



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:18 PM GMT

PDB ID : 1T5O  
Title : Crystal structure of the translation initiation factor eIF-2B, subunit delta, from *A. fulgidus*  
Authors : Malashkevich, V.N.; Almo, S.C.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2004-05-04  
Resolution : 1.90 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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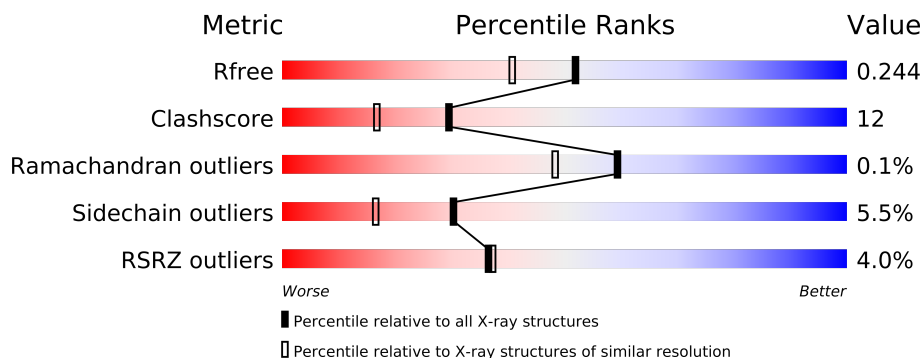
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	351	
1	B	351	
1	C	351	
1	D	351	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12002 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 Translation initiation factor eIF2B, subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2651	1685	453	503	10			
1	B	340	Total	C	N	O	S	0	0	0
			2651	1685	453	503	10			
1	C	340	Total	C	N	O	S	0	0	0
			2651	1685	453	503	10			
1	D	340	Total	C	N	O	S	0	0	0
			2651	1685	453	503	10			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP O29877
A	2	SER	-	CLONING ARTIFACT	UNP O29877
A	3	LEU	-	CLONING ARTIFACT	UNP O29877
A	342	GLU	-	CLONING ARTIFACT	UNP O29877
A	343	GLY	-	CLONING ARTIFACT	UNP O29877
A	344	GLY	-	CLONING ARTIFACT	UNP O29877
A	345	SER	-	CLONING ARTIFACT	UNP O29877
A	346	HIS	-	EXPRESSION TAG	UNP O29877
A	347	HIS	-	EXPRESSION TAG	UNP O29877
A	348	HIS	-	EXPRESSION TAG	UNP O29877
A	349	HIS	-	EXPRESSION TAG	UNP O29877
A	350	HIS	-	EXPRESSION TAG	UNP O29877
A	351	HIS	-	EXPRESSION TAG	UNP O29877
B	1	MET	-	CLONING ARTIFACT	UNP O29877
B	2	SER	-	CLONING ARTIFACT	UNP O29877
B	3	LEU	-	CLONING ARTIFACT	UNP O29877
B	342	GLU	-	CLONING ARTIFACT	UNP O29877
B	343	GLY	-	CLONING ARTIFACT	UNP O29877
B	344	GLY	-	CLONING ARTIFACT	UNP O29877
B	345	SER	-	CLONING ARTIFACT	UNP O29877
B	346	HIS	-	EXPRESSION TAG	UNP O29877

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Chain	Residue	Modelled	Actual	Comment	Reference
B	347	HIS	-	EXPRESSION TAG	UNP O29877
B	348	HIS	-	EXPRESSION TAG	UNP O29877
B	349	HIS	-	EXPRESSION TAG	UNP O29877
B	350	HIS	-	EXPRESSION TAG	UNP O29877
B	351	HIS	-	EXPRESSION TAG	UNP O29877
C	1	MET	-	CLONING ARTIFACT	UNP O29877
C	2	SER	-	CLONING ARTIFACT	UNP O29877
C	3	LEU	-	CLONING ARTIFACT	UNP O29877
C	342	GLU	-	CLONING ARTIFACT	UNP O29877
C	343	GLY	-	CLONING ARTIFACT	UNP O29877
C	344	GLY	-	CLONING ARTIFACT	UNP O29877
C	345	SER	-	CLONING ARTIFACT	UNP O29877
C	346	HIS	-	EXPRESSION TAG	UNP O29877
C	347	HIS	-	EXPRESSION TAG	UNP O29877
C	348	HIS	-	EXPRESSION TAG	UNP O29877
C	349	HIS	-	EXPRESSION TAG	UNP O29877
C	350	HIS	-	EXPRESSION TAG	UNP O29877
C	351	HIS	-	EXPRESSION TAG	UNP O29877
D	1	MET	-	CLONING ARTIFACT	UNP O29877
D	2	SER	-	CLONING ARTIFACT	UNP O29877
D	3	LEU	-	CLONING ARTIFACT	UNP O29877
D	342	GLU	-	CLONING ARTIFACT	UNP O29877
D	343	GLY	-	CLONING ARTIFACT	UNP O29877
D	344	GLY	-	CLONING ARTIFACT	UNP O29877
D	345	SER	-	CLONING ARTIFACT	UNP O29877
D	346	HIS	-	EXPRESSION TAG	UNP O29877
D	347	HIS	-	EXPRESSION TAG	UNP O29877
D	348	HIS	-	EXPRESSION TAG	UNP O29877
D	349	HIS	-	EXPRESSION TAG	UNP O29877
D	350	HIS	-	EXPRESSION TAG	UNP O29877
D	351	HIS	-	EXPRESSION TAG	UNP O29877

- Molecule 2 is water.

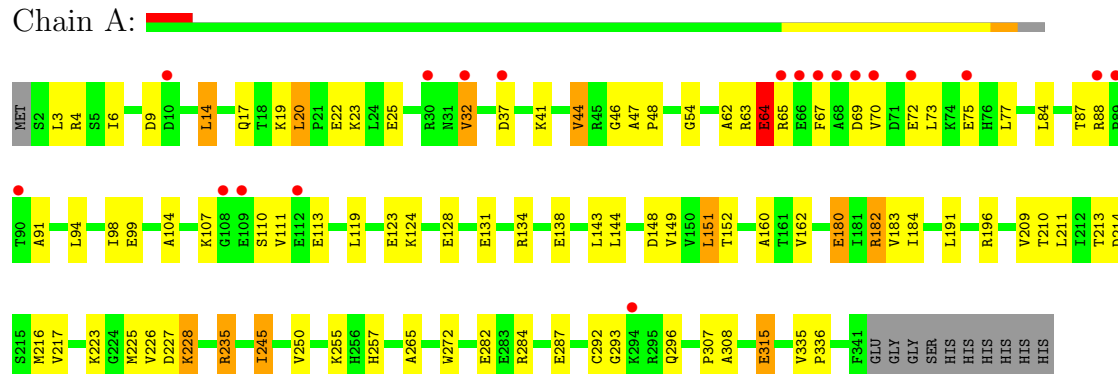
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	325	Total O 325 325	0	0
2	B	396	Total O 396 396	0	0
2	C	374	Total O 374 374	0	0
2	D	303	Total O 303 303	0	0

### 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.

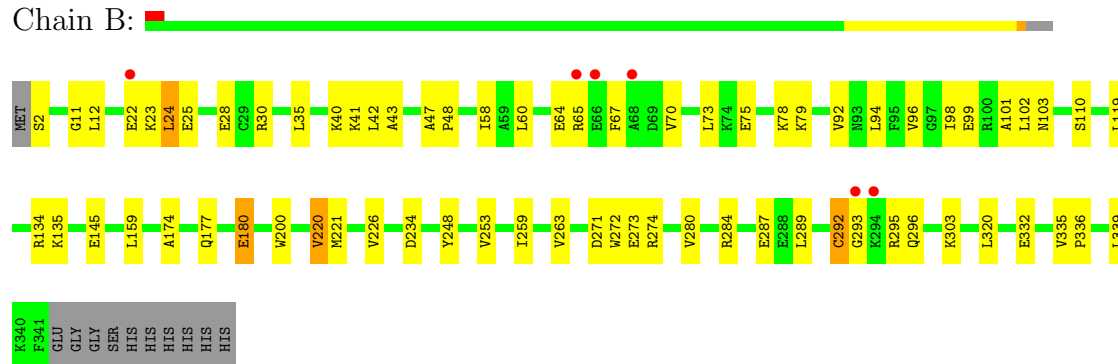
- Molecule 1: Translation initiation factor eIF2B, subunit delta

Chain A:



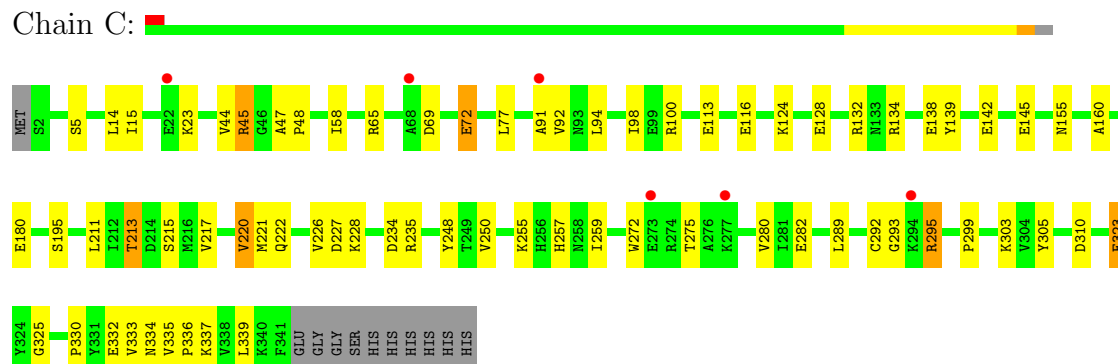
- Molecule 1: Translation initiation factor eIF2B, subunit delta

Chain B:



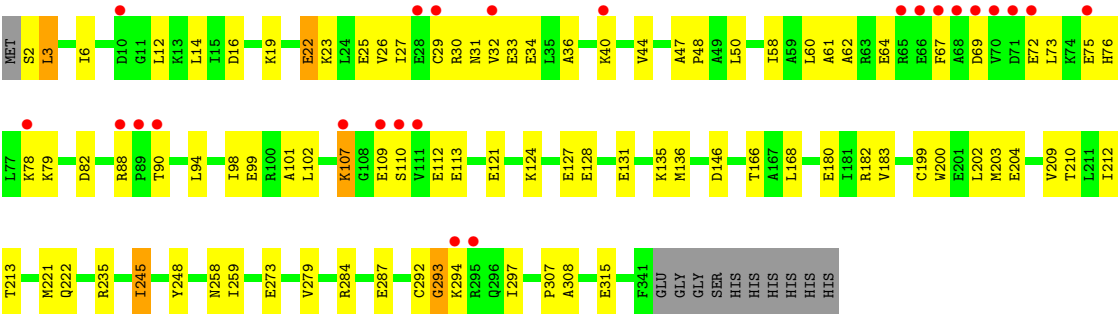
- Molecule 1: Translation initiation factor eIF2B, subunit delta

Chain C:



● Molecule 1: Translation initiation factor eIF2B, subunit delta

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.58Å 110.20Å 141.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.99 – 1.90 24.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (9.99-1.90) 93.5 (24.95-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.197 , 0.246 0.194 , 0.244	Depositor DCC
$R_{free}$ test set	8714 reflections (7.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 51.4	EDS
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 121742 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	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 41.37 % 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 2.3830e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 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	0.54	0/2694	0.74	3/3652 (0.1%)
1	B	0.59	1/2694 (0.0%)	0.75	1/3652 (0.0%)
1	C	0.58	0/2694	0.75	2/3652 (0.1%)
1	D	0.56	0/2694	0.74	1/3652 (0.0%)
All	All	0.57	1/10776 (0.0%)	0.74	7/14608 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	GLU	CB-CG	-5.58	1.41	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	GLY	N-CA-C	-7.31	94.82	113.10
1	A	14	LEU	CA-CB-CG	6.52	130.30	115.30
1	B	293	GLY	N-CA-C	-6.11	97.83	113.10
1	C	310	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	196	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	D	293	GLY	N-CA-C	-5.14	100.25	113.10
1	C	293	GLY	N-CA-C	-5.06	100.45	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the



chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2651	0	2696	88	0
1	B	2651	0	2696	55	0
1	C	2651	0	2696	57	0
1	D	2651	0	2696	84	0
2	A	325	0	0	20	0
2	B	396	0	0	14	0
2	C	374	0	0	10	0
2	D	303	0	0	13	0
All	All	12002	0	10784	258	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 12.

All (258) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:132:ARG:HG3	1:C:323:GLU:HG2	1.32	1.07
1:D:6:ILE:HD12	1:D:14:LEU:HD21	1.44	0.96
1:C:235:ARG:HG2	2:C:699:HOH:O	1.69	0.92
1:D:22:GLU:HG2	2:D:463:HOH:O	1.70	0.91
1:C:299:PRO:HG2	1:D:203:MET:HE3	1.54	0.89
1:A:22:GLU:HG2	1:A:23:LYS:HG3	1.55	0.88
1:C:132:ARG:CG	1:C:323:GLU:HG2	2.02	0.88
1:D:136:MET:CE	1:D:166:THR:HA	2.05	0.86
1:A:182:ARG:HB2	1:A:182:ARG:HH11	1.41	0.84
1:D:315:GLU:HG3	2:D:585:HOH:O	1.77	0.84
1:C:134:ARG:O	1:C:138:GLU:HG2	1.75	0.84
1:C:299:PRO:HG2	1:D:203:MET:CE	2.07	0.84
1:D:245:ILE:HG12	1:D:307:PRO:O	1.77	0.83
1:B:58:ILE:HD12	1:B:101:ALA:HB3	1.61	0.81
1:A:65:ARG:HB2	2:A:519:HOH:O	1.80	0.81
1:A:245:ILE:HG12	1:A:307:PRO:O	1.81	0.80
1:B:23:LYS:HD3	1:B:25:GLU:HG3	1.63	0.80
1:D:14:LEU:HD22	1:D:44:VAL:HG12	1.64	0.80
1:A:149:VAL:HG11	1:A:225:MET:O	1.80	0.79
1:A:296:GLN:OE1	1:B:22:GLU:HG2	1.82	0.79
1:D:22:GLU:HB3	2:D:442:HOH:O	1.83	0.79
1:D:146:ASP:OD1	1:D:180:GLU:HG3	1.82	0.78
1:D:69:ASP:HB3	1:D:72:GLU:HB2	1.67	0.77
1:A:149:VAL:HG12	1:A:227:ASP:OD2	1.86	0.76
1:B:273:GLU:HG2	2:B:612:HOH:O	1.84	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:LEU:O	1:A:228:LYS:HE3	1.88	0.74
1:B:70:VAL:HG23	2:B:402:HOH:O	1.87	0.73
1:A:214:ASP:O	1:A:217:VAL:HG23	1.89	0.72
1:B:23:LYS:HD2	1:B:25:GLU:OE2	1.89	0.72
1:C:282:GLU:CD	1:C:282:GLU:H	1.93	0.71
1:A:75:GLU:HG3	2:A:528:HOH:O	1.90	0.71
1:C:292:CYS:CB	1:D:292:CYS:HG	2.04	0.70
1:D:99:GLU:HG3	2:D:446:HOH:O	1.90	0.70
1:A:113:GLU:HG2	2:A:488:HOH:O	1.90	0.70
1:C:195:SER:HB3	1:D:297:ILE:O	1.92	0.69
1:A:287:GLU:HG3	2:A:648:HOH:O	1.93	0.69
1:A:128:GLU:HA	1:A:131:GLU:HG2	1.72	0.69
1:A:32:VAL:HG13	2:A:552:HOH:O	1.92	0.69
1:D:6:ILE:CD1	1:D:14:LEU:HD21	2.23	0.69
1:A:47:ALA:HB3	1:A:48:PRO:HD3	1.76	0.68
1:A:138:GLU:HG3	2:A:440:HOH:O	1.94	0.68
1:A:69:ASP:OD1	1:A:72:GLU:HG3	1.94	0.68
1:D:36:ALA:O	1:D:40:LYS:HG3	1.94	0.68
1:B:65:ARG:HD3	2:B:725:HOH:O	1.95	0.67
1:A:6:ILE:HG13	1:A:14:LEU:HD23	1.77	0.67
1:D:200:TRP:CZ2	1:D:204:GLU:HG3	2.29	0.67
1:D:136:MET:HE1	1:D:166:THR:HA	1.76	0.66
1:A:265:ALA:HB3	2:A:531:HOH:O	1.94	0.66
1:C:292:CYS:HG	1:D:292:CYS:CB	2.09	0.66
1:C:23:LYS:HE2	2:C:499:HOH:O	1.96	0.65
1:C:221:MET:SD	1:C:259:ILE:HD12	2.38	0.64
1:D:47:ALA:HB3	1:D:48:PRO:HD3	1.79	0.64
1:D:14:LEU:HD22	1:D:44:VAL:CG1	2.26	0.64
1:A:14:LEU:HD13	1:A:44:VAL:HG22	1.79	0.63
1:C:14:LEU:HD22	1:C:44:VAL:HG21	1.79	0.63
1:B:22:GLU:HG3	2:B:404:HOH:O	1.99	0.63
1:A:182:ARG:CB	1:A:182:ARG:HH11	2.12	0.63
1:D:23:LYS:HE2	1:D:25:GLU:HG2	1.81	0.62
1:D:78:LYS:HD3	1:D:78:LYS:O	1.98	0.62
1:C:334:ASN:HA	1:C:337:LYS:HG2	1.81	0.62
1:D:136:MET:HE1	1:D:166:THR:HG22	1.80	0.62
1:D:124:LYS:O	1:D:128:GLU:HG3	2.01	0.61
1:A:180:GLU:HG3	1:A:180:GLU:O	1.99	0.61
1:C:124:LYS:O	1:C:128:GLU:HG3	2.01	0.60
1:C:14:LEU:HD22	1:C:44:VAL:CG2	2.31	0.60
1:A:151:LEU:HD12	1:A:152:THR:N	2.16	0.60
1:B:135:LYS:HD2	2:B:675:HOH:O	2.02	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:11:GLY:HA3	1:B:30:ARG:NH2	2.17	0.59
1:B:47:ALA:HB3	1:B:48:PRO:HD3	1.85	0.59
1:B:332:GLU:OE1	1:B:332:GLU:N	2.29	0.58
1:B:11:GLY:HA3	1:B:30:ARG:HH22	1.69	0.58
1:A:41:LYS:HD3	2:A:529:HOH:O	2.03	0.58
1:A:128:GLU:HA	1:A:131:GLU:CG	2.33	0.58
1:A:94:LEU:O	1:A:98:ILE:HG12	2.04	0.58
1:C:280:VAL:O	1:C:280:VAL:HG23	2.03	0.58
1:D:136:MET:HE3	1:D:166:THR:HA	1.83	0.58
1:D:58:ILE:HD12	1:D:101:ALA:HB3	1.86	0.57
1:C:303:LYS:HD2	2:D:629:HOH:O	2.03	0.57
2:A:493:HOH:O	1:B:303:LYS:HD3	2.04	0.57
1:D:78:LYS:HD3	1:D:78:LYS:C	2.24	0.57
1:D:182:ARG:NH2	2:D:481:HOH:O	2.37	0.56
1:D:61:ALA:HA	1:D:64:GLU:HG3	1.88	0.56
1:C:65:ARG:NH2	2:C:669:HOH:O	2.38	0.56
1:C:333:VAL:HG12	1:C:337:LYS:HE3	1.88	0.56
1:D:273:GLU:HG3	2:D:352:HOH:O	2.05	0.56
1:A:37:ASP:O	1:A:41:LYS:HG3	2.06	0.55
1:B:134:ARG:NH1	2:B:441:HOH:O	2.39	0.55
1:D:30:ARG:N	1:D:34:GLU:OE2	2.39	0.55
1:C:332:GLU:HG2	2:C:385:HOH:O	2.06	0.55
1:C:132:ARG:NH1	2:C:462:HOH:O	2.38	0.55
1:C:91:ALA:O	1:C:92:VAL:HB	2.06	0.55
1:D:109:GLU:HA	1:D:109:GLU:OE2	2.06	0.54
1:A:213:THR:HG22	1:A:216:MET:CG	2.37	0.54
1:C:255:LYS:NZ	2:C:458:HOH:O	2.40	0.54
1:C:217:VAL:HG11	1:C:250:VAL:HG22	1.90	0.53
1:C:128:GLU:HB3	2:C:462:HOH:O	2.07	0.53
1:D:22:GLU:HG3	1:D:23:LYS:N	2.23	0.53
1:C:47:ALA:HB3	1:C:48:PRO:HD3	1.90	0.53
1:A:213:THR:HG22	1:A:216:MET:HG3	1.89	0.53
1:A:70:VAL:HG21	1:A:110:SER:HA	1.90	0.53
1:A:84:LEU:O	1:A:87:THR:HG23	2.08	0.53
1:D:26:VAL:HB	2:D:574:HOH:O	2.08	0.53
1:A:62:ALA:HB2	1:A:77:LEU:HD21	1.90	0.52
1:A:23:LYS:HE3	2:A:549:HOH:O	2.09	0.52
1:B:180:GLU:HG2	2:B:428:HOH:O	2.09	0.52
1:A:88:ARG:HG3	1:A:91:ALA:HB2	1.90	0.52
1:A:235:ARG:HH11	1:A:235:ARG:HG3	1.72	0.52
1:D:110:SER:OG	1:D:113:GLU:HB2	2.09	0.52
1:B:220:VAL:HG13	1:B:226:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:299:PRO:HG2	1:D:203:MET:HE1	1.87	0.52
1:C:58:ILE:HD11	1:C:98:ILE:HG23	1.91	0.52
1:A:227:ASP:C	1:A:228:LYS:HG2	2.31	0.51
1:A:124:LYS:O	1:A:128:GLU:HG3	2.10	0.51
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.92	0.51
1:D:60:LEU:O	1:D:64:GLU:HG3	2.10	0.51
1:B:103:ASN:HB2	2:B:388:HOH:O	2.11	0.51
1:C:292:CYS:SG	1:D:292:CYS:CB	2.99	0.51
1:A:151:LEU:HD12	1:A:152:THR:H	1.75	0.50
1:D:14:LEU:HD13	1:D:44:VAL:CG1	2.41	0.50
1:B:58:ILE:CD1	1:B:98:ILE:O	2.59	0.50
1:C:100:ARG:HH11	1:C:100:ARG:HG2	1.77	0.50
1:A:70:VAL:HG23	2:A:563:HOH:O	2.11	0.50
1:D:16:ASP:HB2	1:D:27:ILE:HG13	1.93	0.49
1:B:22:GLU:HB3	2:B:634:HOH:O	2.13	0.49
1:A:235:ARG:CZ	2:A:624:HOH:O	2.60	0.49
1:B:271:ASP:OD2	1:B:274:ARG:HD2	2.12	0.49
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.95	0.49
1:A:119:LEU:O	1:A:123:GLU:HG3	2.13	0.49
1:B:40:LYS:HE2	2:B:521:HOH:O	2.11	0.49
1:C:299:PRO:CG	1:D:203:MET:HE1	2.42	0.49
1:B:40:LYS:CE	2:B:521:HOH:O	2.59	0.49
1:D:107:LYS:HB2	1:D:107:LYS:NZ	2.27	0.49
1:C:299:PRO:CG	1:D:203:MET:CE	2.86	0.49
1:A:128:GLU:CA	1:A:131:GLU:HG2	2.40	0.49
1:A:88:ARG:HG3	1:A:88:ARG:O	2.12	0.49
1:A:32:VAL:HG22	2:A:552:HOH:O	2.12	0.49
1:C:213:THR:CG2	1:C:215:SER:OG	2.61	0.48
1:A:213:THR:HG22	1:A:216:MET:SD	2.53	0.48
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.95	0.48
1:D:136:MET:HE3	1:D:166:THR:CA	2.44	0.48
1:D:284:ARG:HD2	2:D:385:HOH:O	2.13	0.48
1:A:107:LYS:HE3	2:A:601:HOH:O	2.13	0.48
1:C:295:ARG:HD2	1:D:293:GLY:HA2	1.95	0.48
1:A:23:LYS:HZ2	1:A:25:GLU:HG3	1.79	0.48
1:D:99:GLU:HG3	2:D:434:HOH:O	2.13	0.48
1:B:40:LYS:NZ	2:B:521:HOH:O	2.38	0.48
1:A:17:GLN:HA	1:A:20:LEU:HD22	1.96	0.48
1:A:22:GLU:HB3	2:A:484:HOH:O	2.12	0.48
1:D:58:ILE:CD1	1:D:98:ILE:O	2.62	0.48
1:C:45:ARG:NH2	1:C:155:ASN:OD1	2.46	0.48
1:C:292:CYS:CB	1:D:292:CYS:SG	3.00	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:183:VAL:O	1:D:209:VAL:HA	2.14	0.47
1:A:151:LEU:CD1	1:A:184:ILE:O	2.62	0.47
1:D:75:GLU:HG3	2:D:650:HOH:O	2.13	0.47
1:A:148:ASP:OD1	1:A:228:LYS:HE2	2.15	0.47
1:A:182:ARG:HH11	1:A:182:ARG:CG	2.28	0.47
1:A:128:GLU:O	1:A:131:GLU:HG2	2.15	0.47
1:A:272:TRP:HB3	2:A:556:HOH:O	2.14	0.47
1:A:63:ARG:O	1:A:64:GLU:C	2.51	0.47
1:A:151:LEU:HD12	1:A:184:ILE:O	2.15	0.46
1:B:280:VAL:O	1:B:280:VAL:HG23	2.14	0.46
1:B:295:ARG:HA	1:B:295:ARG:HD2	1.76	0.46
1:C:69:ASP:HB3	1:C:72:GLU:HB2	1.96	0.46
1:A:104:ALA:O	1:A:107:LYS:HB2	2.15	0.46
1:C:45:ARG:NH2	1:C:160:ALA:HB2	2.31	0.46
1:C:5:SER:HA	1:C:15:ILE:HD12	1.98	0.46
1:D:6:ILE:HB	1:D:14:LEU:HD23	1.98	0.46
1:B:58:ILE:HD11	1:B:98:ILE:O	2.16	0.46
1:D:62:ALA:HA	1:D:73:LEU:HD11	1.98	0.46
1:A:70:VAL:HG22	1:A:111:VAL:N	2.31	0.46
1:C:289:LEU:HD11	1:D:213:THR:CG2	2.46	0.46
1:B:2:SER:HB3	2:B:636:HOH:O	2.15	0.45
1:A:315:GLU:OE1	1:D:258:ASN:ND2	2.49	0.45
1:C:303:LYS:HD3	1:D:210:THR:OG1	2.17	0.45
1:D:67:PHE:CE2	1:D:73:LEU:HA	2.51	0.45
1:B:24:LEU:HG	1:B:200:TRP:CZ2	2.51	0.45
1:D:31:ASN:C	1:D:33:GLU:H	2.19	0.45
1:A:88:ARG:HG3	1:A:91:ALA:CB	2.45	0.45
1:A:149:VAL:HG13	1:A:227:ASP:H	1.81	0.45
1:A:46:GLY:HA3	1:A:160:ALA:O	2.16	0.45
1:C:222:GLN:HG3	1:D:248:TYR:CE1	2.51	0.45
1:A:149:VAL:HG13	1:A:226:VAL:HA	1.97	0.45
1:A:128:GLU:HA	1:A:131:GLU:CD	2.36	0.45
1:B:30:ARG:NH2	2:B:412:HOH:O	2.48	0.45
1:D:6:ILE:CB	1:D:14:LEU:HD23	2.47	0.45
1:D:31:ASN:C	1:D:33:GLU:N	2.70	0.45
1:B:78:LYS:HD3	1:B:78:LYS:O	2.16	0.45
1:C:289:LEU:HD11	1:D:213:THR:HG22	1.99	0.45
1:A:223:LYS:NZ	2:A:661:HOH:O	2.39	0.45
1:A:23:LYS:NZ	1:A:25:GLU:HG3	2.32	0.45
1:D:127:GLU:OE2	1:D:131:GLU:OE1	2.34	0.45
1:D:136:MET:CE	1:D:166:THR:CA	2.85	0.44
1:B:28:GLU:CD	1:B:30:ARG:HH21	2.21	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:263:VAL:HB	1:B:320:LEU:HD23	1.99	0.44
1:B:70:VAL:HG21	1:B:110:SER:HA	1.99	0.44
1:A:235:ARG:HG3	1:A:235:ARG:NH1	2.32	0.44
1:C:275:THR:HG21	2:C:670:HOH:O	2.16	0.44
1:B:145:GLU:OE1	1:C:330:PRO:HB2	2.17	0.44
1:A:149:VAL:O	1:A:149:VAL:HG13	2.18	0.44
1:B:67:PHE:CD1	1:B:73:LEU:HD13	2.53	0.44
1:B:58:ILE:HD13	1:B:102:LEU:HB2	2.00	0.44
1:C:139:TYR:CG	1:C:325:GLY:HA2	2.53	0.44
1:D:221:MET:SD	1:D:259:ILE:HD12	2.58	0.44
1:D:199:CYS:O	1:D:203:MET:HE2	2.18	0.44
1:A:54:GLY:O	1:A:98:ILE:HD13	2.17	0.44
1:D:29:CYS:O	1:D:30:ARG:HG3	2.18	0.44
1:C:227:ASP:C	1:C:228:LYS:HG2	2.38	0.44
1:A:4:ARG:HD3	1:A:162:VAL:CG1	2.48	0.43
1:A:257:HIS:HE1	1:B:248:TYR:OH	2.00	0.43
1:D:200:TRP:CE2	1:D:204:GLU:HG3	2.53	0.43
1:A:210:THR:HG23	1:B:303:LYS:HG2	2.00	0.43
1:C:292:CYS:SG	1:D:292:CYS:HB3	2.59	0.43
1:D:58:ILE:HD13	1:D:102:LEU:HB2	2.00	0.43
1:C:248:TYR:CE1	1:D:222:GLN:HG3	2.53	0.43
1:D:245:ILE:HG13	1:D:308:ALA:O	2.18	0.43
1:D:135:LYS:HB2	1:D:135:LYS:HE3	1.77	0.43
1:B:92:VAL:O	1:B:96:VAL:HG23	2.18	0.43
1:B:41:LYS:O	1:B:42:LEU:HB2	2.19	0.42
1:C:142:GLU:HG3	2:C:592:HOH:O	2.20	0.42
1:D:50:LEU:HD23	1:D:50:LEU:HA	1.88	0.42
1:C:305:TYR:HB3	1:D:212:ILE:HG22	2.01	0.42
1:A:70:VAL:O	1:A:73:LEU:HB3	2.20	0.42
1:A:245:ILE:HG13	1:A:308:ALA:O	2.20	0.42
1:D:235:ARG:HH21	1:D:279:VAL:HG22	1.85	0.42
1:D:76:HIS:O	1:D:79:LYS:N	2.53	0.42
1:A:223:LYS:HE2	2:A:661:HOH:O	2.19	0.42
1:C:220:VAL:HG13	1:C:226:VAL:HG23	2.01	0.42
1:A:22:GLU:HG2	1:A:23:LYS:CG	2.38	0.42
1:B:28:GLU:CD	1:B:30:ARG:HE	2.23	0.42
1:A:282:GLU:HG3	1:A:284:ARG:NH1	2.35	0.42
1:B:23:LYS:HD3	1:B:25:GLU:CG	2.42	0.41
1:A:257:HIS:CE1	1:B:248:TYR:OH	2.73	0.41
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.74	0.41
1:B:75:GLU:HG2	1:B:79:LYS:HE2	2.03	0.41
1:C:257:HIS:HE1	2:C:467:HOH:O	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:245:ILE:HG13	1:D:245:ILE:H	1.66	0.41
1:A:67:PHE:CE2	1:A:73:LEU:HA	2.55	0.41
1:A:223:LYS:CE	2:A:661:HOH:O	2.67	0.41
1:B:23:LYS:CD	1:B:25:GLU:OE2	2.66	0.41
1:D:101:ALA:HA	1:D:121:GLU:HG2	2.03	0.41
1:D:94:LEU:C	1:D:94:LEU:HD23	2.41	0.41
1:A:217:VAL:HG21	1:A:250:VAL:HG22	2.03	0.41
1:A:183:VAL:O	1:A:209:VAL:HA	2.20	0.41
1:C:113:GLU:HA	1:C:116:GLU:HG2	2.03	0.41
1:B:221:MET:SD	1:B:253:VAL:HG12	2.61	0.41
1:B:284:ARG:HD3	1:B:284:ARG:HA	1.89	0.41
1:D:3:LEU:HD13	2:D:488:HOH:O	2.21	0.41
1:A:22:GLU:HB2	1:B:296:GLN:OE1	2.21	0.41
1:D:88:ARG:NH2	2:D:620:HOH:O	2.45	0.41
1:D:32:VAL:HG12	1:D:32:VAL:O	2.21	0.40
1:C:295:ARG:HG3	1:C:295:ARG:NH1	2.36	0.40
1:A:134:ARG:HD2	1:A:134:ARG:HH11	1.76	0.40
1:A:245:ILE:HG21	1:A:307:PRO:HG2	2.03	0.40
1:B:41:LYS:HD2	1:B:43:ALA:HB2	2.04	0.40
1:A:292:CYS:CB	1:B:292:CYS:HG	2.26	0.40
1:A:32:VAL:HG23	2:A:479:HOH:O	2.22	0.40
1:B:221:MET:SD	1:B:259:ILE:HD12	2.61	0.40
1:B:174:ALA:O	1:B:177:GLN:HB2	2.22	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	338/351 (96%)	326 (96%)	11 (3%)	1 (0%)	50	37
1	B	338/351 (96%)	328 (97%)	10 (3%)	0	100	100
1	C	338/351 (96%)	327 (97%)	11 (3%)	0	100	100
1	D	338/351 (96%)	324 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1352/1404 (96%)	1305 (96%)	46 (3%)	1 (0%)	59 48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	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	281/290 (97%)	262 (93%)	19 (7%)	22 10
1	B	281/290 (97%)	266 (95%)	15 (5%)	32 18
1	C	281/290 (97%)	267 (95%)	14 (5%)	34 20
1	D	281/290 (97%)	267 (95%)	14 (5%)	34 20
All	All	1124/1160 (97%)	1062 (94%)	62 (6%)	30 16

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	9	ASP
1	A	19	LYS
1	A	20	LEU
1	A	32	VAL
1	A	44	VAL
1	A	64	GLU
1	A	99	GLU
1	A	144	LEU
1	A	151	LEU
1	A	180	GLU
1	A	182	ARG
1	A	191	LEU
1	A	211	LEU
1	A	228	LYS

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Mol	Chain	Res	Type
1	A	235	ARG
1	A	245	ILE
1	A	255	LYS
1	A	315	GLU
1	B	12	LEU
1	B	24	LEU
1	B	35	LEU
1	B	60	LEU
1	B	94	LEU
1	B	99	GLU
1	B	119	LEU
1	B	180	GLU
1	B	220	VAL
1	B	234	ASP
1	B	272	TRP
1	B	287	GLU
1	B	289	LEU
1	B	292	CYS
1	B	339	LEU
1	C	45	ARG
1	C	72	GLU
1	C	77	LEU
1	C	94	LEU
1	C	145	GLU
1	C	180	GLU
1	C	211	LEU
1	C	213	THR
1	C	220	VAL
1	C	234	ASP
1	C	272	TRP
1	C	295	ARG
1	C	323	GLU
1	C	339	LEU
1	D	2	SER
1	D	3	LEU
1	D	12	LEU
1	D	19	LYS
1	D	22	GLU
1	D	82	ASP
1	D	90	THR
1	D	107	LYS
1	D	112	GLU

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Mol	Chain	Res	Type
1	D	168	LEU
1	D	202	LEU
1	D	245	ILE
1	D	287	GLU
1	D	294	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	257	HIS
1	D	256	HIS
1	D	258	ASN
1	D	301	ASN

### 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 ⓘ

There are no ligands in this entry.

## 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	340/351 (96%)	0.22	19 (5%) 24 24	16, 28, 57, 81	0
1	B	340/351 (96%)	-0.11	6 (1%) 65 67	15, 24, 39, 55	0
1	C	340/351 (96%)	-0.04	6 (1%) 65 67	17, 25, 42, 57	0
1	D	340/351 (96%)	0.23	24 (7%) 16 15	17, 30, 61, 82	0
All	All	1360/1404 (96%)	0.08	55 (4%) 36 37	15, 26, 53, 82	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	ALA	11.2
1	A	65	ARG	8.5
1	D	68	ALA	6.4
1	A	67	PHE	5.3
1	D	67	PHE	5.1
1	A	32	VAL	4.5
1	D	70	VAL	4.4
1	D	66	GLU	4.3
1	A	66	GLU	4.1
1	A	109	GLU	4.1
1	A	294	LYS	4.1
1	C	68	ALA	4.1
1	A	70	VAL	3.9
1	A	108	GLY	3.8
1	A	30	ARG	3.7
1	D	294	LYS	3.5
1	C	294	LYS	3.4
1	A	75	GLU	3.4
1	A	90	THR	3.4
1	A	10	ASP	3.4
1	A	72	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	65	ARG	3.2
1	B	294	LYS	3.2
1	A	112	GLU	3.0
1	D	111	VAL	3.0
1	D	109	GLU	2.9
1	B	68	ALA	2.8
1	D	69	ASP	2.8
1	A	69	ASP	2.7
1	C	22	GLU	2.7
1	D	88	ARG	2.6
1	D	78	LYS	2.6
1	D	72	GLU	2.5
1	D	75	GLU	2.5
1	D	40	LYS	2.5
1	C	277	LYS	2.3
1	D	65	ARG	2.3
1	D	90	THR	2.3
1	A	37	ASP	2.3
1	C	91	ALA	2.3
1	D	32	VAL	2.2
1	D	107	LYS	2.2
1	D	71	ASP	2.2
1	D	10	ASP	2.2
1	B	22	GLU	2.2
1	D	89	PRO	2.2
1	B	293	GLY	2.1
1	A	88	ARG	2.1
1	A	89	PRO	2.1
1	B	66	GLU	2.1
1	D	28	GLU	2.1
1	D	295	ARG	2.1
1	C	273	GLU	2.0
1	D	110	SER	2.0
1	D	29	CYS	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

There are no ligands in this entry.

### 6.5 Other polymers

There are no such residues in this entry.