	53	ASP
1	E	152	ILE
1	F	53	ASP
1	F	152	ILE
1	G	53	ASP
1	G	152	ILE
1	G	294	ASP
1	H	53	ASP
1	H	153	ASP
1	I	152	ILE
1	J	53	ASP
1	J	152	ILE
1	A	152	ILE
1	A	153	ASP
1	A	294	ASP
1	B	150	GLU
1	B	153	ASP
1	B	294	ASP
1	C	294	ASP
1	D	53	ASP
1	D	150	GLU
1	D	153	ASP
1	E	153	ASP
1	F	294	ASP
1	G	153	ASP
1	H	150	GLU
1	I	53	ASP
1	I	150	GLU
1	J	153	ASP
1	C	153	ASP
1	E	200	ASN
1	F	150	GLU
1	F	153	ASP
1	J	150	GLU
1	J	294	ASP
1	A	166	ALA
1	C	60	ASN
1	G	150	GLU
1	H	152	ILE
1	I	294	ASP

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Mol	Chain	Res	Type
1	E	150	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	274/275 (100%)	249 (91%)	25 (9%)	14	50
1	B	274/275 (100%)	250 (91%)	24 (9%)	14	52
1	C	274/275 (100%)	248 (90%)	26 (10%)	12	47
1	D	274/275 (100%)	250 (91%)	24 (9%)	14	52
1	E	274/275 (100%)	250 (91%)	24 (9%)	14	52
1	F	274/275 (100%)	250 (91%)	24 (9%)	14	52
1	G	274/275 (100%)	245 (89%)	29 (11%)	10	40
1	H	274/275 (100%)	248 (90%)	26 (10%)	12	47
1	I	274/275 (100%)	245 (89%)	29 (11%)	10	40
1	J	274/275 (100%)	253 (92%)	21 (8%)	18	61
All	All	2740/2750 (100%)	2488 (91%)	252 (9%)	13	49

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	32	THR
1	A	56	LEU
1	A	71	LEU
1	A	118	LEU
1	A	122	ASP
1	A	124	GLN
1	A	130	LEU
1	A	134	SER
1	A	136	ASN
1	A	146	GLN
1	A	165	LYS
1	A	178	LEU

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Mol	Chain	Res	Type
1	A	180	SER
1	A	231	ARG
1	A	238	LEU
1	A	239	MET
1	A	240	LEU
1	A	247	PHE
1	A	286	ARG
1	A	287	GLN
1	A	291	VAL
1	A	297	ILE
1	A	302	LEU
1	A	304	PHE
1	B	29	LEU
1	B	32	THR
1	B	39	ILE
1	B	56	LEU
1	B	71	LEU
1	B	81	VAL
1	B	118	LEU
1	B	122	ASP
1	B	130	LEU
1	B	134	SER
1	B	145	ILE
1	B	146	GLN
1	B	154	ASN
1	B	165	LYS
1	B	169	HIS
1	B	178	LEU
1	B	180	SER
1	B	231	ARG
1	B	238	LEU
1	B	240	LEU
1	B	247	PHE
1	B	287	GLN
1	B	302	LEU
1	B	304	PHE
1	C	29	LEU
1	C	32	THR
1	C	39	ILE
1	C	56	LEU
1	C	71	LEU
1	C	79	ILE

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Mol	Chain	Res	Type
1	C	118	LEU
1	C	122	ASP
1	C	124	GLN
1	C	130	LEU
1	C	134	SER
1	C	136	ASN
1	C	146	GLN
1	C	165	LYS
1	C	178	LEU
1	C	180	SER
1	C	210	LEU
1	C	222	VAL
1	C	238	LEU
1	C	239	MET
1	C	240	LEU
1	C	247	PHE
1	C	287	GLN
1	C	291	VAL
1	C	302	LEU
1	C	304	PHE
1	D	29	LEU
1	D	32	THR
1	D	56	LEU
1	D	71	LEU
1	D	118	LEU
1	D	122	ASP
1	D	124	GLN
1	D	130	LEU
1	D	134	SER
1	D	145	ILE
1	D	146	GLN
1	D	165	LYS
1	D	168	THR
1	D	169	HIS
1	D	178	LEU
1	D	180	SER
1	D	210	LEU
1	D	231	ARG
1	D	238	LEU
1	D	240	LEU
1	D	247	PHE
1	D	287	GLN

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Mol	Chain	Res	Type
1	D	291	VAL
1	D	304	PHE
1	E	29	LEU
1	E	39	ILE
1	E	56	LEU
1	E	71	LEU
1	E	118	LEU
1	E	124	GLN
1	E	130	LEU
1	E	134	SER
1	E	145	ILE
1	E	146	GLN
1	E	157	ILE
1	E	165	LYS
1	E	178	LEU
1	E	180	SER
1	E	219	SER
1	E	231	ARG
1	E	238	LEU
1	E	239	MET
1	E	240	LEU
1	E	247	PHE
1	E	287	GLN
1	E	291	VAL
1	E	302	LEU
1	E	304	PHE
1	F	32	THR
1	F	39	ILE
1	F	40	VAL
1	F	56	LEU
1	F	71	LEU
1	F	118	LEU
1	F	122	ASP
1	F	124	GLN
1	F	130	LEU
1	F	134	SER
1	F	145	ILE
1	F	146	GLN
1	F	165	LYS
1	F	178	LEU
1	F	180	SER
1	F	210	LEU

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Mol	Chain	Res	Type
1	F	238	LEU
1	F	240	LEU
1	F	247	PHE
1	F	258	TYR
1	F	287	GLN
1	F	291	VAL
1	F	302	LEU
1	F	304	PHE
1	G	29	LEU
1	G	32	THR
1	G	56	LEU
1	G	107	LEU
1	G	118	LEU
1	G	122	ASP
1	G	123	ARG
1	G	124	GLN
1	G	130	LEU
1	G	134	SER
1	G	136	ASN
1	G	146	GLN
1	G	154	ASN
1	G	165	LYS
1	G	169	HIS
1	G	174	ARG
1	G	178	LEU
1	G	180	SER
1	G	222	VAL
1	G	231	ARG
1	G	238	LEU
1	G	239	MET
1	G	240	LEU
1	G	247	PHE
1	G	287	GLN
1	G	291	VAL
1	G	293	ASP
1	G	302	LEU
1	G	304	PHE
1	H	29	LEU
1	H	32	THR
1	H	39	ILE
1	H	56	LEU
1	H	71	LEU

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Mol	Chain	Res	Type
1	H	81	VAL
1	H	118	LEU
1	H	122	ASP
1	H	124	GLN
1	H	130	LEU
1	H	134	SER
1	H	136	ASN
1	H	145	ILE
1	H	146	GLN
1	H	154	ASN
1	H	165	LYS
1	H	178	LEU
1	H	180	SER
1	H	219	SER
1	H	231	ARG
1	H	238	LEU
1	H	239	MET
1	H	247	PHE
1	H	287	GLN
1	H	291	VAL
1	H	304	PHE
1	I	28	THR
1	I	29	LEU
1	I	32	THR
1	I	39	ILE
1	I	56	LEU
1	I	71	LEU
1	I	81	VAL
1	I	118	LEU
1	I	122	ASP
1	I	124	GLN
1	I	130	LEU
1	I	134	SER
1	I	145	ILE
1	I	146	GLN
1	I	165	LYS
1	I	167	SER
1	I	169	HIS
1	I	178	LEU
1	I	180	SER
1	I	189	SER
1	I	231	ARG

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Mol	Chain	Res	Type
1	I	238	LEU
1	I	239	MET
1	I	240	LEU
1	I	258	TYR
1	I	287	GLN
1	I	291	VAL
1	I	302	LEU
1	I	304	PHE
1	J	29	LEU
1	J	32	THR
1	J	39	ILE
1	J	56	LEU
1	J	71	LEU
1	J	118	LEU
1	J	130	LEU
1	J	134	SER
1	J	136	ASN
1	J	146	GLN
1	J	165	LYS
1	J	178	LEU
1	J	180	SER
1	J	238	LEU
1	J	239	MET
1	J	240	LEU
1	J	247	PHE
1	J	287	GLN
1	J	291	VAL
1	J	302	LEU
1	J	304	PHE

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 ⓘ

10 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	ZPC	A	1318	-	30,30,30	3.52	10 (33%)	43,43,43	6.27	24 (55%)
2	ZPC	B	1318	-	30,30,30	4.03	11 (36%)	43,43,43	6.49	26 (60%)
2	ZPC	C	1318	-	30,30,30	3.04	11 (36%)	43,43,43	6.77	26 (60%)
2	ZPC	D	1318	-	30,30,30	3.53	9 (30%)	43,43,43	5.97	25 (58%)
2	ZPC	E	1318	-	30,30,30	3.31	10 (33%)	43,43,43	6.15	31 (72%)
2	ZPC	F	1318	-	30,30,30	3.42	10 (33%)	43,43,43	6.25	30 (69%)
2	ZPC	G	1318	-	30,30,30	3.53	9 (30%)	43,43,43	6.44	31 (72%)
2	ZPC	H	1318	-	30,30,30	3.33	10 (33%)	43,43,43	5.16	28 (65%)
2	ZPC	I	1318	-	30,30,30	3.24	9 (30%)	43,43,43	5.24	28 (65%)
2	ZPC	J	1318	-	30,30,30	2.67	11 (36%)	43,43,43	5.33	29 (67%)

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	ZPC	A	1318	-	-	0/12/38/38	0/2/4/4
2	ZPC	B	1318	-	-	0/12/38/38	0/2/4/4
2	ZPC	C	1318	-	-	0/12/38/38	0/2/4/4
2	ZPC	D	1318	-	-	0/12/38/38	0/2/4/4
2	ZPC	E	1318	-	-	0/12/38/38	0/2/4/4
2	ZPC	F	1318	-	-	0/12/38/38	0/2/4/4
2	ZPC	G	1318	-	-	0/12/38/38	0/2/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZPC	H	1318	-	-	1/12/38/38	0/2/4/4
2	ZPC	I	1318	-	-	0/12/38/38	0/2/4/4
2	ZPC	J	1318	-	-	0/12/38/38	0/2/4/4

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1318	ZPC	C13-N12	12.66	1.49	1.38
2	A	1318	ZPC	C13-N12	12.55	1.49	1.38
2	D	1318	ZPC	C13-N12	11.16	1.48	1.38
2	E	1318	ZPC	C13-N12	11.12	1.48	1.38
2	F	1318	ZPC	C13-N12	10.78	1.48	1.38
2	H	1318	ZPC	C21-N12	10.64	1.51	1.41
2	B	1318	ZPC	C20-C11	10.54	1.55	1.50
2	D	1318	ZPC	C21-N12	10.14	1.50	1.41
2	I	1318	ZPC	C13-N12	10.10	1.47	1.38
2	I	1318	ZPC	C21-N12	9.91	1.50	1.41
2	G	1318	ZPC	C20-C11	9.85	1.55	1.50
2	A	1318	ZPC	C21-N12	9.73	1.50	1.41
2	B	1318	ZPC	C21-N12	9.41	1.50	1.41
2	E	1318	ZPC	C21-N12	9.22	1.49	1.41
2	G	1318	ZPC	C13-N12	8.91	1.46	1.38
2	F	1318	ZPC	C21-N12	8.72	1.49	1.41
2	G	1318	ZPC	C21-N12	8.60	1.49	1.41
2	C	1318	ZPC	C21-N12	8.31	1.49	1.41
2	H	1318	ZPC	C13-N12	7.84	1.45	1.38
2	C	1318	ZPC	C13-N12	7.26	1.45	1.38
2	J	1318	ZPC	C13-N12	6.90	1.44	1.38
2	H	1318	ZPC	C20-C11	6.85	1.53	1.50
2	D	1318	ZPC	C20-C11	6.79	1.53	1.50
2	J	1318	ZPC	C21-N12	6.30	1.47	1.41
2	F	1318	ZPC	C20-C11	6.21	1.53	1.50
2	C	1318	ZPC	C08-N05	5.96	1.47	1.35
2	G	1318	ZPC	C08-N05	5.95	1.47	1.35
2	F	1318	ZPC	C08-N05	5.71	1.46	1.35
2	J	1318	ZPC	C08-N05	5.50	1.46	1.35
2	C	1318	ZPC	C20-C11	5.39	1.53	1.50
2	A	1318	ZPC	C08-N05	5.35	1.46	1.35
2	E	1318	ZPC	C08-N05	5.17	1.45	1.35
2	H	1318	ZPC	C20-N19	5.06	1.40	1.34
2	B	1318	ZPC	C20-N19	5.06	1.40	1.34
2	B	1318	ZPC	C08-N05	4.96	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1318	ZPC	C08-N05	4.92	1.45	1.35
2	J	1318	ZPC	C20-N19	4.91	1.40	1.34
2	H	1318	ZPC	C08-N05	4.87	1.45	1.35
2	F	1318	ZPC	C06-N05	-4.63	1.38	1.47
2	G	1318	ZPC	C20-N19	4.58	1.39	1.34
2	E	1318	ZPC	C06-N05	-4.55	1.38	1.47
2	I	1318	ZPC	C06-N05	-4.51	1.38	1.47
2	D	1318	ZPC	C20-N19	4.43	1.39	1.34
2	I	1318	ZPC	C08-N05	4.34	1.44	1.35
2	I	1318	ZPC	C20-C11	4.28	1.52	1.50
2	F	1318	ZPC	C20-N19	4.24	1.39	1.34
2	J	1318	ZPC	C06-N05	-4.16	1.39	1.47
2	A	1318	ZPC	O10-C08	4.13	1.42	1.34
2	I	1318	ZPC	C20-N19	4.13	1.39	1.34
2	C	1318	ZPC	O10-C08	4.13	1.42	1.34
2	A	1318	ZPC	C20-C11	4.10	1.52	1.50
2	J	1318	ZPC	C11-N12	-4.01	1.44	1.47
2	B	1318	ZPC	C06-N05	-4.01	1.39	1.47
2	A	1318	ZPC	C06-N05	-3.79	1.40	1.47
2	H	1318	ZPC	O10-C08	3.78	1.42	1.34
2	F	1318	ZPC	O10-C08	3.73	1.42	1.34
2	D	1318	ZPC	C06-N05	-3.72	1.40	1.47
2	B	1318	ZPC	O10-C08	3.66	1.41	1.34
2	B	1318	ZPC	C11-N12	-3.64	1.45	1.47
2	C	1318	ZPC	C20-N19	3.64	1.38	1.34
2	A	1318	ZPC	C20-N19	3.64	1.38	1.34
2	G	1318	ZPC	C06-N05	-3.56	1.40	1.47
2	H	1318	ZPC	C06-N05	-3.54	1.40	1.47
2	E	1318	ZPC	C20-N19	3.52	1.38	1.34
2	E	1318	ZPC	O10-C08	3.52	1.41	1.34
2	C	1318	ZPC	C06-N05	-3.50	1.40	1.47
2	G	1318	ZPC	O10-C08	3.50	1.41	1.34
2	G	1318	ZPC	C27-C26	3.42	1.45	1.38
2	G	1318	ZPC	C26-C24	3.41	1.44	1.38
2	J	1318	ZPC	C20-C11	3.41	1.52	1.50
2	D	1318	ZPC	O10-C08	3.30	1.41	1.34
2	C	1318	ZPC	C26-C24	3.30	1.44	1.38
2	E	1318	ZPC	C27-C26	3.27	1.45	1.38
2	B	1318	ZPC	C26-C24	3.22	1.44	1.38
2	C	1318	ZPC	C27-C26	3.19	1.44	1.38
2	F	1318	ZPC	C27-C26	3.16	1.44	1.38
2	I	1318	ZPC	O10-C08	3.08	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1318	ZPC	C20-C11	3.05	1.51	1.50
2	I	1318	ZPC	C27-C26	3.00	1.44	1.38
2	H	1318	ZPC	C27-C26	2.90	1.44	1.38
2	A	1318	ZPC	C27-C26	2.86	1.44	1.38
2	D	1318	ZPC	C27-C26	2.69	1.43	1.38
2	I	1318	ZPC	C26-C24	2.62	1.43	1.38
2	B	1318	ZPC	C27-C26	2.61	1.43	1.38
2	C	1318	ZPC	C21-N22	2.54	1.39	1.34
2	J	1318	ZPC	O10-C08	2.54	1.39	1.34
2	H	1318	ZPC	C26-C24	2.52	1.43	1.38
2	J	1318	ZPC	C27-C26	2.45	1.43	1.38
2	F	1318	ZPC	C26-C24	2.44	1.42	1.38
2	A	1318	ZPC	C26-C24	2.40	1.42	1.38
2	D	1318	ZPC	C26-C24	2.24	1.42	1.38
2	F	1318	ZPC	C18-C17	2.24	1.44	1.38
2	H	1318	ZPC	C18-C17	2.20	1.44	1.38
2	E	1318	ZPC	C18-N19	-2.17	1.29	1.34
2	E	1318	ZPC	C26-C24	2.17	1.42	1.38
2	J	1318	ZPC	C26-C24	2.15	1.42	1.38
2	J	1318	ZPC	C18-C17	2.14	1.44	1.38
2	A	1318	ZPC	O10-C11	2.07	1.47	1.43
2	B	1318	ZPC	C18-C17	2.04	1.44	1.38
2	C	1318	ZPC	C18-C17	2.01	1.43	1.38

All (278) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1318	ZPC	O14-C13-N12	29.05	144.49	126.29
2	A	1318	ZPC	O14-C13-N12	28.28	144.01	126.29
2	E	1318	ZPC	O14-C13-N12	27.14	143.29	126.29
2	F	1318	ZPC	O14-C13-N12	24.81	141.84	126.29
2	G	1318	ZPC	O14-C13-N12	23.74	141.16	126.29
2	D	1318	ZPC	O14-C13-N12	23.62	141.09	126.29
2	C	1318	ZPC	O14-C13-N12	21.20	139.57	126.29
2	I	1318	ZPC	O14-C13-N12	20.23	138.96	126.29
2	C	1318	ZPC	O10-C08-N05	18.63	129.03	111.25
2	J	1318	ZPC	O14-C13-N12	18.55	137.91	126.29
2	H	1318	ZPC	O14-C13-N12	17.29	137.12	126.29
2	F	1318	ZPC	O10-C08-N05	16.81	127.29	111.25
2	E	1318	ZPC	O10-C08-N05	15.91	126.43	111.25
2	C	1318	ZPC	C15-C20-N19	-15.09	118.25	123.94
2	D	1318	ZPC	O10-C08-N05	14.97	125.53	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1318	ZPC	O10-C08-N05	14.36	124.96	111.25
2	H	1318	ZPC	O10-C08-N05	13.81	124.43	111.25
2	J	1318	ZPC	O10-C08-N05	13.59	124.22	111.25
2	B	1318	ZPC	C15-C20-N19	-13.28	118.93	123.94
2	B	1318	ZPC	O10-C08-N05	13.21	123.86	111.25
2	G	1318	ZPC	C27-C21-N12	13.19	129.36	122.33
2	G	1318	ZPC	C15-C20-N19	-13.18	118.97	123.94
2	I	1318	ZPC	O10-C11-N12	13.08	128.50	108.95
2	G	1318	ZPC	O10-C08-N05	13.01	123.66	111.25
2	J	1318	ZPC	O10-C11-N12	12.48	127.59	108.95
2	D	1318	ZPC	O10-C11-N12	11.52	126.17	108.95
2	H	1318	ZPC	O10-C11-N12	11.41	125.99	108.95
2	C	1318	ZPC	C06-C07-N02	11.22	123.20	110.82
2	C	1318	ZPC	O10-C11-N12	10.92	125.26	108.95
2	F	1318	ZPC	O10-C11-N12	10.86	125.17	108.95
2	A	1318	ZPC	O10-C11-N12	10.84	125.14	108.95
2	E	1318	ZPC	O10-C11-N12	10.28	124.31	108.95
2	G	1318	ZPC	O10-C11-N12	9.55	123.22	108.95
2	D	1318	ZPC	C15-C20-N19	-9.35	120.41	123.94
2	C	1318	ZPC	C01-N02-C07	9.12	125.63	110.64
2	F	1318	ZPC	C04-N05-C08	-8.98	96.09	121.77
2	A	1318	ZPC	C15-C20-N19	-8.92	120.57	123.94
2	C	1318	ZPC	C04-N05-C08	-8.63	97.08	121.77
2	G	1318	ZPC	C11-C20-N19	8.63	133.42	125.57
2	D	1318	ZPC	N22-C21-N12	8.51	122.33	114.23
2	B	1318	ZPC	C11-C20-N19	8.43	133.24	125.57
2	H	1318	ZPC	C04-N05-C08	-8.36	97.84	121.77
2	C	1318	ZPC	C04-C03-N02	-8.26	101.71	110.82
2	J	1318	ZPC	C04-N05-C08	-8.26	98.13	121.77
2	F	1318	ZPC	C15-C20-N19	-8.23	120.83	123.94
2	C	1318	ZPC	N22-C21-N12	7.93	121.78	114.23
2	E	1318	ZPC	C04-N05-C08	-7.80	99.45	121.77
2	I	1318	ZPC	O10-C08-N05	7.73	118.62	111.25
2	F	1318	ZPC	C06-C07-N02	7.68	119.30	110.82
2	B	1318	ZPC	O10-C11-C20	7.63	119.68	109.38
2	A	1318	ZPC	C04-N05-C08	-7.56	100.13	121.77
2	C	1318	ZPC	C11-C20-N19	7.54	132.43	125.57
2	I	1318	ZPC	C04-N05-C08	-7.53	100.22	121.77
2	F	1318	ZPC	C01-N02-C07	7.51	122.98	110.64
2	J	1318	ZPC	C01-N02-C07	7.50	122.96	110.64
2	C	1318	ZPC	O09-C08-N05	-7.49	109.61	124.36
2	I	1318	ZPC	C15-C20-N19	-7.49	121.11	123.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1318	ZPC	C23-C24-CL	-7.40	111.80	119.86
2	B	1318	ZPC	C04-N05-C08	-7.27	100.98	121.77
2	B	1318	ZPC	C01-N02-C07	7.26	122.57	110.64
2	I	1318	ZPC	C01-N02-C07	7.10	122.31	110.64
2	B	1318	ZPC	O10-C11-N12	7.00	119.41	108.95
2	D	1318	ZPC	C21-N12-C11	6.96	126.22	118.83
2	A	1318	ZPC	C06-C07-N02	6.93	118.47	110.82
2	F	1318	ZPC	C04-C03-N02	-6.91	103.20	110.82
2	D	1318	ZPC	C04-N05-C08	-6.87	102.11	121.77
2	G	1318	ZPC	C21-N12-C11	6.82	126.08	118.83
2	J	1318	ZPC	C11-C20-N19	6.82	131.77	125.57
2	D	1318	ZPC	C06-C07-N02	6.76	118.28	110.82
2	J	1318	ZPC	C21-N12-C11	6.60	125.84	118.83
2	D	1318	ZPC	C01-N02-C07	6.52	121.36	110.64
2	A	1318	ZPC	C11-O10-C08	6.48	126.20	116.43
2	H	1318	ZPC	C27-C21-N12	6.42	125.75	122.33
2	I	1318	ZPC	C01-N02-C03	6.42	121.18	110.64
2	I	1318	ZPC	C21-N12-C11	6.41	125.64	118.83
2	H	1318	ZPC	C11-C20-N19	6.40	131.40	125.57
2	G	1318	ZPC	O10-C11-C20	6.40	118.01	109.38
2	B	1318	ZPC	C01-N02-C03	6.31	121.01	110.64
2	J	1318	ZPC	C15-C20-N19	-6.29	121.57	123.94
2	I	1318	ZPC	C11-C20-N19	6.24	131.25	125.57
2	H	1318	ZPC	O09-C08-N05	-6.10	112.36	124.36
2	E	1318	ZPC	C23-C24-CL	-6.09	113.23	119.86
2	C	1318	ZPC	C07-N02-C03	6.02	117.93	109.54
2	I	1318	ZPC	C11-O10-C08	6.00	125.47	116.43
2	G	1318	ZPC	C04-N05-C08	-6.00	104.62	121.77
2	A	1318	ZPC	C01-N02-C07	5.94	120.40	110.64
2	F	1318	ZPC	C11-C20-N19	5.91	130.94	125.57
2	C	1318	ZPC	O10-C11-C20	5.90	117.35	109.38
2	B	1318	ZPC	C23-C24-CL	-5.90	113.43	119.86
2	D	1318	ZPC	C11-C20-N19	5.90	130.94	125.57
2	C	1318	ZPC	O10-C08-O09	-5.87	112.61	124.67
2	A	1318	ZPC	C01-N02-C03	5.87	120.28	110.64
2	A	1318	ZPC	N22-C21-N12	5.82	119.77	114.23
2	H	1318	ZPC	C11-O10-C08	5.82	125.20	116.43
2	C	1318	ZPC	C24-C23-N22	-5.80	115.22	122.34
2	E	1318	ZPC	C15-C20-N19	-5.79	121.75	123.94
2	E	1318	ZPC	C06-C07-N02	5.76	117.18	110.82
2	H	1318	ZPC	C01-N02-C07	5.70	120.01	110.64
2	F	1318	ZPC	N22-C21-N12	5.67	119.63	114.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1318	ZPC	C15-C20-C11	-5.66	106.30	109.85
2	A	1318	ZPC	O09-C08-N05	-5.65	113.25	124.36
2	B	1318	ZPC	O09-C08-N05	-5.61	113.32	124.36
2	A	1318	ZPC	C03-C04-N05	5.61	124.15	110.58
2	G	1318	ZPC	C03-C04-N05	5.60	124.14	110.58
2	E	1318	ZPC	C27-C21-N12	5.56	125.30	122.33
2	G	1318	ZPC	C01-N02-C07	5.53	119.73	110.64
2	G	1318	ZPC	C26-C24-CL	5.53	128.45	119.34
2	F	1318	ZPC	C23-N22-C21	5.52	128.74	117.77
2	A	1318	ZPC	C11-C20-N19	5.49	130.57	125.57
2	D	1318	ZPC	O09-C08-N05	-5.43	113.66	124.36
2	B	1318	ZPC	C24-C23-N22	-5.32	115.80	122.34
2	J	1318	ZPC	C06-C07-N02	5.31	116.68	110.82
2	B	1318	ZPC	C11-O10-C08	5.30	124.41	116.43
2	E	1318	ZPC	C11-C20-N19	5.28	130.38	125.57
2	F	1318	ZPC	C27-C21-N12	5.27	125.14	122.33
2	G	1318	ZPC	C07-N02-C03	5.27	116.89	109.54
2	C	1318	ZPC	C23-N22-C21	5.23	128.16	117.77
2	J	1318	ZPC	C15-C20-C11	-5.14	106.63	109.85
2	E	1318	ZPC	O09-C08-N05	-5.05	114.42	124.36
2	H	1318	ZPC	C07-N02-C03	5.05	116.58	109.54
2	F	1318	ZPC	C07-N02-C03	4.99	116.50	109.54
2	H	1318	ZPC	O10-C11-C20	4.95	116.07	109.38
2	E	1318	ZPC	C03-C04-N05	4.92	122.50	110.58
2	E	1318	ZPC	C07-N02-C03	4.92	116.41	109.54
2	C	1318	ZPC	C27-C21-N12	-4.92	119.71	122.33
2	I	1318	ZPC	N22-C21-N12	4.88	118.87	114.23
2	D	1318	ZPC	C07-N02-C03	4.85	116.30	109.54
2	G	1318	ZPC	C23-N22-C21	4.84	127.38	117.77
2	D	1318	ZPC	C23-N22-C21	4.80	127.31	117.77
2	E	1318	ZPC	C01-N02-C07	4.80	118.53	110.64
2	G	1318	ZPC	C06-C07-N02	4.79	116.11	110.82
2	B	1318	ZPC	C23-N22-C21	4.77	127.24	117.77
2	D	1318	ZPC	C11-O10-C08	4.75	123.59	116.43
2	A	1318	ZPC	C23-C24-CL	-4.61	114.84	119.86
2	G	1318	ZPC	C11-O10-C08	4.56	123.31	116.43
2	C	1318	ZPC	C06-N05-C08	4.49	134.64	121.77
2	F	1318	ZPC	C26-C24-CL	4.49	126.75	119.34
2	G	1318	ZPC	O10-C08-O09	-4.48	115.46	124.67
2	F	1318	ZPC	O09-C08-N05	-4.45	115.60	124.36
2	I	1318	ZPC	C23-C24-CL	-4.43	115.04	119.86
2	E	1318	ZPC	C01-N02-C03	4.40	117.87	110.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1318	ZPC	C06-N05-C08	4.37	134.28	121.77
2	J	1318	ZPC	N22-C21-N12	4.35	118.38	114.23
2	I	1318	ZPC	C03-C04-N05	4.35	121.09	110.58
2	H	1318	ZPC	C15-C20-N19	-4.34	122.30	123.94
2	B	1318	ZPC	N22-C21-N12	4.34	118.36	114.23
2	F	1318	ZPC	C27-C21-N22	-4.28	115.16	123.08
2	I	1318	ZPC	C07-N02-C03	4.28	115.51	109.54
2	B	1318	ZPC	C03-C04-N05	4.25	120.87	110.58
2	A	1318	ZPC	C23-N22-C21	4.24	126.19	117.77
2	E	1318	ZPC	C18-C17-N16	4.22	127.79	122.28
2	C	1318	ZPC	C03-C04-N05	4.21	120.77	110.58
2	J	1318	ZPC	C23-N22-C21	4.17	126.05	117.77
2	E	1318	ZPC	C26-C24-CL	4.14	126.16	119.34
2	G	1318	ZPC	O09-C08-N05	-4.11	116.27	124.36
2	H	1318	ZPC	C23-N22-C21	4.10	125.90	117.77
2	G	1318	ZPC	C01-N02-C03	4.09	117.37	110.64
2	H	1318	ZPC	C03-C04-N05	4.09	120.47	110.58
2	G	1318	ZPC	C20-C15-N16	4.05	126.56	123.60
2	D	1318	ZPC	C24-C23-N22	-3.98	117.45	122.34
2	J	1318	ZPC	C11-O10-C08	3.97	122.42	116.43
2	E	1318	ZPC	C23-N22-C21	3.97	125.65	117.77
2	F	1318	ZPC	O10-C08-O09	-3.96	116.55	124.67
2	D	1318	ZPC	C27-C21-N22	-3.95	115.77	123.08
2	E	1318	ZPC	C11-O10-C08	3.87	122.27	116.43
2	J	1318	ZPC	O10-C11-C20	3.87	114.60	109.38
2	F	1318	ZPC	C23-C24-CL	-3.78	115.75	119.86
2	J	1318	ZPC	C01-N02-C03	3.77	116.83	110.64
2	H	1318	ZPC	C01-N02-C03	3.76	116.82	110.64
2	I	1318	ZPC	C23-N22-C21	3.73	125.18	117.77
2	H	1318	ZPC	C06-C07-N02	3.70	114.90	110.82
2	J	1318	ZPC	O10-C08-O09	-3.70	117.08	124.67
2	G	1318	ZPC	C24-C23-N22	-3.69	117.81	122.34
2	J	1318	ZPC	C03-C04-N05	3.68	119.48	110.58
2	G	1318	ZPC	C15-C20-C11	-3.60	107.59	109.85
2	G	1318	ZPC	C21-N12-C13	-3.59	123.60	127.46
2	B	1318	ZPC	C26-C24-C23	3.59	121.88	119.41
2	B	1318	ZPC	O14-C13-C15	-3.57	110.83	128.61
2	I	1318	ZPC	C11-N12-C13	-3.55	109.92	112.83
2	I	1318	ZPC	C15-C20-C11	-3.54	107.63	109.85
2	A	1318	ZPC	C26-C24-CL	3.49	125.11	119.34
2	E	1318	ZPC	C21-N12-C11	3.49	122.54	118.83
2	D	1318	ZPC	C21-N12-C13	-3.46	123.75	127.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1318	ZPC	C11-N12-C13	-3.44	110.00	112.83
2	H	1318	ZPC	C23-C24-CL	-3.40	116.16	119.86
2	J	1318	ZPC	C21-N12-C13	-3.37	123.84	127.46
2	I	1318	ZPC	C27-C21-N12	3.37	124.13	122.33
2	A	1318	ZPC	O14-C13-C15	-3.33	112.02	128.61
2	J	1318	ZPC	C04-C03-N02	3.33	114.49	110.82
2	E	1318	ZPC	N22-C21-N12	3.32	117.39	114.23
2	G	1318	ZPC	O14-C13-C15	-3.32	112.10	128.61
2	I	1318	ZPC	C27-C21-N22	-3.30	116.97	123.08
2	F	1318	ZPC	C21-N12-C11	3.30	122.33	118.83
2	F	1318	ZPC	O14-C13-C15	-3.28	112.28	128.61
2	A	1318	ZPC	C24-C23-N22	-3.27	118.32	122.34
2	B	1318	ZPC	C26-C24-CL	3.24	124.68	119.34
2	F	1318	ZPC	O10-C11-C20	3.23	113.75	109.38
2	I	1318	ZPC	C26-C24-CL	3.23	124.66	119.34
2	B	1318	ZPC	C15-C20-C11	-3.22	107.83	109.85
2	D	1318	ZPC	C03-C04-N05	3.21	118.34	110.58
2	E	1318	ZPC	C15-C20-C11	-3.20	107.84	109.85
2	D	1318	ZPC	O14-C13-C15	-3.19	112.74	128.61
2	H	1318	ZPC	C24-C23-N22	-3.19	118.42	122.34
2	J	1318	ZPC	C27-C21-N12	3.17	124.02	122.33
2	E	1318	ZPC	O10-C08-O09	-3.17	118.17	124.67
2	C	1318	ZPC	C20-C15-N16	3.16	125.91	123.60
2	H	1318	ZPC	C11-N12-C13	-3.15	110.24	112.83
2	G	1318	ZPC	C11-N12-C13	-3.15	110.24	112.83
2	F	1318	ZPC	C11-N12-C13	-3.13	110.25	112.83
2	A	1318	ZPC	C27-C21-N22	-3.13	117.30	123.08
2	E	1318	ZPC	O14-C13-C15	-3.13	113.04	128.61
2	E	1318	ZPC	C27-C21-N22	-3.12	117.31	123.08
2	B	1318	ZPC	O10-C08-O09	-3.12	118.26	124.67
2	J	1318	ZPC	C11-N12-C13	-3.06	110.31	112.83
2	E	1318	ZPC	C24-C23-N22	-3.04	118.61	122.34
2	H	1318	ZPC	C27-C21-N22	-3.01	117.52	123.08
2	G	1318	ZPC	C04-C03-N02	2.99	114.12	110.82
2	H	1318	ZPC	C06-N05-C08	2.99	130.32	121.77
2	J	1318	ZPC	O09-C08-N05	-2.99	118.48	124.36
2	J	1318	ZPC	C27-C21-N22	-2.97	117.58	123.08
2	C	1318	ZPC	C01-N02-C03	2.97	115.52	110.64
2	A	1318	ZPC	O10-C08-O09	-2.97	118.57	124.67
2	F	1318	ZPC	C24-C23-N22	-2.96	118.70	122.34
2	H	1318	ZPC	C26-C24-CL	2.96	124.22	119.34
2	J	1318	ZPC	C24-C23-N22	-2.95	118.72	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1318	ZPC	C17-C18-N19	-2.94	118.44	122.28
2	J	1318	ZPC	C07-N02-C03	2.94	113.64	109.54
2	C	1318	ZPC	C11-O10-C08	2.93	120.85	116.43
2	F	1318	ZPC	C20-C15-N16	2.91	125.73	123.60
2	J	1318	ZPC	C26-C24-CL	2.87	124.08	119.34
2	I	1318	ZPC	O09-C08-N05	-2.86	118.73	124.36
2	I	1318	ZPC	O10-C11-C20	2.85	113.23	109.38
2	I	1318	ZPC	C21-N12-C13	-2.84	124.42	127.46
2	F	1318	ZPC	C03-C04-N05	2.82	117.41	110.58
2	C	1318	ZPC	O14-C13-C15	-2.80	114.65	128.61
2	E	1318	ZPC	C04-C03-N02	2.79	113.91	110.82
2	F	1318	ZPC	C26-C24-C23	-2.76	117.50	119.41
2	C	1318	ZPC	C27-C26-C24	2.76	122.30	119.22
2	F	1318	ZPC	C01-N02-C03	2.73	115.12	110.64
2	G	1318	ZPC	C27-C21-N22	-2.71	118.07	123.08
2	C	1318	ZPC	C27-C21-N22	-2.67	118.15	123.08
2	H	1318	ZPC	O10-C08-O09	-2.66	119.20	124.67
2	E	1318	ZPC	C17-N16-C15	-2.61	112.08	116.86
2	F	1318	ZPC	C06-N05-C08	2.61	129.24	121.77
2	F	1318	ZPC	C15-C20-C11	-2.61	108.21	109.85
2	I	1318	ZPC	O14-C13-C15	-2.60	115.65	128.61
2	F	1318	ZPC	C17-N16-C15	-2.54	112.20	116.86
2	A	1318	ZPC	C06-N05-C04	2.51	117.30	112.52
2	B	1318	ZPC	C27-C21-N22	-2.50	118.46	123.08
2	A	1318	ZPC	C07-N02-C03	2.48	112.99	109.54
2	H	1318	ZPC	N22-C21-N12	2.45	116.56	114.23
2	G	1318	ZPC	C17-N16-C15	-2.43	112.41	116.86
2	J	1318	ZPC	O14-C13-C15	-2.43	116.52	128.61
2	I	1318	ZPC	C06-N05-C04	2.41	117.12	112.52
2	B	1318	ZPC	C20-C15-N16	2.35	125.32	123.60
2	J	1318	ZPC	C23-C24-CL	-2.34	117.32	119.86
2	A	1318	ZPC	C06-N05-C08	2.33	128.46	121.77
2	B	1318	ZPC	C18-C17-N16	2.32	125.31	122.28
2	H	1318	ZPC	O14-C13-C15	-2.28	117.28	128.61
2	D	1318	ZPC	O10-C08-O09	-2.27	120.00	124.67
2	E	1318	ZPC	C11-N12-C13	-2.24	110.99	112.83
2	H	1318	ZPC	C21-N12-C13	2.21	129.83	127.46
2	D	1318	ZPC	C20-C15-N16	2.19	125.21	123.60
2	I	1318	ZPC	C24-C23-N22	-2.17	119.67	122.34
2	B	1318	ZPC	C17-C18-N19	-2.17	119.45	122.28
2	E	1318	ZPC	C06-N05-C08	2.17	127.97	121.77
2	D	1318	ZPC	C26-C27-C21	2.15	120.71	117.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1318	ZPC	C26-C27-C21	2.16	120.71	117.65
2	J	1318	ZPC	C17-C18-N19	-2.15	119.48	122.28
2	A	1318	ZPC	C17-N16-C15	-2.14	112.94	116.86
2	H	1318	ZPC	C07-C06-N05	-2.14	105.40	110.58
2	D	1318	ZPC	C17-N16-C15	-2.14	112.95	116.86
2	G	1318	ZPC	C06-N05-C08	2.12	127.85	121.77
2	I	1318	ZPC	C07-C06-N05	-2.08	105.56	110.58
2	B	1318	ZPC	C17-N16-C15	-2.05	113.11	116.86
2	C	1318	ZPC	C21-N12-C11	2.04	120.99	118.83
2	G	1318	ZPC	N22-C21-N12	-2.02	112.31	114.23
2	E	1318	ZPC	C20-C15-C13	2.00	113.10	108.48

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1318	ZPC	N22-C21-N12-C11

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, 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	307/307 (100%)	-0.15	3 (0%) 79 34	74, 118, 187, 217	0
1	B	307/307 (100%)	-0.10	5 (1%) 68 24	71, 108, 171, 263	0
1	C	307/307 (100%)	-0.11	9 (2%) 49 13	71, 107, 186, 232	0
1	D	307/307 (100%)	-0.19	3 (0%) 79 34	74, 104, 186, 263	0
1	E	307/307 (100%)	-0.18	2 (0%) 84 43	73, 113, 188, 233	0
1	F	307/307 (100%)	-0.19	2 (0%) 84 43	78, 118, 190, 276	0
1	G	307/307 (100%)	-0.18	2 (0%) 84 43	75, 108, 171, 236	0
1	H	307/307 (100%)	-0.08	8 (2%) 53 14	75, 111, 187, 279	0
1	I	307/307 (100%)	-0.14	7 (2%) 57 17	76, 106, 192, 274	0
1	J	307/307 (100%)	-0.19	1 (0%) 91 64	77, 115, 203, 261	0
All	All	3070/3070 (100%)	-0.15	42 (1%) 72 26	71, 111, 189, 279	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	317	ILE	7.8
1	E	290	GLY	7.3
1	F	317	ILE	6.0
1	B	290	GLY	4.8
1	C	289	ASN	4.1
1	B	289	ASN	4.0
1	A	153	ASP	4.0
1	C	315	LEU	3.9
1	C	291	VAL	3.9
1	C	314	VAL	3.8
1	B	291	VAL	3.7
1	H	289	ASN	3.5
1	J	153	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	290	GLY	3.2
1	I	153	ASP	3.2
1	C	288	ALA	3.2
1	G	290	GLY	3.1
1	H	150	GLU	3.1
1	E	291	VAL	3.0
1	I	315	LEU	3.0
1	A	152	ILE	3.0
1	C	316	VAL	2.9
1	I	291	VAL	2.8
1	H	315	LEU	2.8
1	H	291	VAL	2.7
1	H	311	ILE	2.6
1	I	290	GLY	2.6
1	I	289	ASN	2.6
1	D	226	GLU	2.5
1	I	317	ILE	2.5
1	H	314	VAL	2.5
1	G	285	HIS	2.4
1	H	153	ASP	2.4
1	D	291	VAL	2.3
1	B	31	GLN	2.2
1	F	315	LEU	2.1
1	B	102	TYR	2.1
1	D	153	ASP	2.1
1	C	311	ILE	2.0
1	H	293	ASP	2.0
1	A	49	LYS	2.0
1	I	154	ASN	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ZPC	A	1318	27/27	0.43	2.09	73,96,144,160	0
2	ZPC	H	1318	27/27	0.27	0.62	52,91,138,212	0
2	ZPC	D	1318	27/27	0.29	0.60	49,74,112,136	0
2	ZPC	C	1318	27/27	0.28	0.55	29,69,126,170	0
2	ZPC	E	1318	27/27	0.18	-0.05	54,79,132,152	0
2	ZPC	F	1318	27/27	0.20	-0.14	33,81,133,160	0
2	ZPC	I	1318	27/27	0.19	-0.26	51,84,125,167	0
2	ZPC	G	1318	27/27	0.15	-0.46	55,91,123,138	0
2	ZPC	B	1318	27/27	0.15	-0.57	55,84,115,171	0
2	ZPC	J	1318	27/27	0.15	-0.59	30,62,129,167	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.