



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:51 PM GMT

PDB ID : 4MZ0  
Title : Structure of a ketosynthase-acyltransferase di-domain from module CurL of the curacin A polyketide synthase  
Authors : Whicher, J.R.; Smaga, S.S.; Smith, J.L.  
Deposited on : 2013-09-28  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

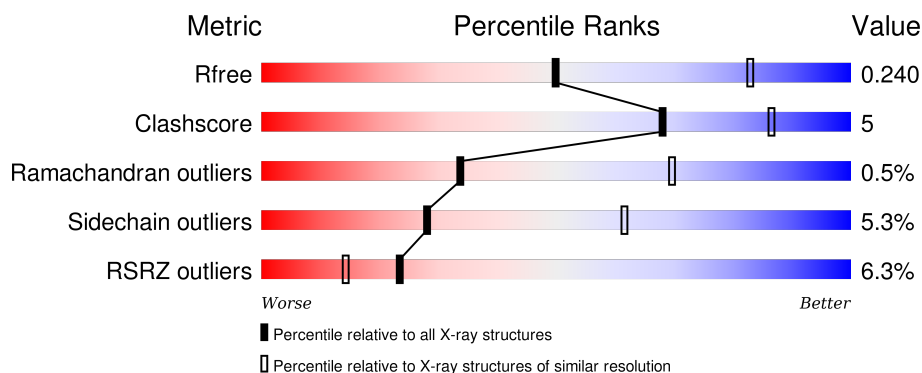
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	938	<div> <div></div> <div>79% 16% . .</div> </div>
1	B	938	<div> <div>10%</div> <div>76% 11% . 12%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13429 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 CurL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	896	Total	C	N	O	S	0	0	0
			6857	4340	1173	1317	27			
1	B	823	Total	C	N	O	S	0	0	0
			6288	3984	1077	1204	23			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

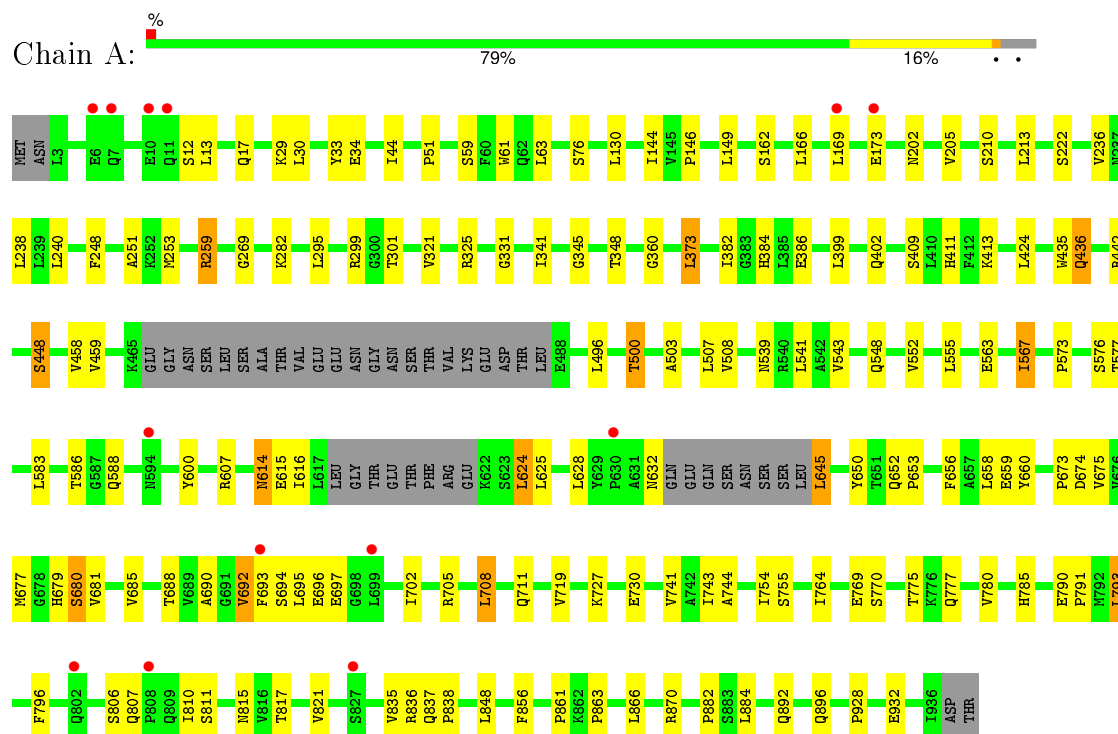
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total	O	0	0
			166	166		
3	B	116	Total	O	0	0
			116	116		

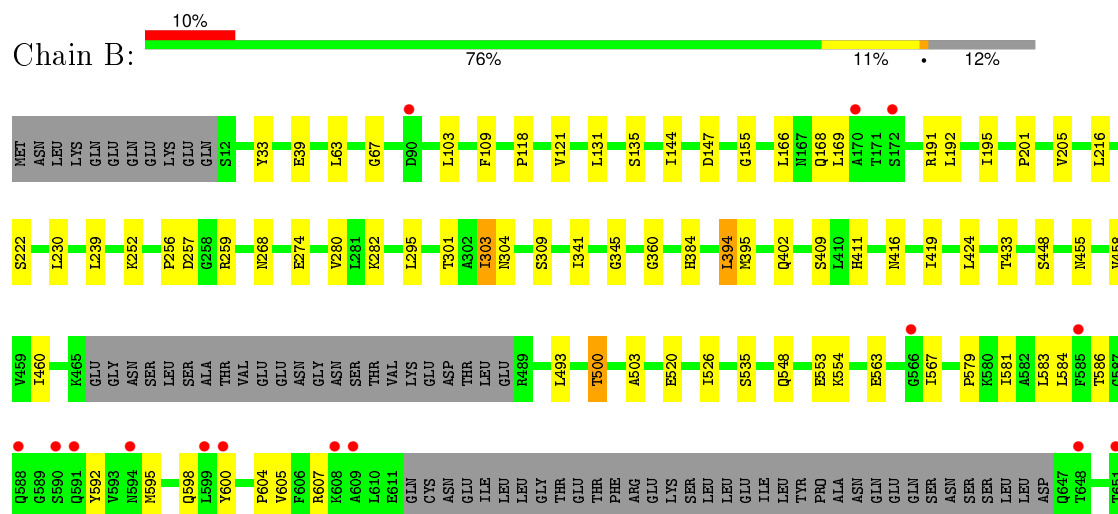
### 3 Residue-property plots

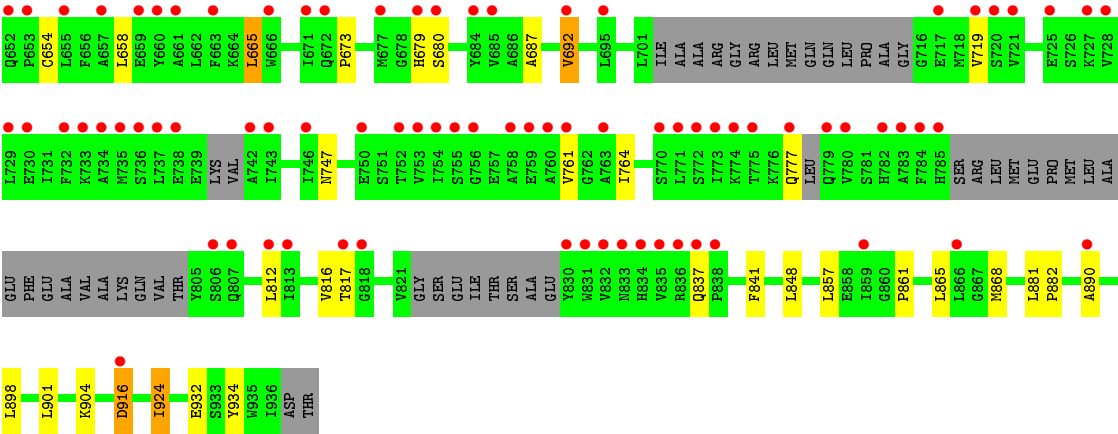
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



#### • Molecule 1: CurL





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.27Å 150.70Å 236.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.99 – 2.80 49.14 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.99-2.80) 99.7 (49.14-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.00 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, $R_{free}$	0.185 , 0.231 0.192 , 0.240	Depositor DCC
$R_{free}$ test set	3118 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 59.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 61618 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA

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	0.52	0/6995	0.73	0/9506
1	B	0.50	0/6417	0.72	1/8722 (0.0%)
All	All	0.51	0/13412	0.72	1/18228 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	916	ASP	CB-CG-OD2	5.21	122.99	118.30

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	6857	0	6816	77	0
1	B	6288	0	6224	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	166	0	0	0	0
3	B	116	0	0	1	0
All	All	13429	0	13040	123	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 5.

All (123) 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:656:PHE:HZ	1:A:688:THR:HG21	1.36	0.90
1:A:675:VAL:HG12	1:A:811:SER:HB2	1.58	0.85
1:A:248:PHE:HD1	1:A:253:MET:SD	2.05	0.80
1:A:202:ASN:H	1:B:303:ILE:HD11	1.48	0.79
1:A:251:ALA:HB3	1:A:253:MET:HE3	1.67	0.77
1:A:248:PHE:CD1	1:A:253:MET:SD	2.85	0.70
1:B:600:TYR:O	1:B:607:ARG:HG2	1.93	0.68
1:A:500:THR:HG22	1:A:503:ALA:H	1.58	0.68
1:A:543:VAL:HG22	1:A:567:ILE:HD12	1.78	0.65
1:B:816:VAL:HG13	1:B:837:GLN:HG2	1.79	0.64
1:A:251:ALA:HB3	1:A:253:MET:CE	2.27	0.63
1:A:248:PHE:HD1	1:A:253:MET:CE	2.12	0.62
1:B:500:THR:HG22	1:B:503:ALA:H	1.64	0.62
1:A:301:THR:HG22	1:A:458:VAL:HG22	1.80	0.62
1:B:166:LEU:HA	1:B:169:LEU:HD12	1.83	0.61
1:A:583:LEU:HD13	1:A:673:PRO:HB3	1.84	0.59
1:B:584:LEU:HB3	1:B:865:LEU:HD23	1.84	0.59
1:B:118:PRO:HA	1:B:121:VAL:HG12	1.83	0.59
1:A:259:ARG:HG2	1:A:411:HIS:NE2	2.17	0.59
1:A:166:LEU:HA	1:A:169:LEU:HD12	1.84	0.59
1:A:541:LEU:HD11	1:A:567:ILE:HD11	1.85	0.58
1:A:863:PRO:HB3	1:A:882:PRO:HB3	1.86	0.58
1:A:650:TYR:O	1:A:653:PRO:HD2	2.04	0.57
1:A:656:PHE:CZ	1:A:688:THR:HG21	2.28	0.57
1:B:605:VAL:HB	1:B:665:LEU:HD23	1.86	0.57
1:B:360:GLY:HA3	1:B:424:LEU:HD23	1.86	0.57
1:A:213:LEU:HD12	1:A:448:SER:HB2	1.87	0.56
1:B:586:THR:HG22	1:B:865:LEU:HD13	1.87	0.55
1:A:435:TRP:O	1:A:442:ARG:NH1	2.40	0.54
1:B:191:ARG:HG2	1:B:195:ILE:HD12	1.90	0.54
1:A:44:ILE:HD13	1:A:282:LYS:HD2	1.91	0.53
1:A:61:TRP:HB2	1:A:399:LEU:HD22	1.90	0.52
1:B:295:LEU:HD22	1:B:402:GLN:HE22	1.73	0.52
1:B:526:ILE:HG23	1:B:924:ILE:HD11	1.90	0.52
1:A:690:ALA:HA	1:A:810:ILE:HD12	1.93	0.51
1:A:680:SER:H	1:A:815:ASN:ND2	2.08	0.51
1:A:360:GLY:HA3	1:A:424:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:719:VAL:HG22	1:A:777:GLN:HA	1.93	0.51
1:A:680:SER:H	1:A:815:ASN:HD21	1.58	0.51
1:A:614:ASN:OD1	1:A:625:LEU:HB2	2.10	0.51
1:B:416:ASN:HB3	1:B:419:ILE:HD12	1.92	0.50
1:A:251:ALA:CB	1:A:253:MET:CE	2.88	0.50
1:B:301:THR:HG22	1:B:458:VAL:HG22	1.92	0.50
1:B:103:LEU:HG	1:B:274:GLU:HG3	1.94	0.50
1:A:694:SER:H	1:A:697:GLU:HB2	1.77	0.50
1:A:321:VAL:O	1:A:325:ARG:HG3	2.11	0.50
1:A:248:PHE:HA	1:A:253:MET:HE3	1.94	0.49
1:A:146:PRO:HA	1:A:149:LEU:HB3	1.94	0.49
1:A:573:PRO:HG2	1:A:576:SER:HB3	1.95	0.49
1:A:692:VAL:HA	1:A:806:SER:O	2.13	0.48
1:B:595:MET:HB3	1:B:658:LEU:HD13	1.95	0.48
1:A:836:ARG:HG3	1:A:837:GLN:HE21	1.77	0.48
1:A:588:GLN:HB2	1:A:681:VAL:HG21	1.96	0.48
1:A:548:GLN:O	1:A:552:VAL:HG23	2.14	0.47
1:B:109:PHE:O	1:B:934:TYR:HE2	1.97	0.47
1:A:624:LEU:HD23	1:A:628:LEU:HD12	1.96	0.47
1:A:251:ALA:CB	1:A:253:MET:HE2	2.44	0.47
1:B:579:PRO:HG3	1:B:904:LYS:HB3	1.96	0.47
1:B:583:LEU:HD13	1:B:673:PRO:HB3	1.97	0.47
1:B:554:LYS:HB3	1:B:567:ILE:HD11	1.97	0.47
1:A:600:TYR:CZ	1:A:625:LEU:HD11	2.50	0.46
1:A:708:LEU:HD23	1:A:796:PHE:HB2	1.97	0.46
1:A:30:LEU:O	1:A:34:GLU:HG2	2.14	0.46
1:A:507:LEU:HD13	1:A:928:PRO:HD3	1.98	0.46
1:A:384:HIS:CD2	1:A:386:GLU:H	2.34	0.46
1:A:688:THR:HG22	1:A:693:PHE:HB2	1.98	0.46
1:A:790:GLU:N	1:A:791:PRO:HD2	2.31	0.46
1:A:708:LEU:O	1:A:711:GLN:HG2	2.15	0.46
1:B:131:LEU:O	1:B:135:SER:OG	2.28	0.46
1:A:744:ALA:HB2	1:A:755:SER:HB2	1.99	0.45
1:A:299:ARG:NH1	1:A:331:GLY:O	2.48	0.45
1:A:861:PRO:HA	1:A:884:LEU:HB2	1.98	0.45
1:B:394:LEU:HD12	1:B:460:ILE:HD11	1.99	0.45
1:A:866:LEU:O	1:A:870:ARG:HG3	2.17	0.45
1:B:841:PHE:CE2	1:B:868:MET:HB3	2.51	0.45
1:B:239:LEU:HG	1:B:274:GLU:HB3	1.99	0.45
1:B:898:LEU:HA	1:B:901:LEU:HD12	1.99	0.45
1:A:33:TYR:HB3	1:B:33:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:VAL:HG21	1:A:764:ILE:HD12	1.99	0.44
1:A:785:HIS:HA	1:A:835:VAL:O	2.17	0.44
1:B:592:TYR:CE1	1:B:861:PRO:HB2	2.52	0.44
1:A:51:PRO:HD2	1:A:382:ILE:HB	1.99	0.44
1:A:653:PRO:HA	1:A:702:ILE:HG23	1.99	0.44
1:A:269:GLY:HA2	1:A:348:THR:HG22	1.99	0.44
1:A:508:VAL:HG13	1:A:555:LEU:HD22	1.99	0.44
1:A:660:TYR:CE2	1:A:695:LEU:HD12	2.52	0.44
1:B:761:VAL:HA	1:B:764:ILE:HD12	2.00	0.44
1:A:743:ILE:O	1:A:838:PRO:HB3	2.18	0.44
1:A:616:ILE:HD11	1:A:696:GLU:HG2	1.99	0.43
1:B:230:LEU:HD13	1:B:282:LYS:HE3	1.99	0.43
1:A:496:LEU:HD12	1:A:541:LEU:HD23	2.00	0.43
1:B:881:LEU:HA	1:B:882:PRO:HD3	1.93	0.43
1:B:604:PRO:HG2	1:B:916:ASP:HB3	1.99	0.43
1:A:659:GLU:OE1	1:A:685:VAL:HG11	2.19	0.43
1:B:295:LEU:HD22	1:B:402:GLN:NE2	2.34	0.42
1:B:598:GLN:HB3	1:B:890:ALA:HB3	2.01	0.42
1:A:295:LEU:HD22	1:A:402:GLN:NE2	2.34	0.42
1:B:67:GLY:HA2	3:B:1106:HOH:O	2.18	0.42
1:A:848:LEU:HD23	1:A:856:PHE:HE1	1.83	0.42
1:A:341:ILE:HD12	1:A:373:LEU:HD21	2.02	0.42
1:B:747:ASN:HB3	1:B:868:MET:HG2	2.01	0.42
1:A:210:SER:HA	1:A:448:SER:HB3	2.01	0.42
1:B:259:ARG:HG2	1:B:411:HIS:NE2	2.35	0.42
1:B:679:HIS:HB2	1:B:865:LEU:HD11	2.01	0.42
1:A:652:GLN:OE1	1:A:705:ARG:HG3	2.20	0.42
1:B:256:PRO:HD2	1:B:268:ASN:ND2	2.35	0.41
1:B:168:GLN:HG2	1:B:168:GLN:H	1.75	0.41
1:A:645:LEU:N	1:A:650:TYR:HD2	2.18	0.41
1:A:144:ILE:HG21	1:A:149:LEU:HD13	2.02	0.41
1:B:719:VAL:HG13	1:B:777:GLN:HB3	2.02	0.41
1:A:436:GLN:HB2	1:A:436:GLN:HE21	1.66	0.41
1:B:144:ILE:HD11	1:B:280:VAL:HG11	2.03	0.41
1:B:493:LEU:HD23	1:B:898:LEU:HD23	2.03	0.41
1:B:581:ILE:HD11	1:B:857:LEU:HB2	2.02	0.41
1:A:727:LYS:O	1:A:730:GLU:HG2	2.21	0.41
1:A:238:LEU:HB3	1:A:240:LEU:HD12	2.03	0.41
1:B:304:ASN:OD1	1:B:455:ASN:HB2	2.21	0.41
1:A:13:LEU:HD23	1:A:13:LEU:HA	1.97	0.41
1:B:687:ALA:HB1	1:B:692:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:GLN:HE21	1:A:896:GLN:HE21	1.68	0.40
1:B:216:LEU:HD11	1:B:394:LEU:HD13	2.02	0.40
1:A:675:VAL:HG12	1:A:811:SER:CB	2.41	0.40
1:B:155:GLY:HA2	1:B:201:PRO:O	2.21	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	888/938 (95%)	843 (95%)	40 (4%)	5 (1%)	30	65
1	B	807/938 (86%)	769 (95%)	35 (4%)	3 (0%)	39	74
All	All	1695/1876 (90%)	1612 (95%)	75 (4%)	8 (0%)	34	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	GLY
1	A	563	GLU
1	A	680	SER
1	A	692	VAL
1	B	309	SER
1	B	345	GLY
1	B	680	SER
1	A	793	LEU

### 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	743/781 (95%)	698 (94%)	45 (6%)	23	55
1	B	681/781 (87%)	651 (96%)	30 (4%)	35	69
All	All	1424/1562 (91%)	1349 (95%)	75 (5%)	28	61

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	17	GLN
1	A	29	LYS
1	A	59	SER
1	A	63	LEU
1	A	76	SER
1	A	130	LEU
1	A	162	SER
1	A	173	GLU
1	A	205	VAL
1	A	222	SER
1	A	236	VAL
1	A	259	ARG
1	A	373	LEU
1	A	409	SER
1	A	413	LYS
1	A	436	GLN
1	A	448	SER
1	A	459	VAL
1	A	500	THR
1	A	539	ASN
1	A	567	ILE
1	A	577	THR
1	A	586	THR
1	A	607	ARG
1	A	614	ASN
1	A	615	GLU
1	A	624	LEU
1	A	632	ASN
1	A	645	LEU
1	A	658	LEU
1	A	674	ASP
1	A	677	MET

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Mol	Chain	Res	Type
1	A	679	HIS
1	A	708	LEU
1	A	754	ILE
1	A	769	GLU
1	A	770	SER
1	A	775	THR
1	A	780	VAL
1	A	793	LEU
1	A	807	GLN
1	A	817	THR
1	A	821	VAL
1	A	932	GLU
1	B	39	GLU
1	B	63	LEU
1	B	147	ASP
1	B	192	LEU
1	B	205	VAL
1	B	222	SER
1	B	252	LYS
1	B	257	ASP
1	B	303	ILE
1	B	341	ILE
1	B	384	HIS
1	B	394	LEU
1	B	395	MET
1	B	409	SER
1	B	433	THR
1	B	448	SER
1	B	500	THR
1	B	520	GLU
1	B	535	SER
1	B	548	GLN
1	B	553	GLU
1	B	563	GLU
1	B	654	CYS
1	B	665	LEU
1	B	692	VAL
1	B	812	LEU
1	B	817	THR
1	B	848	LEU
1	B	924	ILE
1	B	932	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	384	HIS
1	A	402	GLN
1	A	436	GLN
1	A	509	ASN
1	A	512	GLN
1	A	559	GLN
1	A	601	GLN
1	A	807	GLN
1	A	815	ASN
1	A	819	GLN
1	A	837	GLN
1	A	896	GLN
1	B	167	ASN
1	B	226	GLN
1	B	369	GLN
1	B	400	GLN
1	B	402	GLN
1	B	574	ASN
1	B	834	HIS
1	B	896	GLN

### 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

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	896/938 (95%)	0.02	13 (1%) 76 68	29, 50, 94, 123	0
1	B	823/938 (87%)	0.44	95 (11%) 6 3	31, 58, 116, 141	0
All	All	1719/1876 (91%)	0.22	108 (6%) 23 14	29, 54, 110, 141	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	743	ILE	5.5
1	B	742	ALA	5.5
1	B	834	HIS	5.5
1	B	684	TYR	5.4
1	B	588	GLN	5.3
1	B	831	TRP	5.3
1	B	785	HIS	4.8
1	B	784	PHE	4.6
1	B	738	GLU	4.3
1	B	770	SER	4.3
1	B	759	GLU	4.2
1	B	660	TYR	4.1
1	B	655	LEU	4.1
1	B	761	VAL	4.1
1	A	802	GLN	4.1
1	B	806	SER	4.1
1	B	609	ALA	4.1
1	B	732	PHE	4.0
1	B	734	ALA	4.0
1	B	692	VAL	4.0
1	B	755	SER	4.0
1	A	594	ASN	4.0
1	B	837	GLN	4.0
1	B	835	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	833	ASN	3.9
1	B	773	ILE	3.9
1	B	836	ARG	3.9
1	B	830	TYR	3.7
1	A	630	PRO	3.6
1	B	771	LEU	3.5
1	B	590	SER	3.5
1	B	736	SER	3.4
1	B	746	ILE	3.4
1	B	172	SER	3.4
1	B	608	LYS	3.4
1	B	653	PRO	3.4
1	B	807	GLN	3.3
1	B	758	ALA	3.3
1	B	659	GLU	3.3
1	B	763	ALA	3.2
1	B	756	GLY	3.2
1	B	838	PRO	3.2
1	B	772	SER	3.1
1	B	721	VAL	3.1
1	B	754	ILE	3.1
1	B	725	GLU	3.0
1	B	817	THR	3.0
1	B	735	MET	3.0
1	B	737	LEU	3.0
1	B	775	THR	2.9
1	B	782	HIS	2.9
1	A	6	GLU	2.9
1	B	813	ILE	2.8
1	B	859	ILE	2.8
1	B	680	SER	2.8
1	B	728	VAL	2.8
1	B	585	PHE	2.8
1	B	783	ALA	2.8
1	B	720	SER	2.8
1	B	729	LEU	2.8
1	B	661	ALA	2.7
1	B	752	THR	2.7
1	B	760	ALA	2.7
1	A	10	GLU	2.7
1	B	599	LEU	2.6
1	B	750	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	779	GLN	2.6
1	B	717	GLU	2.6
1	B	812	LEU	2.6
1	B	727	LYS	2.6
1	B	719	VAL	2.6
1	B	648	THR	2.5
1	A	699	LEU	2.5
1	B	90	ASP	2.5
1	B	685	VAL	2.5
1	B	832	VAL	2.5
1	A	7	GLN	2.5
1	B	777	GLN	2.4
1	B	594	ASN	2.4
1	B	866	LEU	2.4
1	B	677	MET	2.4
1	B	566	GLY	2.3
1	B	671	ILE	2.3
1	B	651	THR	2.3
1	B	695	LEU	2.3
1	B	818	GLY	2.3
1	B	890	ALA	2.3
1	B	663	PHE	2.3
1	B	666	TRP	2.3
1	A	169	LEU	2.3
1	B	774	LYS	2.2
1	B	591	GLN	2.2
1	B	916	ASP	2.2
1	A	693	PHE	2.2
1	A	827	SER	2.2
1	A	808	PRO	2.2
1	A	11	GLN	2.2
1	B	753	VAL	2.2
1	B	679	HIS	2.1
1	B	657	ALA	2.1
1	B	730	GLU	2.1
1	B	652	GLN	2.1
1	A	173	GLU	2.1
1	B	600	TYR	2.1
1	B	672	GLN	2.1
1	B	780	VAL	2.1
1	B	170	ALA	2.1
1	B	733	LYS	2.1

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	B	1001	1/1	0.96	0.15	-0.19	53,53,53,53	0
2	CA	A	1001	1/1	0.99	0.12	-1.61	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.