



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:17 am BST

PDB ID : 4KS9  
Title : Crystal Structure of Malonyl-CoA decarboxylase (Rmet\_2797) from Cupriavidus metallidurans, Northeast Structural Genomics Consortium Target CrR76  
Authors : Forouhar, F.; Tran, T.H.; Lew, S.; Seetharaman, J.; Xiao, R.; Acton, T.B.; Everett, J.K.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2013-05-17  
Resolution : 2.30 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

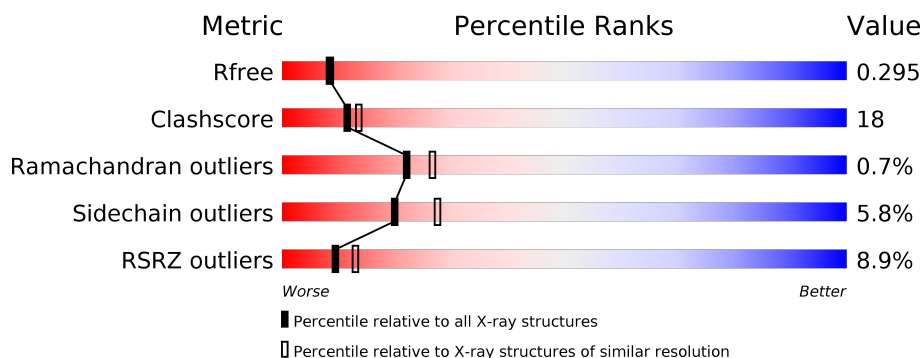
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	428	<div> <div>8%</div> <div> <div></div> <div>62%</div> <div>28%</div> <div>• 8%</div> </div> </div>
1	B	428	<div> <div>9%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>• 8%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6535 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 Malonyl-CoA decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3118	1971	582	553	12			
1	B	395	Total	C	N	O	S	0	0	0
			3140	1985	585	558	12			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ALA	-	EXPRESSION TAG	UNP Q1LJK6
A	475	ALA	-	EXPRESSION TAG	UNP Q1LJK6
A	476	ALA	-	EXPRESSION TAG	UNP Q1LJK6
A	477	LEU	-	EXPRESSION TAG	UNP Q1LJK6
A	478	GLU	-	EXPRESSION TAG	UNP Q1LJK6
A	479	HIS	-	EXPRESSION TAG	UNP Q1LJK6
A	480	HIS	-	EXPRESSION TAG	UNP Q1LJK6
A	481	HIS	-	EXPRESSION TAG	UNP Q1LJK6
A	482	HIS	-	EXPRESSION TAG	UNP Q1LJK6
A	483	HIS	-	EXPRESSION TAG	UNP Q1LJK6
A	484	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	474	ALA	-	EXPRESSION TAG	UNP Q1LJK6
B	475	ALA	-	EXPRESSION TAG	UNP Q1LJK6
B	476	ALA	-	EXPRESSION TAG	UNP Q1LJK6
B	477	LEU	-	EXPRESSION TAG	UNP Q1LJK6
B	478	GLU	-	EXPRESSION TAG	UNP Q1LJK6
B	479	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	480	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	481	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	482	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	483	HIS	-	EXPRESSION TAG	UNP Q1LJK6
B	484	HIS	-	EXPRESSION TAG	UNP Q1LJK6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mg 1	0	0

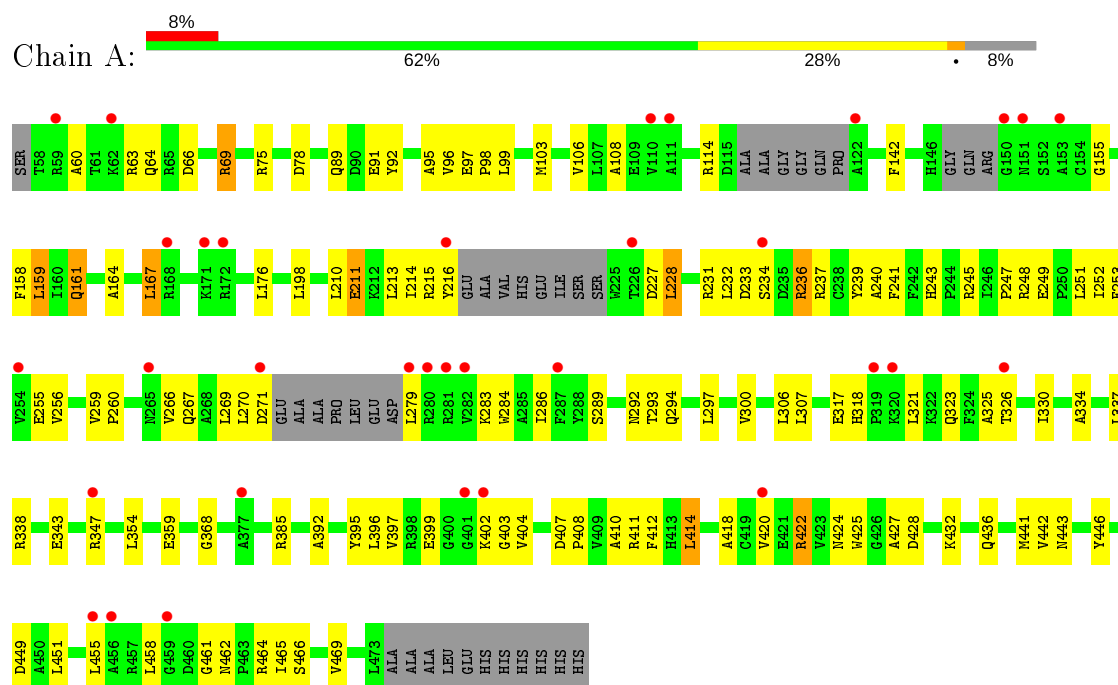
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	127	Total 127	O 127	0	0
3	B	149	Total 149	O 149	0	0

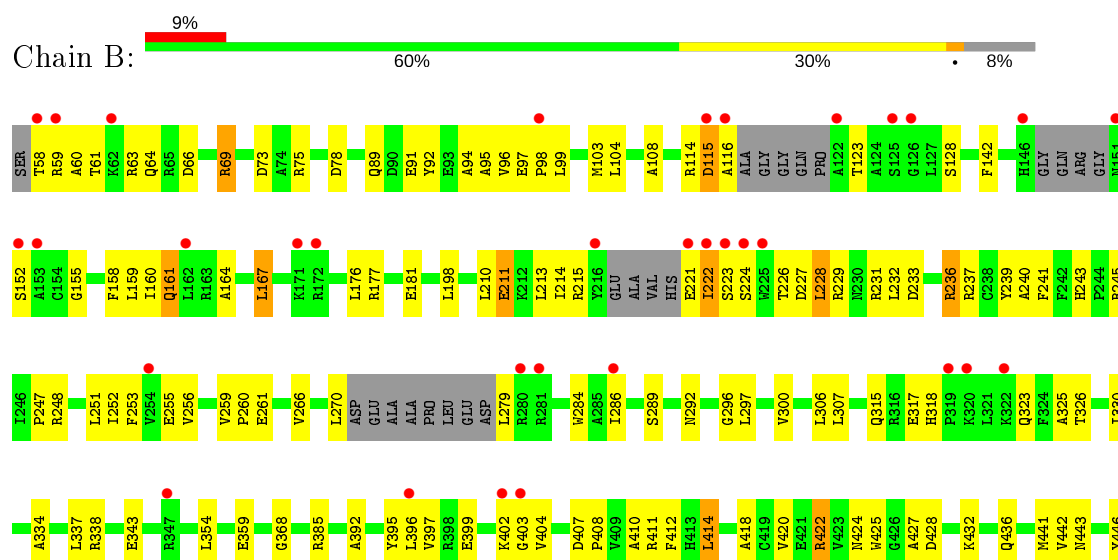
### 3 Residue-property plots

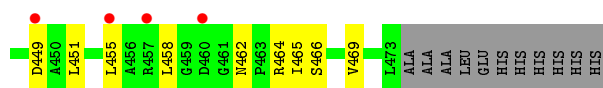
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Malonyl-CoA decarboxylase



#### • Molecule 1: Malonyl-CoA decarboxylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.01Å 69.39Å 74.36Å 90.00° 103.80° 90.00°	Depositor
Resolution (Å)	28.75 – 2.30 28.75 – 2.24	Depositor EDS
% Data completeness (in resolution range)	89.1 (28.75-2.30) 92.1 (28.75-2.24)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.24Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.239 , 0.286 0.250 , 0.295	Depositor DCC
$R_{free}$ test set	4254 reflections (9.61%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.8	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6535	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.37	0/3182	0.58	0/4302
1	B	0.38	0/3204	0.58	0/4332
All	All	0.37	0/6386	0.58	0/8634

There are no bond length outliers.

There are no bond angle outliers.

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	3118	0	3107	110	0
1	B	3140	0	3132	110	0
2	B	1	0	0	0	0
3	A	127	0	0	6	0
3	B	149	0	0	5	0
All	All	6535	0	6239	220	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 (220) 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:A:60:ALA:HB1	1:A:63:ARG:HH12	1.37	0.89
1:B:60:ALA:HB1	1:B:63:ARG:HH12	1.41	0.85
1:A:408:PRO:HA	1:A:411:ARG:HH12	1.42	0.84
1:B:247:PRO:O	1:B:248:ARG:HB2	1.78	0.83
1:B:408:PRO:HA	1:B:411:ARG:HH12	1.44	0.81
1:A:247:PRO:O	1:A:248:ARG:HB2	1.81	0.80
1:A:330:ILE:HD11	1:A:442:VAL:HG23	1.65	0.79
1:B:330:ILE:HD11	1:B:442:VAL:HG23	1.65	0.79
1:B:422:ARG:HD2	1:B:424:ASN:OD1	1.83	0.78
1:A:422:ARG:HD2	1:A:424:ASN:OD1	1.86	0.76
1:A:408:PRO:HA	1:A:411:ARG:NH1	1.99	0.75
1:A:60:ALA:HB1	1:A:63:ARG:NH1	2.01	0.75
1:B:408:PRO:HA	1:B:411:ARG:NH1	2.00	0.74
1:A:259:VAL:CG2	1:A:260:PRO:HD2	2.18	0.74
1:A:228:LEU:HD22	1:A:232:LEU:HD22	1.70	0.73
1:B:228:LEU:HD22	1:B:232:LEU:HD22	1.68	0.73
1:B:259:VAL:CG2	1:B:260:PRO:HD2	2.19	0.73
1:B:60:ALA:HB1	1:B:63:ARG:NH1	2.05	0.72
1:B:128:SER:HB2	3:B:726:HOH:O	1.93	0.69
1:A:266:VAL:HB	1:A:441:MET:SD	2.34	0.68
1:A:286:ILE:HA	1:A:325:ALA:O	1.94	0.68
1:B:286:ILE:HA	1:B:325:ALA:O	1.96	0.66
1:B:231:ARG:HD3	1:B:255:GLU:OE1	1.95	0.65
1:A:269:LEU:HD21	1:A:286:ILE:HD11	1.79	0.65
1:A:214:ILE:HG13	1:A:215:ARG:N	2.12	0.64
1:B:317:GLU:HG3	1:B:318:HIS:CD2	2.32	0.64
1:A:231:ARG:HD3	1:A:255:GLU:OE1	1.97	0.64
1:A:317:GLU:HG3	1:A:318:HIS:CD2	2.33	0.64
1:A:410:ALA:O	1:A:414:LEU:HB2	1.96	0.64
1:B:60:ALA:CB	1:B:63:ARG:HH12	2.09	0.63
1:B:214:ILE:HG13	1:B:215:ARG:N	2.12	0.62
1:B:266:VAL:HB	1:B:441:MET:SD	2.39	0.62
1:B:297:LEU:O	1:B:300:VAL:HG13	1.99	0.62
1:B:396:LEU:HA	3:B:632:HOH:O	1.97	0.62
1:A:297:LEU:O	1:A:300:VAL:HG13	2.00	0.62
1:A:60:ALA:CB	1:A:63:ARG:HH12	2.09	0.61
1:B:410:ALA:O	1:B:414:LEU:HB2	2.00	0.61
1:A:89:GLN:HG3	1:A:158:PHE:CD1	2.36	0.61
1:A:259:VAL:HG23	1:A:260:PRO:HD2	1.82	0.61
1:B:224:SER:HB2	1:B:226:THR:HG22	1.83	0.60
1:B:259:VAL:HG23	1:B:260:PRO:HD2	1.82	0.60
1:B:95:ALA:HB1	1:B:99:LEU:HD23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ALA:HB1	1:A:99:LEU:HD23	1.84	0.59
1:A:240:ALA:HA	1:A:252:ILE:O	2.03	0.59
1:A:231:ARG:O	1:A:236:ARG:HG2	2.02	0.58
1:A:465:ILE:HG23	1:A:469:VAL:HB	1.85	0.58
1:B:465:ILE:HG23	1:B:469:VAL:HB	1.86	0.58
1:A:259:VAL:HG22	1:A:260:PRO:HD2	1.86	0.57
1:B:392:ALA:O	1:B:396:LEU:HG	2.05	0.57
1:A:243:HIS:CE1	1:A:245:ARG:HG2	2.40	0.57
1:B:89:GLN:HG3	1:B:158:PHE:CD1	2.39	0.57
1:B:259:VAL:HG22	1:B:260:PRO:HD2	1.87	0.57
1:A:270:LEU:HD12	1:A:270:LEU:N	2.20	0.56
1:A:269:LEU:CD2	1:A:286:ILE:HD11	2.34	0.56
1:A:89:GLN:HG3	1:A:158:PHE:CE1	2.40	0.56
1:B:231:ARG:O	1:B:236:ARG:HG2	2.05	0.56
1:B:222:ILE:HG22	1:B:224:SER:H	1.71	0.56
1:A:385:ARG:HG3	1:A:425:TRP:CG	2.41	0.55
1:B:240:ALA:HA	1:B:252:ILE:O	2.05	0.55
1:A:142:PHE:O	1:A:155:GLY:HA3	2.07	0.55
1:A:228:LEU:HD22	1:A:232:LEU:CD2	2.36	0.55
1:B:385:ARG:HG3	1:B:425:TRP:CG	2.42	0.55
1:B:228:LEU:HD22	1:B:232:LEU:CD2	2.34	0.55
1:A:330:ILE:HD11	1:A:442:VAL:CG2	2.37	0.54
1:A:392:ALA:O	1:A:396:LEU:HG	2.08	0.54
1:B:243:HIS:CE1	1:B:245:ARG:HG2	2.43	0.54
1:B:89:GLN:HG3	1:B:158:PHE:CE1	2.44	0.53
1:B:236:ARG:HG3	1:B:256:VAL:O	2.08	0.53
1:A:411:ARG:HH11	1:A:411:ARG:HB3	1.74	0.53
1:B:323:GLN:HA	1:B:323:GLN:HE21	1.74	0.52
1:B:330:ILE:CD1	1:B:442:VAL:HG23	2.38	0.52
1:B:60:ALA:HB1	1:B:63:ARG:HH22	1.73	0.52
1:B:152:SER:HB3	1:B:161:GLN:OE1	2.09	0.52
1:A:347:ARG:HD2	3:A:567:HOH:O	2.10	0.52
1:A:395:TYR:O	1:A:399:GLU:HB2	2.10	0.52
1:B:64:GLN:HE21	1:B:91:GLU:CD	2.14	0.52
1:B:58:THR:HA	1:B:61:THR:OG1	2.10	0.51
1:A:397:VAL:HG11	1:A:465:ILE:HD11	1.91	0.51
1:B:92:TYR:HA	1:B:103:MET:HE1	1.92	0.51
1:B:337:LEU:O	1:B:368:GLY:HA3	2.11	0.51
1:B:210:LEU:HG	1:B:228:LEU:HD13	1.92	0.51
1:A:323:GLN:HA	1:A:323:GLN:HE21	1.76	0.51
1:A:330:ILE:CD1	1:A:442:VAL:HG23	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:HG3	1:A:294:GLN:NE2	2.26	0.51
1:A:337:LEU:O	1:A:368:GLY:HA3	2.10	0.51
1:A:64:GLN:HE21	1:A:91:GLU:CD	2.14	0.51
1:A:403:GLY:HA2	1:A:458:LEU:O	2.11	0.50
1:B:411:ARG:HH11	1:B:411:ARG:HB3	1.75	0.50
1:A:266:VAL:HG22	1:A:270:LEU:HD13	1.93	0.50
1:B:108:ALA:HB2	1:B:176:LEU:HD23	1.94	0.50
1:B:334:ALA:O	1:B:338:ARG:HG2	2.11	0.50
1:A:60:ALA:HB1	1:A:63:ARG:HH22	1.77	0.50
1:A:247:PRO:O	1:A:248:ARG:CB	2.56	0.50
1:B:403:GLY:HA2	1:B:458:LEU:O	2.11	0.50
1:A:236:ARG:HG3	1:A:256:VAL:O	2.12	0.50
1:A:418:ALA:HB2	1:A:446:TYR:CZ	2.47	0.50
1:B:395:TYR:O	1:B:399:GLU:HB2	2.12	0.50
1:B:397:VAL:HG11	1:B:465:ILE:HD11	1.93	0.50
1:B:224:SER:CB	1:B:226:THR:HG22	2.42	0.49
1:A:108:ALA:HB2	1:A:176:LEU:HD23	1.95	0.49
1:A:210:LEU:HG	1:A:228:LEU:HD13	1.94	0.49
1:A:334:ALA:O	1:A:338:ARG:HG2	2.12	0.49
1:B:330:ILE:HD11	1:B:442:VAL:CG2	2.39	0.49
1:B:60:ALA:HB1	1:B:63:ARG:NH2	2.28	0.49
1:A:307:LEU:HD22	1:A:446:TYR:CZ	2.48	0.49
1:B:307:LEU:HD22	1:B:446:TYR:CZ	2.48	0.49
1:A:234:SER:O	1:A:279:LEU:HD21	2.14	0.48
1:A:420:VAL:HG12	1:A:464:ARG:O	2.13	0.48
1:B:210:LEU:HG	1:B:228:LEU:CD1	2.43	0.48
1:B:213:LEU:HD12	1:B:253:PHE:CG	2.47	0.48
1:B:418:ALA:HB2	1:B:446:TYR:CZ	2.48	0.48
1:B:420:VAL:HG12	1:B:464:ARG:O	2.14	0.48
1:B:92:TYR:HA	1:B:103:MET:CE	2.43	0.48
1:B:279:LEU:HD22	1:B:279:LEU:N	2.28	0.48
1:B:142:PHE:O	1:B:155:GLY:HA3	2.13	0.48
1:A:407:ASP:HB3	1:A:410:ALA:HB3	1.96	0.48
1:A:227:ASP:O	1:A:231:ARG:HG3	2.14	0.47
1:B:315:GLN:NE2	3:B:693:HOH:O	2.48	0.47
1:A:428:ASP:HB2	1:A:441:MET:SD	2.55	0.47
1:A:432:LYS:HE2	1:A:436:GLN:OE1	2.14	0.47
1:A:404:VAL:HG13	1:A:411:ARG:HD3	1.96	0.47
1:A:427:ALA:CB	1:A:441:MET:HB2	2.44	0.47
1:A:60:ALA:HB1	1:A:63:ARG:NH2	2.30	0.47
1:A:269:LEU:C	1:A:271:ASP:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:VAL:HG13	1:B:411:ARG:HD3	1.97	0.47
1:A:92:TYR:HA	1:A:103:MET:CE	2.45	0.47
1:B:221:GLU:HA	1:B:227:ASP:OD2	2.14	0.46
1:B:432:LYS:HE2	1:B:436:GLN:OE1	2.15	0.46
1:B:213:LEU:N	1:B:213:LEU:HD22	2.31	0.46
1:A:465:ILE:CG2	1:A:469:VAL:HB	2.46	0.46
1:A:397:VAL:CG1	1:A:465:ILE:HD11	2.45	0.46
1:B:306:LEU:HD23	1:B:412:PHE:CE1	2.51	0.46
1:A:279:LEU:HD22	1:A:279:LEU:N	2.30	0.46
1:B:465:ILE:HG22	1:B:466:SER:O	2.15	0.46
1:A:106:VAL:HB	3:A:514:HOH:O	2.14	0.46
1:A:461:GLY:HA2	3:A:517:HOH:O	2.16	0.46
1:B:96:VAL:HG23	1:B:98:PRO:HG2	1.96	0.46
1:A:306:LEU:HD23	1:A:412:PHE:CE1	2.51	0.46
1:B:407:ASP:HB3	1:B:410:ALA:HB3	1.97	0.46
1:B:397:VAL:CG1	1:B:465:ILE:HD11	2.46	0.46
1:A:161:GLN:HB3	1:A:161:GLN:HE21	1.53	0.45
1:B:69:ARG:HD3	1:B:69:ARG:HA	1.76	0.45
1:A:259:VAL:HG22	1:A:260:PRO:CD	2.47	0.45
1:B:95:ALA:CB	1:B:99:LEU:HD23	2.45	0.45
1:A:213:LEU:HD12	1:A:253:PHE:CG	2.51	0.45
1:A:96:VAL:HG23	1:A:98:PRO:HG2	1.98	0.45
1:B:97:GLU:N	1:B:98:PRO:HD2	2.31	0.45
1:B:465:ILE:CG2	1:B:469:VAL:HB	2.47	0.45
1:A:97:GLU:N	1:A:98:PRO:HD2	2.32	0.45
1:B:427:ALA:CB	1:B:441:MET:HB2	2.46	0.45
1:A:213:LEU:N	1:A:213:LEU:HD22	2.31	0.45
1:A:255:GLU:HB2	1:A:289:SER:HB3	1.99	0.45
1:A:465:ILE:HG22	1:A:466:SER:O	2.17	0.45
1:A:60:ALA:HB1	1:A:63:ARG:CZ	2.46	0.45
1:B:214:ILE:CG1	1:B:215:ARG:N	2.80	0.44
1:A:92:TYR:HA	1:A:103:MET:HE1	1.98	0.44
1:A:210:LEU:HG	1:A:228:LEU:CD1	2.47	0.44
1:B:114:ARG:HA	1:B:114:ARG:HD2	1.69	0.44
1:B:259:VAL:HG22	1:B:260:PRO:CD	2.48	0.44
1:B:261:GLU:HB2	3:B:663:HOH:O	2.17	0.44
1:B:73:ASP:OD2	1:B:114:ARG:NH1	2.49	0.44
1:B:451:LEU:O	1:B:455:LEU:HG	2.17	0.44
1:B:60:ALA:HB1	1:B:63:ARG:CZ	2.46	0.44
1:B:222:ILE:HG22	1:B:223:SER:N	2.32	0.44
1:A:326:THR:O	1:A:443:ASN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ASP:O	1:B:231:ARG:HG3	2.17	0.44
1:B:161:GLN:O	1:B:164:ALA:HB3	2.17	0.44
1:A:432:LYS:CE	1:A:436:GLN:OE1	2.66	0.44
1:B:211:GLU:O	1:B:211:GLU:HG3	2.18	0.44
1:B:411:ARG:NH1	1:B:411:ARG:HB3	2.33	0.44
1:A:69:ARG:HA	1:A:69:ARG:HD3	1.77	0.43
1:A:161:GLN:O	1:A:164:ALA:HB3	2.17	0.43
1:A:95:ALA:CB	1:A:99:LEU:HD23	2.46	0.43
1:B:211:GLU:O	1:B:215:ARG:HD3	2.18	0.43
1:B:270:LEU:CD1	1:B:270:LEU:N	2.82	0.43
1:A:306:LEU:HD23	1:A:412:PHE:CZ	2.53	0.43
1:B:428:ASP:HB2	1:B:441:MET:SD	2.59	0.43
1:A:198:LEU:HD13	1:A:241:PHE:CZ	2.54	0.43
1:A:411:ARG:HB3	1:A:411:ARG:NH1	2.32	0.43
1:B:306:LEU:HD23	1:B:412:PHE:CZ	2.53	0.43
1:A:114:ARG:HA	1:A:114:ARG:HD2	1.88	0.43
1:B:326:THR:O	1:B:443:ASN:HA	2.18	0.43
1:A:420:VAL:HG13	1:A:420:VAL:O	2.19	0.43
1:B:420:VAL:HG13	1:B:420:VAL:O	2.19	0.43
1:A:214:ILE:CG1	1:A:215:ARG:N	2.81	0.43
1:A:321:LEU:HD23	3:A:571:HOH:O	2.18	0.43
1:B:177:ARG:O	1:B:181:GLU:HG3	2.18	0.43
1:B:432:LYS:CE	1:B:436:GLN:OE1	2.67	0.43
1:A:396:LEU:HA	3:A:525:HOH:O	2.19	0.42
1:A:451:LEU:O	1:A:455:LEU:HG	2.19	0.42
1:B:75:ARG:HG3	1:B:78:ASP:H	1.84	0.42
1:A:267:GLN:O	1:A:271:ASP:HB3	2.19	0.42
1:A:424:ASN:HB2	1:A:427:ALA:HB2	2.01	0.42
1:B:396:LEU:HD12	1:B:397:VAL:HG23	2.02	0.42
1:A:396:LEU:HD12	1:A:397:VAL:HG23	2.01	0.42
1:B:284:TRP:CE3	1:B:323:GLN:HB3	2.54	0.42
1:A:284:TRP:CE3	1:A:323:GLN:HB3	2.55	0.41
1:A:75:ARG:HG3	1:A:78:ASP:H	1.85	0.41
1:B:92:TYR:HE2	1:B:104:LEU:CD1	2.33	0.41
1:A:211:GLU:HG3	1:A:211:GLU:O	2.16	0.41
1:A:237:ARG:HG2	1:A:239:TYR:OH	2.19	0.41
1:B:167:LEU:HD12	1:B:167:LEU:HA	1.84	0.41
1:A:216:TYR:HB2	1:A:293:THR:HG22	2.02	0.41
1:A:396:LEU:CD2	1:A:442:VAL:HG21	2.50	0.41
1:B:237:ARG:HG2	1:B:239:TYR:OH	2.20	0.41
1:B:226:THR:O	1:B:229:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLU:HB2	1:B:289:SER:HB3	2.01	0.41
1:A:259:VAL:O	1:A:284:TRP:HB2	2.21	0.41
1:B:424:ASN:HB2	1:B:427:ALA:HB2	2.01	0.41
1:B:396:LEU:CD2	1:B:442:VAL:HG21	2.50	0.41
1:A:159:LEU:HA	1:A:159:LEU:HD12	1.86	0.41
1:A:167:LEU:HA	1:A:167:LEU:HD12	1.84	0.41
1:A:96:VAL:HG23	1:A:99:LEU:H	1.85	0.41
1:B:198:LEU:HD13	1:B:241:PHE:CZ	2.55	0.41
1:B:160:ILE:O	1:B:296:GLY:HA3	2.20	0.41
1:A:283:LYS:NZ	3:A:601:HOH:O	2.54	0.40
1:B:94:ALA:HB2	3:B:621:HOH:O	2.20	0.40
1:A:411:ARG:NH1	1:A:411:ARG:CB	2.85	0.40
1:B:115:ASP:HB3	1:B:116:ALA:H	1.67	0.40
1:B:96:VAL:HG23	1:B:99:LEU:H	1.86	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	382/428 (89%)	361 (94%)	20 (5%)	1 (0%)	41	50
1	B	385/428 (90%)	360 (94%)	21 (6%)	4 (1%)	15	17
All	All	767/856 (90%)	721 (94%)	41 (5%)	5 (1%)	22	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	115	ASP
1	B	222	ILE
1	A	402	LYS
1	B	402	LYS

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Mol	Chain	Res	Type
1	B	123	THR

### 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	317/342 (93%)	299 (94%)	18 (6%)	20	28
1	B	320/342 (94%)	301 (94%)	19 (6%)	19	27
All	All	637/684 (93%)	600 (94%)	37 (6%)	20	27

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	A	69	ARG
1	A	159	LEU
1	A	161	GLN
1	A	167	LEU
1	A	211	GLU
1	A	228	LEU
1	A	233	ASP
1	A	236	ARG
1	A	251	LEU
1	A	292	ASN
1	A	343	GLU
1	A	354	LEU
1	A	359	GLU
1	A	414	LEU
1	A	422	ARG
1	A	449	ASP
1	A	462	ASN
1	B	59	ARG
1	B	66	ASP
1	B	69	ARG
1	B	159	LEU

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Mol	Chain	Res	Type
1	B	161	GLN
1	B	167	LEU
1	B	211	GLU
1	B	228	LEU
1	B	233	ASP
1	B	236	ARG
1	B	251	LEU
1	B	292	ASN
1	B	343	GLU
1	B	354	LEU
1	B	359	GLU
1	B	414	LEU
1	B	422	ARG
1	B	449	ASP
1	B	462	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	101	GLN
1	A	161	GLN
1	A	292	ASN
1	A	294	GLN
1	A	318	HIS
1	A	323	GLN
1	A	462	ASN
1	B	67	GLN
1	B	101	GLN
1	B	146	HIS
1	B	161	GLN
1	B	292	ASN
1	B	294	GLN
1	B	315	GLN
1	B	318	HIS
1	B	323	GLN
1	B	462	ASN

### 5.3.3 RNA ⓘ

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 1 ligands modelled in this entry, 1 is 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 [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	392/428 (91%)	0.48	33 (8%) 11 15	23, 43, 70, 97	0
1	B	395/428 (92%)	0.59	37 (9%) 8 11	22, 43, 72, 91	0
All	All	787/856 (91%)	0.53	70 (8%) 9 13	22, 43, 71, 97	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	ILE	6.7
1	B	223	SER	6.4
1	B	116	ALA	6.3
1	B	125	SER	6.3
1	B	280	ARG	5.3
1	B	126	GLY	5.0
1	B	281	ARG	4.9
1	A	216	TYR	4.8
1	A	280	ARG	4.4
1	B	62	LYS	4.4
1	B	151	ASN	4.2
1	A	122	ALA	4.1
1	B	58	THR	4.1
1	B	171	LYS	4.0
1	B	122	ALA	3.8
1	A	401	GLY	3.7
1	A	59	ARG	3.5
1	B	216	TYR	3.4
1	B	460	ASP	3.4
1	B	455	LEU	3.3
1	B	320	LYS	3.1
1	A	254	VAL	3.0
1	B	59	ARG	3.0
1	B	402	LYS	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	98	PRO	2.9
1	B	254	VAL	2.9
1	B	153	ALA	2.8
1	A	347	ARG	2.7
1	B	449	ASP	2.7
1	B	403	GLY	2.7
1	B	457	ARG	2.7
1	A	271	ASP	2.6
1	B	152	SER	2.6
1	A	320	LYS	2.6
1	A	153	ALA	2.6
1	A	377	ALA	2.6
1	A	150	GLY	2.4
1	B	225	TRP	2.4
1	A	455	LEU	2.4
1	A	282	VAL	2.4
1	B	322	LYS	2.3
1	A	319	PRO	2.3
1	B	319	PRO	2.2
1	B	172	ARG	2.2
1	A	62	LYS	2.2
1	A	234	SER	2.2
1	B	224	SER	2.2
1	A	171	LYS	2.2
1	B	347	ARG	2.2
1	B	115	ASP	2.2
1	A	111	ALA	2.2
1	A	279	LEU	2.1
1	B	221	GLU	2.1
1	A	420	VAL	2.1
1	A	281	ARG	2.1
1	A	151	ASN	2.1
1	B	162	LEU	2.1
1	B	396	LEU	2.1
1	A	168	ARG	2.1
1	A	265	ASN	2.1
1	A	287	PHE	2.1
1	A	402	LYS	2.1
1	B	286	ILE	2.1
1	A	326	THR	2.1
1	A	456	ALA	2.1
1	A	110	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	459	GLY	2.0
1	B	146	HIS	2.0
1	A	226	THR	2.0
1	A	172	ARG	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
2	MG	B	501	1/1	0.97	0.11	29,29,29,29	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.