



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 09:51 PM EDT

PDB ID : 1T4D  
Title : Crystal structure of Escherichia coli aspartate beta-semialdehyde dehydrogenase (EcASADH), at 1.95 Angstrom resolution  
Authors : Nichols, C.E.; Dhaliwal, B.; Lockyer, M.; Hawkins, A.R.; Stammers, D.K.  
Deposited on : 2004-04-29  
Resolution : 1.95 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

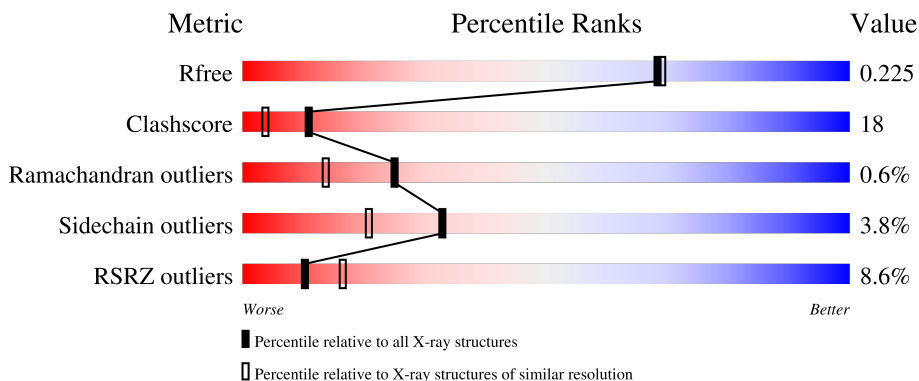
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	367	<div> <div>9%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
1	B	367	<div> <div>8%</div> <div>71%</div> <div>25%</div> <div>..</div> </div>
1	C	367	<div> <div>9%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aspartate-semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2810	1772	490	532	16			
1	B	367	Total	C	N	O	S	0	0	0
			2810	1772	490	532	16			
1	C	367	Total	C	N	O	S	0	0	0
			2810	1772	490	532	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLN	LYS	engineered mutation	UNP P0A9Q9
B	2	GLN	LYS	engineered mutation	UNP P0A9Q9
C	2	GLN	LYS	engineered mutation	UNP P0A9Q9

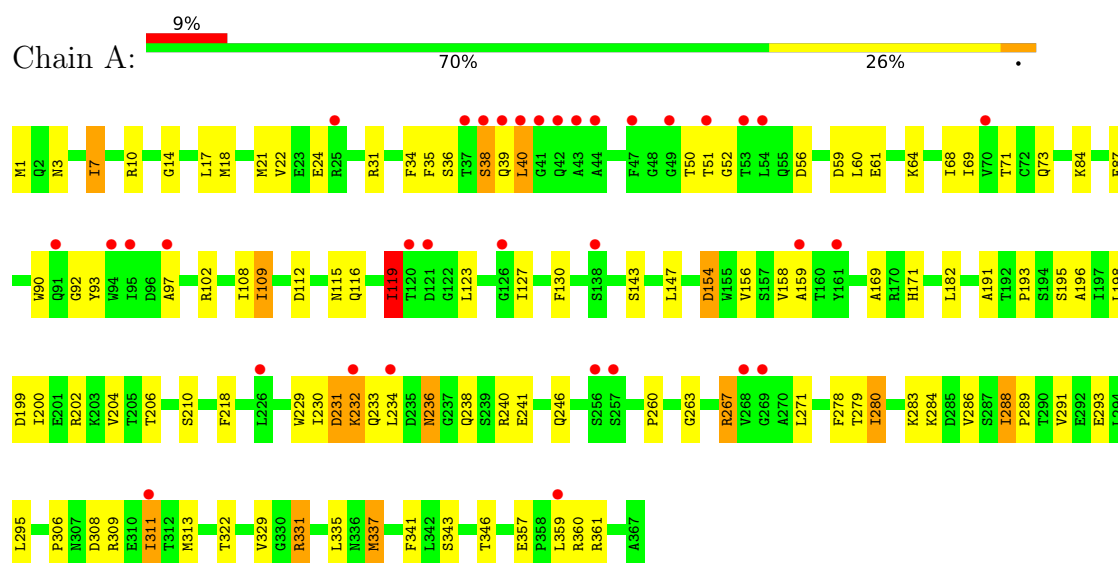
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	285	Total	O	0	0
			285	285		
2	B	293	Total	O	0	0
			293	293		
2	C	284	Total	O	0	0
			284	284		

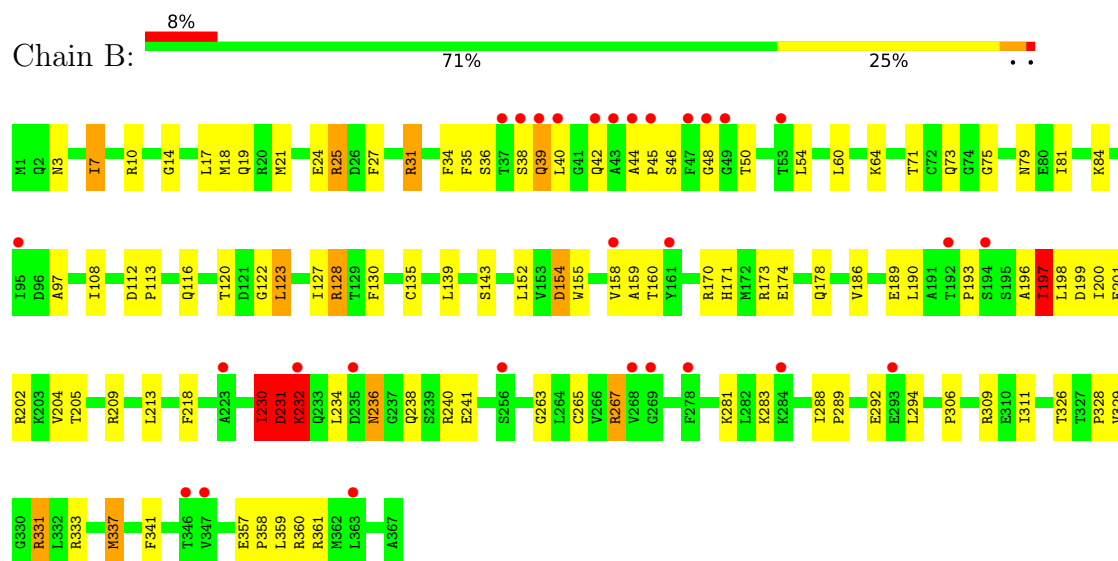
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

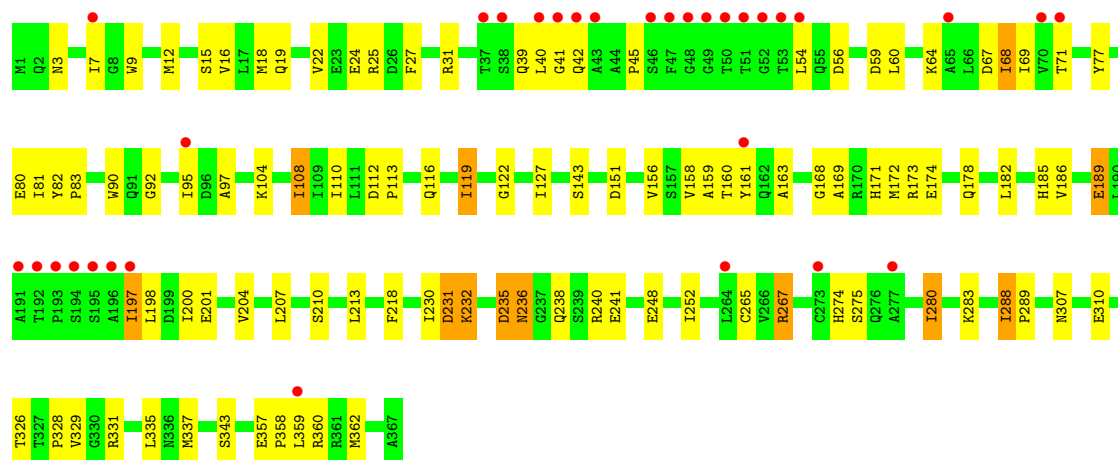
- Molecule 1: Aspartate-semialdehyde dehydrogenase



- Molecule 1: Aspartate-semialdehyde dehydrogenase



- Molecule 1: Aspartate-semialdehyde dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	172.42Å 117.21Å 57.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 1.95 29.72 – 1.95	Depositor EDS
% Data completeness (in resolution range)	90.5 (29.72-1.95) 90.6 (29.72-1.95)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.204 , 0.250 0.204 , 0.225	Depositor DCC
$R_{free}$ test set	7867 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.4	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9292	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.43	3/2863 (0.1%)	0.70	5/3887 (0.1%)
1	B	0.39	1/2863 (0.0%)	0.72	4/3887 (0.1%)
1	C	0.42	2/2863 (0.1%)	0.69	5/3887 (0.1%)
All	All	0.41	6/8589 (0.1%)	0.70	14/11661 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	ILE	CG1-CD1	-6.99	1.02	1.50
1	B	7	ILE	CG1-CD1	-6.45	1.05	1.50
1	A	109	ILE	CG1-CD1	-6.06	1.08	1.50
1	C	119	ILE	CG1-CD1	-5.66	1.11	1.50
1	A	280	ILE	CG1-CD1	-5.08	1.15	1.50
1	C	288	ILE	CG1-CD1	-5.02	1.15	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	ILE	CB-CG1-CD1	10.94	144.53	113.90
1	B	197	ILE	CB-CG1-CD1	9.29	139.91	113.90
1	A	7	ILE	CB-CG1-CD1	9.00	139.09	113.90
1	C	288	ILE	CB-CG1-CD1	8.57	137.89	113.90
1	A	288	ILE	CB-CG1-CD1	7.04	133.61	113.90
1	C	197	ILE	CB-CG1-CD1	6.91	133.25	113.90
1	C	68	ILE	CB-CG1-CD1	6.31	131.56	113.90
1	A	109	ILE	CB-CG1-CD1	6.05	130.83	113.90
1	C	108	ILE	CB-CG1-CD1	5.56	129.48	113.90
1	A	119	ILE	CB-CG1-CD1	5.21	128.48	113.90
1	B	230	ILE	CB-CG1-CD1	5.19	128.44	113.90
1	B	232	LYS	N-CA-C	5.09	124.73	111.00
1	A	279	THR	N-CA-C	-5.08	97.30	111.00
1	C	280	ILE	CB-CG1-CD1	5.04	128.01	113.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2810	0	2816	106	0
1	B	2810	0	2816	122	0
1	C	2810	0	2816	91	0
2	A	285	0	0	6	0
2	B	293	0	0	6	0
2	C	284	0	0	1	0
All	All	9292	0	8448	307	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (307) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ILE:CD1	1:C:230:ILE:CG1	1.75	1.58
1:B:7:ILE:HB	1:B:71:THR:HG22	1.23	1.20
1:B:186:VAL:HG11	1:B:200:ILE:HG23	1.28	1.12
1:B:232:LYS:HA	1:B:232:LYS:HE2	1.27	1.10
1:A:335:LEU:HD21	1:A:343:SER:HB3	1.42	1.01
1:A:232:LYS:HE2	1:A:232:LYS:HA	1.51	0.91
1:C:186:VAL:HG11	1:C:200:ILE:HB	1.51	0.90
1:C:7:ILE:HB	1:C:71:THR:HG22	1.55	0.86
1:C:143:SER:HB3	1:C:329:VAL:HG22	1.58	0.85
1:A:218:PHE:CE1	1:A:267:ARG:HD3	2.11	0.85
2:A:416:HOH:O	1:B:197:ILE:HD11	1.77	0.84
1:C:110:ILE:HG22	1:C:119:ILE:HD12	1.60	0.83
1:C:307:ASN:HD21	1:C:331:ARG:NH1	1.80	0.80
1:C:230:ILE:HD11	1:C:267:ARG:HB2	1.64	0.79
1:A:218:PHE:HE1	1:A:267:ARG:HD3	1.46	0.78
1:C:231:ASP:OD2	1:C:240:ARG:HB3	1.83	0.78
1:A:236:ASN:HD21	1:A:238:GLN:HB3	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ILE:H	1:B:197:ILE:CD1	1.97	0.77
1:A:147:LEU:HG	1:A:295:LEU:HD21	1.67	0.77
1:B:7:ILE:CB	1:B:71:THR:HG22	2.11	0.77
1:C:110:ILE:HG22	1:C:119:ILE:CD1	2.13	0.77
1:A:230:ILE:CG2	1:A:241:GLU:HG3	2.14	0.77
1:C:42:GLN:HB2	1:C:54:LEU:HD12	1.66	0.77
1:B:174:GLU:O	1:B:178:GLN:HG3	1.85	0.76
1:A:60:LEU:O	1:A:64:LYS:HG3	1.86	0.76
1:A:119:ILE:O	1:A:123:LEU:HB2	1.85	0.76
1:C:156:VAL:HG13	1:C:280:ILE:HD13	1.68	0.76
1:A:231:ASP:OD2	1:A:240:ARG:HB3	1.86	0.75
1:B:197:ILE:H	1:B:197:ILE:HD13	1.52	0.75
1:A:154:ASP:OD1	1:A:283:LYS:HG2	1.88	0.74
1:A:112:ASP:HB2	1:A:116:GLN:NE2	2.02	0.74
1:A:112:ASP:HB2	1:A:116:GLN:HE21	1.51	0.73
1:C:230:ILE:CD1	1:C:230:ILE:CB	2.67	0.73
1:A:147:LEU:HD21	1:A:291:VAL:HG13	1.71	0.73
1:A:39:GLN:HG3	1:C:210:SER:O	1.88	0.73
1:B:97:ALA:HB2	1:B:359:LEU:HD11	1.71	0.73
1:B:230:ILE:CG2	1:B:241:GLU:HG3	2.19	0.72
1:C:67:ASP:HB2	1:C:68:ILE:HD12	1.70	0.72
1:B:154:ASP:OD1	1:B:283:LYS:HG2	1.90	0.71
1:B:186:VAL:HG12	1:B:186:VAL:O	1.90	0.71
1:A:198:LEU:HD13	1:B:19:GLN:HE22	1.56	0.71
1:B:186:VAL:HG13	1:B:189:GLU:CG	2.20	0.71
1:B:3:ASN:ND2	1:B:31:ARG:HH11	1.89	0.71
1:A:234:LEU:HB2	1:A:238:GLN:O	1.91	0.71
1:C:97:ALA:HB2	1:C:359:LEU:HD11	1.73	0.70
1:B:288:ILE:HD11	1:B:333:ARG:HA	1.73	0.70
1:C:189:GLU:HG3	1:C:200:ILE:HG22	1.73	0.70
1:A:56:ASP:HB3	1:A:59:ASP:HB2	1.72	0.69
1:B:232:LYS:HE2	1:B:232:LYS:CA	2.16	0.69
1:C:186:VAL:HG12	1:C:186:VAL:O	1.91	0.69
1:B:186:VAL:HG13	1:B:189:GLU:HG2	1.73	0.69
1:C:56:ASP:HB3	1:C:59:ASP:HB2	1.76	0.68
1:A:143:SER:HB3	1:A:329:VAL:HG22	1.74	0.68
1:A:231:ASP:OD2	1:A:232:LYS:N	2.28	0.66
1:C:95:ILE:HG22	1:C:359:LEU:HD22	1.76	0.66
1:C:200:ILE:HD12	1:C:201:GLU:N	2.08	0.66
1:B:234:LEU:HD21	1:B:240:ARG:HA	1.77	0.66
1:A:202:ARG:O	1:A:206:THR:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ALA:O	1:C:173:ARG:HG3	1.96	0.66
1:A:156:VAL:HG22	1:A:280:ILE:HD12	1.78	0.65
1:A:61:GLU:HG2	2:A:548:HOH:O	1.95	0.65
1:A:7:ILE:HB	1:A:71:THR:HG22	1.79	0.65
1:A:158:VAL:HG22	1:A:278:PHE:CD1	2.32	0.65
1:A:284:LYS:O	1:A:286:VAL:HG23	1.97	0.65
1:A:306:PRO:HB2	1:A:311:ILE:CD1	2.26	0.65
1:A:115:ASN:O	1:A:119:ILE:HD13	1.97	0.65
1:A:232:LYS:HE2	1:A:232:LYS:CA	2.27	0.64
1:B:143:SER:HB3	1:B:329:VAL:HG22	1.78	0.64
1:C:60:LEU:O	1:C:64:LYS:HG3	1.97	0.64
1:A:236:ASN:ND2	1:A:238:GLN:H	1.97	0.63
1:B:24:GLU:C	1:B:25:ARG:HD3	2.19	0.63
1:A:50:THR:HG22	1:A:52:GLY:H	1.64	0.63
1:C:197:ILE:O	1:C:200:ILE:HG13	1.97	0.63
1:A:50:THR:HG22	1:A:52:GLY:N	2.12	0.63
1:C:174:GLU:O	1:C:178:GLN:HG3	1.98	0.63
1:C:171:HIS:HB3	1:C:218:PHE:CZ	2.34	0.63
1:A:156:VAL:HG13	1:A:280:ILE:CD1	2.30	0.62
1:B:232:LYS:HA	1:B:232:LYS:CE	2.14	0.62
1:A:335:LEU:CD2	1:A:343:SER:HB3	2.26	0.62
1:B:288:ILE:O	1:B:292:GLU:HG3	2.00	0.62
1:B:231:ASP:OD2	1:B:240:ARG:HB3	2.00	0.62
1:A:236:ASN:ND2	1:A:238:GLN:HB3	2.15	0.61
1:C:331:ARG:HA	1:C:331:ARG:HH11	1.65	0.61
1:A:308:ASP:HB2	1:A:311:ILE:HD11	1.83	0.61
1:A:169:ALA:HB1	1:B:197:ILE:HG13	1.82	0.61
1:C:218:PHE:CE1	1:C:267:ARG:HD3	2.35	0.61
1:B:357:GLU:O	1:B:361:ARG:HG2	2.00	0.61
1:A:230:ILE:HG21	1:A:241:GLU:HG3	1.82	0.60
1:A:7:ILE:HG22	1:A:73:GLN:HB2	1.83	0.60
1:B:123:LEU:HD13	1:B:130:PHE:CZ	2.35	0.60
1:A:156:VAL:HG13	1:A:280:ILE:HD13	1.81	0.60
1:C:186:VAL:CG1	1:C:200:ILE:HB	2.27	0.60
1:C:207:LEU:HG	1:C:213:LEU:HD11	1.83	0.60
1:B:17:LEU:HG	1:B:21:MET:CE	2.32	0.60
1:C:67:ASP:CB	1:C:68:ILE:HD12	2.31	0.60
1:B:331:ARG:CB	1:B:331:ARG:HH11	2.15	0.60
1:C:40:LEU:O	1:C:42:GLN:N	2.35	0.60
1:B:196:ALA:HB3	1:B:199:ASP:OD2	2.02	0.60
1:A:68:ILE:HG12	1:A:93:TYR:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:LEU:CD1	1:B:204:VAL:HG21	2.32	0.59
1:B:3:ASN:HD22	1:B:31:ARG:HH11	1.50	0.59
1:B:288:ILE:CD1	1:B:333:ARG:HA	2.33	0.59
1:B:39:GLN:O	1:B:54:LEU:HD12	2.03	0.59
1:A:1:MET:HB3	1:A:31:ARG:HG3	1.85	0.58
1:A:171:HIS:HB3	1:A:218:PHE:CZ	2.38	0.58
1:B:38:SER:O	1:B:40:LEU:N	2.36	0.58
1:B:331:ARG:HH11	1:B:331:ARG:HB3	1.68	0.58
1:B:331:ARG:HB3	1:B:331:ARG:NH1	2.18	0.58
1:B:44:ALA:HB1	1:B:45:PRO:HD2	1.84	0.58
1:B:128:ARG:HD3	2:B:423:HOH:O	2.03	0.58
1:B:112:ASP:OD1	1:B:113:PRO:HD3	2.05	0.57
1:A:69:ILE:HG22	1:A:71:THR:HG23	1.85	0.57
1:C:81:ILE:HD12	1:C:81:ILE:N	2.20	0.56
1:C:156:VAL:HG13	1:C:280:ILE:CD1	2.35	0.56
1:A:97:ALA:HB2	1:A:359:LEU:HD11	1.88	0.56
1:B:14:GLY:O	1:B:18:MET:HG2	2.06	0.56
1:B:218:PHE:CE1	1:B:267:ARG:HD3	2.40	0.55
1:A:331:ARG:HA	1:A:331:ARG:HH11	1.71	0.55
1:C:201:GLU:O	1:C:204:VAL:HG22	2.07	0.55
1:A:18:MET:O	1:A:22:VAL:HG23	2.06	0.55
1:B:116:GLN:OE1	1:B:120:THR:HG23	2.07	0.55
1:B:7:ILE:HD12	1:B:35:PHE:HB2	1.88	0.55
1:A:50:THR:HG22	1:A:51:THR:N	2.23	0.54
1:B:17:LEU:HG	1:B:21:MET:HE2	1.89	0.54
1:C:112:ASP:HB2	1:C:116:GLN:NE2	2.23	0.54
1:A:14:GLY:O	1:A:18:MET:HG2	2.08	0.54
1:B:306:PRO:HD2	1:B:311:ILE:HD13	1.90	0.54
1:B:326:THR:HG22	1:B:328:PRO:HD3	1.90	0.53
1:B:24:GLU:HG3	1:B:360:ARG:CZ	2.38	0.53
1:C:7:ILE:N	1:C:7:ILE:HD12	2.24	0.53
1:C:77:TYR:O	1:C:81:ILE:HD13	2.09	0.53
1:A:50:THR:HB	2:A:533:HOH:O	2.07	0.53
1:B:42:GLN:O	1:B:54:LEU:HG	2.08	0.53
1:B:288:ILE:HD11	2:B:472:HOH:O	2.09	0.53
1:A:331:ARG:HH11	1:A:331:ARG:CA	2.21	0.53
1:B:218:PHE:HE1	1:B:267:ARG:HD3	1.74	0.53
1:A:169:ALA:CB	1:B:197:ILE:HG13	2.38	0.53
1:C:15:SER:O	1:C:19:GLN:HG3	2.09	0.53
1:C:40:LEU:C	1:C:42:GLN:H	2.12	0.52
1:C:307:ASN:ND2	1:C:331:ARG:NH1	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ASN:ND2	1:C:238:GLN:H	2.08	0.52
1:B:112:ASP:CG	1:B:113:PRO:HD3	2.30	0.52
1:A:196:ALA:O	1:A:200:ILE:CD1	2.59	0.51
1:C:186:VAL:O	1:C:186:VAL:CG1	2.59	0.51
1:A:17:LEU:HG	1:A:21:MET:CE	2.41	0.51
1:C:7:ILE:CD1	1:C:69:ILE:HG23	2.40	0.51
1:B:186:VAL:HG13	1:B:189:GLU:HG3	1.92	0.51
1:A:210:SER:O	1:C:39:GLN:HG3	2.11	0.51
1:A:196:ALA:O	1:A:200:ILE:HD13	2.11	0.51
1:B:230:ILE:HG21	1:B:241:GLU:HG3	1.92	0.51
1:C:197:ILE:HG23	1:C:198:LEU:N	2.26	0.51
1:B:331:ARG:HH11	1:B:331:ARG:CA	2.25	0.50
1:B:7:ILE:HG22	1:B:73:GLN:HB2	1.94	0.50
1:B:152:LEU:HD11	1:B:294:LEU:CD1	2.41	0.50
1:A:158:VAL:HG22	1:A:278:PHE:HD1	1.75	0.50
1:B:186:VAL:CG1	1:B:189:GLU:HG2	2.42	0.50
1:A:331:ARG:HB3	1:A:331:ARG:NH1	2.26	0.50
1:B:18:MET:HE3	1:B:34:PHE:CE1	2.47	0.50
1:B:186:VAL:HG11	1:B:200:ILE:CG2	2.20	0.50
1:B:186:VAL:HG12	1:B:190:LEU:HG	1.93	0.50
1:B:48:GLY:C	1:B:50:THR:N	2.64	0.50
1:C:9:TRP:CZ3	1:C:45:PRO:HG3	2.47	0.49
1:C:335:LEU:HD21	1:C:343:SER:HB3	1.94	0.49
1:A:289:PRO:O	1:A:293:GLU:HG3	2.12	0.49
1:B:186:VAL:O	1:B:186:VAL:CG1	2.60	0.49
1:B:27:PHE:HB3	1:B:48:GLY:HA2	1.93	0.49
1:B:45:PRO:O	1:B:46:SER:OG	2.25	0.49
1:C:122:GLY:HA2	1:C:127:ILE:HD13	1.95	0.49
1:B:158:VAL:O	1:B:263:GLY:HA3	2.12	0.49
1:C:310:GLU:CD	1:C:310:GLU:H	2.15	0.49
1:A:17:LEU:HG	1:A:21:MET:HE2	1.94	0.49
1:C:80:GLU:HG2	1:C:81:ILE:HD12	1.95	0.49
1:A:198:LEU:HD13	1:B:19:GLN:NE2	2.26	0.49
1:A:60:LEU:HD11	1:A:84:LYS:HD3	1.95	0.49
1:A:38:SER:OG	1:A:39:GLN:N	2.46	0.48
1:B:357:GLU:HB3	1:B:358:PRO:HD3	1.95	0.48
1:A:230:ILE:HG22	1:A:241:GLU:HG3	1.94	0.48
1:C:95:ILE:HD12	1:C:362:MET:HG2	1.96	0.48
1:B:198:LEU:O	1:B:202:ARG:HB2	2.14	0.48
1:C:108:ILE:HG21	1:C:119:ILE:HD13	1.95	0.48
1:A:331:ARG:HH11	1:A:331:ARG:CB	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ASN:HD22	1:C:31:ARG:HD2	1.77	0.48
1:A:229:TRP:CZ2	1:A:233:GLN:HG3	2.49	0.48
1:A:40:LEU:HD21	2:A:642:HOH:O	2.13	0.47
1:A:232:LYS:HA	1:A:232:LYS:CE	2.35	0.47
1:B:197:ILE:HD13	1:B:197:ILE:N	2.26	0.47
1:C:7:ILE:HD13	1:C:69:ILE:CG2	2.44	0.47
1:C:110:ILE:HG22	1:C:119:ILE:HD11	1.93	0.47
1:C:18:MET:O	1:C:22:VAL:HG23	2.14	0.47
1:A:102:ARG:O	1:A:109:ILE:HD11	2.15	0.47
1:B:18:MET:HE3	1:B:34:PHE:HE1	1.80	0.47
1:B:331:ARG:HH11	1:B:331:ARG:HA	1.80	0.47
1:A:7:ILE:HD13	1:A:35:PHE:HB2	1.96	0.47
1:A:7:ILE:HB	1:A:71:THR:CG2	2.44	0.46
1:C:25:ARG:HG2	1:C:25:ARG:HH11	1.79	0.46
1:B:197:ILE:CD1	1:B:197:ILE:N	2.74	0.46
1:C:82:TYR:HB3	1:C:83:PRO:CD	2.46	0.46
1:C:81:ILE:N	1:C:81:ILE:CD1	2.79	0.46
1:A:123:LEU:HD13	1:A:130:PHE:CZ	2.51	0.46
1:A:329:VAL:HG13	1:A:346:THR:HG22	1.97	0.46
1:C:189:GLU:CG	1:C:200:ILE:HG22	2.42	0.46
1:C:3:ASN:ND2	1:C:31:ARG:HD2	2.32	0.45
1:B:60:LEU:HD11	1:B:84:LYS:HD3	1.98	0.45
1:B:236:ASN:HD22	1:B:236:ASN:N	2.13	0.45
1:B:3:ASN:ND2	1:B:31:ARG:NH1	2.62	0.45
1:B:10:ARG:NH2	1:B:54:LEU:HD13	2.31	0.45
1:B:24:GLU:HG3	1:B:360:ARG:NE	2.31	0.45
1:B:10:ARG:HH22	1:B:36:SER:CB	2.30	0.45
1:B:60:LEU:O	1:B:64:LYS:HG3	2.16	0.45
1:A:73:GLN:OE1	1:A:73:GLN:HA	2.16	0.45
1:C:27:PHE:HB2	2:C:468:HOH:O	2.17	0.45
1:B:18:MET:CE	1:B:34:PHE:HE1	2.30	0.45
1:A:271:LEU:HD11	1:B:204:VAL:HG21	1.97	0.45
1:B:267:ARG:NH2	2:B:370:HOH:O	2.34	0.45
1:A:196:ALA:HB3	1:A:199:ASP:OD2	2.18	0.44
1:C:31:ARG:O	1:C:31:ARG:HD3	2.18	0.44
1:C:326:THR:HG22	1:C:328:PRO:HD3	2.00	0.44
1:C:163:ALA:H	1:C:274:HIS:HD1	1.66	0.44
1:C:95:ILE:CG2	1:C:359:LEU:HD22	2.47	0.44
1:A:306:PRO:HB2	1:A:311:ILE:HD12	1.97	0.44
1:A:236:ASN:ND2	1:A:238:GLN:CB	2.81	0.44
1:B:7:ILE:HD12	1:B:35:PHE:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ASP:CG	1:C:113:PRO:HD3	2.38	0.44
1:C:158:VAL:HG12	1:C:159:ALA:N	2.33	0.44
1:A:18:MET:HE1	1:A:34:PHE:HE1	1.82	0.44
1:A:234:LEU:HD12	2:A:407:HOH:O	2.17	0.44
2:A:411:HOH:O	1:B:197:ILE:HD12	2.17	0.44
1:A:182:LEU:HD22	1:A:204:VAL:HG13	1.99	0.43
1:A:24:GLU:HG3	1:A:360:ARG:NH2	2.33	0.43
1:A:231:ASP:CG	1:A:232:LYS:N	2.71	0.43
1:B:81:ILE:N	1:B:81:ILE:HD12	2.33	0.43
1:C:160:THR:OG1	1:C:265:CYS:HA	2.19	0.43
1:A:271:LEU:HD12	1:B:204:VAL:HG21	1.98	0.43
1:B:201:GLU:HA	1:B:204:VAL:HG22	2.00	0.43
1:B:236:ASN:ND2	1:B:238:GLN:H	2.15	0.43
1:C:151:ASP:O	1:C:283:LYS:HD2	2.18	0.43
1:C:201:GLU:O	1:C:204:VAL:CG2	2.66	0.43
1:B:171:HIS:HB3	1:B:218:PHE:CZ	2.53	0.43
1:C:182:LEU:HD21	1:C:213:LEU:HD21	1.99	0.43
1:C:357:GLU:HB3	1:C:358:PRO:HD3	1.99	0.43
1:A:108:ILE:HG12	1:A:127:ILE:HG21	2.00	0.43
1:B:160:THR:OG1	1:B:265:CYS:HA	2.18	0.43
1:A:229:TRP:HZ2	1:A:233:GLN:HG3	1.84	0.43
1:B:123:LEU:HD13	1:B:130:PHE:HZ	1.79	0.43
1:C:232:LYS:HA	1:C:232:LYS:HD3	1.85	0.43
1:A:195:SER:OG	1:B:173:ARG:NH2	2.52	0.43
1:A:236:ASN:HD22	1:A:238:GLN:H	1.62	0.43
1:B:40:LEU:C	1:B:42:GLN:H	2.21	0.43
1:B:48:GLY:C	1:B:50:THR:H	2.21	0.43
1:A:200:ILE:HD12	1:A:200:ILE:H	1.83	0.43
1:C:24:GLU:HG3	1:C:360:ARG:HE	1.82	0.43
1:C:189:GLU:CD	1:C:189:GLU:H	2.13	0.43
1:A:3:ASN:ND2	1:A:31:ARG:HD2	2.34	0.43
1:B:230:ILE:CB	1:B:241:GLU:HG3	2.49	0.42
1:C:235:ASP:OD2	1:C:235:ASP:N	2.52	0.42
1:C:288:ILE:N	1:C:289:PRO:CD	2.82	0.42
1:A:246:GLN:OE1	1:A:260:PRO:HA	2.18	0.42
1:A:309:ARG:O	1:A:313:MET:HG3	2.19	0.42
1:B:108:ILE:HD13	2:B:648:HOH:O	2.19	0.42
1:B:158:VAL:HG12	1:B:159:ALA:N	2.34	0.42
1:C:197:ILE:CG2	1:C:198:LEU:N	2.81	0.42
1:A:200:ILE:HD12	1:A:200:ILE:N	2.34	0.42
1:B:288:ILE:HB	1:B:289:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TRP:CZ2	1:A:92:GLY:HA3	2.55	0.42
1:A:191:ALA:O	1:A:193:PRO:HD3	2.20	0.42
1:B:155:TRP:CE2	1:B:281:LYS:HB2	2.55	0.42
1:C:12:MET:O	1:C:16:VAL:HG23	2.20	0.42
1:B:189:GLU:CD	1:B:189:GLU:H	2.23	0.42
1:C:236:ASN:HD21	1:C:238:GLN:HB2	1.85	0.42
1:A:87:GLU:OE1	1:A:87:GLU:HA	2.19	0.42
1:C:236:ASN:C	1:C:236:ASN:HD22	2.23	0.42
1:A:331:ARG:HA	1:A:331:ARG:HD2	1.89	0.42
1:B:357:GLU:O	1:B:361:ARG:CG	2.68	0.42
1:C:60:LEU:HB3	1:C:64:LYS:HE3	2.01	0.42
1:A:158:VAL:O	1:A:263:GLY:HA3	2.20	0.41
1:A:331:ARG:HH11	1:A:331:ARG:HB3	1.85	0.41
1:B:18:MET:CE	1:B:34:PHE:CE1	3.02	0.41
1:B:17:LEU:HG	1:B:21:MET:HE1	2.02	0.41
1:B:309:ARG:NE	2:B:630:HOH:O	2.53	0.41
1:C:161:TYR:HB2	1:C:275:SER:HB2	2.02	0.41
1:B:204:VAL:HG23	1:B:205:THR:N	2.35	0.41
1:A:322:THR:O	1:B:209:ARG:NH2	2.40	0.41
1:B:75:GLY:O	1:B:79:ASN:ND2	2.54	0.41
1:B:230:ILE:HD13	1:B:265:CYS:O	2.20	0.41
1:C:104:LYS:HD3	1:C:104:LYS:HA	1.89	0.41
1:A:7:ILE:CB	1:A:71:THR:HG22	2.49	0.41
1:C:200:ILE:CD1	1:C:201:GLU:N	2.82	0.41
1:B:10:ARG:HH22	1:B:36:SER:HB2	1.84	0.41
1:A:158:VAL:HG12	1:A:159:ALA:N	2.36	0.41
1:B:24:GLU:O	1:B:25:ARG:HG2	2.21	0.41
1:C:168:GLY:O	1:C:172:MET:HG3	2.21	0.41
1:B:10:ARG:HH21	1:B:54:LEU:HD13	1.86	0.41
1:B:48:GLY:O	1:B:50:THR:N	2.53	0.41
1:B:122:GLY:HA3	1:B:127:ILE:HD12	2.03	0.41
1:B:230:ILE:HB	1:B:241:GLU:HG3	2.02	0.41
1:B:331:ARG:HA	1:B:331:ARG:HD2	1.91	0.41
1:C:122:GLY:O	1:C:127:ILE:HD13	2.21	0.41
1:A:337:MET:HG3	1:A:341:PHE:CD2	2.55	0.40
1:B:337:MET:HB2	1:B:341:PHE:CD1	2.55	0.40
1:B:193:PRO:HD2	2:B:526:HOH:O	2.22	0.40
1:C:248:GLU:O	1:C:252:ILE:HG13	2.21	0.40
1:C:230:ILE:CD1	1:C:267:ARG:HD2	2.52	0.40
1:A:195:SER:O	1:B:173:ARG:NH2	2.55	0.40
1:A:357:GLU:O	1:A:361:ARG:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LEU:HD12	1:B:123:LEU:HA	1.96	0.40
1:B:135:CYS:O	1:B:139:LEU:HG	2.22	0.40
1:C:90:TRP:CZ2	1:C:92:GLY:HA3	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	365/367 (100%)	342 (94%)	21 (6%)	2 (0%)	29	17
1	B	365/367 (100%)	346 (95%)	17 (5%)	2 (0%)	29	17
1	C	365/367 (100%)	347 (95%)	15 (4%)	3 (1%)	19	9
All	All	1095/1101 (100%)	1035 (94%)	53 (5%)	7 (1%)	25	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39	GLN
1	A	232	LYS
1	B	231	ASP
1	C	41	GLY
1	C	185	HIS
1	C	232	LYS
1	A	38	SER

### 5.3.2 Protein sidechains [i](#)

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	302/302 (100%)	290 (96%)	12 (4%)	31	19
1	B	302/302 (100%)	287 (95%)	15 (5%)	24	11
1	C	302/302 (100%)	295 (98%)	7 (2%)	50	42
All	All	906/906 (100%)	872 (96%)	34 (4%)	33	21

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	36	SER
1	A	40	LEU
1	A	119	ILE
1	A	154	ASP
1	A	231	ASP
1	A	236	ASN
1	A	267	ARG
1	A	288	ILE
1	A	311	ILE
1	A	331	ARG
1	A	337	MET
1	B	25	ARG
1	B	31	ARG
1	B	123	LEU
1	B	128	ARG
1	B	154	ASP
1	B	170	ARG
1	B	197	ILE
1	B	213	LEU
1	B	230	ILE
1	B	231	ASP
1	B	232	LYS
1	B	236	ASN
1	B	267	ARG
1	B	331	ARG
1	B	337	MET
1	C	189	GLU
1	C	231	ASP
1	C	235	ASP
1	C	236	ASN

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Mol	Chain	Res	Type
1	C	241	GLU
1	C	267	ARG
1	C	337	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	39	GLN
1	A	42	GLN
1	A	116	GLN
1	A	125	ASN
1	A	162	GLN
1	A	181	HIS
1	A	236	ASN
1	A	307	ASN
1	A	365	GLN
1	B	3	ASN
1	B	19	GLN
1	B	79	ASN
1	B	125	ASN
1	B	162	GLN
1	B	181	HIS
1	B	236	ASN
1	B	307	ASN
1	C	3	ASN
1	C	116	GLN
1	C	134	ASN
1	C	162	GLN
1	C	236	ASN
1	C	307	ASN
1	C	365	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	367/367 (100%)	0.57	34 (9%) 8 14	22, 35, 60, 87	0
1	B	367/367 (100%)	0.44	29 (7%) 12 19	21, 32, 58, 91	0
1	C	367/367 (100%)	0.53	32 (8%) 10 16	22, 34, 66, 98	0
All	All	1101/1101 (100%)	0.51	95 (8%) 10 16	21, 34, 62, 98	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	GLY	10.7
1	C	49	GLY	9.3
1	C	50	THR	6.7
1	B	38	SER	6.3
1	C	51	THR	6.0
1	B	40	LEU	5.2
1	B	39	GLN	5.0
1	A	234	LEU	4.9
1	A	40	LEU	4.9
1	B	47	PHE	4.5
1	A	51	THR	4.3
1	A	47	PHE	4.3
1	C	38	SER	4.2
1	C	52	GLY	4.1
1	A	43	ALA	3.9
1	C	191	ALA	3.8
1	A	359	LEU	3.6
1	C	43	ALA	3.5
1	A	42	GLN	3.3
1	A	232	LYS	3.3
1	A	41	GLY	3.3
1	B	268	VAL	3.3
1	A	257	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	95	ILE	3.3
1	C	192	THR	3.3
1	C	40	LEU	3.3
1	C	197	ILE	3.2
1	B	37	THR	3.2
1	B	347	VAL	3.2
1	C	161	TYR	3.1
1	A	126	GLY	3.1
1	C	37	THR	3.1
1	A	54	LEU	3.0
1	C	47	PHE	3.0
1	B	256	SER	3.0
1	A	161	TYR	2.9
1	B	42	GLN	2.9
1	A	95	ILE	2.9
1	A	268	VAL	2.9
1	C	277	ALA	2.8
1	C	70	VAL	2.8
1	A	25	ARG	2.8
1	B	49	GLY	2.8
1	C	41	GLY	2.7
1	B	235	ASP	2.7
1	A	120	THR	2.7
1	B	278	PHE	2.6
1	A	269	GLY	2.6
1	C	193	PRO	2.6
1	A	311	ILE	2.6
1	A	49	GLY	2.6
1	A	38	SER	2.6
1	A	91	GLN	2.6
1	B	346	THR	2.6
1	B	43	ALA	2.5
1	B	45	PRO	2.5
1	C	71	THR	2.5
1	B	194	SER	2.5
1	A	44	ALA	2.5
1	A	70	VAL	2.5
1	B	48	GLY	2.5
1	A	53	THR	2.5
1	B	161	TYR	2.4
1	B	232	LYS	2.4
1	C	359	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	159	ALA	2.4
1	C	194	SER	2.4
1	C	195	SER	2.4
1	C	7	ILE	2.4
1	B	269	GLY	2.4
1	C	42	GLN	2.4
1	C	65	ALA	2.3
1	C	46	SER	2.3
1	B	293	GLU	2.3
1	B	53	THR	2.3
1	A	37	THR	2.2
1	C	95	ILE	2.2
1	C	273	CYS	2.2
1	A	226	LEU	2.2
1	A	121	ASP	2.2
1	B	158	VAL	2.2
1	A	138	SER	2.1
1	C	196	ALA	2.1
1	B	363	LEU	2.1
1	A	94	TRP	2.1
1	A	97	ALA	2.1
1	A	256	SER	2.1
1	B	223	ALA	2.1
1	C	264	LEU	2.1
1	B	192	THR	2.1
1	A	39	GLN	2.1
1	B	44	ALA	2.0
1	C	54	LEU	2.0
1	C	53	THR	2.0
1	B	284	LYS	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.