



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:20 PM UTC

PDB ID : 1YRU / pdb_00001yru
Title : Crystal Structure analysis of the adenylyl cyclase catalytic domain of adenylyl cyclase toxin of Bordetella pertussis in presence of c-terminal calmodulin and 1mM calcium chloride
Authors : Guo, Q.; Shen, Y.; Tang, W.J.
Deposited on : 2005-02-04
Resolution : 2.50 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

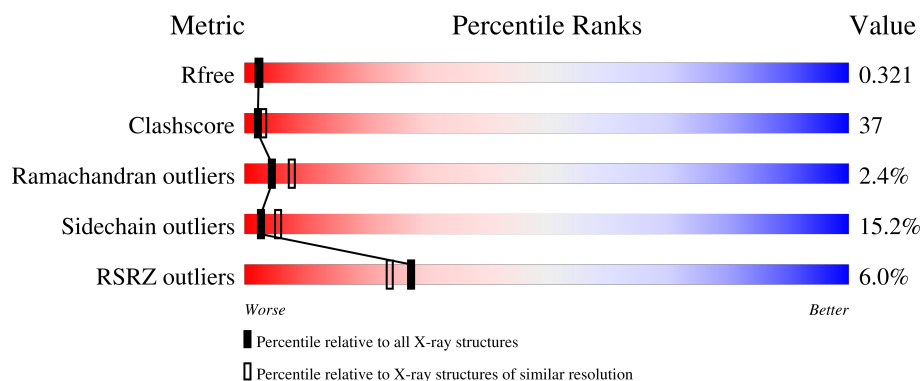
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	364	6% 46% 35% 12% . .
2	B	74	3% 50% 34% 9% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3307 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 Bifunctional hemolysin-adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2684	1664	495	519	6			

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	69	Total	C	N	O	S	0	0	0
			551	335	90	122	4			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		

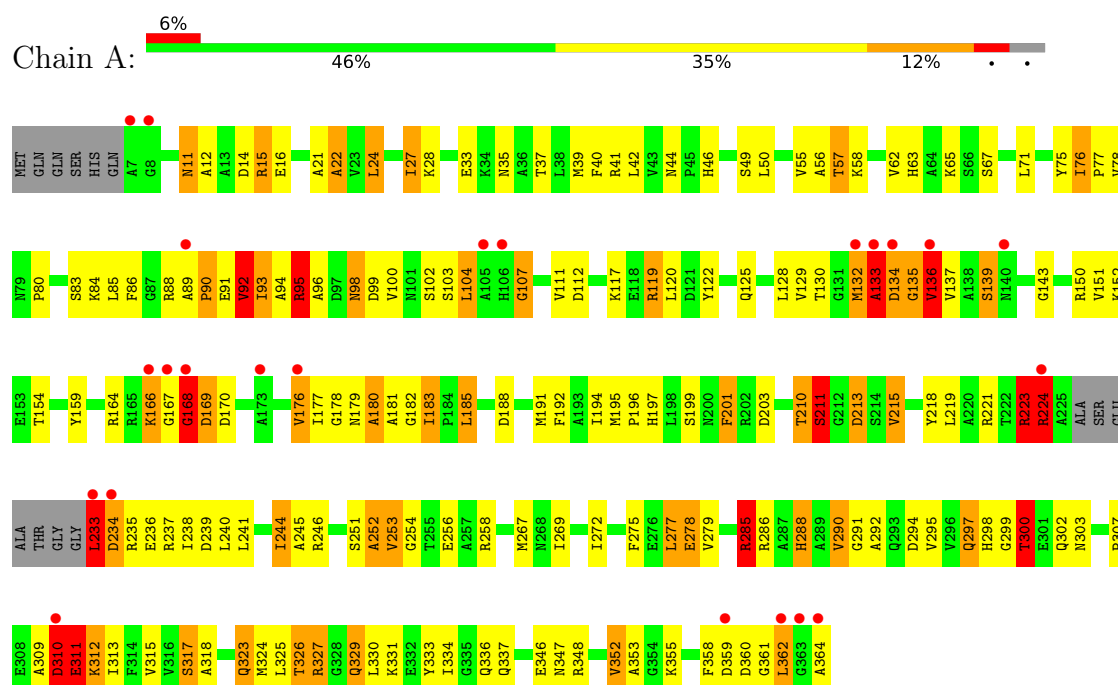
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total	O	0	0
			56	56		
4	B	14	Total	O	0	0
			14	14		

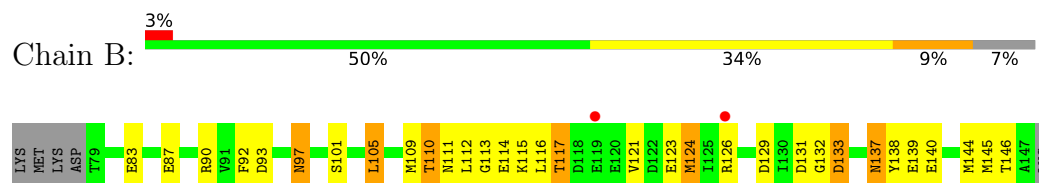
3 Residue-property plots

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: Bifunctional hemolysin-adenylate cyclase



• Molecule 2: Calmodulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	79.44Å 79.44Å 139.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.9 (30.00-2.50) 92.5 (30.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.52 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.308 0.240 , 0.321	Depositor DCC
R_{free} test set	1441 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.4	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	0.91	EDS
Total number of atoms	3307	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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 [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	1.32	12/2728 (0.4%)	1.67	56/3682 (1.5%)
2	B	1.32	1/556 (0.2%)	1.74	10/746 (1.3%)
All	All	1.32	13/3284 (0.4%)	1.68	66/4428 (1.5%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	311	GLU	C-N	-10.54	1.19	1.33
1	A	267	MET	SD-CE	8.19	2.00	1.79
1	A	312	LYS	N-CA	-7.73	1.36	1.46
1	A	223	ARG	CA-C	6.48	1.57	1.53
1	A	169	ASP	N-CA	6.34	1.54	1.46
1	A	55	VAL	CA-CB	-6.12	1.47	1.54
2	B	124	MET	SD-CE	-5.97	1.64	1.79
1	A	309	ALA	C-N	5.89	1.41	1.33
1	A	201	PHE	CA-C	-5.77	1.45	1.52
1	A	133	ALA	C-N	-5.61	1.25	1.33
1	A	295	VAL	CA-CB	-5.55	1.47	1.54
1	A	256	GLU	CA-C	-5.49	1.45	1.52
1	A	252	ALA	C-O	-5.21	1.18	1.24

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LEU	CA-C-N	-20.49	94.64	122.30
1	A	233	LEU	C-N-CA	-20.49	94.64	122.30
2	B	110	THR	N-CA-CB	-19.80	79.55	110.44
1	A	180	ALA	N-CA-C	-14.19	95.90	111.36
1	A	133	ALA	N-CA-C	-12.37	90.67	109.60
2	B	133	ASP	N-CA-C	-12.15	95.46	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	GLN	OE1-CD-NE2	-10.30	112.30	122.60
1	A	292	ALA	N-CA-C	7.89	122.03	110.59
1	A	132	MET	CA-C-N	-7.72	109.53	121.74
1	A	132	MET	C-N-CA	-7.72	109.53	121.74
1	A	311	GLU	N-CA-C	7.60	120.60	110.88
1	A	76	ILE	CA-C-N	7.24	127.64	119.83
1	A	76	ILE	C-N-CA	7.24	127.64	119.83
2	B	113	GLY	N-CA-C	7.23	126.78	113.76
1	A	211	SER	N-CA-C	-7.16	101.07	111.30
1	A	278	GLU	N-CA-C	-6.99	102.72	111.11
1	A	329	GLN	CG-CD-NE2	6.94	126.81	116.40
1	A	44	ASN	CA-C-N	-6.79	112.63	119.56
1	A	44	ASN	C-N-CA	-6.79	112.63	119.56
1	A	312	LYS	N-CA-C	-6.73	96.46	110.80
1	A	254	GLY	N-CA-C	6.54	123.03	113.48
1	A	253	VAL	N-CA-CB	-6.47	102.63	112.15
2	B	133	ASP	CA-C-N	-6.25	109.16	121.41
2	B	133	ASP	C-N-CA	-6.25	109.16	121.41
2	B	111	ASN	N-CA-C	-6.23	104.59	111.82
1	A	210	THR	CA-C-N	-6.05	113.02	123.25
1	A	210	THR	C-N-CA	-6.05	113.02	123.25
2	B	131	ASP	N-CA-C	6.01	120.34	113.19
1	A	40	PHE	N-CA-C	5.93	118.86	109.50
1	A	279	VAL	CB-CA-C	-5.87	104.22	112.14
1	A	310	ASP	N-CA-C	-5.85	101.74	110.23
1	A	234	ASP	CA-CB-CG	-5.83	106.77	112.60
1	A	22	ALA	N-CA-C	5.68	118.41	111.82
1	A	169	ASP	CA-C-N	-5.66	113.03	122.64
1	A	169	ASP	C-N-CA	-5.66	113.03	122.64
1	A	309	ALA	CA-C-N	5.62	128.69	120.71
1	A	309	ALA	C-N-CA	5.62	128.69	120.71
1	A	62	VAL	N-CA-C	5.60	115.63	108.12
1	A	288	HIS	N-CA-C	-5.57	105.29	111.36
1	A	323	GLN	N-CA-C	5.54	117.27	108.79
1	A	326	THR	N-CA-C	-5.51	103.11	110.55
1	A	300	THR	N-CA-CB	-5.47	102.14	110.45
2	B	117	THR	N-CA-C	-5.40	103.56	110.53
1	A	285	ARG	NE-CZ-NH1	-5.40	116.10	121.50
1	A	315	VAL	N-CA-C	5.35	115.61	108.11
1	A	21	ALA	N-CA-C	5.35	120.19	111.37
1	A	57	THR	N-CA-CB	-5.34	102.18	110.57
1	A	63	HIS	N-CA-C	-5.34	106.07	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	133	ASP	CA-C-O	-5.32	115.93	121.99
1	A	154	THR	N-CA-C	-5.27	101.43	108.86
2	B	110	THR	N-CA-C	-5.25	106.72	113.23
1	A	317	SER	N-CA-C	5.24	117.45	110.53
1	A	183	ILE	CB-CA-C	-5.22	105.25	110.89
1	A	58	LYS	N-CA-C	5.22	118.20	110.48
1	A	103	SER	N-CA-C	5.18	117.00	111.36
1	A	203	ASP	CA-C-N	5.13	127.47	120.54
1	A	203	ASP	C-N-CA	5.13	127.47	120.54
1	A	307	PRO	N-CA-C	5.13	118.54	110.80
1	A	168	GLY	O-C-N	-5.10	116.07	122.70
1	A	134	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	294	ASP	CA-C-N	-5.07	115.63	121.71
1	A	294	ASP	C-N-CA	-5.07	115.63	121.71
1	A	95	ARG	N-CA-C	-5.06	105.28	111.75
1	A	290	VAL	CA-C-N	-5.06	109.58	122.78
1	A	290	VAL	C-N-CA	-5.06	109.58	122.78
1	A	182	GLY	N-CA-C	5.02	122.03	115.40

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	2684	0	2624	209	0
2	B	551	0	503	38	0
3	B	2	0	0	0	0
4	A	56	0	0	4	0
4	B	14	0	0	1	0
All	All	3307	0	3127	233	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 37.

All (233) 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:109:MET:HG3	2:B:124:MET:HE1	1.27	1.13
1:A:89:ALA:HB1	1:A:90:PRO:HD2	1.26	1.11
1:A:85:LEU:HD22	1:A:88:ARG:HG3	1.31	1.11
1:A:166:LYS:CD	1:A:166:LYS:O	2.04	1.06
1:A:166:LYS:O	1:A:166:LYS:HD3	1.55	1.06
1:A:311:GLU:O	1:A:311:GLU:HG3	1.31	1.05
1:A:210:THR:CG2	1:A:211:SER:H	1.69	1.04
1:A:151:VAL:CG2	1:A:159:TYR:HB3	1.87	1.04
1:A:89:ALA:HB1	1:A:90:PRO:CD	1.89	1.03
1:A:210:THR:HG22	1:A:211:SER:H	0.87	1.02
1:A:210:THR:HG22	1:A:211:SER:N	1.59	1.00
1:A:300:THR:HG23	1:A:302:GLN:H	1.28	0.95
1:A:311:GLU:O	1:A:311:GLU:CG	2.14	0.94
1:A:132:MET:C	1:A:133:ALA:O	2.03	0.92
1:A:302:GLN:NE2	1:A:347:ASN:H	1.66	0.92
1:A:223:ARG:HE	1:A:223:ARG:HA	1.33	0.91
1:A:93:ILE:O	1:A:96:ALA:HB3	1.71	0.90
1:A:210:THR:CG2	1:A:213:ASP:H	1.87	0.87
1:A:290:VAL:HG12	1:A:291:GLY:H	1.39	0.87
1:A:211:SER:HB2	1:A:221:ARG:HH22	1.37	0.87
1:A:95:ARG:HH11	1:A:98:ASN:ND2	1.73	0.87
1:A:233:LEU:HD22	1:A:235:ARG:HG3	1.57	0.86
1:A:233:LEU:CD2	1:A:235:ARG:HG3	2.05	0.85
1:A:300:THR:CG2	1:A:302:GLN:H	1.89	0.85
1:A:358:PHE:CE2	2:B:90:ARG:HD3	2.14	0.82
1:A:327:ARG:HH11	1:A:327:ARG:HG3	1.43	0.82
2:B:137:ASN:C	2:B:137:ASN:HD22	1.84	0.82
1:A:132:MET:HB2	1:A:133:ALA:O	1.79	0.82
1:A:297:GLN:HE21	1:A:297:GLN:HA	1.42	0.82
1:A:78:VAL:O	1:A:80:PRO:HD3	1.78	0.81
2:B:116:LEU:CD1	2:B:124:MET:HE2	2.09	0.81
1:A:213:ASP:OD2	1:A:221:ARG:NH1	2.14	0.80
1:A:223:ARG:O	1:A:224:ARG:HG3	1.81	0.80
1:A:132:MET:HB3	1:A:137:VAL:HG12	1.65	0.78
1:A:324:MET:O	1:A:325:LEU:HD23	1.84	0.78
2:B:137:ASN:ND2	2:B:140:GLU:H	1.82	0.78
1:A:151:VAL:HG21	1:A:159:TYR:HB3	1.64	0.77
1:A:15:ARG:HG2	1:A:15:ARG:HH11	1.50	0.77
1:A:12:ALA:O	1:A:16:GLU:HG3	1.84	0.77
1:A:269:ILE:HG22	1:A:269:ILE:O	1.85	0.77
1:A:85:LEU:CD2	1:A:88:ARG:HG3	2.13	0.76
1:A:119:ARG:HD3	4:A:374:HOH:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:O	1:A:334:ILE:HG13	1.87	0.74
1:A:362:LEU:HG	2:B:90:ARG:HH22	1.49	0.74
1:A:132:MET:HA	1:A:137:VAL:HA	1.67	0.74
1:A:302:GLN:HE21	1:A:347:ASN:N	1.85	0.73
1:A:197:HIS:HD2	1:A:199:SER:OG	1.71	0.72
1:A:272:ILE:HD13	1:A:277:LEU:HB2	1.71	0.72
1:A:50:LEU:HD21	1:A:119:ARG:HD2	1.71	0.72
1:A:215:VAL:HB	2:B:114:GLU:OE1	1.91	0.71
1:A:237:ARG:NH1	1:A:241:LEU:HD11	2.05	0.71
1:A:167:GLY:O	1:A:168:GLY:O	2.09	0.70
1:A:290:VAL:HG12	1:A:291:GLY:N	2.04	0.70
1:A:41:ARG:HE	1:A:310:ASP:CG	2.00	0.70
1:A:234:ASP:OD2	1:A:237:ARG:HB2	1.92	0.69
2:B:116:LEU:HD11	2:B:124:MET:HE2	1.74	0.69
1:A:135:GLY:HA2	1:A:151:VAL:HG12	1.74	0.69
1:A:164:ARG:HD2	1:A:169:ASP:O	1.91	0.69
1:A:210:THR:HG21	1:A:213:ASP:CA	2.22	0.69
1:A:89:ALA:CB	1:A:90:PRO:CD	2.62	0.69
1:A:210:THR:HG21	1:A:213:ASP:H	1.54	0.69
2:B:93:ASP:OD1	2:B:97:ASN:O	2.11	0.69
1:A:80:PRO:HG3	1:A:100:VAL:HG21	1.73	0.69
1:A:302:GLN:NE2	1:A:347:ASN:N	2.39	0.68
1:A:269:ILE:HG23	1:A:298:HIS:HA	1.75	0.67
1:A:210:THR:HG21	1:A:213:ASP:N	2.10	0.67
1:A:75:TYR:HB3	1:A:176:VAL:HG21	1.76	0.67
1:A:85:LEU:HD13	1:A:92:VAL:HG12	1.77	0.66
1:A:130:THR:OG1	1:A:139:SER:HA	1.94	0.66
2:B:129:ASP:OD1	2:B:133:ASP:O	2.13	0.65
1:A:41:ARG:NE	1:A:310:ASP:OD1	2.30	0.64
1:A:211:SER:HB2	1:A:221:ARG:NH2	2.11	0.64
1:A:22:ALA:CB	1:A:290:VAL:HG11	2.29	0.63
2:B:105:LEU:CD1	2:B:124:MET:HE3	2.29	0.63
1:A:258:ARG:HH22	2:B:87:GLU:CD	2.07	0.62
1:A:178:GLY:HA2	1:A:185:LEU:HG	1.81	0.62
1:A:333:TYR:CE2	1:A:337:GLN:HG3	2.35	0.62
1:A:362:LEU:HD23	1:A:362:LEU:O	2.01	0.61
2:B:137:ASN:C	2:B:137:ASN:ND2	2.58	0.61
1:A:196:PRO:HB3	1:A:275:PHE:CE2	2.36	0.61
1:A:353:ALA:O	1:A:355:LYS:HE3	2.00	0.61
1:A:326:THR:HG23	1:A:329:GLN:OE1	2.00	0.61
1:A:358:PHE:CZ	2:B:90:ARG:HD3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD21	1:A:324:MET:HE1	1.82	0.60
1:A:132:MET:CB	1:A:133:ALA:O	2.48	0.60
1:A:95:ARG:HH11	1:A:98:ASN:HD22	1.47	0.60
1:A:210:THR:HG21	1:A:213:ASP:CB	2.31	0.60
1:A:327:ARG:HH11	1:A:327:ARG:CG	2.14	0.60
1:A:41:ARG:HG2	1:A:310:ASP:OD1	2.01	0.60
1:A:298:HIS:HD2	1:A:299:GLY:O	1.83	0.60
1:A:135:GLY:CA	1:A:151:VAL:HG12	2.32	0.59
1:A:177:ILE:HG22	1:A:185:LEU:HD12	1.83	0.59
1:A:11:ASN:ND2	1:A:14:ASP:H	2.00	0.59
1:A:223:ARG:HA	1:A:223:ARG:NE	2.06	0.59
1:A:15:ARG:HG2	1:A:15:ARG:NH1	2.16	0.59
1:A:210:THR:HG22	1:A:213:ASP:H	1.63	0.59
1:A:133:ALA:HB3	1:A:136:VAL:HG23	1.83	0.58
1:A:24:LEU:HA	1:A:27:ILE:HG13	1.83	0.58
1:A:327:ARG:HG3	1:A:327:ARG:NH1	2.18	0.58
1:A:352:VAL:HG12	1:A:352:VAL:O	2.02	0.58
1:A:269:ILE:O	1:A:269:ILE:CG2	2.51	0.57
1:A:135:GLY:O	1:A:150:ARG:HA	2.05	0.57
1:A:57:THR:HG23	1:A:188:ASP:CB	2.35	0.57
1:A:98:ASN:O	1:A:102:SER:N	2.30	0.56
1:A:92:VAL:O	1:A:93:ILE:C	2.48	0.56
1:A:133:ALA:C	1:A:135:GLY:H	2.13	0.56
1:A:238:ILE:HD11	2:B:123:GLU:HB3	1.88	0.56
1:A:300:THR:CG2	1:A:302:GLN:N	2.65	0.56
1:A:362:LEU:HG	2:B:90:ARG:NH2	2.20	0.56
1:A:80:PRO:HG3	1:A:100:VAL:CG2	2.35	0.55
1:A:237:ARG:HH11	1:A:241:LEU:HD11	1.70	0.55
1:A:46:HIS:CE1	1:A:128:LEU:HD11	2.42	0.55
1:A:302:GLN:HE21	1:A:346:GLU:HA	1.72	0.55
1:A:167:GLY:C	1:A:168:GLY:O	2.49	0.55
1:A:95:ARG:NH1	1:A:98:ASN:ND2	2.50	0.54
2:B:137:ASN:HD21	2:B:140:GLU:H	1.52	0.54
1:A:151:VAL:HG23	1:A:159:TYR:HB3	1.84	0.54
2:B:115:LYS:O	2:B:116:LEU:HD23	2.08	0.54
1:A:166:LYS:O	1:A:166:LYS:HD2	2.02	0.53
1:A:100:VAL:O	1:A:104:LEU:HD12	2.08	0.53
1:A:78:VAL:HG13	1:A:100:VAL:HG11	1.91	0.53
1:A:132:MET:CA	1:A:137:VAL:HA	2.38	0.53
1:A:201:PHE:CZ	1:A:252:ALA:HA	2.44	0.53
1:A:323:GLN:HG3	1:A:325:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LYS:HG2	1:A:159:TYR:HE1	1.74	0.53
1:A:71:LEU:HD11	1:A:137:VAL:HG21	1.91	0.53
1:A:179:ASN:HB3	1:A:181:ALA:N	2.24	0.52
1:A:22:ALA:HB3	1:A:290:VAL:HG11	1.92	0.52
1:A:95:ARG:HH11	1:A:98:ASN:HD21	1.52	0.52
1:A:197:HIS:CD2	1:A:199:SER:OG	2.59	0.52
1:A:364:ALA:HA	2:B:138:TYR:CD2	2.45	0.52
1:A:210:THR:HG21	1:A:213:ASP:HB2	1.92	0.52
2:B:101:SER:HB3	4:B:42:HOH:O	2.09	0.52
2:B:105:LEU:HD11	2:B:124:MET:CE	2.40	0.52
2:B:116:LEU:HD12	2:B:124:MET:HE2	1.90	0.52
1:A:277:LEU:O	1:A:278:GLU:C	2.52	0.51
1:A:57:THR:HG22	1:A:297:GLN:CG	2.41	0.51
1:A:24:LEU:HD22	1:A:28:LYS:HE3	1.91	0.51
1:A:179:ASN:HB2	1:A:183:ILE:H	1.76	0.51
2:B:109:MET:HG3	2:B:124:MET:CE	2.20	0.51
1:A:78:VAL:HG13	1:A:100:VAL:CG1	2.42	0.50
1:A:272:ILE:CD1	1:A:277:LEU:HB2	2.39	0.50
1:A:89:ALA:O	1:A:92:VAL:N	2.45	0.50
1:A:111:VAL:CG1	1:A:112:ASP:N	2.74	0.49
1:A:86:PHE:CZ	1:A:143:GLY:HA2	2.47	0.49
1:A:166:LYS:CD	1:A:166:LYS:C	2.72	0.49
1:A:327:ARG:CG	1:A:327:ARG:NH1	2.72	0.49
1:A:24:LEU:HD22	1:A:28:LYS:CE	2.43	0.49
1:A:90:PRO:O	1:A:94:ALA:CB	2.61	0.49
1:A:39:MET:O	1:A:192:PHE:N	2.45	0.49
1:A:151:VAL:HG22	1:A:152:LYS:N	2.27	0.48
1:A:352:VAL:O	1:A:352:VAL:CG1	2.60	0.48
1:A:11:ASN:HD22	1:A:14:ASP:H	1.62	0.48
1:A:57:THR:HG22	1:A:297:GLN:HG3	1.95	0.48
2:B:117:THR:O	2:B:121:VAL:HG23	2.14	0.48
1:A:67:SER:HB2	1:A:77:PRO:HG3	1.94	0.48
1:A:310:ASP:OD2	1:A:310:ASP:N	2.45	0.47
2:B:105:LEU:HD12	2:B:124:MET:HE3	1.96	0.47
1:A:80:PRO:HB3	1:A:96:ALA:HB1	1.97	0.47
1:A:129:VAL:HG12	1:A:129:VAL:O	2.13	0.47
1:A:132:MET:HB3	1:A:137:VAL:HA	1.95	0.47
1:A:233:LEU:CD2	1:A:235:ARG:CG	2.85	0.47
1:A:211:SER:CB	1:A:221:ARG:HH22	2.19	0.47
1:A:233:LEU:HD21	1:A:235:ARG:HG3	1.90	0.47
2:B:105:LEU:CD1	2:B:124:MET:CE	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:MET:HE3	2:B:144:MET:HA	1.95	0.47
1:A:234:ASP:HB3	1:A:237:ARG:HB3	1.96	0.47
1:A:98:ASN:OD1	1:A:98:ASN:N	2.48	0.47
1:A:177:ILE:HG22	1:A:185:LEU:CD1	2.44	0.47
1:A:238:ILE:CD1	2:B:123:GLU:HB3	2.45	0.47
1:A:133:ALA:C	1:A:135:GLY:N	2.73	0.46
1:A:135:GLY:HA2	1:A:151:VAL:CG1	2.44	0.46
1:A:22:ALA:HB1	1:A:290:VAL:HG11	1.96	0.46
1:A:210:THR:CG2	1:A:213:ASP:N	2.65	0.46
1:A:246:ARG:HD3	4:A:391:HOH:O	2.15	0.46
2:B:146:THR:HG22	2:B:146:THR:O	2.14	0.46
1:A:151:VAL:HG22	1:A:159:TYR:HB3	1.90	0.46
1:A:176:VAL:HG22	4:A:382:HOH:O	2.16	0.46
1:A:211:SER:HB2	1:A:221:ARG:HH12	1.80	0.46
1:A:245:ALA:HB1	2:B:92:PHE:CZ	2.51	0.46
1:A:285:ARG:HH11	1:A:285:ARG:HD3	1.59	0.46
1:A:195:MET:HE1	1:A:337:GLN:HB2	1.98	0.46
1:A:84:LYS:C	1:A:86:PHE:H	2.25	0.45
1:A:210:THR:CG2	1:A:211:SER:N	2.33	0.45
1:A:50:LEU:HD23	1:A:50:LEU:HA	1.67	0.45
1:A:56:ALA:O	1:A:185:LEU:HA	2.16	0.45
1:A:191:MET:HE1	1:A:194:ILE:HD11	1.97	0.45
1:A:14:ASP:OD2	1:A:28:LYS:NZ	2.49	0.45
1:A:35:ASN:HD22	1:A:318:ALA:HB1	1.80	0.45
2:B:126:ARG:HE	2:B:126:ARG:HB2	1.53	0.44
1:A:133:ALA:O	1:A:135:GLY:N	2.50	0.44
1:A:179:ASN:HB2	1:A:183:ILE:N	2.32	0.44
1:A:210:THR:HG21	1:A:213:ASP:C	2.42	0.44
1:A:241:LEU:HD22	2:B:109:MET:HE2	2.00	0.44
1:A:22:ALA:HB1	1:A:290:VAL:HG21	1.98	0.44
1:A:119:ARG:O	1:A:119:ARG:HG3	2.16	0.44
1:A:360:ASP:O	1:A:361:GLY:C	2.60	0.44
1:A:286:ARG:HD2	1:A:286:ARG:HA	1.65	0.44
1:A:76:ILE:HA	1:A:77:PRO:HD2	1.72	0.44
1:A:302:GLN:NE2	1:A:346:GLU:HA	2.32	0.44
1:A:179:ASN:HB3	1:A:181:ALA:H	1.82	0.44
1:A:223:ARG:HD3	1:A:236:GLU:OE1	2.17	0.43
1:A:219:LEU:O	1:A:223:ARG:HB2	2.17	0.43
1:A:210:THR:HG23	1:A:218:TYR:CD1	2.54	0.43
1:A:285:ARG:HE	1:A:285:ARG:HB3	1.65	0.43
1:A:95:ARG:HD3	1:A:95:ARG:HA	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:GLY:O	1:A:180:ALA:HA	2.18	0.42
1:A:169:ASP:C	1:A:169:ASP:OD2	2.60	0.42
1:A:91:GLU:OE2	1:A:95:ARG:HG2	2.19	0.42
1:A:15:ARG:HH11	1:A:15:ARG:CG	2.20	0.42
1:A:244:ILE:HD12	2:B:112:LEU:HB3	2.01	0.42
1:A:272:ILE:HD13	1:A:277:LEU:CB	2.47	0.42
1:A:333:TYR:O	1:A:334:ILE:C	2.63	0.42
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.64	0.42
1:A:15:ARG:NH1	1:A:15:ARG:CG	2.80	0.42
1:A:258:ARG:HD3	1:A:303:ASN:HD21	1.84	0.42
1:A:132:MET:HB3	1:A:137:VAL:CG1	2.44	0.42
1:A:317:SER:OG	1:A:333:TYR:OH	2.27	0.42
1:A:151:VAL:HG21	1:A:159:TYR:CB	2.43	0.41
1:A:95:ARG:NH1	1:A:98:ASN:HD21	2.17	0.41
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.76	0.41
2:B:137:ASN:HD22	2:B:140:GLU:H	1.63	0.41
1:A:288:HIS:O	1:A:290:VAL:O	2.37	0.41
1:A:246:ARG:HG3	2:B:145:MET:SD	2.60	0.41
2:B:132:GLY:C	2:B:133:ASP:O	2.52	0.41
1:A:96:ALA:O	1:A:99:ASP:HB2	2.21	0.40
1:A:119:ARG:NH2	1:A:122:TYR:CE2	2.90	0.40
1:A:331:LYS:HE2	1:A:331:LYS:HB3	1.75	0.40
2:B:109:MET:CG	2:B:124:MET:HE1	2.20	0.40
1:A:42:LEU:CD2	1:A:324:MET:HE1	2.48	0.40
1:A:85:LEU:HD13	1:A:92:VAL:CG1	2.48	0.40
1:A:300:THR:HG21	4:A:367:HOH:O	2.20	0.40
1:A:348:ARG:HD3	2:B:83:GLU:CD	2.46	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	347/364 (95%)	309 (89%)	29 (8%)	9 (3%)	4	7
2	B	67/74 (90%)	59 (88%)	7 (10%)	1 (2%)	8	16
All	All	414/438 (94%)	368 (89%)	36 (9%)	10 (2%)	4	8

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97	ASN
1	A	134	ASP
1	A	168	GLY
1	A	135	GLY
1	A	107	GLY
1	A	133	ALA
1	A	224	ARG
1	A	92	VAL
1	A	352	VAL
1	A	136	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	271/280 (97%)	225 (83%)	46 (17%)	2	4
2	B	59/64 (92%)	55 (93%)	4 (7%)	14	31
All	All	330/344 (96%)	280 (85%)	50 (15%)	3	5

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	15	ARG
1	A	24	LEU
1	A	27	ILE
1	A	33	GLU
1	A	37	THR

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Mol	Chain	Res	Type
1	A	49	SER
1	A	65	LYS
1	A	83	SER
1	A	90	PRO
1	A	92	VAL
1	A	93	ILE
1	A	95	ARG
1	A	98	ASN
1	A	104	LEU
1	A	119	ARG
1	A	125	GLN
1	A	136	VAL
1	A	139	SER
1	A	166	LYS
1	A	170	ASP
1	A	176	VAL
1	A	185	LEU
1	A	211	SER
1	A	213	ASP
1	A	215	VAL
1	A	223	ARG
1	A	224	ARG
1	A	233	LEU
1	A	239	ASP
1	A	240	LEU
1	A	244	ILE
1	A	251	SER
1	A	253	VAL
1	A	277	LEU
1	A	285	ARG
1	A	297	GLN
1	A	300	THR
1	A	310	ASP
1	A	311	GLU
1	A	312	LYS
1	A	313	ILE
1	A	327	ARG
1	A	336	GLN
1	A	359	ASP
1	A	362	LEU
2	B	105	LEU
2	B	110	THR

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Mol	Chain	Res	Type
2	B	137	ASN
2	B	139	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	35	ASN
1	A	108	HIS
1	A	140	ASN
1	A	197	HIS
1	A	260	GLN
1	A	281	ASN
1	A	297	GLN
1	A	298	HIS
1	A	302	GLN
1	A	304	ASN
1	A	337	GLN
2	B	107	HIS
2	B	111	ASN
2	B	135	GLN
2	B	137	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	311:GLU	C	312:LYS	N	1.18

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	351/364 (96%)	0.40	23 (6%) 24 21	11, 34, 59, 72	0
2	B	69/74 (93%)	0.14	2 (2%) 53 49	18, 30, 47, 56	0
All	All	420/438 (95%)	0.35	25 (5%) 27 24	11, 33, 58, 72	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	LEU	6.2
1	A	133	ALA	4.9
1	A	363	GLY	3.7
1	A	310	ASP	3.6
1	A	168	GLY	3.2
1	A	364	ALA	3.1
1	A	7	ALA	3.0
1	A	224	ARG	2.9
2	B	126	ARG	2.8
1	A	8	GLY	2.7
1	A	140	ASN	2.6
1	A	136	VAL	2.6
1	A	105	ALA	2.6
1	A	134	ASP	2.4
1	A	234	ASP	2.4
1	A	106	HIS	2.3
1	A	173	ALA	2.2
1	A	362	LEU	2.2
1	A	167	GLY	2.1
1	A	176	VAL	2.1
1	A	166	LYS	2.1
1	A	132	MET	2.0
1	A	89	ALA	2.0
2	B	119	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	359	ASP	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	CA	B	800	1/1	0.97	0.04	31,31,31,31	0
3	CA	B	801	1/1	0.98	0.04	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.