



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:05 am BST

PDB ID : 4IG2  
Title : 1.80 Angstroms X-ray crystal structure of R51A and R239A heterodimer 2-amino-3-carboxymuconate-6-semialdehyde decarboxylase from *Pseudomonas fluorescens*  
Authors : Huo, L.; Davis, I.; Chen, L.; Liu, A.  
Deposited on : 2012-12-15  
Resolution : 1.80 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	:	2.11
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)	:	2.11

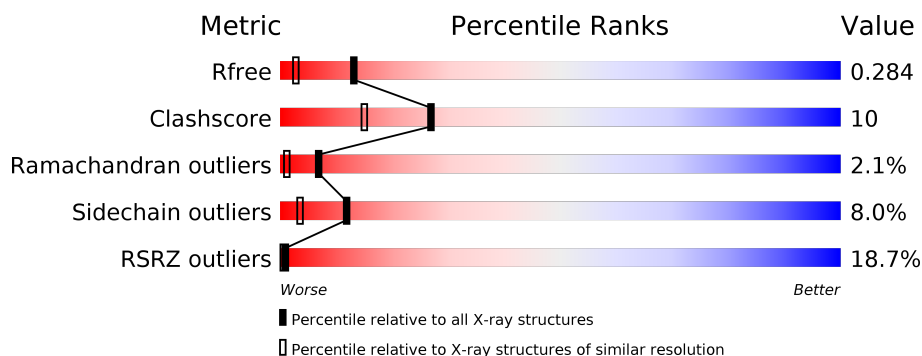
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	331	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
2	B	331	<div> <div>34%</div> <div> <div>59%</div> <div>33%</div> <div>7%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5316 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 2-amino-3-carboxymuconate 6-semialdehyde decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	1	0
			2582	1648	447	469	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	ALA	ARG	engineered mutation	UNP Q83V25

- Molecule 2 is a protein called 2-amino-3-carboxymuconate 6-semialdehyde decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	331	Total	C	N	O	S	0	2	0
			2591	1652	451	470	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	51	ALA	ARG	engineered mutation	UNP Q83V25

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		

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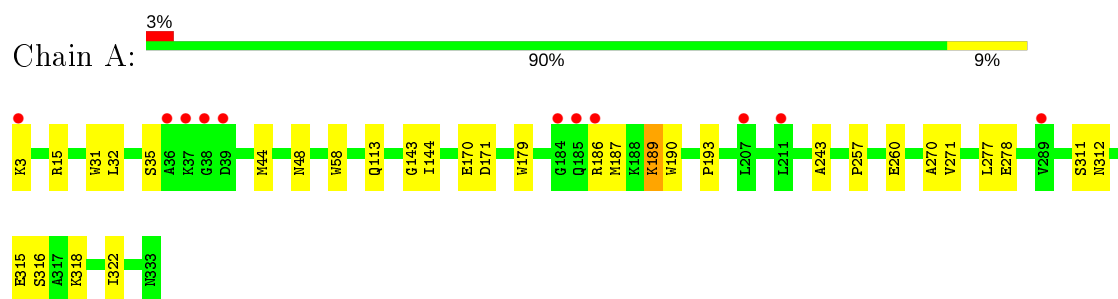
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	24	Total	O	0	0
			24	24		

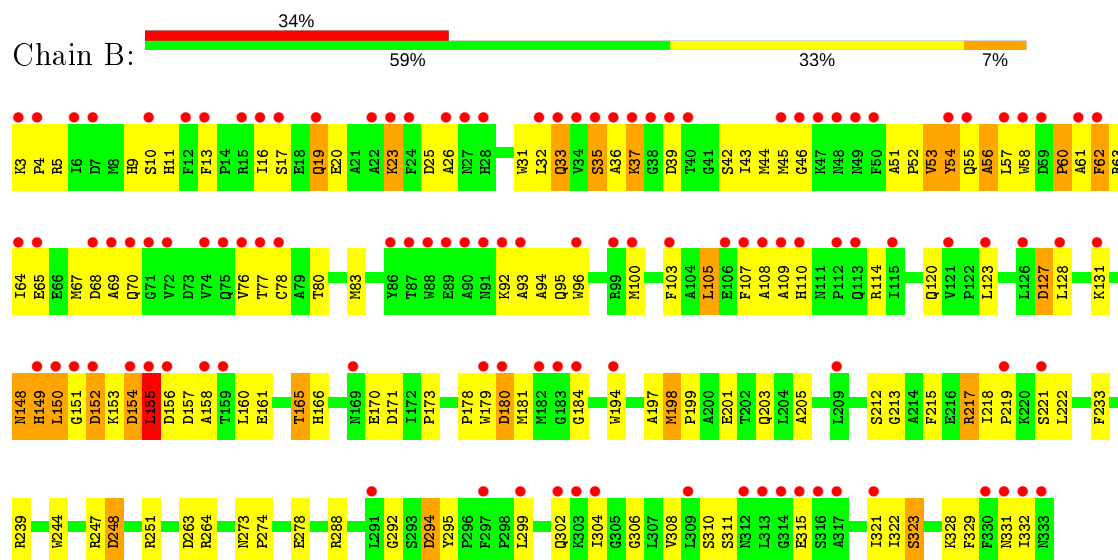
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: 2-amino-3-carboxymuconate 6-semialdehyde decarboxylase



- Molecule 2: 2-amino-3-carboxymuconate 6-semialdehyde decarboxylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.10Å 48.52Å 109.83Å 90.00° 126.80° 90.00°	Depositor
Resolution (Å)	20.78 – 1.80 20.78 – 1.80	Depositor EDS
% Data completeness (in resolution range)	86.0 (20.78-1.80) 81.1 (20.78-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, $R_{free}$	0.232 , 0.282 0.234 , 0.284	Depositor DCC
$R_{free}$ test set	2591 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.9	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.4	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	5316	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.49	0/2656	0.60	0/3599
2	B	0.41	1/2667 (0.0%)	0.60	1/3614 (0.0%)
All	All	0.45	1/5323 (0.0%)	0.60	1/7213 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	332	ILE	C-N	5.45	1.46	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	155	LEU	CA-CB-CG	5.30	127.48	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2582	0	2521	18	0
2	B	2591	0	2535	90	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	117	0	0	3	0
4	B	24	0	0	6	0
All	All	5316	0	5056	104	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 10.

All (104) 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)
2:B:158:ALA:HA	2:B:161:GLU:HB2	1.51	0.89
1:A:170:GLU:OE1	4:A:599:HOH:O	1.93	0.84
1:A:113:GLN:O	4:A:570:HOH:O	1.97	0.82
2:B:78:CYS:SG	4:B:515:HOH:O	2.38	0.81
2:B:123:LEU:HB3	2:B:150:LEU:HD11	1.62	0.81
2:B:215:PHE:O	2:B:264:ARG:NH1	2.17	0.78
2:B:105:LEU:O	2:B:109:ALA:N	2.21	0.73
2:B:10:SER:O	4:B:515:HOH:O	2.05	0.73
2:B:53:VAL:HG21	2:B:57:LEU:HD22	1.68	0.73
1:A:189:LYS:HE3	1:A:190:TRP:H	1.53	0.72
2:B:70:GLN:NE2	2:B:302:GLN:O	2.23	0.72
2:B:150:LEU:HB2	2:B:153:LYS:HD2	1.72	0.71
2:B:248:ASP:N	2:B:248:ASP:OD1	2.21	0.71
2:B:127:ASP:N	2:B:127:ASP:OD1	2.22	0.70
2:B:60:PRO:O	2:B:63:ARG:N	2.21	0.70
2:B:161:GLU:O	2:B:165:THR:OG1	2.10	0.69
2:B:110:HIS:NE2	4:B:522:HOH:O	2.29	0.66
2:B:263:ASP:O	2:B:288:ARG:NH2	2.31	0.64
2:B:94:ALA:HB2	2:B:128:LEU:HD13	1.81	0.63
2:B:198:MET:HG3	2:B:199:PRO:HD3	1.80	0.62
1:A:270:ALA:O	2:B:239[A]:ARG:NH2	2.33	0.61
2:B:53:VAL:HG22	2:B:54:TYR:H	1.66	0.61
2:B:67:MET:HE2	2:B:114:ARG:HH21	1.66	0.60
2:B:11:HIS:O	2:B:63:ARG:NH2	2.33	0.60
2:B:148:ASN:HD21	2:B:178:PRO:HA	1.66	0.60
2:B:212:SER:O	4:B:506:HOH:O	2.16	0.59
2:B:149:HIS:NE2	2:B:180:ASP:O	2.36	0.58
2:B:244:TRP:CE2	2:B:251:ARG:HG2	2.38	0.58
2:B:306:GLY:O	2:B:310:SER:OG	2.21	0.57
2:B:37:LYS:NZ	2:B:39:ASP:OD2	2.36	0.57
2:B:292:GLY:O	4:B:510:HOH:O	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:GLY:O	2:B:217:ARG:HD2	2.05	0.56
1:A:278:GLU:OE2	1:A:312:ASN:ND2	2.30	0.56
2:B:17:SER:OG	2:B:19:GLN:HG3	2.05	0.56
1:A:15:ARG:HD3	1:A:58:TRP:CD1	2.41	0.56
1:A:315:GLU:OE2	4:A:560:HOH:O	2.18	0.55
2:B:68:ASP:OD1	2:B:114:ARG:NH2	2.26	0.55
1:A:277:LEU:HD23	1:A:311:SER:OG	2.07	0.54
2:B:153:LYS:NZ	2:B:160:LEU:HD23	2.23	0.54
2:B:110:HIS:CE1	4:B:522:HOH:O	2.61	0.53
2:B:149:HIS:HE1	2:B:201:GLU:CD	2.12	0.53
1:A:271:VAL:HG12	2:B:239[B]:ARG:HH21	1.76	0.51
2:B:93:ALA:HA	2:B:96:TRP:HB3	1.93	0.51
2:B:35:SER:OG	2:B:36:ALA:N	2.41	0.50
1:A:257:PRO:HG2	1:A:260:GLU:HG3	1.92	0.50
2:B:154:ASP:N	2:B:154:ASP:OD2	2.44	0.50
2:B:60:PRO:O	2:B:62:PHE:N	2.45	0.49
2:B:153:LYS:HG2	2:B:154:ASP:N	2.27	0.49
1:A:15:ARG:HD2	1:A:32:LEU:HD23	1.94	0.49
2:B:96:TRP:O	2:B:100:MET:HG2	2.12	0.49
2:B:151:GLY:HA2	2:B:179:TRP:CH2	2.48	0.48
2:B:5:ARG:HA	2:B:322:ILE:HG22	1.95	0.48
1:A:243:ALA:HA	2:B:299:LEU:HD22	1.95	0.48
2:B:63:ARG:HD3	2:B:295:TYR:HE2	1.79	0.48
2:B:10:SER:OG	2:B:76:VAL:O	2.30	0.48
1:A:143:GLY:O	1:A:144:ILE:HD13	2.14	0.48
1:A:271:VAL:HG12	2:B:239[B]:ARG:NH2	2.30	0.47
2:B:65:GLU:O	2:B:69:ALA:N	2.44	0.47
2:B:155:LEU:H	2:B:155:LEU:HD12	1.79	0.47
2:B:181:MET:HB3	2:B:197:ALA:HB1	1.97	0.47
2:B:123:LEU:CB	2:B:150:LEU:HD11	2.40	0.46
2:B:150:LEU:HA	2:B:150:LEU:HD13	1.55	0.46
1:A:187:MET:O	1:A:193:PRO:HD3	2.16	0.46
2:B:150:LEU:HD23	2:B:153:LYS:NZ	2.31	0.46
2:B:218:ILE:HG21	2:B:222:LEU:HD22	1.98	0.46
2:B:274:PRO:O	2:B:278:GLU:HG3	2.15	0.46
2:B:3:LYS:HB3	2:B:4:PRO:HD2	1.99	0.45
2:B:13:PHE:CE2	2:B:32:LEU:HB2	2.51	0.45
2:B:203:GLN:HG3	2:B:233:PHE:HA	1.99	0.45
2:B:218:ILE:HA	2:B:218:ILE:HD13	1.78	0.45
2:B:37:LYS:HZ3	2:B:39:ASP:H	1.65	0.45
2:B:273:ASN:HA	2:B:274:PRO:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:LYS:HD3	2:B:155:LEU:HA	1.98	0.44
2:B:153:LYS:HZ3	2:B:160:LEU:HD23	1.81	0.44
2:B:9:HIS:NE2	2:B:294:ASP:OD1	2.50	0.44
1:A:31:TRP:CE2	1:A:44:MET:HB2	2.52	0.44
2:B:58:TRP:HA	2:B:107:PHE:CE1	2.53	0.44
1:A:318:LYS:O	1:A:322:ILE:HG12	2.18	0.44
2:B:67:MET:HB3	2:B:67:MET:HE3	1.88	0.44
2:B:13:PHE:HE2	2:B:32:LEU:HB2	1.83	0.44
2:B:165:THR:HG23	2:B:219:PRO:HD3	2.00	0.44
2:B:54:TYR:O	2:B:56:ALA:N	2.48	0.44
2:B:105:LEU:HA	2:B:108:ALA:HB3	1.99	0.43
2:B:4:PRO:HG2	2:B:323:SER:HB3	1.98	0.43
2:B:31:TRP:CZ2	2:B:44:MET:HG3	2.54	0.43
2:B:53:VAL:CG2	2:B:57:LEU:HD22	2.44	0.43
2:B:17:SER:OG	2:B:20:GLU:HG2	2.19	0.43
2:B:33:GLN:HB3	2:B:44:MET:HE2	2.01	0.43
1:A:189:LYS:HD2	1:A:189:LYS:HA	1.63	0.43
2:B:148:ASN:HB3	2:B:205:ALA:HB2	2.01	0.42
2:B:173:PRO:HB3	2:B:329:PHE:CE1	2.54	0.42
2:B:166:HIS:O	2:B:170:GLU:HG2	2.20	0.41
2:B:150:LEU:H	2:B:153:LYS:HB3	1.85	0.41
2:B:92:LYS:HA	2:B:95:GLN:HB2	2.03	0.41
2:B:181:MET:HB3	2:B:197:ALA:CB	2.50	0.41
2:B:51:ALA:HA	2:B:52:PRO:HD2	1.91	0.41
2:B:60:PRO:HG3	2:B:107:PHE:CE1	2.56	0.41
2:B:23:LYS:HD3	2:B:23:LYS:HA	1.80	0.41
2:B:328:LYS:HE3	2:B:328:LYS:HB2	1.61	0.41
2:B:64:ILE:HA	2:B:67:MET:HB2	2.03	0.40
2:B:219:PRO:HB2	2:B:221:SER:OG	2.21	0.40
2:B:155:LEU:HD21	2:B:205:ALA:HA	2.02	0.40
2:B:308:VAL:O	2:B:311:SER:OG	2.25	0.40
2:B:26:ALA:O	2:B:46:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	330/331 (100%)	321 (97%)	8 (2%)	1 (0%)	41	27
2	B	331/331 (100%)	295 (89%)	22 (7%)	14 (4%)	3	0
All	All	661/662 (100%)	616 (93%)	30 (4%)	15 (2%)	7	1

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	61	ALA
2	B	35	SER
2	B	55	GLN
2	B	56	ALA
2	B	60	PRO
2	B	184	GLY
2	B	304	ILE
1	A	35	SER
2	B	37	LYS
2	B	149	HIS
2	B	152	ASP
2	B	331[A]	ASN
2	B	331[B]	ASN
2	B	180	ASP
2	B	53	VAL

### 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	271/270 (100%)	264 (97%)	7 (3%)	46	32
2	B	272/270 (101%)	236 (87%)	36 (13%)	4	1
All	All	543/540 (101%)	500 (92%)	43 (8%)	12	4

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	48	ASN
1	A	171	ASP
1	A	179	TRP
1	A	186	ARG
1	A	189	LYS
1	A	316	SER
2	B	16	ILE
2	B	19	GLN
2	B	23	LYS
2	B	25	ASP
2	B	33	GLN
2	B	42	SER
2	B	43	ILE
2	B	45	MET
2	B	54	TYR
2	B	62	PHE
2	B	77	THR
2	B	80	THR
2	B	83	MET
2	B	103	PHE
2	B	105	LEU
2	B	120	GLN
2	B	127	ASP
2	B	131	LYS
2	B	148	ASN
2	B	150	LEU
2	B	152	ASP
2	B	154	ASP
2	B	155	LEU
2	B	156	ASP
2	B	157	ASP
2	B	165	THR
2	B	171	ASP
2	B	194	TRP
2	B	198	MET
2	B	217	ARG
2	B	247	ARG
2	B	248	ASP
2	B	294	ASP
2	B	315	GLU
2	B	321	ILE

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Mol	Chain	Res	Type
2	B	323	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	148	ASN
2	B	149	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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.

No monomer is involved in short contacts.

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

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	331/331 (100%)	0.28	11 (3%) 46 40	22, 34, 57, 82	0
2	B	331/331 (100%)	1.63	113 (34%) 0 0	25, 63, 84, 94	0
All	All	662/662 (100%)	0.96	124 (18%) 1 0	22, 45, 81, 94	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	ALA	7.0
2	B	36	ALA	6.9
2	B	38	GLY	6.9
2	B	150	LEU	6.8
2	B	333	ASN	6.7
2	B	58	TRP	6.4
2	B	112	PRO	6.3
2	B	109	ALA	6.3
2	B	54	TYR	6.1
2	B	309	LEU	6.1
2	B	155	LEU	5.9
2	B	158	ALA	5.8
2	B	154	ASP	5.6
2	B	35	SER	5.1
1	A	36	ALA	5.1
2	B	99	ARG	5.1
2	B	317	ALA	5.0
2	B	314	GLY	5.0
2	B	68	ASP	5.0
2	B	69	ALA	4.8
2	B	107	PHE	4.8
2	B	45	MET	4.7
2	B	149	HIS	4.5
2	B	291	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	90	ALA	4.4
1	A	185	GLN	4.4
2	B	179	TRP	4.3
2	B	46	GLY	4.3
2	B	19	GLN	4.2
2	B	48	ASN	4.1
1	A	37	LYS	4.1
2	B	184	GLY	4.1
2	B	27	ASN	4.0
2	B	91	ASN	4.0
2	B	93	ALA	4.0
2	B	39	ASP	3.8
2	B	156	ASP	3.7
2	B	74	VAL	3.6
2	B	26	ALA	3.6
2	B	4	PRO	3.6
2	B	22	ALA	3.6
2	B	50	PHE	3.5
2	B	152	ASP	3.5
1	A	186	ARG	3.5
2	B	70	GLN	3.4
2	B	34	VAL	3.4
1	A	184	GLY	3.4
2	B	47	LYS	3.4
2	B	151	GLY	3.4
2	B	297	PHE	3.4
2	B	183	GLY	3.3
2	B	331[A]	ASN	3.3
2	B	64	ILE	3.3
2	B	37	LYS	3.2
2	B	89	GLU	3.2
2	B	87	THR	3.2
2	B	33	GLN	3.2
2	B	3	LYS	3.2
2	B	6	ILE	3.2
2	B	113	GLN	3.1
2	B	96	TRP	3.1
2	B	302	GLN	3.1
2	B	106	GLU	3.1
2	B	312	ASN	3.1
2	B	88	TRP	3.0
2	B	92	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	299	LEU	3.0
2	B	57	LEU	2.9
2	B	209	LEU	2.9
2	B	332	ILE	2.9
2	B	303	LYS	2.9
2	B	24	PHE	2.9
2	B	180	ASP	2.9
2	B	77	THR	2.8
2	B	55	GLN	2.8
2	B	49	ASN	2.8
2	B	71	GLY	2.7
2	B	128	LEU	2.7
2	B	40	THR	2.6
2	B	59	ASP	2.6
2	B	76	VAL	2.6
2	B	316	SER	2.6
2	B	169	ASN	2.6
2	B	182	MET	2.6
2	B	28	HIS	2.6
2	B	78	CYS	2.6
2	B	108	ALA	2.5
2	B	315	GLU	2.5
1	A	211	LEU	2.5
2	B	13	PHE	2.5
2	B	159	THR	2.4
2	B	72	VAL	2.4
2	B	194	TRP	2.4
2	B	65	GLU	2.4
2	B	330	PHE	2.4
2	B	110	HIS	2.4
2	B	75	GLN	2.4
1	A	38	GLY	2.3
1	A	3	LYS	2.3
2	B	219	PRO	2.3
2	B	62	PHE	2.3
1	A	39	ASP	2.3
2	B	15	ARG	2.2
1	A	207	LEU	2.2
2	B	32	LEU	2.2
2	B	126	LEU	2.2
2	B	12	PHE	2.2
2	B	221	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	321	ILE	2.2
2	B	123	LEU	2.2
2	B	16	ILE	2.1
2	B	23	LYS	2.1
2	B	86	TYR	2.1
2	B	115	ILE	2.1
2	B	17	SER	2.1
2	B	7	ASP	2.1
2	B	103	PHE	2.1
2	B	10	SER	2.1
2	B	304	ILE	2.1
2	B	313	LEU	2.1
2	B	131	LYS	2.1
1	A	289	VAL	2.1
2	B	121	VAL	2.1
2	B	100	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	401	1/1	0.96	0.04	46,46,46,46	0
3	ZN	A	401	1/1	1.00	0.09	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.