



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:19 PM UTC

PDB ID : 3UNG / pdb_00003ung
Title : Structure of the Cmr2 subunit of the CRISPR RNA silencing complex
Authors : Cocozaki, A.I.; Ramia, N.F.; Shao, Y.; Hale, C.R.; Terns, R.M.; Terns, M.P.;
Li, H.
Deposited on : 2011-11-15
Resolution : 2.31 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

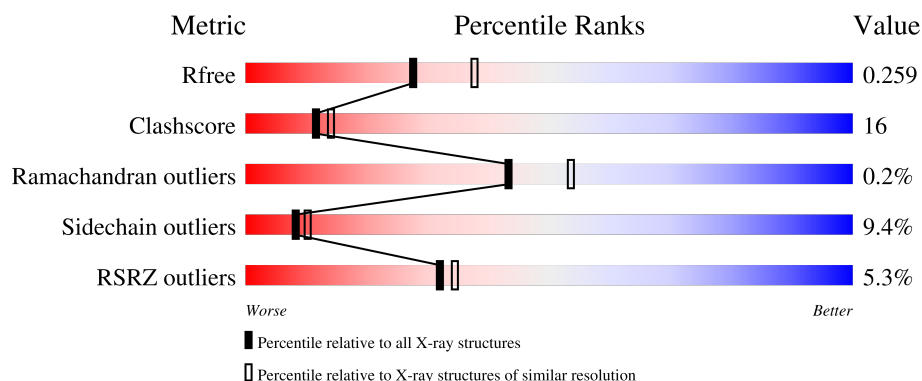
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	C	693	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4534 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 Cmr2dHD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	548	Total	C	N	O	S	0	0	0
			4469	2905	740	811	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	179	MET	-	expression tag	UNP Q8U1S6
C	180	ARG	-	expression tag	UNP Q8U1S6
C	181	GLY	-	expression tag	UNP Q8U1S6
C	182	SER	-	expression tag	UNP Q8U1S6
C	183	HIS	-	expression tag	UNP Q8U1S6
C	184	HIS	-	expression tag	UNP Q8U1S6
C	185	HIS	-	expression tag	UNP Q8U1S6
C	186	HIS	-	expression tag	UNP Q8U1S6
C	187	HIS	-	expression tag	UNP Q8U1S6
C	188	HIS	-	expression tag	UNP Q8U1S6
C	189	GLY	-	expression tag	UNP Q8U1S6
C	190	MET	-	expression tag	UNP Q8U1S6
C	191	ALA	-	expression tag	UNP Q8U1S6
C	192	SER	-	expression tag	UNP Q8U1S6
C	193	MET	-	expression tag	UNP Q8U1S6
C	194	THR	-	expression tag	UNP Q8U1S6
C	195	GLY	-	expression tag	UNP Q8U1S6
C	196	GLY	-	expression tag	UNP Q8U1S6
C	197	GLN	-	expression tag	UNP Q8U1S6
C	198	GLN	-	expression tag	UNP Q8U1S6
C	199	MET	-	expression tag	UNP Q8U1S6
C	200	GLY	-	expression tag	UNP Q8U1S6
C	201	ARG	-	expression tag	UNP Q8U1S6
C	202	ASP	-	expression tag	UNP Q8U1S6
C	203	LEU	-	expression tag	UNP Q8U1S6
C	204	TYR	-	expression tag	UNP Q8U1S6
C	205	ASP	-	expression tag	UNP Q8U1S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	206	ASP	-	expression tag	UNP Q8U1S6
C	207	ASP	-	expression tag	UNP Q8U1S6
C	208	ASP	-	expression tag	UNP Q8U1S6
C	209	LYS	-	expression tag	UNP Q8U1S6
C	210	ASP	-	expression tag	UNP Q8U1S6
C	211	HIS	-	expression tag	UNP Q8U1S6
C	212	PRO	-	expression tag	UNP Q8U1S6
C	213	PHE	-	expression tag	UNP Q8U1S6
C	214	THR	-	expression tag	UNP Q8U1S6

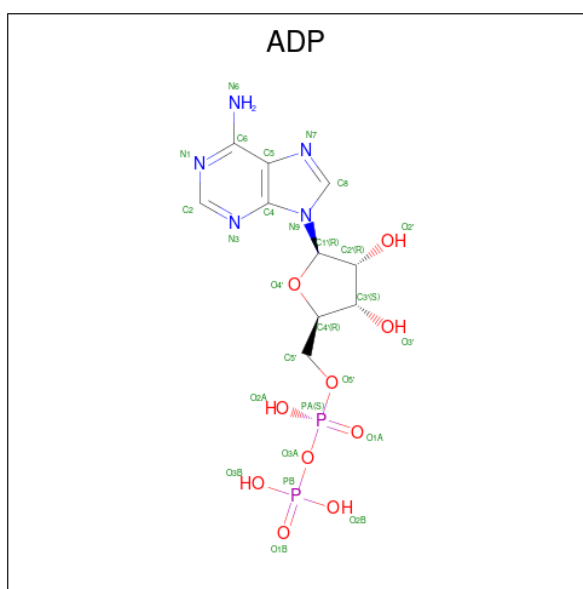
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Ca 2 2	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

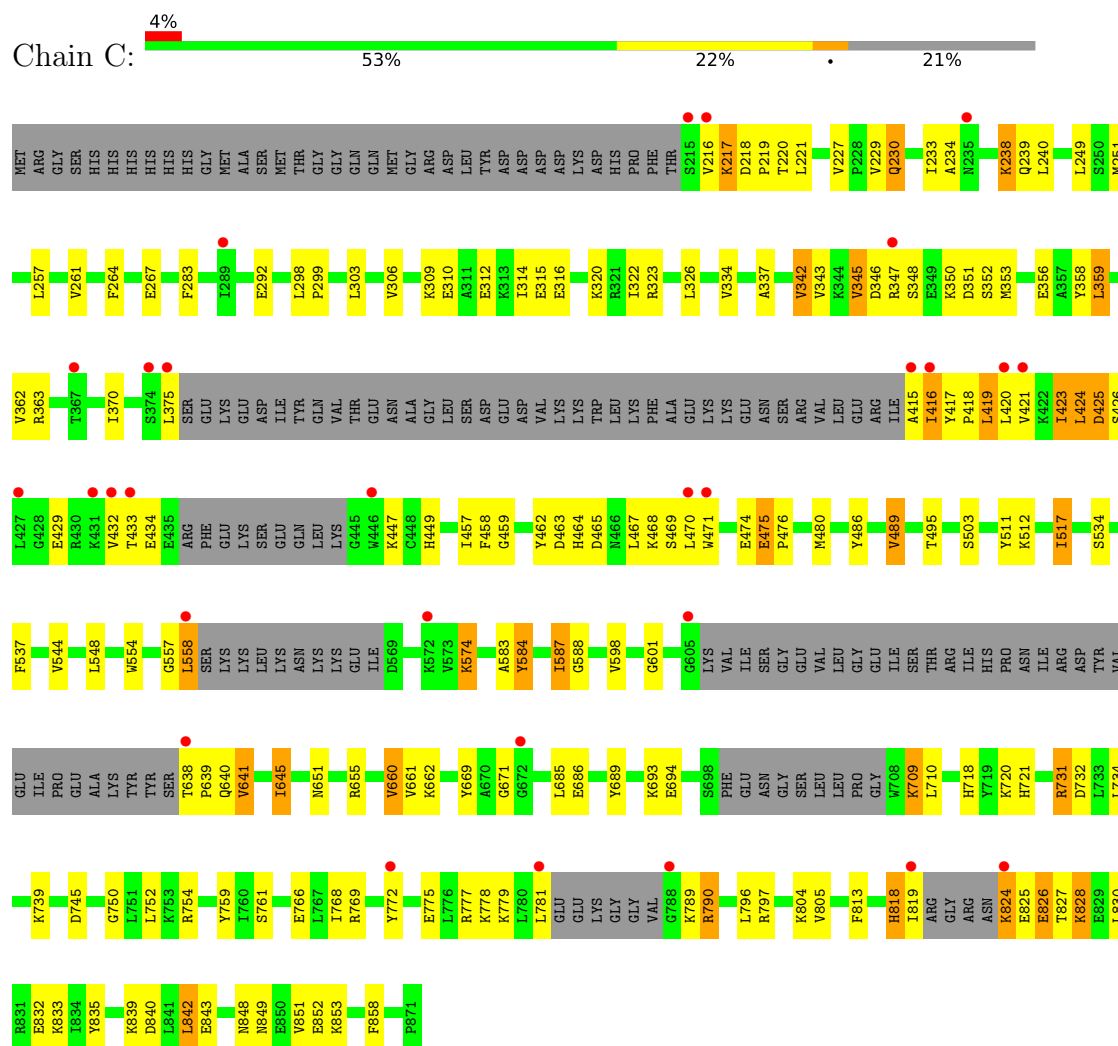
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	35	Total	O	0	0
			35	35		

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: Cmr2dHD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.17Å 85.07Å 140.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 2.31 29.61 – 2.31	Depositor EDS
% Data completeness (in resolution range)	79.9 (29.61-2.31) 78.6 (29.61-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.203 , 0.264 0.199 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (5.68%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 75.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4534	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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, ZN, ADP

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	C	0.55	0/4558	0.90	6/6145 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	495	THR	N-CA-C	-6.97	99.65	109.69
1	C	423	ILE	N-CA-C	6.26	116.90	110.82
1	C	584	TYR	N-CA-C	-5.15	105.58	111.14
1	C	475	GLU	CA-C-N	5.04	124.94	119.85
1	C	475	GLU	C-N-CA	5.04	124.94	119.85
1	C	660	VAL	N-CA-C	5.02	116.47	111.00

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	C	4469	0	4567	145	0
2	C	2	0	0	0	0
3	C	1	0	0	0	0
4	C	27	0	12	1	0
5	C	35	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4534	0	4579	145	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 16.

All (145) 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:C:517:ILE:HG13	1:C:587:ILE:HD11	1.23	1.10
1:C:230:GLN:O	1:C:234:ALA:HB2	1.55	1.05
1:C:219:PRO:HB2	1:C:375:LEU:HD12	1.48	0.92
1:C:731:ARG:HG2	1:C:731:ARG:HH11	1.34	0.90
1:C:362:VAL:HA	1:C:480:MET:CE	2.03	0.89
1:C:775:GLU:HB3	1:C:779:LYS:HE2	1.54	0.89
1:C:766:GLU:H	1:C:766:GLU:CD	1.85	0.85
1:C:230:GLN:O	1:C:234:ALA:CB	2.28	0.82
1:C:601:GLY:HA2	1:C:710:LEU:HD12	1.61	0.81
1:C:775:GLU:O	1:C:779:LYS:HD2	1.82	0.79
1:C:731:ARG:HH11	1:C:731:ARG:CG	1.95	0.79
1:C:238:LYS:HE2	1:C:503:SER:HA	1.66	0.76
1:C:315:GLU:HG3	1:C:370:ILE:HB	1.69	0.73
1:C:517:ILE:HG13	1:C:587:ILE:CD1	2.13	0.72
1:C:468:LYS:O	1:C:474:GLU:HA	1.93	0.69
1:C:458:PHE:HB3	1:C:462:TYR:HD2	1.59	0.67
1:C:358:TYR:CZ	1:C:457:ILE:O	2.49	0.66
1:C:217:LYS:HZ2	1:C:217:LYS:HB2	1.61	0.65
1:C:825:GLU:O	1:C:828:LYS:HG3	1.97	0.65
1:C:824:LYS:HD2	1:C:824:LYS:C	2.22	0.64
1:C:347:ARG:HH11	1:C:350:LYS:HD3	1.62	0.63
1:C:419:LEU:O	1:C:423:ILE:HD13	1.99	0.63
1:C:334:VAL:HB	1:C:353:MET:HE3	1.80	0.63
1:C:557:GLY:O	1:C:558:LEU:HD22	1.99	0.62
1:C:323:ARG:HG3	1:C:363:ARG:HG3	1.81	0.62
1:C:417:TYR:O	1:C:421:VAL:HG23	2.01	0.61
1:C:216:VAL:HB	1:C:217:LYS:HZ1	1.65	0.61
1:C:216:VAL:HB	1:C:217:LYS:HB2	1.83	0.60
1:C:709:LYS:HE2	1:C:745:ASP:HB2	1.82	0.60
1:C:220:THR:HB	1:C:306:VAL:O	2.02	0.59
1:C:459:GLY:HA2	1:C:467:LEU:HD22	1.85	0.59
1:C:718:HIS:CD2	1:C:754:ARG:HD3	2.38	0.59
1:C:830:LEU:HA	1:C:833:LYS:HE3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:ILE:O	1:C:426:SER:HB3	2.02	0.59
1:C:415:ALA:C	1:C:417:TYR:H	2.12	0.58
1:C:362:VAL:HA	1:C:480:MET:HE3	1.82	0.58
1:C:238:LYS:HE3	1:C:239:GLN:H	1.66	0.58
1:C:789:LYS:HB3	1:C:790:ARG:NH2	2.19	0.58
1:C:825:GLU:CD	1:C:828:LYS:HD3	2.28	0.58
1:C:217:LYS:HB2	1:C:217:LYS:NZ	2.19	0.58
1:C:463:ASP:OD1	1:C:464:HIS:N	2.36	0.58
1:C:778:LYS:HE3	1:C:779:LYS:NZ	2.19	0.57
1:C:343:VAL:O	1:C:343:VAL:HG13	2.04	0.57
1:C:709:LYS:HB2	1:C:709:LYS:NZ	2.20	0.57
1:C:347:ARG:HH11	1:C:350:LYS:CD	2.17	0.57
1:C:574:LYS:HA	1:C:574:LYS:HE2	1.87	0.57
1:C:465:ASP:OD1	1:C:468:LYS:HE2	2.05	0.56
1:C:651:ASN:O	1:C:655:ARG:HB2	2.04	0.56
1:C:337:ALA:HB1	1:C:342:VAL:HG22	1.88	0.56
1:C:534:SER:HB3	1:C:537:PHE:CE2	2.41	0.56
1:C:257:LEU:O	1:C:261:VAL:HG23	2.05	0.55
1:C:315:GLU:HA	1:C:370:ILE:HD12	1.88	0.55
1:C:471:TRP:CD1	1:C:476:PRO:HB3	2.42	0.55
1:C:641:VAL:O	1:C:645:ILE:HG23	2.08	0.54
1:C:251:MET:HE1	1:C:283:PHE:CE2	2.43	0.54
1:C:835:TYR:O	1:C:839:LYS:HG2	2.08	0.54
1:C:694:GLU:OE2	1:C:694:GLU:HA	2.06	0.54
1:C:824:LYS:O	1:C:827:THR:HG23	2.07	0.53
1:C:238:LYS:CE	1:C:239:GLN:H	2.20	0.53
1:C:345:VAL:HG13	1:C:346:ASP:O	2.08	0.53
1:C:458:PHE:HB2	1:C:467:LEU:CD1	2.39	0.53
1:C:661:VAL:C	1:C:662:LYS:HG2	2.33	0.53
1:C:638:THR:N	1:C:639:PRO:CD	2.72	0.53
1:C:777:ARG:HH11	1:C:777:ARG:HG2	1.74	0.53
1:C:417:TYR:N	1:C:418:PRO:HD2	2.24	0.52
1:C:601:GLY:CA	1:C:710:LEU:HD12	2.35	0.52
1:C:768:ILE:O	1:C:772:TYR:HB2	2.10	0.52
1:C:818:HIS:CE1	5:C:1030:HOH:O	2.63	0.52
1:C:818:HIS:O	1:C:819:ILE:C	2.52	0.52
1:C:221:LEU:HD22	1:C:424:LEU:HD11	1.93	0.51
1:C:475:GLU:O	1:C:475:GLU:HG3	2.11	0.51
1:C:718:HIS:CD2	1:C:720:LYS:H	2.29	0.50
1:C:830:LEU:C	1:C:830:LEU:HD23	2.37	0.50
1:C:238:LYS:HE3	1:C:239:GLN:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:689:TYR:CE2	1:C:693:LYS:HD2	2.47	0.49
1:C:731:ARG:CG	1:C:731:ARG:NH1	2.65	0.49
1:C:238:LYS:HG3	1:C:240:LEU:H	1.76	0.49
1:C:819:ILE:HD13	1:C:827:THR:HG22	1.95	0.49
1:C:813:PHE:CD2	1:C:813:PHE:C	2.91	0.49
1:C:468:LYS:HG3	1:C:469:SER:N	2.28	0.49
1:C:734:LEU:O	1:C:739:LYS:HG2	2.13	0.49
1:C:750:GLY:HA2	1:C:759:TYR:O	2.13	0.48
1:C:217:LYS:O	1:C:218:ASP:HB3	2.14	0.48
1:C:358:TYR:CE1	1:C:457:ILE:O	2.66	0.48
1:C:548:LEU:HD22	1:C:554:TRP:CZ2	2.49	0.48
1:C:825:GLU:C	1:C:827:THR:N	2.71	0.48
1:C:511:TYR:CE2	1:C:512:LYS:HD3	2.49	0.48
1:C:669:TYR:CZ	1:C:671:GLY:HA3	2.48	0.47
1:C:640:GLN:HG2	1:C:641:VAL:N	2.29	0.47
1:C:731:ARG:HG2	1:C:731:ARG:NH1	2.13	0.47
1:C:267:GLU:H	1:C:267:GLU:CD	2.23	0.47
1:C:721:HIS:CE1	1:C:752:LEU:HD21	2.50	0.47
1:C:825:GLU:C	1:C:827:THR:H	2.22	0.46
1:C:424:LEU:H	1:C:424:LEU:HD12	1.81	0.46
1:C:819:ILE:HD13	1:C:827:THR:CG2	2.47	0.45
1:C:356:GLU:OE2	1:C:363:ARG:NH2	2.39	0.45
1:C:417:TYR:CE2	1:C:421:VAL:HG21	2.52	0.45
1:C:465:ASP:O	1:C:469:SER:HB3	2.16	0.45
1:C:583:ALA:O	1:C:587:ILE:HG22	2.17	0.45
1:C:229:VAL:HA	1:C:249:LEU:HD11	1.99	0.44
1:C:227:VAL:HG21	1:C:432:VAL:HG23	2.00	0.44
1:C:432:VAL:HG13	1:C:433:THR:HG23	1.99	0.44
1:C:334:VAL:HB	1:C:353:MET:CE	2.47	0.44
1:C:778:LYS:HE3	1:C:779:LYS:HZ3	1.81	0.44
1:C:312:GLU:H	1:C:312:GLU:CD	2.26	0.44
1:C:731:ARG:HH11	1:C:731:ARG:CB	2.31	0.43
1:C:218:ASP:O	1:C:218:ASP:CG	2.61	0.43
1:C:842:LEU:HD12	1:C:842:LEU:HA	1.88	0.43
1:C:638:THR:N	1:C:639:PRO:HD3	2.34	0.43
1:C:796:LEU:HG	1:C:858:PHE:HB3	2.00	0.43
1:C:465:ASP:HA	1:C:468:LYS:HG2	2.01	0.43
1:C:598:VAL:HG12	1:C:734:LEU:HD22	2.00	0.43
1:C:359:LEU:HA	1:C:359:LEU:HD12	1.73	0.43
1:C:233:ILE:HD13	4:C:904:ADP:C2	2.54	0.42
1:C:558:LEU:HD13	1:C:558:LEU:HA	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LEU:HA	1:C:299:PRO:HD3	1.68	0.42
1:C:548:LEU:HD22	1:C:554:TRP:CE2	2.54	0.42
1:C:826:GLU:HA	1:C:828:LYS:HZ1	1.84	0.42
1:C:216:VAL:HB	1:C:217:LYS:NZ	2.31	0.42
1:C:415:ALA:C	1:C:417:TYR:N	2.75	0.42
1:C:772:TYR:O	1:C:777:ARG:HD3	2.20	0.42
1:C:849:ASN:O	1:C:853:LYS:HG2	2.20	0.42
1:C:362:VAL:HA	1:C:480:MET:HE1	1.97	0.42
1:C:416:ILE:HG23	1:C:419:LEU:HD12	2.02	0.42
1:C:486:TYR:CE1	1:C:489:VAL:HG22	2.54	0.42
1:C:777:ARG:HG2	1:C:777:ARG:NH1	2.34	0.42
1:C:425:ASP:O	1:C:429:GLU:HB2	2.20	0.41
1:C:470:LEU:C	1:C:470:LEU:HD12	2.45	0.41
1:C:471:TRP:CD2	1:C:476:PRO:HA	2.56	0.41
1:C:346:ASP:HB3	1:C:348:SER:OG	2.20	0.41
1:C:537:PHE:C	1:C:544:VAL:HG13	2.45	0.41
1:C:309:LYS:HE2	1:C:310:GLU:OE2	2.20	0.41
1:C:326:LEU:HA	1:C:326:LEU:HD23	1.84	0.41
1:C:826:GLU:HA	1:C:828:LYS:HE2	2.02	0.41
1:C:824:LYS:C	1:C:824:LYS:CD	2.91	0.41
1:C:264:PHE:HE2	1:C:314:ILE:HD11	1.86	0.41
1:C:709:LYS:NZ	1:C:709:LYS:CB	2.83	0.41
1:C:840:ASP:O	1:C:843:GLU:HB2	2.21	0.41
1:C:511:TYR:CZ	1:C:512:LYS:HD3	2.56	0.41
1:C:352:SER:OG	1:C:458:PHE:HE1	2.04	0.40
1:C:449:HIS:ND1	1:C:476:PRO:HD2	2.35	0.40
1:C:238:LYS:HG3	1:C:239:GLN:N	2.36	0.40
1:C:766:GLU:HA	1:C:769:ARG:CG	2.51	0.40
1:C:429:GLU:O	1:C:432:VAL:HG12	2.21	0.40
1:C:584:TYR:O	1:C:588:GLY:N	2.47	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	C	532/693 (77%)	511 (96%)	20 (4%)	1 (0%)	43	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	416	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	C	489/617 (79%)	443 (91%)	46 (9%)	8	10

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	217	LYS
1	C	230	GLN
1	C	238	LYS
1	C	292	GLU
1	C	303	LEU
1	C	316	GLU
1	C	320	LYS
1	C	322	ILE
1	C	342	VAL
1	C	345	VAL
1	C	351	ASP
1	C	359	LEU
1	C	419	LEU
1	C	420	LEU
1	C	424	LEU
1	C	425	ASP
1	C	434	GLU
1	C	447	LYS

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Mol	Chain	Res	Type
1	C	489	VAL
1	C	517	ILE
1	C	558	LEU
1	C	574	LYS
1	C	587	ILE
1	C	641	VAL
1	C	645	ILE
1	C	660	VAL
1	C	685	LEU
1	C	686	GLU
1	C	709	LYS
1	C	731	ARG
1	C	732	ASP
1	C	761	SER
1	C	781	LEU
1	C	790	ARG
1	C	797	ARG
1	C	804	LYS
1	C	805	VAL
1	C	818	HIS
1	C	824	LYS
1	C	826	GLU
1	C	828	LYS
1	C	832	GLU
1	C	842	LEU
1	C	848	ASN
1	C	851	VAL
1	C	852	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	718	HIS
1	C	740	ASN
1	C	794	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ADP	C	904	2	28,29,29	1.55	5 (17%)	43,45,45	1.79	10 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	C	904	2	-	3/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	904	ADP	C5-C4	5.31	1.48	1.39
4	C	904	ADP	C5-C6	2.98	1.49	1.41
4	C	904	ADP	C8-N7	2.71	1.36	1.31
4	C	904	ADP	PA-O3A	2.29	1.62	1.59
4	C	904	ADP	C5-N7	-2.07	1.35	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	904	ADP	C5-C4-N3	-5.60	119.01	126.72
4	C	904	ADP	N3-C4-N9	3.98	133.94	127.17
4	C	904	ADP	C2-N3-C4	3.59	120.60	111.83
4	C	904	ADP	C4-C5-N7	-3.57	106.50	110.58
4	C	904	ADP	N3-C2-N1	-3.26	123.64	128.58
4	C	904	ADP	O4'-C1'-N9	2.62	113.13	108.09
4	C	904	ADP	C2-N1-C6	2.48	122.80	118.73
4	C	904	ADP	C3'-C2'-C1'	2.29	105.79	101.46
4	C	904	ADP	C6-C5-N7	2.25	136.43	132.09
4	C	904	ADP	C5-N7-C8	2.21	106.92	103.45

There are no chirality outliers.

All (3) torsion outliers are listed below:

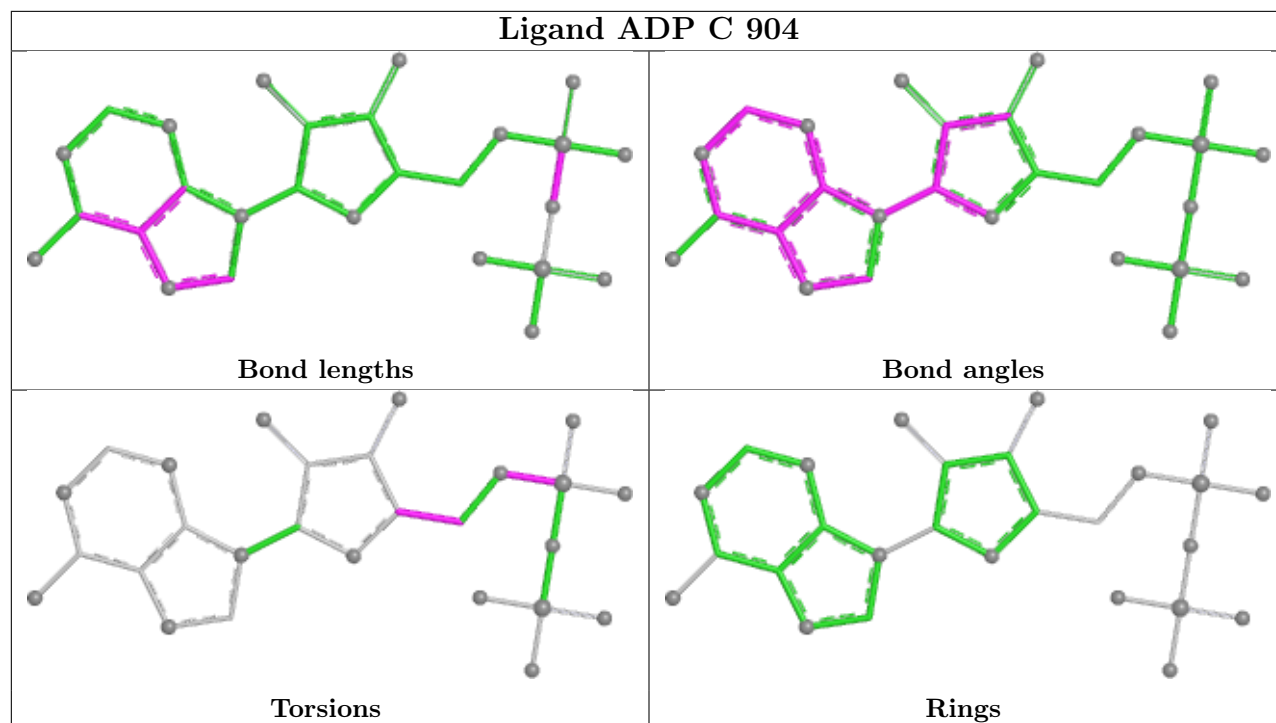
Mol	Chain	Res	Type	Atoms
4	C	904	ADP	C5'-O5'-PA-O2A
4	C	904	ADP	O4'-C4'-C5'-O5'
4	C	904	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	904	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	C	548/693 (79%)	0.32	29 (5%) 32 34	44, 75, 138, 184	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	781	LEU	6.1
1	C	819	ILE	5.6
1	C	215	SER	4.6
1	C	558	LEU	4.4
1	C	427	LEU	4.4
1	C	788	GLY	4.4
1	C	421	VAL	4.1
1	C	216	VAL	3.8
1	C	470	LEU	3.4
1	C	605	GLY	3.3
1	C	416	ILE	3.2
1	C	374	SER	3.1
1	C	672	GLY	3.0
1	C	471	TRP	3.0
1	C	415	ALA	3.0
1	C	772	TYR	3.0
1	C	420	LEU	2.9
1	C	432	VAL	2.9
1	C	638	THR	2.9
1	C	446	TRP	2.8
1	C	572	LYS	2.7
1	C	375	LEU	2.5
1	C	347	ARG	2.5
1	C	824	LYS	2.4
1	C	367	THR	2.2
1	C	289	ILE	2.2
1	C	433	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	235	ASN	2.1
1	C	431	LYS	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](#)

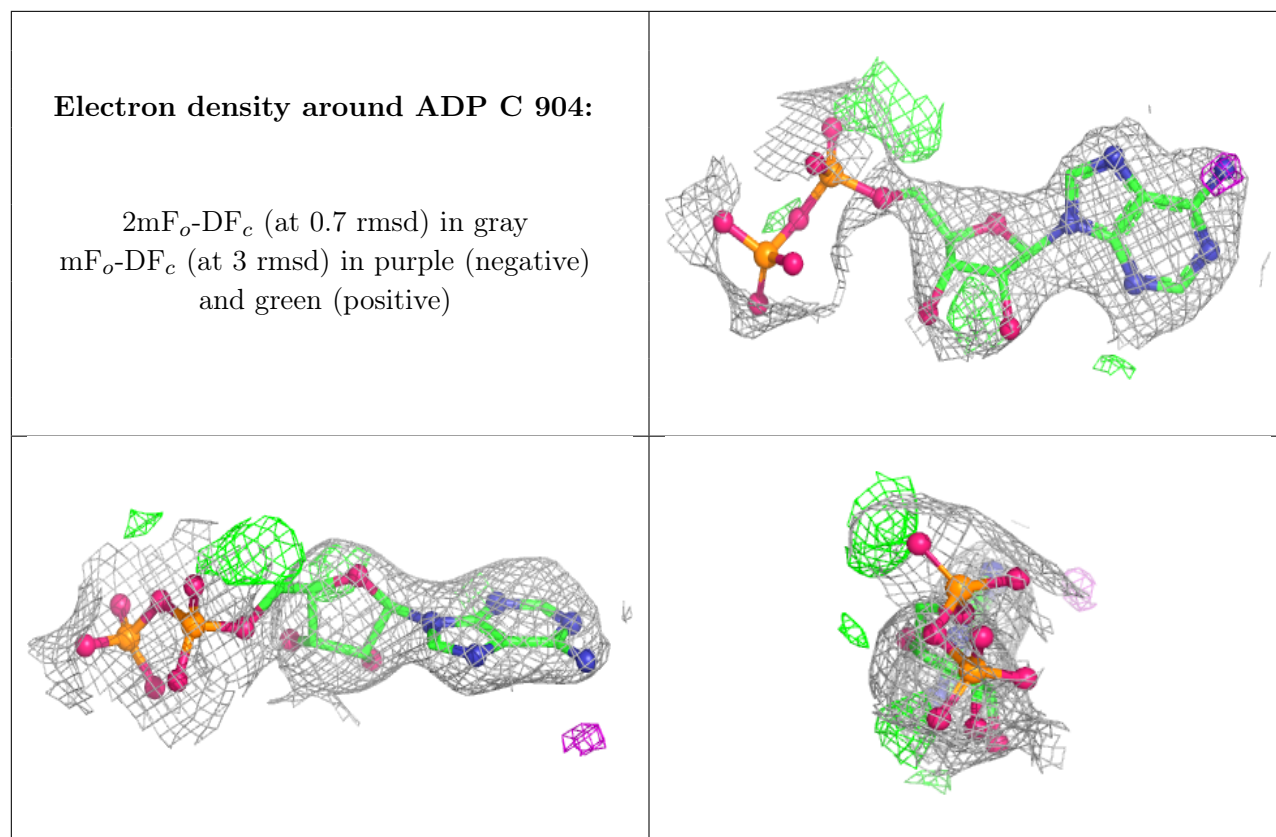
There are no oligosaccharides in this entry.

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
4	ADP	C	904	27/27	0.86	0.13	55,97,173,263	0
2	CA	C	902	1/1	0.96	0.07	86,86,86,86	0
2	CA	C	901	1/1	0.98	0.06	85,85,85,85	0
3	ZN	C	903	1/1	0.99	0.03	79,79,79,79	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.