



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5HUL / pdb_00005hul
Title : Crystal Structure of NadC Deletion Mutant in Cubic Space Group
Authors : Booth, W.T.; Chruszcz, M.
Deposited on : 2016-01-27
Resolution : 2.85 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

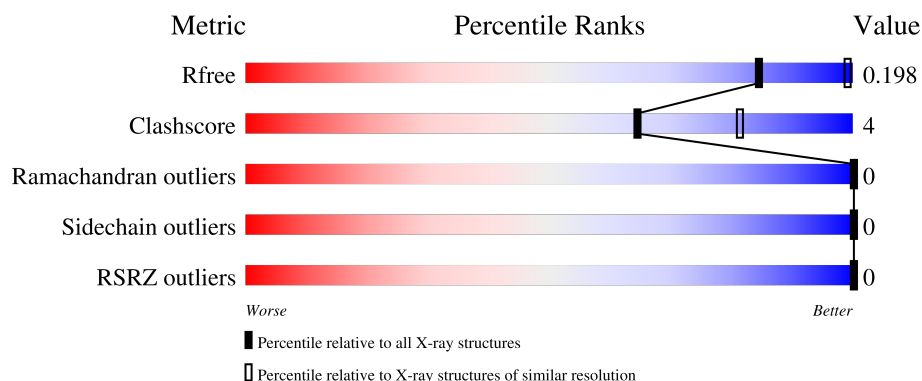
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	314	 82% 8% 10%
1	B	314	 81% 9% 10%
1	C	314	 82% 9% 10%
1	D	314	 78% 12% 10%

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	PO4	A	305	-	X	-	-
2	PO4	D	304	-	X	-	-
2	PO4	D	305	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8671 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 Quinolate phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2139	1346	361	423	9			
1	B	283	Total	C	N	O	S	0	0	0
			2149	1353	370	417	9			
1	C	283	Total	C	N	O	S	0	0	0
			2128	1341	361	417	9			
1	D	284	Total	C	N	O	S	0	0	0
			2157	1359	371	418	9			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
A	-23	HIS	-	expression tag	UNP A0A0H3BVM1
A	-22	HIS	-	expression tag	UNP A0A0H3BVM1
A	-21	HIS	-	expression tag	UNP A0A0H3BVM1
A	-20	HIS	-	expression tag	UNP A0A0H3BVM1
A	-19	HIS	-	expression tag	UNP A0A0H3BVM1
A	-18	HIS	-	expression tag	UNP A0A0H3BVM1
A	-17	SER	-	expression tag	UNP A0A0H3BVM1
A	-16	SER	-	expression tag	UNP A0A0H3BVM1
A	-15	GLY	-	expression tag	UNP A0A0H3BVM1
A	-14	VAL	-	expression tag	UNP A0A0H3BVM1
A	-13	ASP	-	expression tag	UNP A0A0H3BVM1
A	-12	LEU	-	expression tag	UNP A0A0H3BVM1
A	-11	GLY	-	expression tag	UNP A0A0H3BVM1
A	-10	THR	-	expression tag	UNP A0A0H3BVM1
A	-9	GLU	-	expression tag	UNP A0A0H3BVM1
A	-8	ASN	-	expression tag	UNP A0A0H3BVM1
A	-7	LEU	-	expression tag	UNP A0A0H3BVM1
A	-6	TYR	-	expression tag	UNP A0A0H3BVM1
A	-5	PHE	-	expression tag	UNP A0A0H3BVM1
A	-4	GLN	-	expression tag	UNP A0A0H3BVM1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP A0A0H3BVM1
A	-2	GLY	-	expression tag	UNP A0A0H3BVM1
A	-1	SER	-	expression tag	UNP A0A0H3BVM1
A	0	GLY	-	expression tag	UNP A0A0H3BVM1
A	?	-	UNK	deletion	UNP A0A0H3BVM1
B	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
B	-23	HIS	-	expression tag	UNP A0A0H3BVM1
B	-22	HIS	-	expression tag	UNP A0A0H3BVM1
B	-21	HIS	-	expression tag	UNP A0A0H3BVM1
B	-20	HIS	-	expression tag	UNP A0A0H3BVM1
B	-19	HIS	-	expression tag	UNP A0A0H3BVM1
B	-18	HIS	-	expression tag	UNP A0A0H3BVM1
B	-17	SER	-	expression tag	UNP A0A0H3BVM1
B	-16	SER	-	expression tag	UNP A0A0H3BVM1
B	-15	GLY	-	expression tag	UNP A0A0H3BVM1
B	-14	VAL	-	expression tag	UNP A0A0H3BVM1
B	-13	ASP	-	expression tag	UNP A0A0H3BVM1
B	-12	LEU	-	expression tag	UNP A0A0H3BVM1
B	-11	GLY	-	expression tag	UNP A0A0H3BVM1
B	-10	THR	-	expression tag	UNP A0A0H3BVM1
B	-9	GLU	-	expression tag	UNP A0A0H3BVM1
B	-8	ASN	-	expression tag	UNP A0A0H3BVM1
B	-7	LEU	-	expression tag	UNP A0A0H3BVM1
B	-6	TYR	-	expression tag	UNP A0A0H3BVM1
B	-5	PHE	-	expression tag	UNP A0A0H3BVM1
B	-4	GLN	-	expression tag	UNP A0A0H3BVM1
B	-3	SER	-	expression tag	UNP A0A0H3BVM1
B	-2	GLY	-	expression tag	UNP A0A0H3BVM1
B	-1	SER	-	expression tag	UNP A0A0H3BVM1
B	0	GLY	-	expression tag	UNP A0A0H3BVM1
B	?	-	UNK	deletion	UNP A0A0H3BVM1
C	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
C	-23	HIS	-	expression tag	UNP A0A0H3BVM1
C	-22	HIS	-	expression tag	UNP A0A0H3BVM1
C	-21	HIS	-	expression tag	UNP A0A0H3BVM1
C	-20	HIS	-	expression tag	UNP A0A0H3BVM1
C	-19	HIS	-	expression tag	UNP A0A0H3BVM1
C	-18	HIS	-	expression tag	UNP A0A0H3BVM1
C	-17	SER	-	expression tag	UNP A0A0H3BVM1
C	-16	SER	-	expression tag	UNP A0A0H3BVM1
C	-15	GLY	-	expression tag	UNP A0A0H3BVM1
C	-14	VAL	-	expression tag	UNP A0A0H3BVM1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	ASP	-	expression tag	UNP A0A0H3BVM1
C	-12	LEU	-	expression tag	UNP A0A0H3BVM1
C	-11	GLY	-	expression tag	UNP A0A0H3BVM1
C	-10	THR	-	expression tag	UNP A0A0H3BVM1
C	-9	GLU	-	expression tag	UNP A0A0H3BVM1
C	-8	ASN	-	expression tag	UNP A0A0H3BVM1
C	-7	LEU	-	expression tag	UNP A0A0H3BVM1
C	-6	TYR	-	expression tag	UNP A0A0H3BVM1
C	-5	PHE	-	expression tag	UNP A0A0H3BVM1
C	-4	GLN	-	expression tag	UNP A0A0H3BVM1
C	-3	SER	-	expression tag	UNP A0A0H3BVM1
C	-2	GLY	-	expression tag	UNP A0A0H3BVM1
C	-1	SER	-	expression tag	UNP A0A0H3BVM1
C	0	GLY	-	expression tag	UNP A0A0H3BVM1
C	?	-	UNK	deletion	UNP A0A0H3BVM1
D	-24	MET	-	initiating methionine	UNP A0A0H3BVM1
D	-23	HIS	-	expression tag	UNP A0A0H3BVM1
D	-22	HIS	-	expression tag	UNP A0A0H3BVM1
D	-21	HIS	-	expression tag	UNP A0A0H3BVM1
D	-20	HIS	-	expression tag	UNP A0A0H3BVM1
D	-19	HIS	-	expression tag	UNP A0A0H3BVM1
D	-18	HIS	-	expression tag	UNP A0A0H3BVM1
D	-17	SER	-	expression tag	UNP A0A0H3BVM1
D	-16	SER	-	expression tag	UNP A0A0H3BVM1
D	-15	GLY	-	expression tag	UNP A0A0H3BVM1
D	-14	VAL	-	expression tag	UNP A0A0H3BVM1
D	-13	ASP	-	expression tag	UNP A0A0H3BVM1
D	-12	LEU	-	expression tag	UNP A0A0H3BVM1
D	-11	GLY	-	expression tag	UNP A0A0H3BVM1
D	-10	THR	-	expression tag	UNP A0A0H3BVM1
D	-9	GLU	-	expression tag	UNP A0A0H3BVM1
D	-8	ASN	-	expression tag	UNP A0A0H3BVM1
D	-7	LEU	-	expression tag	UNP A0A0H3BVM1
D	-6	TYR	-	expression tag	UNP A0A0H3BVM1
D	-5	PHE	-	expression tag	UNP A0A0H3BVM1
D	-4	GLN	-	expression tag	UNP A0A0H3BVM1
D	-3	SER	-	expression tag	UNP A0A0H3BVM1
D	-2	GLY	-	expression tag	UNP A0A0H3BVM1
D	-1	SER	-	expression tag	UNP A0A0H3BVM1
D	0	GLY	-	expression tag	UNP A0A0H3BVM1
D	?	-	UNK	deletion	UNP A0A0H3BVM1

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	1	Total	O	0	0
			1	1		

- Molecule 1: Quinolate phosphoribosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, α , β , γ	179.63Å 179.63Å 179.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.20 – 2.85 39.20 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.20-2.85) 99.8 (39.20-2.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.170 , 0.205 0.165 , 0.198	Depositor DCC
R_{free} test set	2269 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	74.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.249 for l,-k,h	Xtriage
Reported twinning fraction	0.730 for H, K, L 0.270 for K, H, -L	Depositor
Outliers	0 of 44916 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	8671	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% 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: PO4

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	1.10	0/2169	1.19	8/2940 (0.3%)
1	B	1.09	0/2178	1.18	7/2945 (0.2%)
1	C	1.12	1/2158 (0.0%)	1.18	3/2925 (0.1%)
1	D	1.10	0/2189	1.21	10/2964 (0.3%)
All	All	1.10	1/8694 (0.0%)	1.19	28/11774 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	164	ASN	C-O	-5.39	1.19	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	ILE	CB-CA-C	-7.80	102.85	111.35
1	A	139	ARG	NE-CZ-NH2	7.42	125.88	119.20
1	D	40	GLY	N-CA-C	-6.49	100.14	111.62
1	B	258	ARG	N-CA-C	5.85	118.13	111.11
1	A	139	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	D	39	HIS	N-CA-C	-5.80	102.61	110.68
1	D	258	ARG	N-CA-C	5.68	117.93	111.11
1	D	253	THR	N-CA-C	5.60	117.83	111.11
1	B	194	PRO	CA-C-N	-5.47	113.66	122.24
1	B	194	PRO	C-N-CA	-5.47	113.66	122.24
1	C	253	THR	N-CA-C	5.46	117.93	111.33
1	A	178	ALA	N-CA-C	5.36	117.88	111.71
1	D	37	ASP	N-CA-C	-5.28	105.43	111.14
1	C	183	GLN	N-CA-C	5.22	116.97	111.28
1	A	35	ILE	CB-CA-C	-5.21	105.37	111.94
1	D	131	ASP	N-CA-C	5.18	117.67	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	THR	CB-CA-C	-5.18	102.14	110.74
1	B	35	ILE	N-CA-C	5.17	115.05	108.12
1	D	194	PRO	CA-C-N	-5.16	114.08	121.98
1	D	194	PRO	C-N-CA	-5.16	114.08	121.98
1	A	194	PRO	CA-C-N	-5.14	114.22	122.08
1	A	194	PRO	C-N-CA	-5.14	114.22	122.08
1	D	253	THR	CB-CA-C	-5.07	102.69	110.81
1	A	142	THR	N-CA-C	-5.06	103.28	109.65
1	C	164	ASN	N-CA-C	5.05	114.50	107.73
1	B	253	THR	N-CA-C	5.05	117.17	111.11
1	D	13	ILE	N-CA-C	5.04	118.93	113.43
1	B	182	VAL	N-CA-C	-5.01	106.18	110.74

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	2139	0	2090	13	0
1	B	2149	0	2134	14	1
1	C	2128	0	2086	17	0
1	D	2157	0	2127	22	0
2	A	25	0	0	1	1
2	B	25	0	0	0	0
2	C	20	0	0	1	0
2	D	25	0	0	2	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
All	All	8671	0	8437	66	1

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 4.

All (66) 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:D:54:LEU:HB2	1:D:84:LEU:HD21	1.61	0.82
1:D:222:LEU:HD13	1:D:230:ILE:HG22	1.74	0.69
1:B:48:ALA:HB2	1:B:84:LEU:HD23	1.78	0.65
1:D:9:THR:HG22	1:D:11:PHE:H	1.63	0.63
1:D:6:THR:HG22	1:D:7:ASP:O	2.04	0.57
1:D:36:PHE:CD2	1:D:97:VAL:HG11	2.39	0.57
1:A:6:THR:HG22	1:A:7:ASP:O	2.05	0.56
1:A:9:THR:HG22	1:A:11:PHE:H	1.71	0.55
1:C:203:VAL:HG13	1:C:208:ALA:HB3	1.89	0.55
1:D:140:LYS:NZ	2:D:301:PO4:O2	2.34	0.55
1:B:60:PHE:CE2	1:B:93:ILE:HD11	2.42	0.54
1:B:130:ASP:OD2	1:B:258:ARG:O	2.25	0.54
1:D:287:LEU:HD12	1:D:287:LEU:N	2.22	0.54
1:D:54:LEU:HB2	1:D:84:LEU:CD2	2.35	0.54
1:D:130:ASP:OD2	1:D:258:ARG:O	2.26	0.53
1:C:35:ILE:HG22	1:C:35:ILE:O	2.07	0.53
1:C:60:PHE:CE2	1:C:93:ILE:HD11	2.43	0.53
1:A:60:PHE:CE2	1:A:93:ILE:HD11	2.44	0.53
1:B:48:ALA:CB	1:B:84:LEU:HD23	2.38	0.53
1:C:225:MET:HE3	1:C:229:GLN:HB3	1.91	0.53
1:D:60:PHE:CE2	1:D:93:ILE:HD11	2.44	0.53
1:B:225:MET:HE3	1:B:229:GLN:HB3	1.90	0.52
1:B:203:VAL:HG13	1:B:208:ALA:HB3	1.92	0.51
1:D:225:MET:HE3	1:D:229:GLN:HB3	1.93	0.51
1:A:225:MET:HE3	1:A:229:GLN:HB3	1.93	0.51
1:B:9:THR:HG22	1:B:11:PHE:H	1.75	0.51
1:A:203:VAL:HG13	1:A:208:ALA:HB3	1.92	0.50
1:D:203:VAL:HG13	1:D:208:ALA:HB3	1.93	0.49
1:D:213:ALA:HB3	1:D:240:ARG:HH11	1.77	0.49
1:C:6:THR:O	1:C:6:THR:HG22	2.12	0.49
1:C:35:ILE:O	1:C:37:ASP:N	2.39	0.49
1:B:60:PHE:CD1	1:B:107:ALA:HB1	2.48	0.48
1:B:85:THR:HG22	1:B:86:SER:N	2.28	0.48
1:C:54:LEU:HB2	1:C:84:LEU:HD11	1.96	0.47
1:D:49:LYS:HG3	2:D:304:PO4:O3	2.15	0.47
1:C:9:THR:HG22	1:C:11:PHE:H	1.79	0.47
1:B:250:ASP:OD1	1:B:251:MET:N	2.48	0.46
1:B:44:VAL:HG23	1:B:100:LEU:HD13	1.98	0.46
1:B:114:LEU:HD21	1:B:148:PHE:HB3	1.98	0.45
1:D:35:ILE:HG22	1:D:35:ILE:O	2.16	0.45
1:D:44:VAL:HG23	1:D:100:LEU:HD13	1.98	0.45
1:A:164:ASN:HB3	1:A:166:SER:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ARG:C	1:C:84:LEU:HD12	2.42	0.45
1:C:114:LEU:HD21	1:C:148:PHE:HB3	2.00	0.44
1:A:44:VAL:HG23	1:A:100:LEU:HD13	2.00	0.44
1:A:85:THR:HG22	1:A:86:SER:N	2.32	0.43
1:C:60:PHE:CD1	1:C:107:ALA:HB1	2.53	0.43
1:C:35:ILE:O	1:C:35:ILE:CG2	2.65	0.43
1:A:114:LEU:HD21	1:A:148:PHE:HB3	2.01	0.43
1:D:114:LEU:HD21	1:D:148:PHE:HB3	2.01	0.43
1:A:78:PHE:CD2	1:A:90:VAL:HA	2.54	0.42
1:C:35:ILE:C	1:C:37:ASP:H	2.27	0.42
1:C:44:VAL:HG23	1:C:100:LEU:HD13	2.00	0.42
1:C:250:ASP:OD1	1:C:251:MET:N	2.51	0.42
1:A:60:PHE:CD1	1:A:107:ALA:HB1	2.55	0.42
1:D:222:LEU:CD1	1:D:230:ILE:HG22	2.47	0.41
1:A:139:ARG:N	2:A:304:PO4:O1	2.53	0.41
1:B:164:ASN:OD1	1:B:164:ASN:C	2.64	0.41
1:C:172:LYS:NZ	2:C:303:PO4:O3	2.46	0.41
1:D:60:PHE:HE2	1:D:93:ILE:HD11	1.86	0.41
1:B:54:LEU:HB2	1:B:84:LEU:HD13	2.01	0.41
1:D:60:PHE:CD1	1:D:107:ALA:HB1	2.56	0.41
1:C:85:THR:HG22	1:C:86:SER:N	2.35	0.40
1:A:93:ILE:HG22	1:A:100:LEU:HD22	2.03	0.40
1:D:36:PHE:CG	1:D:97:VAL:HG11	2.57	0.40
1:D:164:ASN:HB3	1:D:166:SER:H	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LYS:NZ	2:A:305:PO4:O4[5_555]	2.06	0.14

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	282/314 (90%)	275 (98%)	7 (2%)	0	100	100
1	B	279/314 (89%)	269 (96%)	10 (4%)	0	100	100
1	C	281/314 (90%)	273 (97%)	8 (3%)	0	100	100
1	D	282/314 (90%)	273 (97%)	9 (3%)	0	100	100
All	All	1124/1256 (90%)	1090 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	224/260 (86%)	224 (100%)	0	100	100
1	B	227/260 (87%)	227 (100%)	0	100	100
1	C	222/260 (85%)	222 (100%)	0	100	100
1	D	227/260 (87%)	227 (100%)	0	100	100
All	All	900/1040 (86%)	900 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	HIS
1	B	76	HIS
1	B	112	GLN
1	C	112	GLN
1	D	39	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

19 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	PO4	B	301	-	4,4,4	0.85	0	6,6,6	0.91	0
2	PO4	B	302	-	4,4,4	0.90	0	6,6,6	0.51	0
2	PO4	D	305	-	4,4,4	10.05	4 (100%)	6,6,6	0.51	0
2	PO4	D	303	-	4,4,4	1.19	0	6,6,6	1.71	2 (33%)
2	PO4	A	301	-	4,4,4	1.41	0	6,6,6	0.91	0
2	PO4	B	305	-	4,4,4	0.89	0	6,6,6	0.59	0
2	PO4	B	303	-	4,4,4	0.91	0	6,6,6	0.71	0
2	PO4	A	302	-	4,4,4	0.83	0	6,6,6	1.26	1 (16%)
2	PO4	C	303	-	4,4,4	0.90	0	6,6,6	1.33	1 (16%)
2	PO4	B	304	-	4,4,4	0.91	0	6,6,6	1.36	1 (16%)
2	PO4	A	304	-	4,4,4	0.81	0	6,6,6	2.11	2 (33%)
2	PO4	C	301	-	4,4,4	0.80	0	6,6,6	0.78	0
2	PO4	C	302	-	4,4,4	0.93	0	6,6,6	0.39	0
2	PO4	D	302	-	4,4,4	0.70	0	6,6,6	0.69	0
2	PO4	D	304	-	4,4,4	8.66	4 (100%)	6,6,6	1.10	0
2	PO4	D	301	-	4,4,4	1.20	0	6,6,6	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	A	305	-	4,4,4	9.61	4 (100%)	6,6,6	0.37	0
2	PO4	C	304	-	4,4,4	0.90	0	6,6,6	0.52	0
2	PO4	A	303	-	4,4,4	0.94	0	6,6,6	0.56	0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	305	PO4	P-O1	13.14	1.81	1.50
2	D	305	PO4	P-O1	12.96	1.80	1.50
2	D	304	PO4	P-O1	10.97	1.76	1.50
2	D	305	PO4	P-O3	9.49	1.82	1.54
2	D	305	PO4	P-O4	9.42	1.82	1.54
2	A	305	PO4	P-O4	8.36	1.79	1.54
2	A	305	PO4	P-O2	8.10	1.78	1.54
2	D	304	PO4	P-O4	7.87	1.77	1.54
2	D	304	PO4	P-O3	7.84	1.77	1.54
2	A	305	PO4	P-O3	7.82	1.77	1.54
2	D	305	PO4	P-O2	7.57	1.76	1.54
2	D	304	PO4	P-O2	7.48	1.76	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	304	PO4	O4-P-O3	3.59	119.09	107.91
2	D	303	PO4	O4-P-O1	2.63	120.26	110.95
2	A	304	PO4	O2-P-O1	-2.53	102.02	110.95
2	C	303	PO4	O2-P-O1	-2.42	102.39	110.95
2	B	304	PO4	O3-P-O1	-2.34	102.67	110.95
2	A	302	PO4	O4-P-O2	2.24	114.88	107.91
2	D	303	PO4	O3-P-O2	2.06	114.32	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	303	PO4	1	0
2	A	304	PO4	1	0
2	D	304	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	PO4	1	0
2	A	305	PO4	0	1

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	284/314 (90%)	-1.60	0 100 100	128, 149, 184, 278	0
1	B	283/314 (90%)	-1.47	0 100 100	116, 145, 207, 240	0
1	C	283/314 (90%)	-1.57	0 100 100	125, 155, 193, 252	0
1	D	284/314 (90%)	-1.50	0 100 100	121, 146, 205, 232	0
All	All	1134/1256 (90%)	-1.54	0 100 100	116, 149, 202, 278	0

There are no RSRZ outliers to report.

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
2	PO4	B	302	5/5	0.91	0.03	187,208,222,249	0
2	PO4	C	304	5/5	0.94	0.03	209,218,243,245	0
2	PO4	A	303	5/5	0.95	0.03	136,137,140,147	5
2	PO4	A	305	5/5	0.95	0.15	72,73,75,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	B	305	5/5	0.97	0.05	254,258,278,294	0
2	PO4	C	302	5/5	0.97	0.03	219,240,254,257	0
2	PO4	A	302	5/5	0.97	0.07	119,129,145,160	5
2	PO4	D	302	5/5	0.97	0.04	113,130,139,147	5
2	PO4	D	304	5/5	0.97	0.22	73,74,74,76	0
2	PO4	A	304	5/5	0.98	0.04	120,128,175,193	5
2	PO4	C	301	5/5	0.98	0.03	180,186,196,216	0
2	PO4	D	303	5/5	0.98	0.05	137,145,169,170	5
2	PO4	B	303	5/5	0.98	0.06	189,206,215,235	0
2	PO4	D	305	5/5	0.98	0.11	72,73,75,77	0
2	PO4	A	301	5/5	0.99	0.03	126,127,140,146	5
2	PO4	C	303	5/5	0.99	0.05	116,123,151,154	5
2	PO4	B	301	5/5	0.99	0.04	117,118,141,149	5
2	PO4	D	301	5/5	0.99	0.03	115,135,143,145	5
2	PO4	B	304	5/5	1.00	0.04	129,152,185,204	5

6.5 Other polymers [i](#)

There are no such residues in this entry.