



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:36 PM UTC

PDB ID : 4ONJ / pdb_00004onj
Title : Crystal structure of the catalytic domain of ntDRM
Authors : Du, J.; Patel, D.J.
Deposited on : 2014-01-28
Resolution : 2.81 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

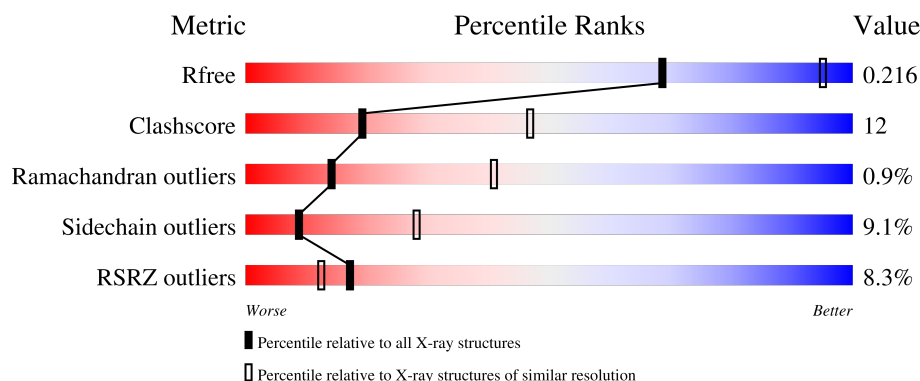
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	357	9% 65% 24% 7%
1	B	357	6% 72% 17% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SFG	A	700	-	-	X	-
2	SFG	B	700	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 5386 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.

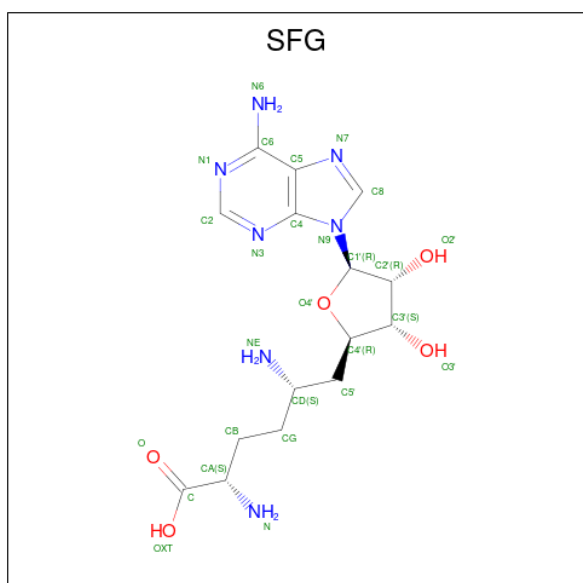
- Molecule 1 is a protein called DNA methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2660	1714	466	472	8			
1	B	333	Total	C	N	O	S	0	0	0
			2672	1721	467	475	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	252	SER	-	expression tag	UNP Q76KU6
A	253	GLU	-	expression tag	UNP Q76KU6
A	254	PHE	-	expression tag	UNP Q76KU6
B	252	SER	-	expression tag	UNP Q76KU6
B	253	GLU	-	expression tag	UNP Q76KU6
B	254	PHE	-	expression tag	UNP Q76KU6

- Molecule 2 is SINEFUNGIN (CCD ID: SFG) (formula: C₁₅H₂₃N₇O₅).

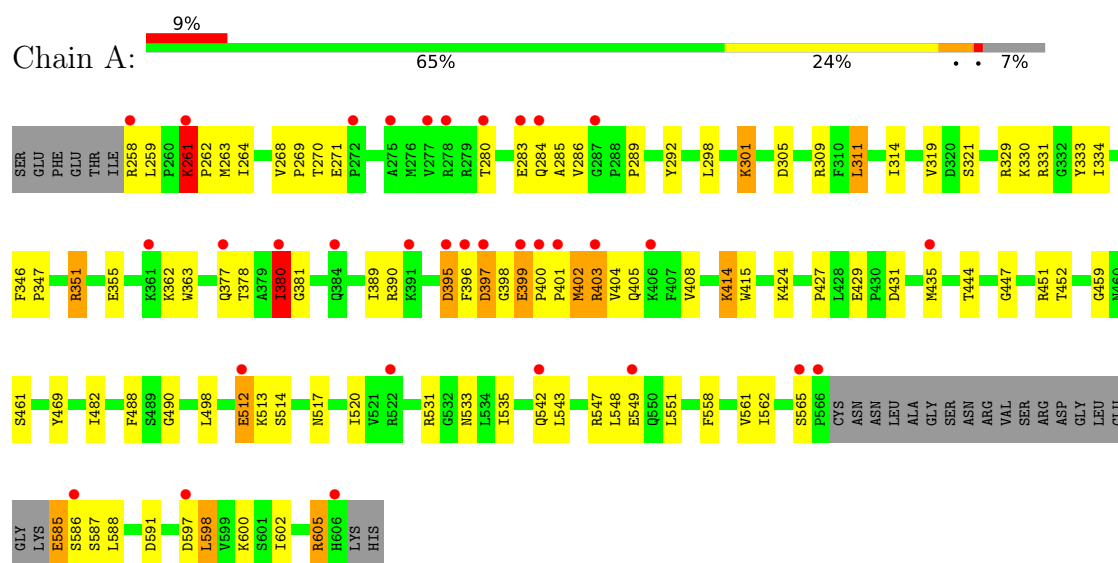


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	15	7	5		
2	B	1	Total	C	N	O	0	0
			27	15	7	5		

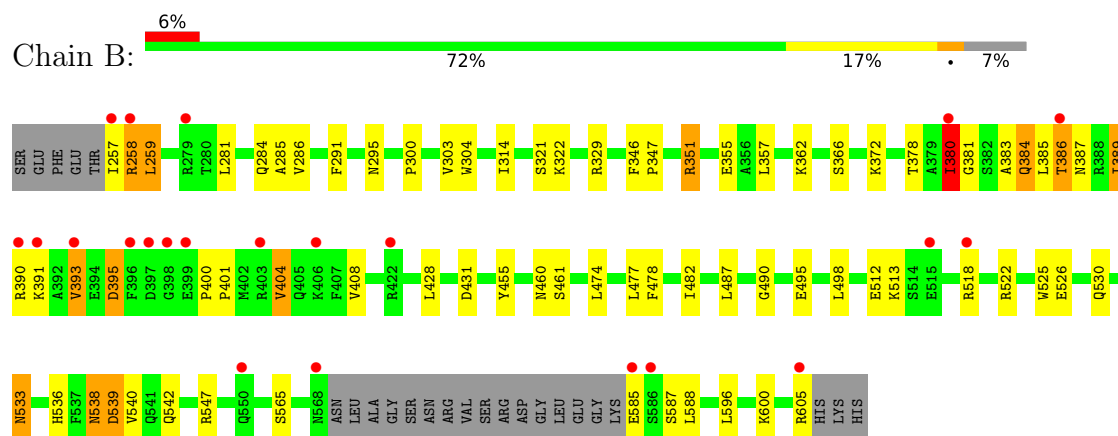
3 Residue-property plots [i](#)

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: DNA methyltransferase



• Molecule 1: DNA methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.32Å 153.32Å 148.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.51 – 2.81 46.51 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.51-2.81) 99.4 (46.51-2.81)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.201 , 0.221 0.199 , 0.216	Depositor DCC
R_{free} test set	2510 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5386	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 3.59% 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: SFG

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	0.34	0/2733	0.80	3/3712 (0.1%)
1	B	0.39	1/2744 (0.0%)	0.79	2/3727 (0.1%)
All	All	0.36	1/5477 (0.0%)	0.79	5/7439 (0.1%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	393	VAL	CA-CB	5.10	1.59	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	598	LEU	N-CA-C	-6.06	104.58	111.07
1	A	380	ILE	N-CA-C	6.04	116.32	108.35
1	A	395	ASP	N-CA-C	-5.99	101.44	110.24
1	B	380	ILE	N-CA-C	5.22	117.28	108.81
1	B	540	VAL	N-CA-C	-5.10	104.67	111.05

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	GLY	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	2660	0	2654	74	0
1	B	2672	0	2669	53	0
2	A	27	0	22	12	0
2	B	27	0	22	10	0
All	All	5386	0	5367	126	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 12.

All (126) 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:261:LYS:HB2	1:A:262:PRO:CD	1.40	1.51
1:B:461:SER:HA	2:B:700:SFG:O	1.48	1.11
1:A:512:GLU:OE2	1:A:513:LYS:N	1.84	1.09
1:A:261:LYS:HB2	1:A:262:PRO:HD2	1.17	1.07
1:A:261:LYS:CB	1:A:262:PRO:CD	2.32	1.06
1:A:261:LYS:HB2	1:A:262:PRO:HD3	1.36	1.02
1:A:512:GLU:OE2	1:A:512:GLU:C	2.06	0.97
1:A:490:GLY:HA2	2:A:700:SFG:O3'	1.65	0.96
1:A:488:PHE:HB3	2:A:700:SFG:O4'	1.73	0.89
1:B:461:SER:CA	2:B:700:SFG:O	2.30	0.80
1:A:261:LYS:CB	1:A:262:PRO:HD3	2.11	0.76
1:B:461:SER:HA	2:B:700:SFG:C	2.15	0.75
1:A:329:ARG:NH1	1:A:461:SER:O	2.20	0.74
1:B:588:LEU:HD11	2:B:700:SFG:HN61	1.51	0.74
1:A:261:LYS:CB	1:A:262:PRO:HD2	2.09	0.72
1:A:512:GLU:OE2	1:A:514:SER:N	2.23	0.72
1:A:512:GLU:OE1	1:A:517:ASN:HB2	1.89	0.72
1:B:565:SER:O	2:B:700:SFG:NE	2.23	0.72
1:B:387:ASN:OD1	1:B:390:ARG:NH1	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:NH1	1:B:461:SER:O	2.25	0.69
1:B:518:ARG:HH22	1:B:522:ARG:HH21	1.39	0.68
1:A:597:ASP:HA	1:A:600:LYS:HB3	1.77	0.67
1:A:402:MET:HA	1:A:405:GLN:HB2	1.76	0.66
1:B:538:ASN:OD1	1:B:538:ASN:N	2.30	0.64
1:A:512:GLU:OE1	1:A:517:ASN:CB	2.45	0.64
1:B:512:GLU:OE2	2:B:700:SFG:H1'	1.97	0.64
1:B:389:ILE:HD13	1:B:408:VAL:HG23	1.80	0.61
1:A:390:ARG:HH11	1:A:424:LYS:HZ3	1.49	0.60
1:A:605:ARG:NH2	1:B:284:GLN:OE1	2.32	0.60
1:A:268:VAL:HG23	1:A:271:GLU:HB2	1.82	0.60
1:A:488:PHE:HA	2:A:700:SFG:H1'	1.84	0.58
1:A:512:GLU:OE1	2:A:700:SFG:O2'	2.21	0.57
1:A:390:ARG:HH11	1:A:424:LYS:NZ	2.02	0.57
1:A:284:GLN:HG3	1:B:605:ARG:NH2	2.20	0.57
1:B:285:ALA:HB1	1:B:314:ILE:HD11	1.87	0.57
1:B:257:ILE:HG22	1:B:258:ARG:H	1.70	0.56
1:B:539:ASP:O	1:B:542:GLN:HG2	2.04	0.56
1:A:258:ARG:HG3	1:A:259:LEU:HG	1.87	0.56
1:A:263:MET:HE1	1:A:330:LYS:HD3	1.86	0.56
1:A:292:TYR:HB3	1:A:562:ILE:HG13	1.88	0.56
1:A:321:SER:OG	1:A:329:ARG:HB3	2.06	0.56
1:B:512:GLU:OE2	1:B:513:LYS:N	2.39	0.55
1:A:488:PHE:CB	2:A:700:SFG:O4'	2.52	0.55
1:B:383:ALA:HA	1:B:386:THR:HG23	1.87	0.55
1:A:362:LYS:HE2	1:A:363:TRP:NE1	2.22	0.54
1:A:585:GLU:HB3	1:A:588:LEU:HG	1.90	0.54
1:A:380:ILE:HG13	1:A:427:PRO:HB3	1.90	0.54
1:A:490:GLY:CA	2:A:700:SFG:O3'	2.49	0.54
1:B:588:LEU:CD1	2:B:700:SFG:HN61	2.18	0.54
1:B:321:SER:HB2	1:B:329:ARG:HB3	1.90	0.54
1:A:402:MET:SD	1:A:402:MET:N	2.81	0.53
1:A:351:ARG:NH1	1:A:355:GLU:OE2	2.42	0.52
1:A:285:ALA:HB1	1:A:314:ILE:HD11	1.91	0.52
1:B:588:LEU:CD1	2:B:700:SFG:N6	2.73	0.52
1:A:399:GLU:O	1:A:405:GLN:NE2	2.43	0.51
1:A:380:ILE:HD12	1:A:381:GLY:H	1.76	0.51
1:B:588:LEU:HD11	2:B:700:SFG:N6	2.24	0.51
1:B:380:ILE:HD12	1:B:381:GLY:H	1.76	0.50
1:A:377:GLN:N	1:A:377:GLN:OE1	2.45	0.50
1:A:401:PRO:HB2	1:A:403:ARG:HG2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:SER:CB	2:B:700:SFG:O	2.59	0.50
1:B:495:GLU:N	1:B:495:GLU:OE1	2.42	0.49
1:A:319:VAL:HG22	1:A:333:TYR:HE2	1.77	0.49
1:A:399:GLU:H	1:A:400:PRO:CD	2.26	0.49
1:B:257:ILE:HG22	1:B:258:ARG:HG2	1.95	0.49
1:B:533:ASN:OD1	1:B:533:ASN:N	2.33	0.49
1:B:257:ILE:C	1:B:259:LEU:H	2.21	0.48
1:B:585:GLU:HG3	1:B:587:SER:H	1.78	0.48
1:A:396:PHE:CG	1:A:397:ASP:N	2.81	0.48
1:A:378:THR:HG22	1:A:459:GLY:HA3	1.95	0.48
2:A:700:SFG:H4'	2:A:700:SFG:HG2	1.37	0.48
1:A:488:PHE:HA	2:A:700:SFG:C1'	2.43	0.48
1:A:512:GLU:CD	2:A:700:SFG:O2'	2.57	0.47
1:B:387:ASN:O	1:B:391:LYS:HD3	2.14	0.47
1:B:351:ARG:NH1	1:B:355:GLU:OE2	2.47	0.47
1:A:429:GLU:OE1	1:A:451:ARG:NH2	2.46	0.47
1:B:490:GLY:HA2	1:B:512:GLU:OE1	2.14	0.47
1:B:395:ASP:OD2	1:B:400:PRO:HB3	2.15	0.47
1:A:269:PRO:HG3	1:A:469:TYR:CE1	2.50	0.46
1:B:384:GLN:CD	1:B:384:GLN:H	2.23	0.46
1:B:585:GLU:HB3	1:B:588:LEU:HG	1.97	0.46
1:A:262:PRO:HB2	1:A:264:ILE:HG23	1.97	0.45
1:B:257:ILE:C	1:B:259:LEU:N	2.74	0.45
1:A:512:GLU:OE2	1:A:512:GLU:CA	2.62	0.45
1:B:482:ILE:HD11	1:B:498:LEU:HD13	1.99	0.45
1:B:257:ILE:HG22	1:B:258:ARG:N	2.31	0.45
1:A:289:PRO:HB3	1:A:558:PHE:O	2.16	0.45
1:A:490:GLY:HA2	2:A:700:SFG:HO3'	1.75	0.45
1:A:380:ILE:HG13	1:A:427:PRO:CB	2.46	0.45
1:A:399:GLU:N	1:A:400:PRO:CD	2.80	0.45
1:A:305:ASP:O	1:A:309:ARG:HG3	2.17	0.44
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.90	0.44
1:A:301:LYS:H	1:A:301:LYS:HG2	1.51	0.44
1:A:435:MET:HE2	1:A:435:MET:HB3	1.79	0.44
1:A:542:GLN:HE21	1:A:547:ARG:NH2	2.15	0.43
1:B:596:LEU:O	1:B:600:LYS:HB2	2.18	0.43
1:A:585:GLU:OE1	1:A:587:SER:OG	2.25	0.43
1:B:393:VAL:C	1:B:395:ASP:H	2.26	0.43
1:A:598:LEU:O	1:A:602:ILE:HG13	2.19	0.43
1:A:444:THR:HG22	1:A:520:ILE:HD13	2.00	0.43
1:A:311:LEU:HD13	1:A:311:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:MET:HE3	1:A:263:MET:HB2	1.78	0.42
1:A:389:ILE:HG23	1:A:408:VAL:HG22	2.02	0.42
1:A:565:SER:O	2:A:700:SFG:NE	2.52	0.42
1:A:588:LEU:HD11	2:A:700:SFG:HN61	1.84	0.42
1:B:428:LEU:O	1:B:455:TYR:OH	2.29	0.42
1:A:351:ARG:HD3	1:A:355:GLU:OE1	2.19	0.42
1:A:403:ARG:HG3	1:A:404:VAL:H	1.85	0.42
1:B:300:PRO:HG2	1:B:303:VAL:HG21	2.02	0.42
1:B:384:GLN:CD	1:B:384:GLN:N	2.78	0.42
1:B:518:ARG:HG3	1:B:536:HIS:CE1	2.55	0.41
1:B:525:TRP:CH2	1:B:530:GLN:HG2	2.55	0.41
1:B:395:ASP:OD1	1:B:395:ASP:C	2.63	0.41
1:A:414:LYS:HG3	1:A:415:TRP:N	2.35	0.41
1:B:322:LYS:HB2	1:B:372:LYS:HE2	2.01	0.41
1:B:404:VAL:O	1:B:408:VAL:HG12	2.20	0.41
1:A:262:PRO:HG2	1:A:264:ILE:HD13	2.02	0.41
1:A:346:PHE:HA	1:A:347:PRO:C	2.46	0.41
1:A:482:ILE:HD11	1:A:498:LEU:HD13	2.03	0.41
1:B:295:ASN:HB3	1:B:304:TRP:CZ2	2.56	0.41
1:B:474:LEU:HD22	1:B:478:PHE:HE2	1.86	0.41
1:A:543:LEU:HD23	1:A:543:LEU:HA	1.92	0.40
1:B:526:GLU:H	1:B:526:GLU:HG2	1.78	0.40
1:B:291:PHE:HZ	1:B:314:ILE:HD12	1.86	0.40
1:A:319:VAL:HG22	1:A:333:TYR:CE2	2.56	0.40
1:B:346:PHE:HA	1:B:347:PRO:C	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	327/357 (92%)	313 (96%)	10 (3%)	4 (1%)	10	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	329/357 (92%)	315 (96%)	12 (4%)	2 (1%)	21	51
All	All	656/714 (92%)	628 (96%)	22 (3%)	6 (1%)	14	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	LYS
1	A	399	GLU
1	A	447	GLY
1	B	258	ARG
1	B	401	PRO
1	A	286	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	290/312 (93%)	260 (90%)	30 (10%)	7	23
1	B	292/312 (94%)	269 (92%)	23 (8%)	11	35
All	All	582/624 (93%)	529 (91%)	53 (9%)	9	28

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	LYS
1	A	270	THR
1	A	280	THR
1	A	283	GLU
1	A	298	LEU
1	A	301	LYS
1	A	311	LEU
1	A	331	ARG
1	A	334	ILE
1	A	351	ARG

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Mol	Chain	Res	Type
1	A	380	ILE
1	A	395	ASP
1	A	397	ASP
1	A	402	MET
1	A	403	ARG
1	A	414	LYS
1	A	431	ASP
1	A	452	THR
1	A	512	GLU
1	A	531	ARG
1	A	533	ASN
1	A	535	ILE
1	A	548	LEU
1	A	549	GLU
1	A	551	LEU
1	A	561	VAL
1	A	585	GLU
1	A	586	SER
1	A	591	ASP
1	A	605	ARG
1	B	259	LEU
1	B	281	LEU
1	B	286	VAL
1	B	351	ARG
1	B	357	LEU
1	B	362	LYS
1	B	366	SER
1	B	378	THR
1	B	380	ILE
1	B	384	GLN
1	B	385	LEU
1	B	386	THR
1	B	389	ILE
1	B	395	ASP
1	B	404	VAL
1	B	431	ASP
1	B	460	ASN
1	B	477	LEU
1	B	487	LEU
1	B	533	ASN
1	B	538	ASN
1	B	539	ASP

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Mol	Chain	Res	Type
1	B	547	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	284	GLN
1	A	483	ASN
1	A	517	ASN
1	A	533	ASN
1	A	542	GLN
1	B	341	ASN
1	B	354	HIS
1	B	423	ASN
1	B	529	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](#)

2 ligands are modelled in this entry.

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
2	SFG	B	700	-	28,29,29	1.40	4 (14%)	34,42,42	2.01	9 (26%)
2	SFG	A	700	-	28,29,29	1.40	4 (14%)	34,42,42	2.01	9 (26%)

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
2	SFG	B	700	-	-	6/17/33/33	0/3/3/3
2	SFG	A	700	-	-	8/17/33/33	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	SFG	C5-C4	4.77	1.47	1.39
2	A	700	SFG	C5-C4	4.76	1.47	1.39
2	B	700	SFG	C5-C6	2.77	1.48	1.41
2	A	700	SFG	C5-C6	2.75	1.48	1.41
2	A	700	SFG	C8-N7	2.39	1.36	1.31
2	B	700	SFG	C8-N7	2.38	1.36	1.31
2	A	700	SFG	C5-N7	-2.25	1.35	1.39
2	B	700	SFG	C5-N7	-2.22	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	SFG	C5-C4-N3	-5.84	118.68	126.72
2	A	700	SFG	C5-C4-N3	-5.83	118.69	126.72
2	B	700	SFG	N3-C4-N9	4.63	135.04	127.17
2	A	700	SFG	N3-C4-N9	4.62	135.03	127.17
2	A	700	SFG	C2-N3-C4	3.70	120.87	111.83
2	B	700	SFG	C2-N3-C4	3.70	120.86	111.83
2	B	700	SFG	C4-C5-N7	-3.47	106.61	110.58
2	A	700	SFG	C4-C5-N7	-3.46	106.62	110.58
2	A	700	SFG	N3-C2-N1	-3.22	123.70	128.58
2	B	700	SFG	N3-C2-N1	-3.21	123.73	128.58
2	A	700	SFG	C4-N9-C8	2.64	108.51	105.74
2	B	700	SFG	C4-N9-C8	2.63	108.50	105.74
2	A	700	SFG	C3'-C2'-C1'	2.57	106.32	101.46
2	B	700	SFG	C3'-C2'-C1'	2.55	106.29	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	700	SFG	C5-N7-C8	2.54	107.45	103.45
2	A	700	SFG	C5-N7-C8	2.53	107.42	103.45
2	B	700	SFG	C6-C5-N7	2.09	136.12	132.09
2	A	700	SFG	C6-C5-N7	2.07	136.08	132.09

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	SFG	NE-CD-CG-CB
2	A	700	SFG	C5'-CD-CG-CB
2	A	700	SFG	C4'-C5'-CD-CG
2	A	700	SFG	O4'-C4'-C5'-CD
2	A	700	SFG	C3'-C4'-C5'-CD
2	B	700	SFG	C5'-CD-CG-CB
2	A	700	SFG	O-C-CA-CB
2	A	700	SFG	OXT-C-CA-CB
2	B	700	SFG	NE-CD-CG-CB
2	B	700	SFG	OXT-C-CA-CB
2	B	700	SFG	O-C-CA-CB
2	B	700	SFG	O4'-C4'-C5'-CD
2	B	700	SFG	C3'-C4'-C5'-CD
2	A	700	SFG	C4'-C5'-CD-NE

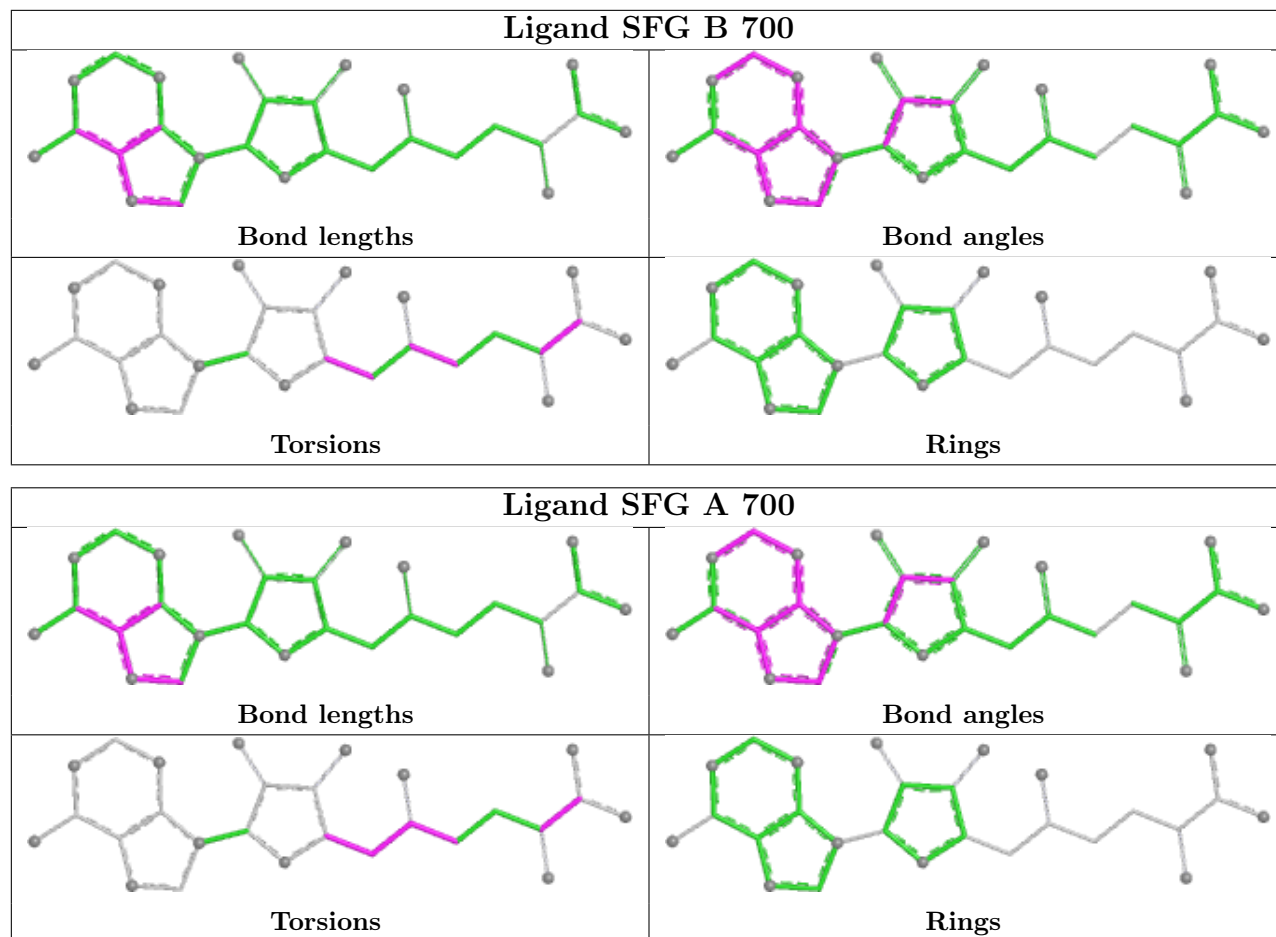
There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	700	SFG	10	0
2	A	700	SFG	12	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	A	331/357 (92%)	0.46	33 (9%) 12 9	51, 75, 136, 184	0
1	B	333/357 (93%)	0.22	22 (6%) 24 18	41, 68, 138, 206	0
All	All	664/714 (92%)	0.34	55 (8%) 17 12	41, 72, 138, 206	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	396	PHE	7.7
1	A	396	PHE	7.1
1	B	568	ASN	6.7
1	A	606	HIS	6.6
1	A	261	LYS	5.6
1	A	391	LYS	5.1
1	B	257	ILE	4.9
1	A	395	ASP	4.9
1	A	384	GLN	4.6
1	A	586	SER	4.2
1	A	400	PRO	4.2
1	B	258	ARG	4.0
1	A	277	VAL	3.8
1	A	377	GLN	3.8
1	A	406	LYS	3.8
1	A	361	LYS	3.6
1	A	258	ARG	3.6
1	B	550	GLN	3.4
1	A	512	GLU	3.2
1	A	275	ALA	3.2
1	B	398	GLY	3.2
1	B	380	ILE	3.1
1	A	542	GLN	3.1
1	A	549	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	518	ARG	3.1
1	A	380	ILE	3.1
1	B	403	ARG	3.1
1	A	397	ASP	3.0
1	B	406	LYS	3.0
1	A	283	GLU	3.0
1	B	397	ASP	2.9
1	A	435	MET	2.9
1	B	586	SER	2.7
1	A	284	GLN	2.7
1	B	391	LYS	2.7
1	A	566	PRO	2.7
1	B	605	ARG	2.6
1	A	403	ARG	2.6
1	B	390	ARG	2.5
1	A	280	THR	2.5
1	A	287	GLY	2.3
1	A	399	GLU	2.3
1	A	565	SER	2.3
1	B	399	GLU	2.3
1	B	585	GLU	2.2
1	A	597	ASP	2.2
1	A	272	PRO	2.1
1	A	278	ARG	2.1
1	B	422	ARG	2.1
1	A	401	PRO	2.1
1	B	279	ARG	2.1
1	B	386	THR	2.0
1	B	515	GLU	2.0
1	A	522	ARG	2.0
1	B	393	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 ⓘ

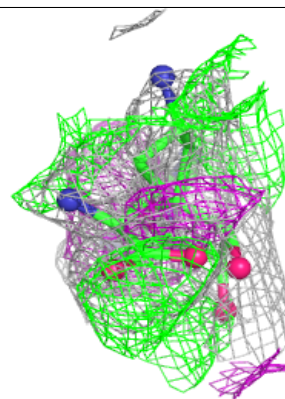
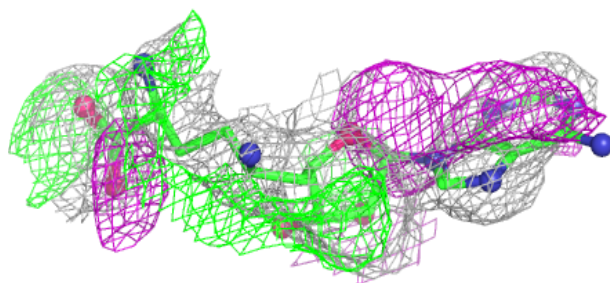
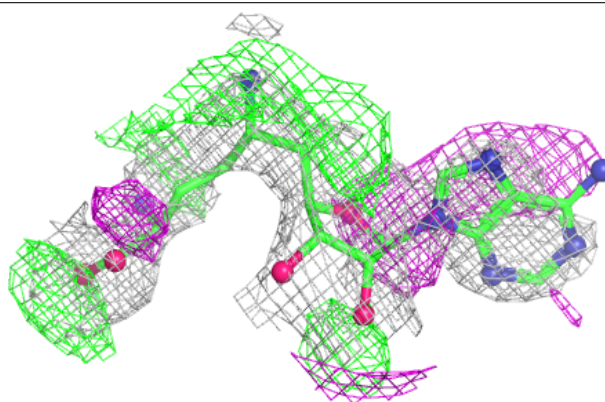
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SFG	A	700	27/27	0.65	0.34	81,126,147,153	0
2	SFG	B	700	27/27	0.71	0.27	79,98,132,148	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.

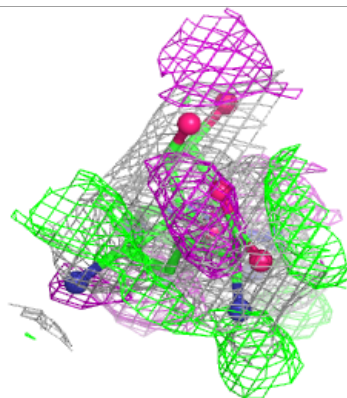
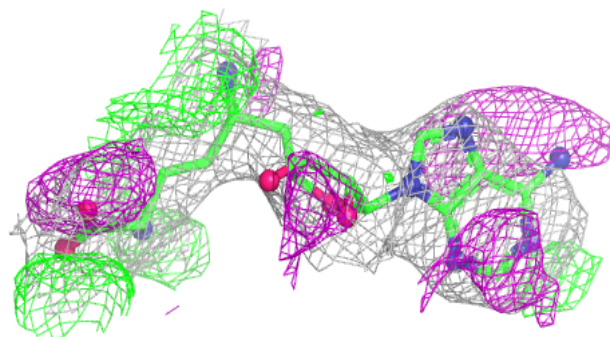
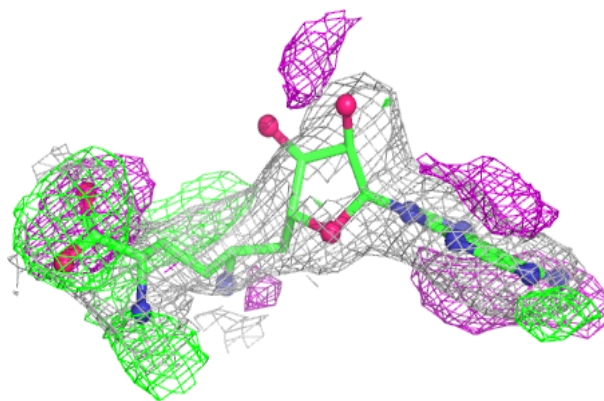
Electron density around SFG A 700:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SFG B 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.