



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:51 AM UTC

PDB ID : 5CXC / pdb_00005cxc
Title : Structure of Ytm1 bound to the C-terminal domain of Erb1 in P 65 2 2 space group
Authors : Wegrecki, M.; Bravo, J.
Deposited on : 2015-07-28
Resolution : 3.10 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

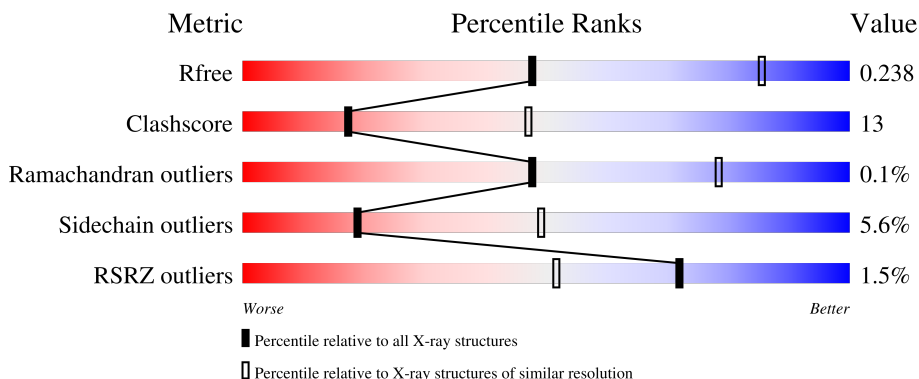
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	510	64% 22% • 11%
2	B	369	2% 65% 25% • • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6170 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 Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3418	2139	598	675	6			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP G0SFB5
A	-13	ALA	-	expression tag	UNP G0SFB5
A	-12	HIS	-	expression tag	UNP G0SFB5
A	-11	HIS	-	expression tag	UNP G0SFB5
A	-10	HIS	-	expression tag	UNP G0SFB5
A	-9	HIS	-	expression tag	UNP G0SFB5
A	-8	HIS	-	expression tag	UNP G0SFB5
A	-7	HIS	-	expression tag	UNP G0SFB5
A	-6	SER	-	expression tag	UNP G0SFB5
A	-5	SER	-	expression tag	UNP G0SFB5
A	-4	GLY	-	expression tag	UNP G0SFB5
A	-3	LEU	-	expression tag	UNP G0SFB5
A	-2	GLU	-	expression tag	UNP G0SFB5
A	-1	VAL	-	expression tag	UNP G0SFB5
A	0	LEU	-	expression tag	UNP G0SFB5

- Molecule 2 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	348	Total	C	N	O	S	0	1	0
			2750	1754	505	485	6			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	169.11Å 169.11Å 154.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.82 – 3.10 48.82 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.82-3.10) 99.9 (48.82-3.10)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.194 , 0.239 0.197 , 0.238	Depositor DCC
R_{free} test set	1237 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	97.2	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 102.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6170	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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:
CL

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	0.39	0/3490	0.91	7/4753 (0.1%)
2	B	0.45	0/2823	1.02	19/3837 (0.5%)
All	All	0.42	0/6313	0.96	26/8590 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	7
All	All	0	9

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	438	LEU	N-CA-C	-13.16	86.76	108.34
1	A	37	VAL	CA-C-N	-9.00	108.59	119.84
1	A	37	VAL	C-N-CA	-9.00	108.59	119.84
2	B	627	ILE	CA-C-N	8.87	129.30	120.52
2	B	627	ILE	C-N-CA	8.87	129.30	120.52
1	A	33	ARG	N-CA-C	8.26	122.19	112.93
2	B	749	VAL	CA-C-N	-6.06	113.29	119.83
2	B	749	VAL	C-N-CA	-6.06	113.29	119.83
2	B	795	GLY	N-CA-C	-5.99	106.46	115.32
2	B	439	LYS	CA-C-N	5.97	127.30	119.84
2	B	439	LYS	C-N-CA	5.97	127.30	119.84
1	A	33	ARG	CG-CD-NE	5.94	125.07	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	754	LEU	CB-CA-C	-5.76	104.12	109.83
2	B	631	LYS	N-CA-C	5.72	122.98	110.80
2	B	436	ASP	CA-C-N	-5.66	114.82	122.86
2	B	436	ASP	C-N-CA	-5.66	114.82	122.86
2	B	729	GLY	N-CA-C	5.62	122.51	114.64
1	A	471	LEU	N-CA-C	-5.61	105.08	111.14
2	B	607	SER	CA-C-N	5.56	125.66	119.32
2	B	607	SER	C-N-CA	5.56	125.66	119.32
2	B	439	LYS	N-CA-C	5.55	122.08	109.81
2	B	756	ASN	N-CA-C	-5.36	103.18	110.36
2	B	630	ARG	CB-CA-C	5.34	121.04	110.42
1	A	457	ALA	CB-CA-C	-5.23	110.53	116.54
1	A	153	GLY	N-CA-C	-5.23	107.83	115.72
2	B	756	ASN	N-CA-CB	5.04	115.59	109.74

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	170	SER	Peptide
1	A	33	ARG	Peptide
2	B	436	ASP	Peptide
2	B	437	GLU	Peptide
2	B	438	LEU	Peptide
2	B	439	LYS	Peptide
2	B	440	PRO	Peptide
2	B	630	ARG	Peptide
2	B	753	GLN	Peptide

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	3418	0	3363	81	0
2	B	2750	0	2763	78	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
All	All	6170	0	6126	154	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 13.

All (154) 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:756:ASN:HD22	2:B:756:ASN:N	1.68	0.92
2:B:756:ASN:HD22	2:B:756:ASN:H	1.18	0.90
2:B:612:ARG:HG3	2:B:630:ARG:HG3	1.57	0.84
1:A:77:GLU:HA	1:A:80:LEU:HG	1.59	0.82
2:B:612:ARG:CG	2:B:630:ARG:HG3	2.10	0.82
2:B:672:PRO:HG3	2:B:677:ILE:HD11	1.62	0.81
1:A:31:SER:HA	1:A:33:ARG:HD2	1.66	0.77
2:B:631:LYS:NZ	2:B:665:GLU:OE2	2.19	0.76
1:A:230:TRP:HB3	1:A:243:ALA:HB3	1.75	0.69
2:B:660:ASP:OD2	2:B:663:LYS:NZ	2.28	0.67
2:B:459:VAL:HG13	2:B:791:ALA:HB2	1.77	0.66
1:A:187:THR:HG23	1:A:190:ARG:H	1.60	0.65
2:B:540:ARG:HG2	2:B:582:LEU:HD11	1.78	0.64
2:B:459:VAL:HG12	2:B:470:THR:HG22	1.80	0.64
2:B:569:TRP:HE1	2:B:625:THR:HG23	1.63	0.64
2:B:768:HIS:ND1	2:B:794:ASP:OD2	2.31	0.63
2:B:708:ARG:HG2	2:B:709:PRO:HD2	1.80	0.62
2:B:612:ARG:HH12	2:B:632:LEU:HB2	1.63	0.62
2:B:523:LEU:HB2	2:B:583:LEU:HB2	1.81	0.61
1:A:308:ARG:NH1	1:A:354:THR:HA	2.16	0.60
2:B:519:GLU:OE2	2:B:589:SER:N	2.34	0.60
2:B:772:ASN:C	2:B:773:LYS:HG3	2.26	0.60
1:A:67:ILE:HG12	1:A:93:LEU:HD22	1.83	0.60
2:B:510:THR:O	2:B:539:SER:OG	2.19	0.60
2:B:753:GLN:CD	2:B:754:LEU:H	2.10	0.59
1:A:42:ARG:NH2	1:A:73:ARG:O	2.35	0.59
2:B:612:ARG:NH1	2:B:632:LEU:HB2	2.18	0.59
1:A:197:ASP:OD2	1:A:201:ARG:NH1	2.35	0.58
2:B:438:LEU:O	2:B:439:LYS:HB2	2.03	0.58
2:B:753:GLN:NE2	2:B:754:LEU:H	2.02	0.58
2:B:612:ARG:HD2	2:B:630:ARG:O	2.04	0.57
1:A:426:LYS:HB2	1:A:427:GLU:OE1	2.05	0.57
1:A:116:ALA:HB3	1:A:149:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:629:PHE:C	2:B:631:LYS:HG2	2.30	0.56
1:A:51:ASN:HB3	1:A:59:GLY:HA2	1.87	0.56
1:A:76:LEU:O	1:A:79:TYR:HB3	2.05	0.56
1:A:109:GLU:N	1:A:109:GLU:OE1	2.38	0.56
1:A:73:ARG:O	1:A:73:ARG:HG3	2.06	0.56
2:B:464:THR:O	2:B:784:ARG:NH2	2.39	0.56
1:A:103:VAL:HG22	1:A:104:TYR:H	1.72	0.54
1:A:152:ASP:HB3	1:A:154:LEU:HD23	1.89	0.54
2:B:671:GLN:O	2:B:708:ARG:HG3	2.07	0.54
1:A:425:THR:OG1	1:A:426:LYS:N	2.40	0.54
2:B:612:ARG:HG2	2:B:630:ARG:HG3	1.90	0.54
2:B:633[A]:ASN:OD1	2:B:633[A]:ASN:N	2.29	0.54
2:B:756:ASN:H	2:B:756:ASN:ND2	1.96	0.54
1:A:367:ILE:HB	1:A:384:LEU:HB2	1.90	0.54
1:A:196:MET:HB3	2:B:529:PRO:HG3	1.90	0.53
2:B:611:GLN:CD	2:B:612:ARG:H	2.16	0.53
1:A:152:ASP:OD2	1:A:156:ARG:NH2	2.40	0.53
1:A:36:LEU:HD21	1:A:41:ILE:HG12	1.90	0.53
2:B:756:ASN:N	2:B:756:ASN:ND2	2.42	0.53
1:A:234:ASP:OD2	1:A:237:SER:HB3	2.09	0.52
2:B:519:GLU:HG2	2:B:590:THR:HA	1.90	0.52
1:A:390:LYS:HE2	2:B:446:GLN:HB3	1.92	0.52
2:B:447:THR:HB	2:B:799:LEU:HB3	1.92	0.52
1:A:262:PRO:HD3	1:A:287:ARG:HA	1.93	0.50
2:B:618:HIS:ND1	2:B:625:THR:HG22	2.27	0.50
1:A:427:GLU:OE1	1:A:427:GLU:N	2.45	0.50
2:B:543:LEU:HD12	2:B:582:LEU:HD12	1.94	0.50
2:B:742:LEU:HD21	2:B:790:SER:HB3	1.94	0.49
1:A:387:HIS:HA	1:A:414:ARG:NH1	2.27	0.49
1:A:389:ASN:HB2	1:A:410:ASP:HB3	1.93	0.49
1:A:401:GLU:OE1	1:A:401:GLU:N	2.31	0.49
1:A:147:LEU:HD11	1:A:155:LEU:HD23	1.94	0.49
1:A:225:THR:O	1:A:246:ASP:HB3	2.12	0.49
2:B:435:PRO:HB2	2:B:438:LEU:HG	1.94	0.49
2:B:665:GLU:HG3	2:B:666:LEU:H	1.78	0.49
2:B:735:ASP:OD1	2:B:743:GLN:HB3	2.12	0.49
1:A:175:GLY:HA2	1:A:203:TRP:HH2	1.78	0.49
1:A:51:ASN:OD1	1:A:58:THR:OG1	2.31	0.48
2:B:567:GLY:HA3	2:B:625:THR:HG21	1.94	0.48
1:A:302:ALA:HB3	1:A:316:ALA:HB3	1.95	0.48
2:B:521:ILE:HD13	2:B:605:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:TRP:CE2	1:A:478:GLU:HG3	2.48	0.48
1:A:256:LYS:O	1:A:287:ARG:NH1	2.41	0.48
2:B:569:TRP:NE1	2:B:625:THR:HG23	2.29	0.48
1:A:265:SER:O	2:B:533:PRO:HG2	2.13	0.47
2:B:628:PRO:HG2	2:B:629:PHE:CE2	2.48	0.47
1:A:31:SER:O	1:A:31:SER:OG	2.29	0.47
1:A:390:LYS:NZ	2:B:483:LEU:O	2.47	0.47
1:A:422:ARG:O	1:A:434:VAL:N	2.44	0.47
2:B:726:HIS:HE1	2:B:730:LEU:HD12	1.79	0.47
1:A:306:ASP:HB3	1:A:309:ASP:O	2.14	0.47
1:A:237:SER:C	1:A:238:LYS:HG3	2.40	0.47
1:A:392:VAL:HG21	1:A:409:HIS:NE2	2.30	0.47
2:B:715:PHE:CZ	2:B:761:PRO:HG3	2.50	0.47
2:B:568:LYS:HE3	2:B:570:ALA:HB2	1.96	0.46
1:A:46:LEU:HB3	1:A:65:PHE:CZ	2.50	0.46
2:B:510:THR:HB	2:B:512:ILE:HG13	1.96	0.46
2:B:612:ARG:HD3	2:B:612:ARG:HA	1.70	0.46
1:A:31:SER:HA	1:A:33:ARG:CD	2.43	0.46
1:A:79:TYR:O	1:A:83:ASN:ND2	2.47	0.46
1:A:198:ARG:HG2	1:A:226:GLY:O	2.16	0.45
1:A:341:PRO:HG2	1:A:363:SER:OG	2.17	0.45
1:A:389:ASN:HA	2:B:446:GLN:HE22	1.82	0.45
2:B:726:HIS:ND1	2:B:730:LEU:HB2	2.32	0.45
2:B:799:LEU:HD21	2:B:801:MET:HE3	1.99	0.45
2:B:435:PRO:HG3	2:B:441:PHE:HE1	1.80	0.45
1:A:261:GLU:HG3	1:A:262:PRO:HD2	1.97	0.45
1:A:308:ARG:HH12	1:A:354:THR:HA	1.81	0.45
2:B:747:GLY:HA2	2:B:758:THR:O	2.16	0.45
2:B:737:SER:OG	2:B:739:ASP:OD1	2.29	0.44
1:A:121:SER:O	1:A:127:GLY:HA3	2.18	0.44
1:A:412:THR:HG21	1:A:414:ARG:NH1	2.33	0.44
1:A:16:LYS:HA	1:A:35:LEU:HA	1.99	0.44
1:A:301:THR:HG21	1:A:343:LEU:HA	1.99	0.44
2:B:589:SER:CB	2:B:610:GLY:HA2	2.47	0.44
1:A:97:ARG:HE	1:A:97:ARG:HB2	1.48	0.43
1:A:410:ASP:OD1	1:A:412:THR:HG22	2.18	0.43
2:B:478:ARG:HG2	2:B:490:SER:HB3	2.00	0.43
1:A:41:ILE:HG13	1:A:46:LEU:HD12	2.00	0.43
1:A:17:VAL:HG23	1:A:93:LEU:HG	2.00	0.43
2:B:519:GLU:OE2	2:B:587:VAL:HG23	2.18	0.43
2:B:726:HIS:CE1	2:B:730:LEU:HD12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:PRO:CB	2:B:786:PRO:HG3	2.49	0.43
2:B:642:HIS:HA	2:B:643:PRO:HD3	1.90	0.43
2:B:745:PHE:HA	2:B:761:PRO:HA	2.01	0.43
2:B:755:GLU:N	2:B:755:GLU:OE2	2.51	0.43
1:A:407:GLY:HA3	1:A:466:VAL:HG21	2.01	0.43
1:A:38:PRO:HA	1:A:41:ILE:HG21	2.00	0.43
1:A:384:LEU:HB3	1:A:416:TRP:CE3	2.54	0.43
2:B:776:VAL:HA	2:B:792:GLY:HA2	2.01	0.42
1:A:31:SER:C	1:A:33:ARG:H	2.27	0.42
1:A:443:ARG:HH11	1:A:479:ASP:CG	2.27	0.42
1:A:15:VAL:H	1:A:38:PRO:HD3	1.84	0.42
1:A:308:ARG:CZ	1:A:354:THR:HA	2.49	0.42
1:A:320:HIS:CE1	1:A:341:PRO:HD3	2.55	0.42
2:B:567:GLY:HA2	2:B:586:THR:O	2.20	0.42
1:A:155:LEU:HB2	1:A:168:SER:HB3	2.02	0.42
1:A:343:LEU:HD12	1:A:390:LYS:HB3	2.02	0.42
2:B:438:LEU:HD12	2:B:762:VAL:HG12	2.01	0.42
2:B:794:ASP:N	2:B:794:ASP:OD1	2.52	0.42
2:B:665:GLU:HG3	2:B:666:LEU:N	2.34	0.42
1:A:121:SER:HB3	1:A:124:SER:HB3	2.01	0.42
1:A:205:TYR:OH	1:A:207:GLU:OE1	2.30	0.42
1:A:324:THR:HB	1:A:334:SER:HB3	2.02	0.41
2:B:575:ARG:O	2:B:579:GLU:HG2	2.20	0.41
2:B:714:ARG:O	2:B:714:ARG:HG3	2.20	0.41
1:A:230:TRP:CD1	1:A:303:ALA:H	2.39	0.41
1:A:469:ASP:O	1:A:472:GLY:HA2	2.20	0.41
2:B:672:PRO:HA	2:B:701:HIS:NE2	2.34	0.41
1:A:33:ARG:H	1:A:33:ARG:HG3	1.25	0.41
1:A:382:MET:HE2	1:A:435:SER:HB2	2.02	0.41
1:A:48:ARG:HD3	1:A:48:ARG:HA	1.65	0.41
1:A:14:GLN:HA	1:A:38:PRO:HD2	2.02	0.41
1:A:34:GLN:NE2	1:A:55:MET:HE1	2.36	0.41
2:B:612:ARG:CZ	2:B:632:LEU:H	2.34	0.41
2:B:571:ARG:H	2:B:571:ARG:HG2	1.72	0.41
1:A:241:LEU:HG	1:A:305:PHE:CE2	2.55	0.40
1:A:42:ARG:NH2	1:A:74:SER:HA	2.37	0.40
2:B:631:LYS:HE3	2:B:631:LYS:HB2	1.93	0.40
2:B:522:PHE:CE1	2:B:584:ARG:HD3	2.57	0.40
1:A:31:SER:O	1:A:34:GLN:NE2	2.42	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	440/510 (86%)	417 (95%)	22 (5%)	1 (0%)	43	73
2	B	343/369 (93%)	322 (94%)	21 (6%)	0	100	100
All	All	783/879 (89%)	739 (94%)	43 (6%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	473	ILE

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	378/423 (89%)	357 (94%)	21 (6%)	19	49
2	B	296/310 (96%)	278 (94%)	18 (6%)	17	46
All	All	674/733 (92%)	635 (94%)	39 (6%)	19	48

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	28	LEU
1	A	31	SER
1	A	33	ARG
1	A	36	LEU

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Mol	Chain	Res	Type
1	A	37	VAL
1	A	43	ARG
1	A	48	ARG
1	A	67	ILE
1	A	77	GLU
1	A	170	SER
1	A	219	LEU
1	A	280	SER
1	A	294	SER
1	A	339	THR
1	A	354	THR
1	A	362	THR
1	A	373	ARG
1	A	404	LEU
1	A	470	LYS
1	A	473	ILE
2	B	509	ASP
2	B	519	GLU
2	B	521	ILE
2	B	537	GLN
2	B	574	THR
2	B	577	GLU
2	B	588	ARG
2	B	627	ILE
2	B	633[A]	ASN
2	B	633[B]	ASN
2	B	691	VAL
2	B	699	LEU
2	B	708	ARG
2	B	713	MET
2	B	756	ASN
2	B	779	ILE
2	B	784	ARG
2	B	794	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	34	GLN
1	A	134	ASN
1	A	286	GLN

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Mol	Chain	Res	Type
1	A	340	HIS
2	B	602	HIS
2	B	753	GLN
2	B	756	ASN

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 oligosaccharides 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	452/510 (88%)	0.08	6 (1%)	75 56	64, 93, 158, 182	2 (0%)
2	B	348/369 (94%)	0.09	6 (1%)	69 48	65, 98, 142, 195	5 (1%)
All	All	800/879 (91%)	0.09	12 (1%)	72 52	64, 95, 154, 195	7 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	633[A]	ASN	4.1
2	B	771	VAL	3.2
1	A	374	ALA	2.8
1	A	31	SER	2.5
1	A	282	VAL	2.5
2	B	629	PHE	2.4
1	A	57	ASP	2.3
1	A	298	ALA	2.2
2	B	718	GLU	2.1
2	B	735	ASP	2.1
1	A	411	GLY	2.1
2	B	634	GLY	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(Å ²)	Q<0.9
3	CL	B	901	1/1	0.95	0.11	93,93,93,93	0
3	CL	A	501	1/1	0.96	0.04	98,98,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.