



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:13 PM UTC

PDB ID : 4MZ0 / pdb_00004mz0
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

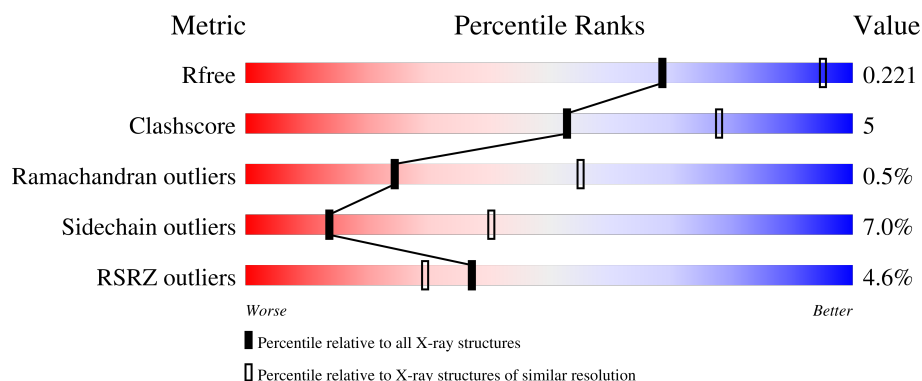
1 Overall quality at a glance

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	938	4% 75% 17% • •
1	B	938	4% 73% 14% • 12%

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 (CCD ID: CA) (formula: Ca).

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

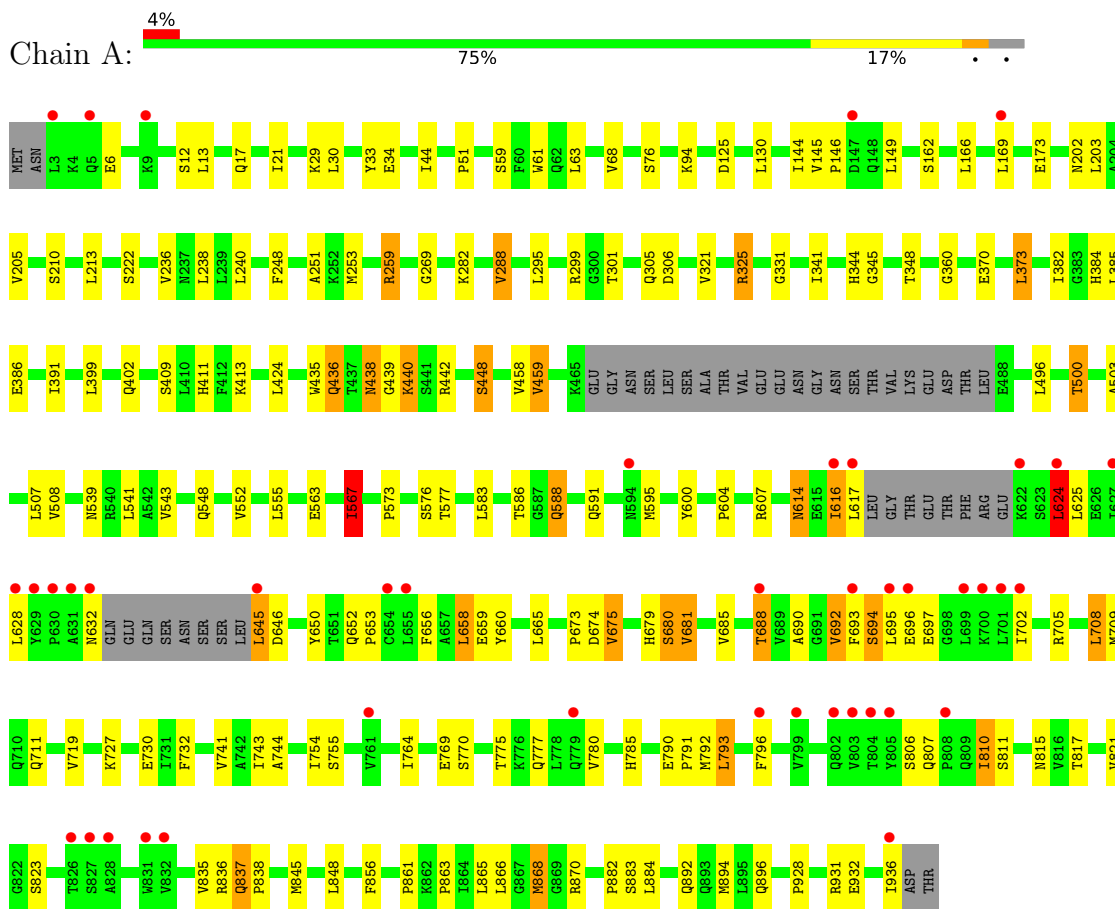
- Molecule 3 is water.

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

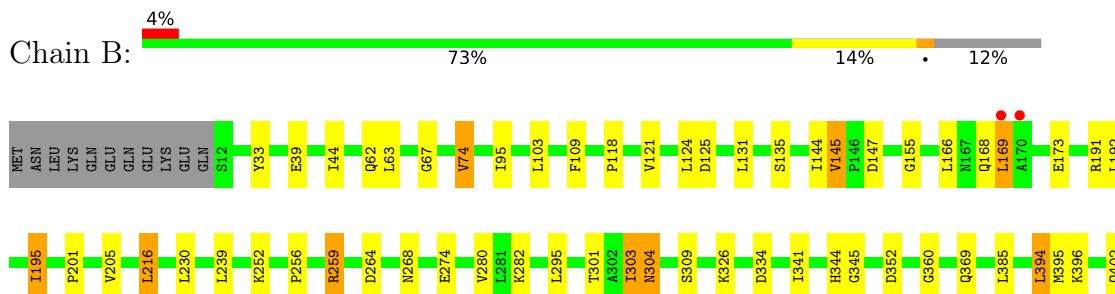
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: CurL



• Molecule 1: CurL





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.27Å 150.70Å 236.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.99 – 2.80 40.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.99-2.80) 99.7 (40.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.185 , 0.231 (Not available) , 0.221	Depositor DCC
R_{free} test set	3118 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 55.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13429	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.88	1/6995 (0.0%)	1.41	35/9506 (0.4%)
1	B	0.86	0/6417	1.40	34/8722 (0.4%)
All	All	0.87	1/13412 (0.0%)	1.40	69/18228 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	845	MET	SD-CE	-6.08	1.64	1.79

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ASP	CA-CB-CG	8.56	121.16	112.60
1	A	588	GLN	N-CA-C	7.93	119.62	110.97
1	B	334	ASP	CA-CB-CG	7.57	120.17	112.60
1	A	288	VAL	N-CA-CB	7.24	121.45	110.58
1	B	173	GLU	N-CA-C	7.08	118.50	108.74
1	A	732	PHE	CA-CB-CG	6.89	120.69	113.80
1	A	674	ASP	CA-C-N	6.71	130.96	121.96
1	A	674	ASP	C-N-CA	6.71	130.96	121.96
1	A	591	GLN	N-CA-C	6.68	119.44	110.35
1	A	125	ASP	CA-CB-CG	6.58	119.18	112.60
1	A	624	LEU	CA-C-N	6.44	128.91	120.28
1	A	624	LEU	C-N-CA	6.44	128.91	120.28
1	A	883	SER	N-CA-C	-6.39	104.18	112.68
1	A	344	HIS	N-CA-C	-6.15	104.58	111.28
1	A	439	GLY	CA-C-N	5.99	129.62	121.05
1	A	439	GLY	C-N-CA	5.99	129.62	121.05
1	A	145	VAL	N-CA-CB	5.92	118.51	111.23
1	A	688	THR	CA-C-N	5.89	128.53	120.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	688	THR	C-N-CA	5.89	128.53	120.46
1	B	44	ILE	N-CA-C	5.83	118.61	112.83
1	A	459	VAL	N-CA-CB	5.83	118.03	111.21
1	A	732	PHE	CA-C-N	5.81	128.34	120.44
1	A	732	PHE	C-N-CA	5.81	128.34	120.44
1	B	74	VAL	N-CA-CB	5.77	119.29	111.21
1	A	604	PRO	N-CA-C	5.76	121.43	113.65
1	A	6	GLU	CA-C-N	5.74	127.90	120.44
1	A	6	GLU	C-N-CA	5.74	127.90	120.44
1	B	935	TRP	CA-C-N	5.68	131.92	121.70
1	B	935	TRP	C-N-CA	5.68	131.92	121.70
1	A	646	ASP	N-CA-C	-5.66	106.14	113.16
1	B	695	LEU	N-CA-C	-5.66	105.20	111.36
1	B	169	LEU	CA-C-N	5.65	128.41	120.28
1	B	169	LEU	C-N-CA	5.65	128.41	120.28
1	B	931	ARG	N-CA-C	5.64	118.45	110.50
1	B	538	ASN	N-CA-C	5.62	117.86	111.11
1	B	591	GLN	N-CA-C	5.59	117.51	110.24
1	B	304	ASN	CA-CB-CG	5.55	118.15	112.60
1	B	815	ASN	CA-C-N	5.53	127.46	120.72
1	B	815	ASN	C-N-CA	5.53	127.46	120.72
1	A	823	SER	CA-C-N	5.50	127.92	120.38
1	A	823	SER	C-N-CA	5.50	127.92	120.38
1	B	439	GLY	CA-C-N	5.45	128.82	120.82
1	B	439	GLY	C-N-CA	5.45	128.82	120.82
1	A	306	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	931	ARG	N-CA-C	5.34	118.64	110.20
1	B	145	VAL	N-CA-CB	5.33	118.67	111.21
1	A	567	ILE	CB-CA-C	5.31	116.46	110.41
1	A	837	GLN	N-CA-C	5.27	117.94	110.24
1	A	868	MET	CA-C-N	5.25	125.76	119.94
1	A	868	MET	C-N-CA	5.25	125.76	119.94
1	A	675	VAL	N-CA-CB	5.24	118.76	111.05
1	B	697	GLU	CA-C-N	5.20	125.71	119.94
1	B	697	GLU	C-N-CA	5.20	125.71	119.94
1	B	344	HIS	N-CA-C	-5.18	105.75	111.71
1	B	806	SER	N-CA-C	5.17	117.51	109.60
1	B	95	ILE	CA-C-N	5.16	127.71	120.28
1	B	95	ILE	C-N-CA	5.16	127.71	120.28
1	B	264	ASP	CA-C-N	5.15	127.70	120.28
1	B	264	ASP	C-N-CA	5.15	127.70	120.28
1	B	124	LEU	CA-C-N	5.13	128.17	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	LEU	C-N-CA	5.13	128.17	120.83
1	B	352	ASP	CA-CB-CG	5.10	117.70	112.60
1	B	695	LEU	CA-C-N	5.10	127.07	120.44
1	B	695	LEU	C-N-CA	5.10	127.07	120.44
1	B	571	GLU	CB-CG-CD	5.09	121.25	112.60
1	A	391	ILE	N-CA-CB	5.08	118.20	110.58
1	A	203	LEU	N-CA-C	5.06	116.93	108.99
1	B	537	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	694	SER	N-CA-C	-5.01	103.05	110.46

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	6857	0	6816	82	0
1	B	6288	0	6224	50	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	130	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 (130) 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:251:ALA:HB3	1:A:253:MET:HE3	1.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:251:ALA:HB3	1:A:253:MET:CE	2.27	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:166:LEU:HA	1:A:169:LEU:HD12	1.84	0.59
1:A:259:ARG:HG2	1:A:411:HIS:NE2	2.17	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:709:MET:HG3	1:A:792:MET:HE3	1.89	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:680:SER:H	1:A:815:ASN:ND2	2.08	0.51
1:A:690:ALA:HA	1:A:810:ILE:HD12	1.93	0.51
1:A:360:GLY:HA3	1:A:424:LEU:HD22	1.92	0.51
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:103:LEU:HG	1:B:274:GLU:HG3	1.94	0.50
1:B:301:THR:HG22	1:B:458:VAL:HG22	1.92	0.50
1:A:321:VAL:O	1:A:325:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:SER:H	1:A:697:GLU:HB2	1.77	0.50
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:A:665:LEU:HD23	1:A:894:MET:HE2	1.95	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:865:LEU:HD12	1:A:868:MET:HE2	1.95	0.48
1:B:665:LEU:HD12	1:B:894:MET:HE2	1.96	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:B:579:PRO:HG3	1:B:904:LYS:HB3	1.96	0.47
1:B:554:LYS:HB3	1:B:567:ILE:HD11	1.97	0.47
1:B:583:LEU:HD13	1:B:673:PRO:HB3	1.97	0.47
1:A:600:TYR:CZ	1:A:625:LEU:HD11	2.50	0.46
1:A:30:LEU:O	1:A:34:GLU:HG2	2.14	0.46
1:A:708:LEU:HD23	1:A:796:PHE:HB2	1.97	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:A:866:LEU:O	1:A:870:ARG:HG3	2.17	0.45
1:B:394:LEU:HD12	1:B:460:ILE:HD11	1.99	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:A:33:TYR:HB3	1:B:33:TYR:CE1	2.51	0.45
1:B:898:LEU:HA	1:B:901:LEU:HD12	1.99	0.45
1:A:741:VAL:HG21	1:A:764:ILE:HD12	1.99	0.44
1:A:438:ASN:C	1:A:440:LYS:H	2.25	0.44
1:A:51:PRO:HD2	1:A:382:ILE:HB	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:695:LEU:C	1:A:695:LEU:HD23	2.44	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:A:848:LEU:HD23	1:A:856:PHE:HE1	1.83	0.42
1:B:67:GLY:HA2	3:B:1106:HOH:O	2.18	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:A:652:GLN:OE1	1:A:705:ARG:HG3	2.20	0.42
1:B:679:HIS:HB2	1:B:865:LEU:HD11	2.01	0.42
1:B:256:PRO:HD2	1:B:268:ASN:ND2	2.35	0.41
1:B:168:GLN:H	1:B:168:GLN:HG2	1.75	0.41
1:B:677:MET:HE1	1:B:844:SER:HB3	2.02	0.41
1:A:144:ILE:HG21	1:A:149:LEU:HD13	2.02	0.41
1:A:645:LEU:N	1:A:650:TYR:HD2	2.18	0.41
1:B:719:VAL:HG13	1:B:777:GLN:HB3	2.02	0.41
1:A:436:GLN:HE21	1:A:436:GLN:HB2	1.66	0.41
1:B:144:ILE:HD11	1:B:280:VAL:HG11	2.03	0.41
1:A:727:LYS:O	1:A:730:GLU:HG2	2.21	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:251:ALA:CB	1:A:253:MET:HE3	2.35	0.41
1:A:13:LEU:HD23	1:A:13:LEU:HA	1.97	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:892:GLN:HE21	1:A:896:GLN:HE21	1.68	0.40
1:B:687:ALA:HB1	1:B:692:VAL:HG12	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:MET:HE3	1:A:658:LEU:HD22	2.04	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%)	21	51
1	B	807/938 (86%)	769 (95%)	35 (4%)	3 (0%)	30	60
All	All	1695/1876 (90%)	1612 (95%)	75 (4%)	8 (0%)	24	55

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%)	686 (92%)	57 (8%)	12	36
1	B	681/781 (87%)	638 (94%)	43 (6%)	16	45
All	All	1424/1562 (91%)	1324 (93%)	100 (7%)	14	40

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	17	GLN
1	A	21	ILE
1	A	29	LYS
1	A	59	SER
1	A	63	LEU
1	A	68	VAL
1	A	76	SER
1	A	94	LYS
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	288	VAL
1	A	305	GLN
1	A	325	ARG
1	A	370	GLU
1	A	373	LEU
1	A	385	LEU
1	A	409	SER
1	A	413	LYS
1	A	436	GLN
1	A	438	ASN
1	A	440	LYS
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

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Mol	Chain	Res	Type
1	A	607	ARG
1	A	614	ASN
1	A	616	ILE
1	A	617	LEU
1	A	624	LEU
1	A	632	ASN
1	A	645	LEU
1	A	658	LEU
1	A	679	HIS
1	A	681	VAL
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	810	ILE
1	A	817	THR
1	A	821	VAL
1	A	932	GLU
1	A	936	ILE
1	B	39	GLU
1	B	62	GLN
1	B	63	LEU
1	B	74	VAL
1	B	145	VAL
1	B	147	ASP
1	B	192	LEU
1	B	195	ILE
1	B	205	VAL
1	B	216	LEU
1	B	252	LYS
1	B	259	ARG
1	B	303	ILE
1	B	326	LYS
1	B	341	ILE
1	B	369	GLN
1	B	385	LEU
1	B	394	LEU
1	B	395	MET

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Mol	Chain	Res	Type
1	B	396	LYS
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	553	GLU
1	B	563	GLU
1	B	654	CYS
1	B	665	LEU
1	B	679	HIS
1	B	683	GLU
1	B	688	THR
1	B	692	VAL
1	B	746	ILE
1	B	773	ILE
1	B	812	LEU
1	B	817	THR
1	B	848	LEU
1	B	868	MET
1	B	871	GLN
1	B	924	ILE
1	B	932	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	167	ASN
1	A	226	GLN
1	A	268	ASN
1	A	290	ASN
1	A	402	GLN
1	A	436	GLN
1	A	509	ASN
1	A	512	GLN
1	A	539	ASN
1	A	557	GLN
1	A	559	GLN
1	A	560	GLN
1	A	594	ASN

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Mol	Chain	Res	Type
1	A	601	GLN
1	A	815	ASN
1	A	819	GLN
1	A	837	GLN
1	A	849	HIS
1	A	896	GLN
1	B	143	ASN
1	B	176	GLN
1	B	202	ASN
1	B	226	GLN
1	B	290	ASN
1	B	369	GLN
1	B	400	GLN
1	B	402	GLN
1	B	403	HIS
1	B	501	GLN
1	B	539	ASN
1	B	574	ASN
1	B	602	GLN
1	B	679	HIS
1	B	747	ASN
1	B	767	HIS
1	B	833	ASN
1	B	834	HIS
1	B	896	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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, 95th 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 ²)	Q<0.9
1	A	896/938 (95%)	-0.03	42 (4%) 36 29	29, 50, 94, 123	0
1	B	823/938 (87%)	0.13	37 (4%) 38 30	31, 58, 116, 141	0
All	All	1719/1876 (91%)	0.04	79 (4%) 37 29	29, 54, 110, 141	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	802	GLN	6.7
1	B	588	GLN	5.9
1	A	645	LEU	5.7
1	A	936	ILE	5.1
1	A	617	LEU	4.8
1	B	916	ASP	4.4
1	A	702	ILE	3.9
1	A	693	PHE	3.8
1	B	609	ALA	3.5
1	B	742	ALA	3.5
1	A	622	LYS	3.4
1	B	660	TYR	3.4
1	B	936	ILE	3.4
1	B	701	LEU	3.2
1	A	700	LYS	3.2
1	A	828	ALA	3.2
1	B	760	ALA	3.1
1	A	808	PRO	3.1
1	B	684	TYR	3.1
1	A	805	TYR	3.1
1	A	831	TRP	3.0
1	B	805	TYR	3.0
1	A	147	ASP	3.0
1	B	832	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	688	THR	2.9
1	A	632	ASN	2.9
1	A	3	LEU	2.8
1	A	699	LEU	2.8
1	B	784	PHE	2.7
1	A	594	ASN	2.6
1	B	600	TYR	2.6
1	A	169	LEU	2.6
1	A	655	LEU	2.6
1	B	608	LYS	2.5
1	B	170	ALA	2.5
1	B	758	ALA	2.5
1	A	696	GLU	2.5
1	B	716	GLY	2.4
1	A	629	TYR	2.4
1	A	804	THR	2.4
1	A	701	LEU	2.4
1	A	624	LEU	2.4
1	A	9	LYS	2.4
1	B	651	THR	2.4
1	B	727	LYS	2.4
1	B	649	ALA	2.4
1	B	768	LEU	2.4
1	A	627	ILE	2.4
1	B	821	VAL	2.3
1	A	695	LEU	2.3
1	B	657	ALA	2.3
1	B	169	LEU	2.3
1	A	654	CYS	2.3
1	A	616	ILE	2.3
1	B	680	SER	2.3
1	B	658	LEU	2.3
1	B	838	PRO	2.3
1	B	743	ILE	2.2
1	A	796	PHE	2.2
1	B	686	ALA	2.2
1	B	817	THR	2.2
1	A	832	VAL	2.2
1	B	831	TRP	2.2
1	B	810	ILE	2.2
1	A	826	THR	2.2
1	A	827	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	610	LEU	2.2
1	B	890	ALA	2.2
1	A	5	GLN	2.1
1	A	779	GLN	2.1
1	A	628	LEU	2.1
1	A	803	VAL	2.1
1	B	605	VAL	2.1
1	A	630	PRO	2.1
1	B	738	GLU	2.1
1	A	799	VAL	2.1
1	B	770	SER	2.0
1	A	631	ALA	2.0
1	A	761	VAL	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 oligosaccharides 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, 95th 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	CA	B	1001	1/1	0.98	0.04	53,53,53,53	0
2	CA	A	1001	1/1	1.00	0.01	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.