



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:27 PM GMT

PDB ID : 4E2F  
Title : Crystal Structure of E. coli Aspartate Transcarbamoylase K164E/E239K Mutant in an intermediate state  
Authors : Guo, W.; Kantrowitz, E.R.  
Deposited on : 2012-03-08  
Resolution : 2.80 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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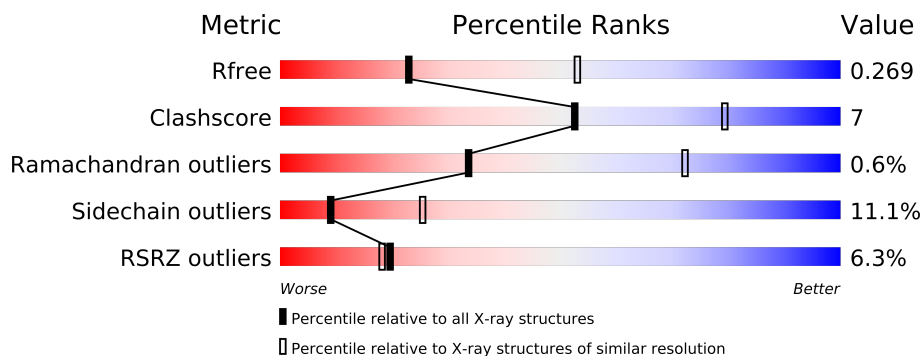
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	310	
1	C	310	
1	E	310	
1	G	310	
1	I	310	
1	K	310	
2	B	153	
2	D	153	
2	F	153	
2	H	153	
2	J	153	
2	L	153	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21764 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 Aspartate carbamoyltransferase catalytic chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	K	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	G	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	E	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	164	GLU	LYS	ENGINEERED MUTATION	UNP P0A786
I	239	LYS	GLU	ENGINEERED MUTATION	UNP P0A786
K	164	GLU	LYS	ENGINEERED MUTATION	UNP P0A786
K	239	LYS	GLU	ENGINEERED MUTATION	UNP P0A786
G	164	GLU	LYS	ENGINEERED MUTATION	UNP P0A786
G	239	LYS	GLU	ENGINEERED MUTATION	UNP P0A786
C	164	GLU	LYS	ENGINEERED MUTATION	UNP P0A786
C	239	LYS	GLU	ENGINEERED MUTATION	UNP P0A786
A	164	GLU	LYS	ENGINEERED MUTATION	UNP P0A786
A	239	LYS	GLU	ENGINEERED MUTATION	UNP P0A786
E	164	GLU	LYS	ENGINEERED MUTATION	UNP P0A786
E	239	LYS	GLU	ENGINEERED MUTATION	UNP P0A786

- Molecule 2 is a protein called Aspartate carbamoyltransferase regulatory chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	144	Total	C	N	O	S	0	0	0
			1127	707	199	216	5			
2	B	144	Total	C	N	O	S	0	0	0
			1127	707	199	216	5			
2	J	144	Total	C	N	O	S	0	0	0
			1127	707	199	216	5			
2	L	144	Total	C	N	O	S	0	0	0
			1127	707	199	216	5			
2	H	144	Total	C	N	O	S	0	0	0
			1127	707	199	216	5			
2	F	144	Total	C	N	O	S	0	0	0
			1127	707	199	216	5			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	L	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	49	Total	O	0	0
			49	49		
4	K	44	Total	O	0	0
			44	44		
4	G	41	Total	O	0	0
			41	41		
4	C	52	Total	O	0	0
			52	52		
4	A	78	Total	O	0	0
			78	78		
4	D	32	Total	O	0	0
			32	32		

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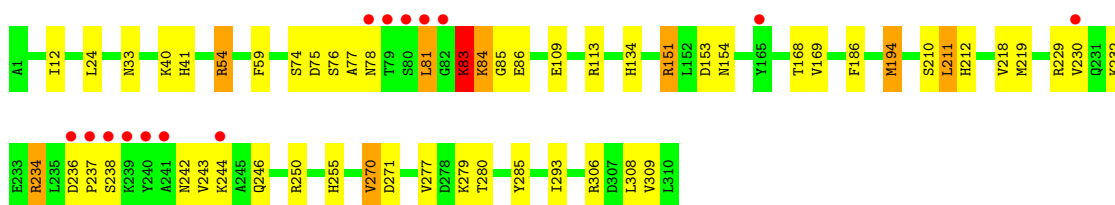
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	35	Total 35	O 35	0	0
4	E	71	Total 71	O 71	0	0
4	J	21	Total 21	O 21	0	0
4	L	26	Total 26	O 26	0	0
4	H	16	Total 16	O 16	0	0
4	F	41	Total 41	O 41	0	0

### 3 Residue-property plots

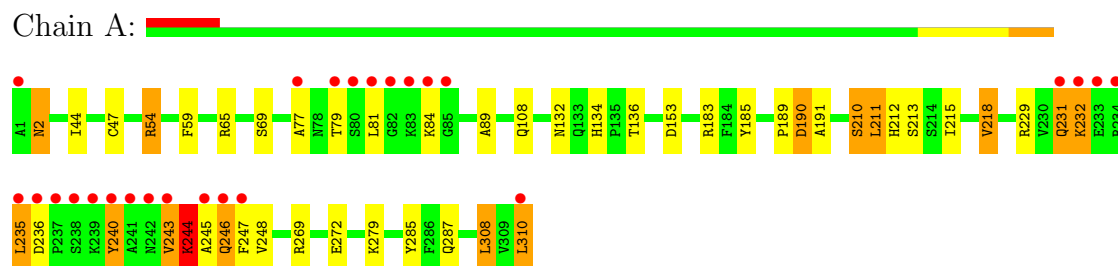
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Aspartate carbamoyltransferase catalytic chain

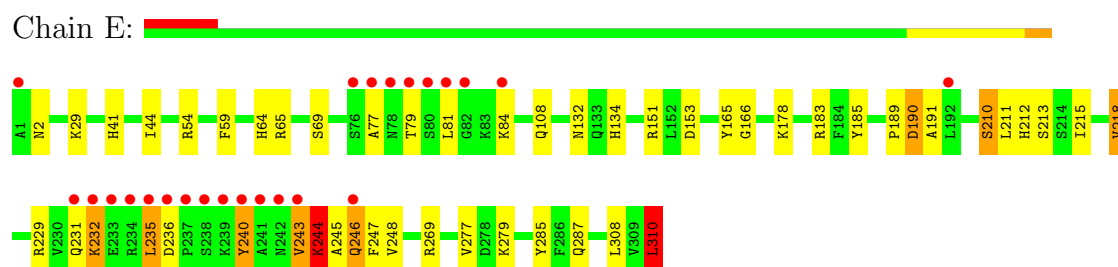
Chain I: 



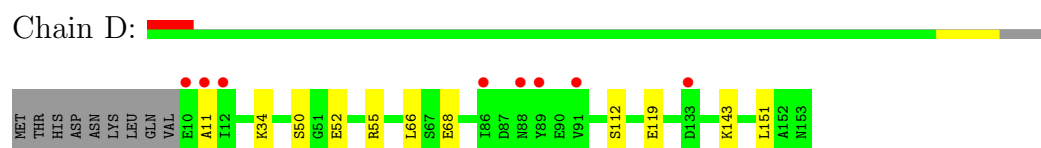
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



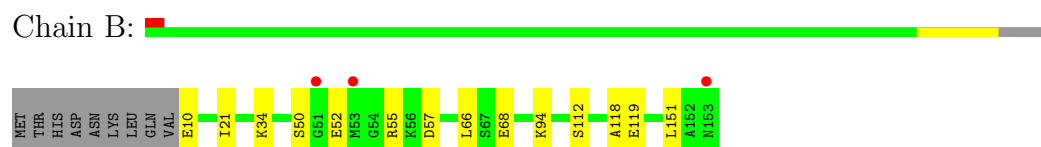
- Molecule 1: Aspartate carbamoyltransferase catalytic chain



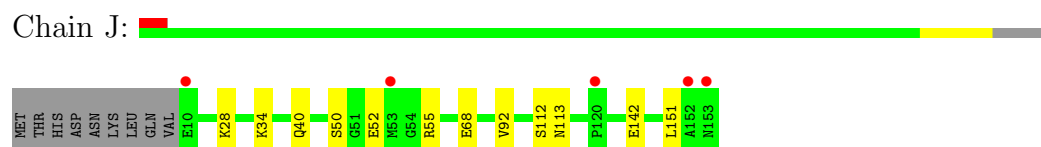
- Molecule 2: Aspartate carbamoyltransferase regulatory chain



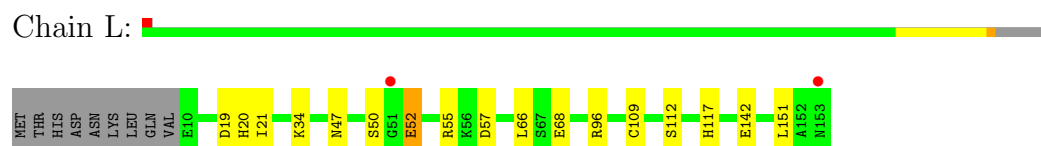
- Molecule 2: Aspartate carbamoyltransferase regulatory chain



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- Molecule 2: Aspartate carbamoyltransferase regulatory chain



- Molecule 2: Aspartate carbamoyltransferase regulatory chain





● Molecule 2: Aspartate carbamoyltransferase regulatory chain

Chain F: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.09Å 144.81Å 203.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 2.80 29.89 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.89-2.80) 92.4 (29.89-2.80)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.214 , 0.274 0.207 , 0.269	Depositor DCC
$R_{free}$ test set	4205 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 83807 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21764	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: ZN

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	0.73	1/2461 (0.0%)	0.86	3/3339 (0.1%)
1	C	0.59	0/2461	0.70	2/3339 (0.1%)
1	E	0.76	0/2461	0.89	3/3339 (0.1%)
1	G	0.63	3/2461 (0.1%)	1.02	13/3339 (0.4%)
1	I	0.60	0/2461	0.72	2/3339 (0.1%)
1	K	0.60	0/2461	0.79	6/3339 (0.2%)
2	B	0.61	0/1144	0.67	0/1546
2	D	0.65	0/1144	0.69	0/1546
2	F	0.65	0/1144	0.69	0/1546
2	H	0.64	0/1144	0.71	0/1546
2	J	0.64	0/1144	0.72	1/1546 (0.1%)
2	L	0.62	0/1144	0.70	0/1546
All	All	0.65	4/21630 (0.0%)	0.79	30/29310 (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	C	0	1
2	H	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	83	LYS	C-O	-8.77	1.06	1.23
1	G	82	GLY	CA-C	6.28	1.61	1.51
1	G	234	ARG	CZ-NH1	6.09	1.41	1.33
1	A	47	CYS	CB-SG	-5.86	1.72	1.81

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	234	ARG	NE-CZ-NH2	-30.54	105.03	120.30
1	G	234	ARG	NE-CZ-NH1	15.91	128.25	120.30
1	K	236	ASP	CB-CG-OD1	-14.09	105.62	118.30
1	G	17	ARG	NE-CZ-NH2	10.36	125.48	120.30
1	G	17	ARG	NE-CZ-NH1	-10.35	115.13	120.30
1	E	310	LEU	CB-CG-CD1	-9.31	95.17	111.00
1	G	234	ARG	CG-CD-NE	7.61	127.77	111.80
1	G	234	ARG	CA-CB-CG	7.49	129.87	113.40
1	G	234	ARG	CD-NE-CZ	7.19	133.67	123.60
1	G	81	LEU	CA-CB-CG	7.00	131.39	115.30
1	G	83	LYS	O-C-N	-6.86	111.72	122.70
1	G	84	LYS	N-CA-CB	-6.73	98.48	110.60
1	K	236	ASP	CB-CG-OD2	6.71	124.34	118.30
1	G	17	ARG	CD-NE-CZ	6.67	132.94	123.60
1	G	234	ARG	NH1-CZ-NH2	6.41	126.45	119.40
1	I	83	LYS	CD-CE-NZ	6.39	126.40	111.70
1	K	236	ASP	N-CA-CB	5.90	121.22	110.60
1	C	234	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	310	LEU	CA-C-O	5.81	132.30	120.10
1	K	82	GLY	C-N-CA	-5.78	107.26	121.70
1	A	244	LYS	CD-CE-NZ	5.68	124.76	111.70
1	K	234	ARG	CG-CD-NE	5.61	123.57	111.80
1	G	83	LYS	CA-C-N	5.54	129.39	117.20
2	J	92	VAL	CG1-CB-CG2	5.50	119.71	110.90
1	I	234	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	E	308	LEU	CA-CB-CG	-5.27	103.18	115.30
1	C	234	ARG	CG-CD-NE	5.22	122.75	111.80
1	K	234	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	244	LYS	CA-CB-CG	5.08	124.58	113.40
1	E	244	LYS	CD-CE-NZ	5.06	123.33	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	82	GLY	Peptide
2	H	11	ALA	Peptide
2	H	12	ILE	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	2415	0	0	29	0
1	C	2415	0	0	19	0
1	E	2415	0	0	31	0
1	G	2415	0	0	17	0
1	I	2415	0	0	21	0
1	K	2415	0	0	18	0
2	B	1127	0	0	5	0
2	D	1127	0	0	3	0
2	F	1127	0	0	1	0
2	H	1127	0	0	5	0
2	J	1127	0	0	4	0
2	L	1127	0	0	8	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	A	78	0	0	5	0
4	B	35	0	0	3	0
4	C	52	0	0	3	0
4	D	32	0	0	1	0
4	E	71	0	0	4	0
4	F	41	0	0	1	0
4	G	41	0	0	4	0
4	H	16	0	0	2	0
4	I	49	0	0	3	0
4	J	21	0	0	1	0
4	K	44	0	0	4	0
4	L	26	0	0	4	0
All	All	21764	0	0	150	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 7.

All (150) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:236:ASP:OD1	1:E:165:TYR:OH	1.64	1.13
1:E:189:PRO:CB	1:E:247:PHE:CZ	2.44	1.01
1:A:189:PRO:CB	1:A:247:PHE:CZ	2.47	0.96
1:E:240:TYR:CE1	1:E:244:LYS:NZ	2.34	0.95
1:A:240:TYR:CE1	1:A:244:LYS:NZ	2.42	0.88
1:K:236:ASP:OD1	1:E:165:TYR:CZ	2.28	0.87
1:A:244:LYS:CE	1:A:247:PHE:CB	2.55	0.84
1:K:236:ASP:CB	1:K:237:PRO:CD	2.62	0.77
1:C:54:ARG:NE	4:C:413:HOH:O	2.16	0.77
1:E:189:PRO:O	1:E:191:ALA:N	2.19	0.75
1:A:240:TYR:CD1	1:A:244:LYS:NZ	2.53	0.75
1:K:78:ASN:CG	1:K:80:SER:O	2.26	0.74
1:E:244:LYS:CE	1:E:247:PHE:CB	2.66	0.73
1:G:77:ALA:O	1:G:78:ASN:C	2.27	0.73
1:I:236:ASP:OD2	1:C:165:TYR:OH	2.07	0.72
1:E:240:TYR:CD1	1:E:244:LYS:NZ	2.59	0.71
1:A:213:SER:O	1:A:246:GLN:OE1	2.08	0.70
1:E:245:ALA:O	1:E:248:VAL:N	2.25	0.69
2:J:28:LYS:NZ	4:J:318:HOH:O	2.26	0.69
1:A:189:PRO:O	1:A:191:ALA:N	2.26	0.69
1:E:213:SER:O	1:E:246:GLN:OE1	2.11	0.68
1:E:151:ARG:NH1	4:E:462:HOH:O	2.28	0.67
1:I:151:ARG:NH2	4:I:446:HOH:O	2.28	0.65
1:G:120:GLY:N	4:G:410:HOH:O	2.30	0.64
1:C:293:ILE:CD1	4:C:408:HOH:O	2.45	0.64
2:H:12:ILE:CG2	2:H:89:TYR:CA	2.75	0.64
2:D:11:ALA:CB	4:D:323:HOH:O	2.46	0.63
1:C:270:VAL:CG2	1:C:271:ASP:N	2.65	0.60
1:K:113:ARG:NH2	2:L:142:GLU:OE2	2.35	0.59
1:E:210:SER:CB	1:E:212:HIS:CE1	2.87	0.58
1:G:78:ASN:O	1:G:80:SER:O	2.22	0.57
2:F:66:LEU:N	4:F:337:HOH:O	2.37	0.57
1:K:10:ILE:N	4:K:423:HOH:O	2.37	0.57
1:I:270:VAL:CG2	1:I:271:ASP:N	2.67	0.57
1:A:244:LYS:O	1:A:244:LYS:CE	2.53	0.56
1:I:113:ARG:NH2	2:J:142:GLU:OE2	2.38	0.56
1:E:185:TYR:CD2	1:E:218:VAL:CG2	2.88	0.56
1:C:186:PHE:CE1	1:C:194:MET:SD	2.99	0.56
1:I:236:ASP:CB	1:I:237:PRO:CD	2.83	0.55
1:E:245:ALA:O	1:E:248:VAL:O	2.25	0.55
1:K:77:ALA:O	1:K:78:ASN:CB	2.54	0.55
1:A:210:SER:CB	1:A:212:HIS:CE1	2.89	0.55
1:A:245:ALA:O	1:A:248:VAL:O	2.25	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:185:TYR:CD2	1:A:218:VAL:CG2	2.90	0.55
1:K:270:VAL:CG2	1:K:271:ASP:N	2.70	0.55
1:I:109:GLU:OE1	2:J:113:ASN:ND2	2.40	0.55
1:G:188:ALA:N	4:G:434:HOH:O	2.40	0.54
4:K:418:HOH:O	1:C:54:ARG:CG	2.56	0.54
1:C:76:SER:O	1:C:78:ASN:O	2.24	0.54
1:C:211:LEU:C	1:C:212:HIS:CD2	2.81	0.54
1:E:244:LYS:O	1:E:244:LYS:CD	2.56	0.54
1:A:235:LEU:CD1	4:A:467:HOH:O	2.56	0.54
1:E:244:LYS:O	1:E:244:LYS:CE	2.56	0.54
2:H:12:ILE:CG2	2:H:86:ILE:CG2	2.86	0.54
1:G:78:ASN:ND2	1:G:107:PRO:CG	2.71	0.53
1:G:79:THR:O	1:G:80:SER:CB	2.56	0.53
1:C:212:HIS:CD2	1:C:212:HIS:N	2.75	0.53
2:H:55:ARG:C	4:H:312:HOH:O	2.46	0.53
1:E:310:LEU:CD1	1:E:310:LEU:N	2.70	0.53
1:I:33:ASN:CB	4:I:407:HOH:O	2.57	0.52
1:G:151:ARG:NH1	1:G:154:ASN:O	2.42	0.52
1:A:244:LYS:O	1:A:244:LYS:CD	2.56	0.52
1:A:54:ARG:CG	4:E:468:HOH:O	2.56	0.52
1:E:243:VAL:O	1:E:247:PHE:CE2	2.62	0.52
1:A:245:ALA:O	1:A:248:VAL:N	2.42	0.52
1:E:64:HIS:CD2	4:E:417:HOH:O	2.63	0.52
1:K:186:PHE:CE1	1:K:194:MET:SD	3.03	0.51
2:B:118:ALA:N	4:B:315:HOH:O	2.43	0.51
1:G:270:VAL:CG2	1:G:271:ASP:N	2.73	0.51
1:K:83:LYS:O	1:K:85:GLY:N	2.44	0.51
1:G:77:ALA:O	1:G:79:THR:N	2.44	0.51
1:E:244:LYS:O	1:E:247:PHE:CB	2.59	0.51
1:E:244:LYS:CE	1:E:247:PHE:CD2	2.94	0.50
1:I:54:ARG:CG	4:A:457:HOH:O	2.59	0.50
1:G:77:ALA:C	1:G:79:THR:N	2.62	0.50
1:C:151:ARG:NH1	1:C:154:ASN:O	2.45	0.50
1:A:236:ASP:N	1:A:236:ASP:OD1	2.45	0.50
1:K:211:LEU:C	1:K:212:HIS:CD2	2.85	0.50
1:G:78:ASN:OD1	1:G:78:ASN:O	2.29	0.50
1:A:308:LEU:CD1	4:A:455:HOH:O	2.59	0.49
1:E:244:LYS:CA	1:E:247:PHE:CD2	2.96	0.49
1:G:211:LEU:CA	4:G:427:HOH:O	2.61	0.49
1:I:211:LEU:C	1:I:212:HIS:CD2	2.87	0.48
1:E:244:LYS:CE	1:E:247:PHE:CG	2.97	0.48
1:K:212:HIS:CD2	1:K:212:HIS:N	2.81	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:78:ASN:O	1:C:79:THR:CG2	2.61	0.48
1:I:81:LEU:CD1	1:I:84:LYS:CG	2.92	0.48
1:G:212:HIS:CD2	1:G:212:HIS:N	2.80	0.47
1:E:236:ASP:OD1	1:E:236:ASP:N	2.46	0.47
1:A:136:THR:N	4:A:405:HOH:O	2.46	0.47
1:A:244:LYS:O	1:A:247:PHE:CB	2.63	0.47
1:A:244:LYS:CA	1:A:247:PHE:CD2	2.97	0.47
1:G:211:LEU:C	1:G:212:HIS:CD2	2.88	0.47
1:I:186:PHE:CE1	1:I:194:MET:SD	3.07	0.47
1:I:186:PHE:CD2	1:I:186:PHE:N	2.82	0.47
1:A:243:VAL:O	1:A:247:PHE:CE2	2.67	0.47
1:A:89:ALA:N	2:B:119:GLU:OE1	2.48	0.46
1:I:77:ALA:O	1:I:78:ASN:CB	2.63	0.46
1:I:40:LYS:O	1:I:41:HIS:CB	2.64	0.46
1:I:151:ARG:NH1	1:I:154:ASN:O	2.49	0.46
1:C:83:LYS:O	1:C:85:GLY:N	2.49	0.46
2:H:55:ARG:NH2	4:H:313:HOH:O	2.47	0.46
1:C:236:ASP:CB	1:C:237:PRO:CD	2.93	0.46
1:E:245:ALA:O	1:E:248:VAL:CA	2.63	0.46
1:I:212:HIS:N	1:I:212:HIS:CD2	2.81	0.46
1:G:236:ASP:CB	1:G:237:PRO:CD	2.93	0.46
2:B:118:ALA:CB	4:B:315:HOH:O	2.65	0.45
1:E:29:LYS:NZ	1:E:310:LEU:CD2	2.80	0.45
2:L:96:ARG:NE	4:L:307:HOH:O	2.49	0.45
2:B:21:ILE:O	2:B:57:ASP:N	2.50	0.45
1:A:244:LYS:CE	1:A:247:PHE:CG	3.00	0.45
1:I:232:LYS:CA	4:I:432:HOH:O	2.65	0.44
1:I:236:ASP:OD2	1:C:165:TYR:CZ	2.70	0.44
1:C:5:TYR:CD1	1:C:306:ARG:CA	3.00	0.44
1:A:272:GLU:N	1:A:272:GLU:OE1	2.51	0.44
1:E:245:ALA:O	1:E:248:VAL:C	2.56	0.44
1:C:78:ASN:CG	1:C:79:THR:N	2.72	0.43
1:E:232:LYS:O	1:E:235:LEU:O	2.36	0.43
1:A:232:LYS:O	1:A:235:LEU:O	2.37	0.43
2:J:40:GLN:O	2:L:47:ASN:ND2	2.52	0.43
2:L:21:ILE:O	2:L:57:ASP:N	2.52	0.43
1:K:78:ASN:ND2	1:K:80:SER:O	2.52	0.43
1:A:231:GLN:N	4:A:453:HOH:O	2.52	0.42
1:E:29:LYS:CD	1:E:310:LEU:CB	2.97	0.42
1:C:237:PRO:O	4:C:437:HOH:O	2.22	0.42
1:I:83:LYS:O	1:I:85:GLY:N	2.52	0.42
1:E:287:GLN:N	1:E:287:GLN:OE1	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:230:VAL:CG1	4:K:444:HOH:O	2.67	0.42
1:C:186:PHE:CD2	1:C:186:PHE:N	2.88	0.42
1:A:211:LEU:C	1:A:212:HIS:ND1	2.73	0.42
1:E:178:LYS:CE	4:E:431:HOH:O	2.67	0.42
2:L:109:CYS:N	4:L:316:HOH:O	2.52	0.42
1:A:287:GLN:OE1	1:A:287:GLN:N	2.52	0.42
1:K:263:VAL:N	1:K:282:HIS:O	2.52	0.42
2:B:94:LYS:NZ	4:B:318:HOH:O	2.52	0.42
1:K:151:ARG:NH1	1:K:154:ASN:O	2.52	0.42
1:I:238:SER:OG	2:D:143:LYS:CD	2.68	0.42
1:A:2:ASN:OD1	1:A:2:ASN:C	2.58	0.42
2:H:67:SER:N	2:H:70:GLN:OE1	2.53	0.41
2:L:52:GLU:CB	4:L:314:HOH:O	2.69	0.41
1:K:41:HIS:N	4:K:424:HOH:O	2.54	0.41
2:L:19:ASP:OD2	2:L:20:HIS:N	2.54	0.41
1:K:278:ASP:OD1	1:K:285:TYR:OH	2.39	0.41
2:L:117:HIS:ND1	4:L:313:HOH:O	2.37	0.41
1:G:186:PHE:CD2	1:G:186:PHE:N	2.89	0.41
1:I:218:VAL:O	1:I:219:MET:C	2.60	0.40
1:G:106:HIS:N	4:G:403:HOH:O	2.54	0.40
1:C:88:LEU:N	2:D:119:GLU:OE2	2.54	0.40
1:E:41:HIS:N	1:E:41:HIS:CD2	2.89	0.40
1:A:244:LYS:CE	1:A:247:PHE:CD2	3.04	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	308/310 (99%)	281 (91%)	24 (8%)	3 (1%)	22 60
1	C	308/310 (99%)	281 (91%)	25 (8%)	2 (1%)	33 72
1	E	308/310 (99%)	285 (92%)	19 (6%)	4 (1%)	18 51
1	G	308/310 (99%)	284 (92%)	21 (7%)	3 (1%)	22 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	308/310 (99%)	281 (91%)	27 (9%)	0	100	100
1	K	308/310 (99%)	285 (92%)	20 (6%)	3 (1%)	22	60
2	B	142/153 (93%)	137 (96%)	5 (4%)	0	100	100
2	D	142/153 (93%)	136 (96%)	6 (4%)	0	100	100
2	F	142/153 (93%)	136 (96%)	6 (4%)	0	100	100
2	H	142/153 (93%)	131 (92%)	11 (8%)	0	100	100
2	J	142/153 (93%)	135 (95%)	7 (5%)	0	100	100
2	L	142/153 (93%)	135 (95%)	7 (5%)	0	100	100
All	All	2700/2778 (97%)	2507 (93%)	178 (7%)	15 (1%)	33	72

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	78	ASN
1	C	80	SER
1	A	190	ASP
1	E	190	ASP
1	K	77	ALA
1	K	80	SER
1	G	80	SER
1	A	132	ASN
1	G	83	LYS
1	A	77	ALA
1	E	77	ALA
1	E	132	ASN
1	G	219	MET
1	C	78	ASN
1	E	166	GLY

### 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	261/261 (100%)	230 (88%)	31 (12%)	8	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	261/261 (100%)	223 (85%)	38 (15%)	5	13
1	E	261/261 (100%)	230 (88%)	31 (12%)	8	22
1	G	261/261 (100%)	223 (85%)	38 (15%)	5	13
1	I	261/261 (100%)	224 (86%)	37 (14%)	5	14
1	K	261/261 (100%)	223 (85%)	38 (15%)	5	13
2	B	128/137 (93%)	119 (93%)	9 (7%)	21	52
2	D	128/137 (93%)	120 (94%)	8 (6%)	25	59
2	F	128/137 (93%)	120 (94%)	8 (6%)	25	59
2	H	128/137 (93%)	121 (94%)	7 (6%)	30	65
2	J	128/137 (93%)	121 (94%)	7 (6%)	30	65
2	L	128/137 (93%)	120 (94%)	8 (6%)	25	59
All	All	2334/2388 (98%)	2074 (89%)	260 (11%)	9	25

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	12	ILE
1	I	24	LEU
1	I	54	ARG
1	I	59	PHE
1	I	74	SER
1	I	75	ASP
1	I	76	SER
1	I	81	LEU
1	I	83	LYS
1	I	84	LYS
1	I	86	GLU
1	I	134	HIS
1	I	151	ARG
1	I	153	ASP
1	I	168	THR
1	I	169	VAL
1	I	194	MET
1	I	210	SER
1	I	211	LEU
1	I	229	ARG
1	I	230	VAL
1	I	234	ARG

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Mol	Chain	Res	Type
1	I	242	ASN
1	I	243	VAL
1	I	244	LYS
1	I	246	GLN
1	I	250	ARG
1	I	255	HIS
1	I	270	VAL
1	I	277	VAL
1	I	279	LYS
1	I	280	THR
1	I	285	TYR
1	I	293	ILE
1	I	306	ARG
1	I	308	LEU
1	I	309	VAL
1	K	24	LEU
1	K	54	ARG
1	K	59	PHE
1	K	74	SER
1	K	75	ASP
1	K	76	SER
1	K	79	THR
1	K	80	SER
1	K	84	LYS
1	K	86	GLU
1	K	134	HIS
1	K	140	LEU
1	K	151	ARG
1	K	153	ASP
1	K	168	THR
1	K	169	VAL
1	K	194	MET
1	K	210	SER
1	K	211	LEU
1	K	229	ARG
1	K	230	VAL
1	K	234	ARG
1	K	236	ASP
1	K	242	ASN
1	K	243	VAL
1	K	244	LYS
1	K	246	GLN

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Mol	Chain	Res	Type
1	K	250	ARG
1	K	255	HIS
1	K	270	VAL
1	K	277	VAL
1	K	279	LYS
1	K	280	THR
1	K	285	TYR
1	K	293	ILE
1	K	306	ARG
1	K	308	LEU
1	K	309	VAL
1	G	12	ILE
1	G	24	LEU
1	G	54	ARG
1	G	59	PHE
1	G	74	SER
1	G	75	ASP
1	G	76	SER
1	G	79	THR
1	G	80	SER
1	G	83	LYS
1	G	84	LYS
1	G	86	GLU
1	G	134	HIS
1	G	140	LEU
1	G	151	ARG
1	G	153	ASP
1	G	168	THR
1	G	169	VAL
1	G	194	MET
1	G	210	SER
1	G	211	LEU
1	G	229	ARG
1	G	230	VAL
1	G	234	ARG
1	G	242	ASN
1	G	243	VAL
1	G	244	LYS
1	G	246	GLN
1	G	250	ARG
1	G	255	HIS
1	G	270	VAL

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Mol	Chain	Res	Type
1	G	279	LYS
1	G	280	THR
1	G	285	TYR
1	G	293	ILE
1	G	306	ARG
1	G	308	LEU
1	G	309	VAL
1	C	12	ILE
1	C	24	LEU
1	C	54	ARG
1	C	59	PHE
1	C	74	SER
1	C	75	ASP
1	C	76	SER
1	C	81	LEU
1	C	83	LYS
1	C	84	LYS
1	C	86	GLU
1	C	134	HIS
1	C	140	LEU
1	C	151	ARG
1	C	153	ASP
1	C	168	THR
1	C	169	VAL
1	C	194	MET
1	C	210	SER
1	C	211	LEU
1	C	229	ARG
1	C	230	VAL
1	C	234	ARG
1	C	242	ASN
1	C	243	VAL
1	C	244	LYS
1	C	246	GLN
1	C	250	ARG
1	C	255	HIS
1	C	270	VAL
1	C	277	VAL
1	C	279	LYS
1	C	280	THR
1	C	285	TYR
1	C	293	ILE

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Mol	Chain	Res	Type
1	C	306	ARG
1	C	308	LEU
1	C	309	VAL
1	A	2	ASN
1	A	44	ILE
1	A	54	ARG
1	A	59	PHE
1	A	65	ARG
1	A	69	SER
1	A	79	THR
1	A	81	LEU
1	A	84	LYS
1	A	108	GLN
1	A	134	HIS
1	A	153	ASP
1	A	183	ARG
1	A	190	ASP
1	A	210	SER
1	A	211	LEU
1	A	215	ILE
1	A	218	VAL
1	A	229	ARG
1	A	231	GLN
1	A	232	LYS
1	A	235	LEU
1	A	240	TYR
1	A	243	VAL
1	A	244	LYS
1	A	246	GLN
1	A	269	ARG
1	A	279	LYS
1	A	285	TYR
1	A	308	LEU
1	A	310	LEU
2	D	34	LYS
2	D	50	SER
2	D	52	GLU
2	D	55	ARG
2	D	66	LEU
2	D	68	GLU
2	D	112	SER
2	D	151	LEU

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Mol	Chain	Res	Type
2	B	10	GLU
2	B	34	LYS
2	B	50	SER
2	B	52	GLU
2	B	55	ARG
2	B	66	LEU
2	B	68	GLU
2	B	112	SER
2	B	151	LEU
1	E	2	ASN
1	E	44	ILE
1	E	54	ARG
1	E	59	PHE
1	E	65	ARG
1	E	69	SER
1	E	79	THR
1	E	81	LEU
1	E	84	LYS
1	E	108	GLN
1	E	134	HIS
1	E	153	ASP
1	E	183	ARG
1	E	190	ASP
1	E	210	SER
1	E	211	LEU
1	E	215	ILE
1	E	218	VAL
1	E	229	ARG
1	E	231	GLN
1	E	232	LYS
1	E	235	LEU
1	E	240	TYR
1	E	243	VAL
1	E	244	LYS
1	E	246	GLN
1	E	269	ARG
1	E	277	VAL
1	E	279	LYS
1	E	285	TYR
1	E	310	LEU
2	J	34	LYS
2	J	50	SER

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Mol	Chain	Res	Type
2	J	52	GLU
2	J	55	ARG
2	J	68	GLU
2	J	112	SER
2	J	151	LEU
2	L	34	LYS
2	L	50	SER
2	L	52	GLU
2	L	55	ARG
2	L	66	LEU
2	L	68	GLU
2	L	112	SER
2	L	151	LEU
2	H	34	LYS
2	H	50	SER
2	H	55	ARG
2	H	66	LEU
2	H	68	GLU
2	H	112	SER
2	H	151	LEU
2	F	10	GLU
2	F	34	LYS
2	F	50	SER
2	F	55	ARG
2	F	66	LEU
2	F	68	GLU
2	F	112	SER
2	F	151	LEU

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 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	310/310 (100%)	0.02	26 (8%)	11 9	42, 61, 202, 311	0
1	C	310/310 (100%)	0.15	28 (9%)	10 8	51, 79, 210, 318	0
1	E	310/310 (100%)	0.14	24 (7%)	13 12	41, 60, 201, 335	0
1	G	310/310 (100%)	0.05	26 (8%)	11 9	55, 79, 205, 316	0
1	I	310/310 (100%)	-0.20	14 (4%)	32 33	43, 70, 204, 320	0
1	K	310/310 (100%)	0.24	29 (9%)	9 7	51, 78, 203, 307	0
2	B	144/153 (94%)	-0.48	3 (2%)	60 61	51, 71, 121, 189	0
2	D	144/153 (94%)	-0.12	8 (5%)	24 23	57, 78, 136, 190	0
2	F	144/153 (94%)	-0.45	2 (1%)	72 72	52, 72, 125, 189	0
2	H	144/153 (94%)	-0.14	4 (2%)	50 52	63, 84, 128, 189	0
2	J	144/153 (94%)	-0.16	5 (3%)	42 42	50, 74, 124, 188	0
2	L	144/153 (94%)	-0.38	2 (1%)	72 72	55, 73, 127, 190	0
All	All	2724/2778 (98%)	-0.05	171 (6%)	19 18	41, 74, 189, 335	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	236	ASP	15.0
1	E	241	ALA	12.6
1	E	235	LEU	12.6
1	E	237	PRO	11.3
1	K	242	ASN	11.2
1	A	242	ASN	10.5
1	E	79	THR	10.3
1	K	246	GLN	10.1
1	K	245	ALA	9.9
1	C	246	GLN	9.8
1	C	242	ASN	9.8

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Mol	Chain	Res	Type	RSRZ
1	A	82	GLY	9.1
1	E	82	GLY	9.0
1	C	236	ASP	8.8
1	G	241	ALA	8.5
1	E	234	ARG	8.5
1	E	238	SER	8.5
1	E	78	ASN	8.3
1	C	191	ALA	8.1
1	C	245	ALA	8.1
1	C	243	VAL	8.1
1	A	240	TYR	8.1
1	E	81	LEU	8.1
1	K	80	SER	8.0
1	K	243	VAL	7.8
1	K	191	ALA	7.6
1	K	81	LEU	7.5
1	K	79	THR	7.5
1	C	77	ALA	7.4
1	E	77	ALA	7.4
1	E	80	SER	7.2
1	A	81	LEU	7.2
1	A	243	VAL	7.1
1	A	235	LEU	7.0
2	H	153	ASN	6.7
1	G	81	LEU	6.7
1	K	236	ASP	6.5
1	C	235	LEU	6.5
1	A	241	ALA	6.5
1	C	79	THR	6.3
2	B	153	ASN	6.3
1	E	239	LYS	6.2
1	C	82	GLY	6.2
1	K	239	LYS	6.1
1	A	85	GLY	6.0
2	J	153	ASN	6.0
1	K	238	SER	5.8
1	G	85	GLY	5.8
1	E	240	TYR	5.8
1	K	310	LEU	5.7
1	K	82	GLY	5.6
2	D	89	TYR	5.5
1	A	237	PRO	5.5

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Mol	Chain	Res	Type	RSRZ
1	I	240	TYR	5.4
1	A	245	ALA	5.3
1	K	77	ALA	5.3
1	C	237	PRO	5.3
1	C	241	ALA	5.2
1	A	80	SER	5.2
1	K	241	ALA	5.2
1	K	235	LEU	5.1
1	C	240	TYR	5.1
2	B	51	GLY	5.1
1	A	236	ASP	5.1
1	A	246	GLN	5.1
1	C	76	SER	5.0
2	D	11	ALA	5.0
1	K	78	ASN	5.0
1	I	237	PRO	4.9
1	E	231	GLN	4.9
1	I	80	SER	4.9
1	C	247	PHE	4.9
1	K	234	ARG	4.9
1	A	234	ARG	4.9
1	G	237	PRO	4.9
1	K	237	PRO	4.9
1	G	83	LYS	4.8
1	E	246	GLN	4.8
1	C	239	LYS	4.7
1	C	80	SER	4.7
1	A	239	LYS	4.7
1	E	232	LYS	4.6
1	A	79	THR	4.6
1	I	81	LEU	4.4
1	I	79	THR	4.3
2	L	51	GLY	4.3
1	K	240	TYR	4.3
1	E	233	GLU	4.2
1	G	82	GLY	4.2
2	L	153	ASN	4.2
1	A	83	LYS	4.1
1	K	190	ASP	4.1
2	F	153	ASN	4.1
1	I	236	ASP	4.0
1	C	230	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	78	ASN	4.0
1	G	235	LEU	4.0
1	E	192	LEU	3.9
1	C	238	SER	3.9
1	G	84	LYS	3.8
1	G	77	ALA	3.8
1	G	78	ASN	3.8
1	K	233	GLU	3.6
1	E	76	SER	3.5
2	D	91	VAL	3.5
2	B	53	MET	3.5
1	A	1	ALA	3.4
1	C	234	ARG	3.4
1	A	232	LYS	3.3
2	D	12	ILE	3.3
1	A	77	ALA	3.2
2	J	152	ALA	3.1
1	I	244	LYS	3.1
2	D	86	ILE	3.1
2	H	131	ALA	3.1
2	J	120	PRO	3.1
1	E	242	ASN	3.0
1	I	78	ASN	3.0
1	A	238	SER	3.0
2	J	10	GLU	3.0
1	I	238	SER	3.0
1	C	81	LEU	2.9
2	D	88	ASN	2.9
1	I	82	GLY	2.9
1	G	232	LYS	2.9
1	G	180	ASP	2.8
1	G	242	ASN	2.8
1	K	76	SER	2.8
1	E	243	VAL	2.8
1	A	233	GLU	2.8
1	A	247	PHE	2.7
1	I	230	VAL	2.7
1	G	246	GLN	2.7
2	F	53	MET	2.7
1	G	239	LYS	2.6
1	G	255	HIS	2.6
1	A	231	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	192	LEU	2.5
1	E	1	ALA	2.5
1	A	84	LYS	2.5
1	I	165	TYR	2.5
1	G	54	ARG	2.5
1	C	83	LYS	2.5
1	G	236	ASP	2.4
1	E	84	LYS	2.4
1	K	196	GLN	2.4
1	C	232	LYS	2.3
1	C	207	ILE	2.3
1	G	234	ARG	2.3
1	G	193	ALA	2.3
1	K	232	LYS	2.3
2	J	53	MET	2.3
1	K	83	LYS	2.3
1	C	190	ASP	2.2
1	G	80	SER	2.2
1	G	207	ILE	2.2
2	D	133	ASP	2.2
1	I	239	LYS	2.2
1	I	241	ALA	2.2
2	D	10	GLU	2.2
1	G	203	ASP	2.1
2	H	10	GLU	2.1
1	A	310	LEU	2.1
1	K	74	SER	2.1
1	G	252	SER	2.1
1	C	309	VAL	2.1
2	H	93	GLY	2.1
1	K	1	ALA	2.0
1	K	309	VAL	2.0
1	G	208	ALA	2.0
1	C	85	GLY	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
3	ZN	H	201	1/1	0.14	-0.22	98,98,98,98	0
3	ZN	F	201	1/1	0.11	-0.70	58,58,58,58	0
3	ZN	J	201	1/1	0.10	-0.74	75,75,75,75	0
3	ZN	B	201	1/1	0.07	-1.47	59,59,59,59	0
3	ZN	D	201	1/1	0.08	-1.62	59,59,59,59	0
3	ZN	L	201	1/1	0.07	-1.69	57,57,57,57	0

### 6.5 Other polymers

There are no such residues in this entry.