



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:24 AM UTC

PDB ID : 363D / pdb_0000363d
Title : High-resolution crystal structure of a fully modified N3'-> P5' phosphoramidate DNA dodecamer duplex
Authors : Tereshko, V.; Gryaznov, S.; Egli, M.
Deposited on : 1997-11-26
Resolution : 2.00 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
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

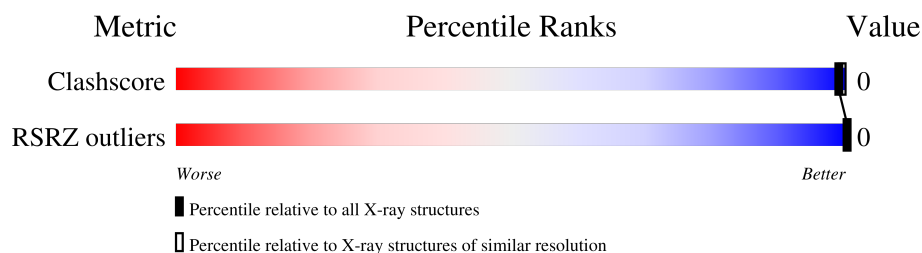
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

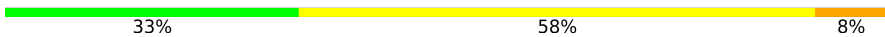
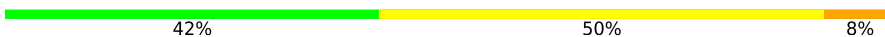
The reported resolution of this entry is 2.00 Å.

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))
Clashscore	190562	11152 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	12	 33% 58% 8%
1	B	12	 42% 50% 8%
1	C	12	 42% 50% 8%
1	D	12	 25% 75%
1	E	12	 50% 50%
1	F	12	 58% 33% 8%

2 Entry composition [i](#)

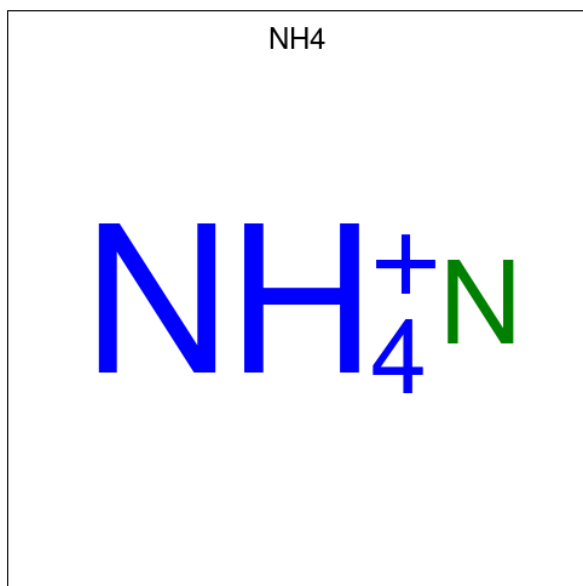
There are 4 unique types of molecules in this entry. The entry contains 1760 atoms, of which 66 are hydrogens and 0 are deuteriums.

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 DNA chain called 5'-D*(C42)P*(G38)P*(C42)P*(G38)P*(A43)P*(A43)P*(NYM)P*(NYM)P*(C42)P*(G38)P*(C42)P*(DG)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	12	Total	C	H	N	O	P	11	0	0
			254	116	11	57	59	11			
1	B	12	Total	C	H	N	O	P	11	0	0
			254	116	11	57	59	11			
1	C	12	Total	C	H	N	O	P	11	0	0
			254	116	11	57	59	11			
1	D	12	Total	C	H	N	O	P	11	0	0
			254	116	11	57	59	11			
1	E	12	Total	C	H	N	O	P	11	0	0
			254	116	11	57	59	11			
1	F	12	Total	C	H	N	O	P	11	0	0
			254	116	11	57	59	11			

- Molecule 2 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total N 1 1	1	0
2	A	1	Total N 1 1	1	0
2	A	1	Total N 1 1	0	0
2	A	1	Total N 1 1	0	0
2	B	1	Total N 1 1	1	0
2	B	1	Total N 1 1	1	0
2	B	1	Total N 1 1	0	0
2	B	1	Total N 1 1	0	0
2	C	1	Total N 1 1	1	0
2	C	1	Total N 1 1	1	0
2	C	1	Total N 1 1	1	0
2	C	1	Total N 1 1	1	0
2	D	1	Total N 1 1	1	0
2	D	1	Total N 1 1	1	0
2	D	1	Total N 1 1	1	0
2	D	1	Total N 1 1	1	0
2	E	1	Total N 1 1	0	0
2	E	1	Total N 1 1	0	0
2	E	1	Total N 1 1	0	0
2	E	1	Total N 1 1	0	0
2	F	1	Total N 1 1	0	0
2	F	1	Total N 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total N 1 1	0	0
2	F	1	Total N 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	1	0
3	B	2	Total Cl 2 2	1	0
3	C	2	Total Cl 2 2	2	0
3	D	2	Total Cl 2 2	2	0
3	E	2	Total Cl 2 2	0	0
3	F	2	Total Cl 2 2	0	0

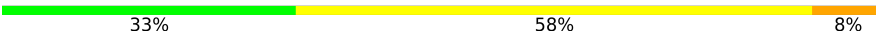
- Molecule 4 is water.

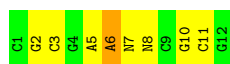
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	36	Total O 36 36	17	0
4	B	34	Total O 34 34	16	0
4	C	30	Total O 30 30	25	0
4	D	36	Total O 36 36	35	0
4	E	37	Total O 37 37	1	0
4	F	27	Total O 27 27	4	0

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: 5'-D*(C42)P*(G38)P*(C42)P*(G38)P*(A43)P*(A43)P*(NYM)P*(NYM)P*(C42)P*(G38)P*(C42)P*DG)-3'

Chain A: 



- Molecule 1: 5'-D*(C42)P*(G38)P*(C42)P*(G38)P*(A43)P*(A43)P*(NYM)P*(NYM)P*(C42)P*(G38)P*(C42)P*DG)-3'

Chain B: 



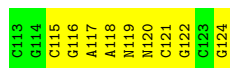
- Molecule 1: 5'-D*(C42)P*(G38)P*(C42)P*(G38)P*(A43)P*(A43)P*(NYM)P*(NYM)P*(C42)P*(G38)P*(C42)P*DG)-3'

Chain C: 



- Molecule 1: 5'-D*(C42)P*(G38)P*(C42)P*(G38)P*(A43)P*(A43)P*(NYM)P*(NYM)P*(C42)P*(G38)P*(C42)P*DG)-3'

Chain D: 



- Molecule 1: 5'-D*(C42)P*(G38)P*(C42)P*(G38)P*(A43)P*(A43)P*(NYM)P*(NYM)P*(C42)P*(G38)P*(C42)P*DG)-3'

Chain E: 



- Molecule 1: 5'-D^{*}(C42)P^{*}(G38)P^{*}(C42)P^{*}(G38)P^{*}(A43)P^{*}(A43)P^{*}(NYM)P^{*}(NYM)P^{*}(C42)P^{*}(G38)P^{*}(C42)P^{*}DG)-3'

Chain F:
58% 33% 8%

Chain F quality score bar chart. The bar is divided into three segments: 58% (green), 33% (yellow), and 8% (orange).



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	40.15Å 40.15Å 304.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.00 8.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.9 (8.00-2.00) 92.0 (8.00-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.192 , 0.247 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	1760	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2356e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: C42, G38, NH4, NYM, A43, 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	0.52	0/24	0.89	0/35
1	B	0.80	0/24	0.56	0/35
1	C	0.42	0/24	0.78	0/35
1	D	0.50	0/24	1.16	1/35 (2.9%)
1	E	0.51	0/24	0.65	0/35
1	F	0.53	0/24	0.82	0/35
All	All	0.56	0/144	0.83	1/210 (0.5%)

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	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	124	DG	C2'-C3'-O3'	5.23	119.35	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	112	DG	Sidechain

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	243	11	140	0	5
1	B	243	11	140	0	5
1	C	243	11	140	0	4
1	D	243	11	140	0	0
1	E	243	11	140	0	0
1	F	243	11	140	0	4
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	36	0	0	0	0
4	B	34	0	0	0	0
4	C	30	0	0	0	0
4	D	36	0	0	0	0
4	E	37	0	0	0	0
4	F	27	0	0	1	0
All	All	1694	66	840	1	9

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 0.

All (1) 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:F:236:NH4:N	4:F:362:HOH:O	2.31	0.63

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:NYM:N3	1:F:220:NYM:N3[12_555]	0.34	1.86
1:A:6:A43:O5'	1:B:19:NYM:O5'[12_555]	0.54	1.66
1:A:6:A43:P	1:B:19:NYM:O5'[12_555]	1.32	0.88
1:C:107:NYM:C4	1:F:220:NYM:N3[12_555]	1.32	0.88
1:C:107:NYM:C2	1:F:220:NYM:N3[12_555]	1.68	0.52
1:A:6:A43:C5'	1:B:19:NYM:O5'[12_555]	1.73	0.47
1:C:107:NYM:O4	1:F:220:NYM:N3[12_555]	2.04	0.16
1:A:6:A43:O2P	1:B:19:NYM:O5'[12_555]	2.14	0.06
1:A:6:A43:O1P	1:B:19:NYM:O5'[12_555]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

66 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	NYM	D	119	1	18,21,22	0.57	0	22,30,33	0.67	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	G38	A	2	1	21,24,25	0.52	0	27,35,38	0.64	1 (3%)
1	NYM	B	20	1	18,21,22	0.62	0	22,30,33	0.75	1 (4%)
1	G38	F	214	1	21,24,25	0.53	0	27,35,38	0.50	0
1	NYM	C	107	1	18,21,22	0.55	0	22,30,33	0.68	1 (4%)
1	G38	B	14	1	21,24,25	0.64	0	27,35,38	0.57	1 (3%)
1	A43	B	17	1	20,23,24	0.41	0	25,33,36	0.49	0
1	A43	F	217	1	20,23,24	0.41	0	25,33,36	0.64	1 (4%)
1	A43	E	205	1	20,23,24	0.42	0	25,33,36	0.75	2 (8%)
1	C42	A	3	1	17,20,21	0.61	0	20,28,31	0.82	1 (5%)
1	G38	A	4	1	21,24,25	0.48	0	27,35,38	0.54	0
1	A43	A	6	1	20,23,24	0.50	0	25,33,36	0.64	1 (4%)
1	C42	D	113	1	17,17,21	0.57	0	21,24,31	0.59	0
1	C42	D	121	1	17,20,21	0.54	0	20,28,31	0.66	1 (5%)
1	G38	D	122	1	21,24,25	0.65	0	27,35,38	0.60	1 (3%)
1	C42	E	201	1	17,17,21	0.46	0	21,24,31	0.64	0
1	G38	A	10	1	21,24,25	0.68	0	27,35,38	0.70	1 (3%)
1	G38	C	104	1	21,24,25	0.60	0	27,35,38	0.75	1 (3%)
1	G38	C	102	1	21,24,25	0.50	0	27,35,38	0.66	1 (3%)
1	A43	D	117	1	20,23,24	0.45	0	25,33,36	0.51	1 (4%)
1	A43	C	106	1	20,23,24	0.50	0	25,33,36	0.49	0
1	NYM	F	220	1	18,21,22	0.69	0	22,30,33	0.73	1 (4%)
1	A43	C	105	1	20,23,24	0.32	0	25,33,36	0.56	0
1	A43	E	206	1	20,23,24	0.48	0	25,33,36	0.79	2 (8%)
1	C42	E	209	1	17,20,21	0.60	0	20,28,31	0.74	1 (5%)
1	C42	D	123	1	17,20,21	0.66	0	20,28,31	0.66	0
1	C42	E	211	1	17,20,21	0.43	0	20,28,31	0.54	0
1	A43	D	118	1	20,23,24	0.50	0	25,33,36	0.75	1 (4%)
1	C42	A	9	1	17,20,21	0.46	0	20,28,31	0.59	0
1	C42	C	111	1	17,20,21	0.62	0	20,28,31	0.67	0
1	G38	F	222	1	21,24,25	0.57	0	27,35,38	0.62	1 (3%)
1	NYM	A	7	1	18,21,22	0.58	0	22,30,33	0.70	1 (4%)
1	G38	F	216	1	21,24,25	0.55	0	27,35,38	0.67	1 (3%)
1	C42	A	11	1	17,20,21	0.56	0	20,28,31	0.80	2 (10%)
1	C42	B	15	1	17,20,21	0.52	0	20,28,31	0.88	2 (10%)
1	G38	B	16	1	21,24,25	0.62	0	27,35,38	0.68	1 (3%)
1	G38	B	22	1	21,24,25	0.57	0	27,35,38	0.69	1 (3%)
1	C42	B	23	1	17,20,21	0.62	0	20,28,31	0.80	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	C42	C	101	1	17,17,21	0.45	0	21,24,31	0.57	0
1	NYM	C	108	1	18,21,22	0.60	0	22,30,33	0.81	1 (4%)
1	C42	B	21	1	17,20,21	0.42	0	20,28,31	0.57	0
1	G38	C	110	1	21,24,25	0.51	0	27,35,38	0.67	0
1	G38	E	210	1	21,24,25	0.54	0	27,35,38	0.72	2 (7%)
1	C42	E	203	1	17,20,21	0.56	0	20,28,31	0.79	1 (5%)
1	C42	A	1	1	17,17,21	0.45	0	21,24,31	0.43	0
1	A43	B	18	1	20,23,24	0.42	0	25,33,36	0.54	0
1	NYM	E	207	1	18,21,22	0.63	0	22,30,33	0.67	0
1	G38	D	116	1	21,24,25	0.58	0	27,35,38	0.65	1 (3%)
1	NYM	D	120	1	18,21,22	0.64	0	22,30,33	0.73	1 (4%)
1	A43	F	218	1	20,23,24	0.50	0	25,33,36	0.56	0
1	C42	F	223	1	17,20,21	0.40	0	20,28,31	0.43	0
1	A43	A	5	1	20,23,24	0.40	0	25,33,36	0.67	1 (4%)
1	NYM	F	219	1	18,21,22	0.53	0	22,30,33	0.53	0
1	C42	C	109	1	17,20,21	0.52	0	20,28,31	0.63	1 (5%)
1	NYM	A	8	1	18,21,22	0.58	0	22,30,33	0.71	1 (4%)
1	C42	F	213	1	17,17,21	0.44	0	21,24,31	0.63	0
1	G38	D	114	1	21,24,25	0.46	0	27,35,38	0.63	0
1	C42	F	215	1	17,20,21	0.51	0	20,28,31	0.86	2 (10%)
1	C42	C	103	1	17,20,21	0.49	0	20,28,31	0.63	1 (5%)
1	G38	E	204	1	21,24,25	0.50	0	27,35,38	0.48	0
1	NYM	B	19	1	18,21,22	0.64	0	22,30,33	0.74	1 (4%)
1	NYM	E	208	1	18,21,22	0.64	0	22,30,33	0.64	0
1	C42	B	13	1	17,17,21	0.41	0	21,24,31	0.51	0
1	C42	D	115	1	17,20,21	0.43	0	20,28,31	0.60	1 (5%)
1	C42	F	221	1	17,20,21	0.57	0	20,28,31	0.72	0
1	G38	E	202	1	21,24,25	0.56	0	27,35,38	0.69	1 (3%)

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
1	NYM	D	119	1	-	0/7/21/22	0/2/2/2
1	G38	A	2	1	-	0/7/21/22	0/3/3/3
1	NYM	B	20	1	-	0/7/21/22	0/2/2/2
1	G38	F	214	1	-	0/7/21/22	0/3/3/3
1	NYM	C	107	1	-	0/7/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G38	B	14	1	-	0/7/21/22	0/3/3/3
1	A43	B	17	1	-	0/7/21/22	0/3/3/3
1	A43	F	217	1	-	0/7/21/22	0/3/3/3
1	A43	E	205	1	-	0/7/21/22	0/3/3/3
1	C42	A	3	1	-	0/7/21/22	0/2/2/2
1	G38	A	4	1	-	0/7/21/22	0/3/3/3
1	A43	A	6	1	-	0/7/21/22	0/3/3/3
1	C42	D	113	1	-	0/6/18/22	0/2/2/2
1	C42	D	121	1	-	0/7/21/22	0/2/2/2
1	G38	D	122	1	-	0/7/21/22	0/3/3/3
1	C42	E	201	1	-	0/6/18/22	0/2/2/2
1	G38	A	10	1	-	0/7/21/22	0/3/3/3
1	G38	C	104	1	-	0/7/21/22	0/3/3/3
1	G38	C	102	1	-	1/7/21/22	0/3/3/3
1	A43	D	117	1	-	2/7/21/22	0/3/3/3
1	A43	C	106	1	-	0/7/21/22	0/3/3/3
1	NYM	F	220	1	-	0/7/21/22	0/2/2/2
1	A43	C	105	1	-	0/7/21/22	0/3/3/3
1	A43	E	206	1	-	0/7/21/22	0/3/3/3
1	C42	E	209	1	-	0/7/21/22	0/2/2/2
1	C42	D	123	1	-	0/7/21/22	0/2/2/2
1	C42	E	211	1	-	0/7/21/22	0/2/2/2
1	A43	D	118	1	-	0/7/21/22	0/3/3/3
1	C42	A	9	1	-	0/7/21/22	0/2/2/2
1	C42	C	111	1	-	0/7/21/22	0/2/2/2
1	G38	F	222	1	-	0/7/21/22	0/3/3/3
1	NYM	A	7	1	-	0/7/21/22	0/2/2/2
1	G38	F	216	1	-	0/7/21/22	0/3/3/3
1	C42	A	11	1	-	0/7/21/22	0/2/2/2
1	C42	B	15	1	-	0/7/21/22	0/2/2/2
1	G38	B	16	1	-	0/7/21/22	0/3/3/3
1	G38	B	22	1	-	0/7/21/22	0/3/3/3
1	C42	B	23	1	-	0/7/21/22	0/2/2/2
1	C42	C	101	1	-	0/6/18/22	0/2/2/2
1	NYM	C	108	1	-	0/7/21/22	0/2/2/2
1	C42	B	21	1	-	0/7/21/22	0/2/2/2
1	G38	C	110	1	-	0/7/21/22	0/3/3/3
1	G38	E	210	1	-	0/7/21/22	0/3/3/3
1	C42	E	203	1	-	0/7/21/22	0/2/2/2
1	C42	A	1	1	-	0/6/18/22	0/2/2/2
1	A43	B	18	1	-	0/7/21/22	0/3/3/3
1	NYM	E	207	1	-	0/7/21/22	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	G38	D	116	1	-	0/7/21/22	0/3/3/3
1	NYM	D	120	1	-	0/7/21/22	0/2/2/2
1	A43	F	218	1	-	0/7/21/22	0/3/3/3
1	C42	F	223	1	-	0/7/21/22	0/2/2/2
1	A43	A	5	1	-	0/7/21/22	0/3/3/3
1	NYM	F	219	1	-	0/7/21/22	0/2/2/2
1	C42	C	109	1	-	0/7/21/22	0/2/2/2
1	NYM	A	8	1	-	0/7/21/22	0/2/2/2
1	C42	F	213	1	-	0/6/18/22	0/2/2/2
1	G38	D	114	1	-	0/7/21/22	0/3/3/3
1	C42	F	215	1	-	0/7/21/22	0/2/2/2
1	C42	C	103	1	-	0/7/21/22	0/2/2/2
1	G38	E	204	1	-	0/7/21/22	0/3/3/3
1	NYM	B	19	1	-	0/7/21/22	0/2/2/2
1	NYM	E	208	1	-	0/7/21/22	0/2/2/2
1	C42	B	13	1	-	1/6/18/22	0/2/2/2
1	C42	D	115	1	-	0/7/21/22	0/2/2/2
1	C42	F	221	1	-	0/7/21/22	0/2/2/2
1	G38	E	202	1	-	0/7/21/22	0/3/3/3

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	NYM	C2'-C3'-C4'	-3.02	99.09	103.06
1	C	104	G38	C2'-C3'-C4'	-2.90	99.25	103.06
1	E	203	C42	C2'-C3'-C4'	-2.79	99.39	103.06
1	B	15	C42	C2'-C3'-C4'	-2.74	99.46	103.06
1	B	16	G38	C2'-C3'-C4'	-2.72	99.49	103.06
1	D	118	A43	C2'-C3'-C4'	-2.70	99.52	103.06
1	A	2	G38	C2'-C3'-C4'	-2.66	99.56	103.06
1	B	20	NYM	C2'-C3'-C4'	-2.65	99.57	103.06
1	E	205	A43	C2'-C3'-C4'	-2.65	99.58	103.06
1	A	3	C42	C2'-C3'-C4'	-2.65	99.58	103.06
1	B	22	G38	C2'-C3'-C4'	-2.58	99.67	103.06
1	D	116	G38	C2'-C3'-C4'	-2.58	99.67	103.06
1	A	5	A43	C2'-C3'-C4'	-2.52	99.75	103.06
1	F	215	C42	C2'-C3'-C4'	-2.52	99.75	103.06
1	F	222	G38	C2'-C3'-C4'	-2.51	99.76	103.06
1	A	8	NYM	C2'-C3'-C4'	-2.48	99.80	103.06
1	B	23	C42	C2'-C3'-C4'	-2.47	99.81	103.06
1	E	202	G38	C2'-C3'-C4'	-2.46	99.82	103.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	108	NYM	C2'-C3'-C4'	-2.46	99.82	103.06
1	A	6	A43	C2'-C3'-C4'	-2.42	99.88	103.06
1	F	216	G38	C1'-C2'-C3'	-2.40	98.39	102.93
1	D	122	G38	C2'-C3'-C4'	-2.38	99.93	103.06
1	E	206	A43	C2'-C3'-C4'	-2.35	99.97	103.06
1	A	7	NYM	C2'-C3'-C4'	-2.34	99.99	103.06
1	C	109	C42	C2'-C3'-C4'	-2.31	100.03	103.06
1	F	215	C42	C1'-C2'-C3'	-2.30	98.58	102.93
1	E	209	C42	C2'-C3'-C4'	-2.30	100.04	103.06
1	F	220	NYM	C2'-C3'-C4'	-2.29	100.05	103.06
1	B	15	C42	C1'-C2'-C3'	-2.29	98.61	102.93
1	B	14	G38	C2'-C3'-C4'	-2.23	100.13	103.06
1	A	10	G38	C2'-C3'-C4'	-2.20	100.16	103.06
1	A	11	C42	C2'-C3'-C4'	-2.19	100.18	103.06
1	D	119	NYM	C2'-C3'-C4'	-2.18	100.20	103.06
1	E	210	G38	C1'-C2'-C3'	-2.17	98.82	102.93
1	C	102	G38	C1'-C2'-C3'	-2.17	98.83	102.93
1	E	210	G38	C2'-C3'-C4'	-2.16	100.23	103.06
1	C	107	NYM	C2'-C3'-C4'	-2.16	100.23	103.06
1	E	205	A43	C1'-C2'-C3'	-2.14	98.89	102.93
1	D	115	C42	C2'-C3'-C4'	-2.14	100.25	103.06
1	E	206	A43	C1'-C2'-C3'	-2.09	98.99	102.93
1	A	11	C42	C1'-C2'-C3'	-2.08	98.99	102.93
1	D	121	C42	C2'-C3'-C4'	-2.08	100.33	103.06
1	D	120	NYM	C2'-C3'-C4'	-2.04	100.38	103.06
1	F	217	A43	C2'-C3'-C4'	-2.03	100.39	103.06
1	C	103	C42	C2'-C3'-C4'	-2.03	100.40	103.06
1	D	117	A43	C2'-C3'-C4'	-2.02	100.41	103.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	117	A43	O4'-C1'-N9-C8
1	B	13	C42	C3'-C4'-C5'-O5'
1	C	102	G38	O4'-C1'-N9-C4
1	D	117	A43	C2'-C1'-N9-C8

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	107	NYM	0	4
1	A	6	A43	0	5
1	F	220	NYM	0	4
1	B	19	NYM	0	5

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are modelled with single atom and 12 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 ⓘ

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	1/12 (8%)	-0.34	0 100 100	11, 11, 11, 11	1 (100%)
1	B	1/12 (8%)	-0.84	0 100 100	10, 10, 10, 10	1 (100%)
1	C	1/12 (8%)	-0.81	0 100 100	8, 8, 8, 8	1 (100%)
1	D	1/12 (8%)	-0.02	0 100 100	13, 13, 13, 13	1 (100%)
1	E	1/12 (8%)	0.09	0 100 100	15, 15, 15, 15	1 (100%)
1	F	1/12 (8%)	-0.92	0 100 100	7, 7, 7, 7	1 (100%)
All	All	6/72 (8%)	-0.47	0 100 100	7, 10, 13, 15	6 (100%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
1	C42	C	101	16/20	0.84	0.09	20,39,50,50	17
1	G38	C	102	22/23	0.84	0.10	19,31,47,50	23
1	G38	F	214	22/23	0.84	0.09	20,35,50,50	23
1	C42	F	215	19/20	0.85	0.09	20,40,49,50	20
1	C42	F	213	16/20	0.86	0.10	14,28,47,50	17
1	C42	C	103	19/20	0.87	0.08	13,24,41,43	20
1	C42	E	211	19/20	0.89	0.09	15,27,38,39	20
1	G38	F	216	22/23	0.90	0.09	16,26,44,47	23
1	C42	A	1	16/20	0.91	0.07	14,22,31,32	17
1	G38	B	14	22/23	0.91	0.07	10,18,32,34	23
1	C42	E	201	16/20	0.92	0.07	11,17,24,25	17

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	C42	D	113	16/20	0.92	0.06	11,19,31,39	17
1	G38	D	114	22/23	0.92	0.07	14,20,26,29	23
1	A43	B	17	21/22	0.93	0.07	13,24,28,29	22
1	A43	C	105	21/22	0.93	0.07	14,20,30,33	22
1	A43	F	218	21/22	0.93	0.06	5,16,28,32	22
1	G38	A	4	22/23	0.94	0.07	10,21,29,34	23
1	G38	C	104	22/23	0.94	0.06	2,18,29,32	23
1	G38	A	2	22/23	0.94	0.06	10,14,30,36	23
1	A43	F	217	21/22	0.94	0.06	12,20,32,34	22
1	C42	B	15	19/20	0.94	0.06	12,22,43,45	20
1	G38	D	116	22/23	0.95	0.06	2,17,28,32	23
1	C42	C	109	19/20	0.95	0.06	12,17,30,30	20
1	C42	E	203	19/20	0.95	0.06	16,24,30,31	20
1	C42	B	21	19/20	0.95	0.06	12,17,22,24	20
1	C42	A	11	19/20	0.95	0.06	3,21,29,31	20
1	G38	F	222	22/23	0.95	0.06	19,23,30,35	23
1	NYM	A	8	20/21	0.95	0.06	7,16,26,28	21
1	G38	E	204	22/23	0.96	0.06	5,11,15,20	23
1	G38	E	210	22/23	0.96	0.06	4,15,20,25	23
1	A43	C	106	21/22	0.96	0.06	2,9,19,22	22
1	C42	D	115	19/20	0.96	0.06	15,21,28,31	20
1	G38	B	22	22/23	0.96	0.05	2,9,16,20	23
1	A43	D	117	21/22	0.96	0.06	5,11,20,25	22
1	C42	D	121	19/20	0.96	0.05	7,13,20,23	20
1	C42	D	123	19/20	0.96	0.06	8,16,25,29	20
1	C42	C	111	19/20	0.96	0.05	5,15,20,21	20
1	G38	E	202	22/23	0.96	0.05	2,20,29,34	23
1	NYM	E	207	20/21	0.96	0.05	9,17,24,28	21
1	NYM	F	219	20/21	0.96	0.06	2,12,18,22	21
1	C42	B	13	16/20	0.96	0.07	14,23,33,38	17
1	NYM	E	208	20/21	0.96	0.05	2,12,20,27	21
1	G38	C	110	22/23	0.97	0.05	7,12,17,20	23
1	G38	B	16	22/23	0.97	0.05	10,19,28,34	23
1	A43	D	118	21/22	0.97	0.04	7,12,15,20	22
1	A43	E	205	21/22	0.97	0.04	7,11,17,20	22
1	A43	E	206	21/22	0.97	0.05	8,13,17,20	22
1	C42	F	223	19/20	0.97	0.05	11,16,29,30	20
1	NYM	C	107	20/21	0.97	0.05	8,12,16,20	21
1	NYM	D	119	20/21	0.97	0.05	5,9,18,27	21
1	A43	A	5	21/22	0.97	0.05	5,12,17,22	22
1	G38	D	122	22/23	0.97	0.05	2,7,13,20	23
1	A43	B	18	21/22	0.97	0.05	8,14,19,20	22

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	NYM	B	20	20/21	0.97	0.05	4,13,16,21	21
1	NYM	D	120	20/21	0.97	0.04	4,13,17,20	21
1	C42	A	9	19/20	0.97	0.05	10,15,20,22	20
1	NYM	F	220	20/21	0.97	0.05	8,13,17,20	20
1	C42	A	3	19/20	0.98	0.05	10,16,22,23	20
1	G38	A	10	22/23	0.98	0.04	4,10,16,20	23
1	C42	F	221	19/20	0.98	0.04	9,16,22,28	20
1	C42	B	23	19/20	0.98	0.05	5,11,18,20	20
1	C42	E	209	19/20	0.98	0.04	5,14,17,20	20
1	NYM	C	108	20/21	0.98	0.05	2,11,18,22	21
1	NYM	A	7	20/21	0.98	0.05	6,11,20,23	21
1	NYM	B	19	20/21	0.98	0.04	9,12,17,22	20
1	A43	A	6	21/22	0.98	0.05	2,10,12,20	22

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NH4	A	237	1/1	-	-	16,16,16,16	1
2	NH4	A	239	1/1	-	-	13,13,13,13	1
2	NH4	B	225	1/1	0.02	0.23	16,16,16,16	1
2	NH4	A	226	1/1	0.48	0.23	17,17,17,17	1
2	NH4	B	238	1/1	-	-	17,17,17,17	1
2	NH4	B	240	1/1	-	-	13,13,13,13	1
2	NH4	F	231	1/1	0.49	0.10	15,15,15,15	1
3	CL	A	250	1/1	0.70	0.06	9,9,9,9	1
2	NH4	C	243	1/1	-	-	15,15,15,15	1
2	NH4	C	245	1/1	-	-	15,15,15,15	1
2	NH4	C	244	1/1	-	-	15,15,15,15	1
2	NH4	C	248	1/1	-	-	15,15,15,15	1
2	NH4	D	242	1/1	-	-	15,15,15,15	1
2	NH4	D	246	1/1	-	-	15,15,15,15	1
2	NH4	D	241	1/1	-	-	16,16,16,16	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NH4	D	247	1/1	-	-	14,14,14,14	1
2	NH4	E	235	1/1	0.73	0.07	14,14,14,14	1
2	NH4	E	229	1/1	0.75	0.16	16,16,16,16	1
3	CL	F	253	1/1	0.79	0.05	12,12,12,12	1
3	CL	E	252	1/1	0.84	0.07	15,15,15,15	1
2	NH4	E	230	1/1	0.84	0.10	15,15,15,15	1
2	NH4	A	228	1/1	0.87	0.07	13,13,13,13	1
3	CL	F	254	1/1	0.89	0.11	12,12,12,12	1
2	NH4	F	233	1/1	0.89	0.05	15,15,15,15	1
3	CL	A	255	1/1	-	-	10,10,10,10	1
2	NH4	F	232	1/1	0.94	0.06	15,15,15,15	1
3	CL	B	256	1/1	-	-	9,9,9,9	1
2	NH4	E	234	1/1	0.97	0.03	15,15,15,15	1
3	CL	C	259	1/1	-	-	12,12,12,12	1
3	CL	C	260	1/1	-	-	12,12,12,12	1
3	CL	D	258	1/1	-	-	15,15,15,15	1
3	CL	D	257	1/1	-	-	14,14,14,14	1
2	NH4	B	227	1/1	0.99	0.06	13,13,13,13	1
2	NH4	F	236	1/1	0.99	0.12	15,15,15,15	1
3	CL	E	251	1/1	0.99	0.02	14,14,14,14	1
3	CL	B	249	1/1	1.00	0.01	10,10,10,10	1

6.5 Other polymers

There are no such residues in this entry.