Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 11:38 AM JST

|		
PDB ID	:	5Z2L
Title	:	Crystal structure of BdcA in complex with NADPH
Authors	:	Yang, W.S.; Hou, Y.J.; Li, D.F.; Wang, D.C.
Deposited on	:	2018-01-03
Resolution	:	1.70 Å(reported)

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 1.70 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.
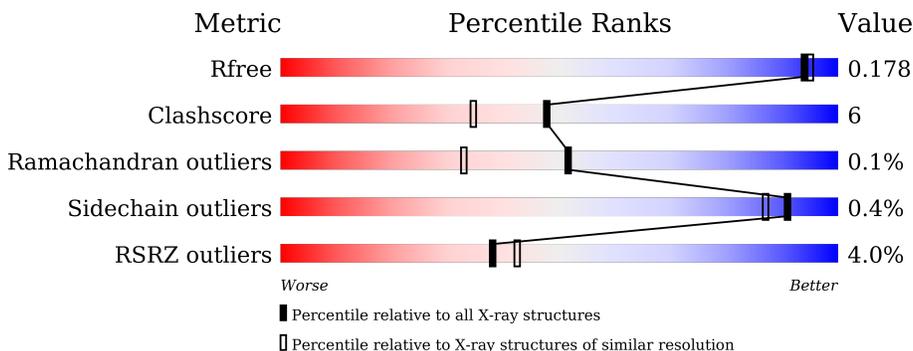
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	245	3% / 90% / 7% ·
1	B	245	3% / 89% / 10% ·
1	C	245	2% / 85% / 12% ··
1	D	245	% / 89% / 9% ·
1	E	245	3% / 86% / 12% ·
1	F	245	4% / 88% / 10% ·

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Mol	Chain	Length	Quality of chain
1	G	245	16% · · · 77% · · · 20%
1	H	245	13% · · · 83% · · · 14%
1	I	245	.% · · · 90% · · · 8%
1	J	245	.% · · · 91% · · · 7%
1	K	245	.% · · · 91% · · · 9%
1	L	245	91% · · · 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
7	PG4	F	301	-	-	-	X

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 25111 atoms, of which 404 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 Cyclic-di-GMP-binding biofilm dispersal mediator protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	10	0
			1784	1111	330	332	11			
1	D	240	Total	C	N	O	S	0	7	0
			1776	1103	333	329	11			
1	B	243	Total	C	N	O	S	0	11	0
			1823	1130	349	333	11			
1	C	241	Total	C	N	O	S	0	17	0
			1842	1143	345	342	12			
1	E	239	Total	C	N	O	S	0	6	0
			1772	1100	335	328	9			
1	J	242	Total	C	N	O	S	0	12	0
			1815	1125	340	339	11			
1	H	239	Total	C	N	O	S	0	5	0
			1757	1094	324	328	11			
1	K	244	Total	C	N	O	S	0	19	0
			1882	1167	360	343	12			
1	I	241	Total	C	N	O	S	0	9	0
			1786	1112	330	333	11			
1	F	239	Total	C	N	O	S	0	8	0
			1768	1103	326	328	11			
1	G	239	Total	C	N	O	S	0	9	0
			1769	1102	325	331	11			
1	L	239	Total	C	N	O	S	0	11	0
			1777	1103	331	332	11			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	LEU	-	expression tag	UNP P39333
A	239	GLU	-	expression tag	UNP P39333
A	240	HIS	-	expression tag	UNP P39333
A	241	HIS	-	expression tag	UNP P39333
A	242	HIS	-	expression tag	UNP P39333

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Chain	Residue	Modelled	Actual	Comment	Reference
A	243	HIS	-	expression tag	UNP P39333
A	244	HIS	-	expression tag	UNP P39333
A	245	HIS	-	expression tag	UNP P39333
D	238	LEU	-	expression tag	UNP P39333
D	239	GLU	-	expression tag	UNP P39333
D	240	HIS	-	expression tag	UNP P39333
D	241	HIS	-	expression tag	UNP P39333
D	242	HIS	-	expression tag	UNP P39333
D	243	HIS	-	expression tag	UNP P39333
D	244	HIS	-	expression tag	UNP P39333
D	245	HIS	-	expression tag	UNP P39333
B	238	LEU	-	expression tag	UNP P39333
B	239	GLU	-	expression tag	UNP P39333
B	240	HIS	-	expression tag	UNP P39333
B	241	HIS	-	expression tag	UNP P39333
B	242	HIS	-	expression tag	UNP P39333
B	243	HIS	-	expression tag	UNP P39333
B	244	HIS	-	expression tag	UNP P39333
B	245	HIS	-	expression tag	UNP P39333
C	238	LEU	-	expression tag	UNP P39333
C	239	GLU	-	expression tag	UNP P39333
C	240	HIS	-	expression tag	UNP P39333
C	241	HIS	-	expression tag	UNP P39333
C	242	HIS	-	expression tag	UNP P39333
C	243	HIS	-	expression tag	UNP P39333
C	244	HIS	-	expression tag	UNP P39333
C	245	HIS	-	expression tag	UNP P39333
E	238	LEU	-	expression tag	UNP P39333
E	239	GLU	-	expression tag	UNP P39333
E	240	HIS	-	expression tag	UNP P39333
E	241	HIS	-	expression tag	UNP P39333
E	242	HIS	-	expression tag	UNP P39333
E	243	HIS	-	expression tag	UNP P39333
E	244	HIS	-	expression tag	UNP P39333
E	245	HIS	-	expression tag	UNP P39333
J	238	LEU	-	expression tag	UNP P39333
J	239	GLU	-	expression tag	UNP P39333
J	240	HIS	-	expression tag	UNP P39333
J	241	HIS	-	expression tag	UNP P39333
J	242	HIS	-	expression tag	UNP P39333
J	243	HIS	-	expression tag	UNP P39333
J	244	HIS	-	expression tag	UNP P39333

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Chain	Residue	Modelled	Actual	Comment	Reference
J	245	HIS	-	expression tag	UNP P39333
H	238	LEU	-	expression tag	UNP P39333
H	239	GLU	-	expression tag	UNP P39333
H	240	HIS	-	expression tag	UNP P39333
H	241	HIS	-	expression tag	UNP P39333
H	242	HIS	-	expression tag	UNP P39333
H	243	HIS	-	expression tag	UNP P39333
H	244	HIS	-	expression tag	UNP P39333
H	245	HIS	-	expression tag	UNP P39333
K	238	LEU	-	expression tag	UNP P39333
K	239	GLU	-	expression tag	UNP P39333
K	240	HIS	-	expression tag	UNP P39333
K	241	HIS	-	expression tag	UNP P39333
K	242	HIS	-	expression tag	UNP P39333
K	243	HIS	-	expression tag	UNP P39333
K	244	HIS	-	expression tag	UNP P39333
K	245	HIS	-	expression tag	UNP P39333
I	238	LEU	-	expression tag	UNP P39333
I	239	GLU	-	expression tag	UNP P39333
I	240	HIS	-	expression tag	UNP P39333
I	241	HIS	-	expression tag	UNP P39333
I	242	HIS	-	expression tag	UNP P39333
I	243	HIS	-	expression tag	UNP P39333
I	244	HIS	-	expression tag	UNP P39333
I	245	HIS	-	expression tag	UNP P39333
F	238	LEU	-	expression tag	UNP P39333
F	239	GLU	-	expression tag	UNP P39333
F	240	HIS	-	expression tag	UNP P39333
F	241	HIS	-	expression tag	UNP P39333
F	242	HIS	-	expression tag	UNP P39333
F	243	HIS	-	expression tag	UNP P39333
F	244	HIS	-	expression tag	UNP P39333
F	245	HIS	-	expression tag	UNP P39333
G	238	LEU	-	expression tag	UNP P39333
G	239	GLU	-	expression tag	UNP P39333
G	240	HIS	-	expression tag	UNP P39333
G	241	HIS	-	expression tag	UNP P39333
G	242	HIS	-	expression tag	UNP P39333
G	243	HIS	-	expression tag	UNP P39333
G	244	HIS	-	expression tag	UNP P39333
G	245	HIS	-	expression tag	UNP P39333
L	238	LEU	-	expression tag	UNP P39333

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Chain	Residue	Modelled	Actual	Comment	Reference
L	239	GLU	-	expression tag	UNP P39333
L	240	HIS	-	expression tag	UNP P39333
L	241	HIS	-	expression tag	UNP P39333
L	242	HIS	-	expression tag	UNP P39333
L	243	HIS	-	expression tag	UNP P39333
L	244	HIS	-	expression tag	UNP P39333
L	245	HIS	-	expression tag	UNP P39333

- Molecule 2 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 20	C 5	H 12	O 3	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	D	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	B	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	C	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	E	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	J	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	H	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	K	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	I	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	F	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	G	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		
3	L	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1
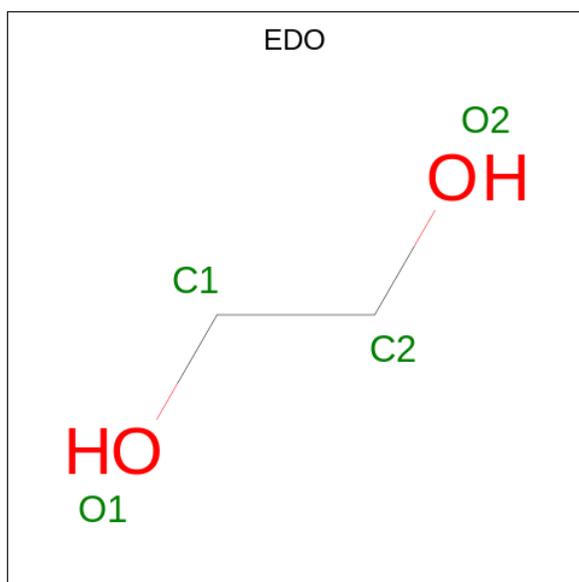
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 10	C 2	H 6	O 2	0	0
4	C	1	Total 10	C 2	H 6	O 2	0	0
4	C	1	Total 10	C 2	H 6	O 2	0	0
4	E	1	Total 10	C 2	H 6	O 2	0	0
4	I	1	Total 10	C 2	H 6	O 2	0	0
4	G	1	Total 10	C 2	H 6	O 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
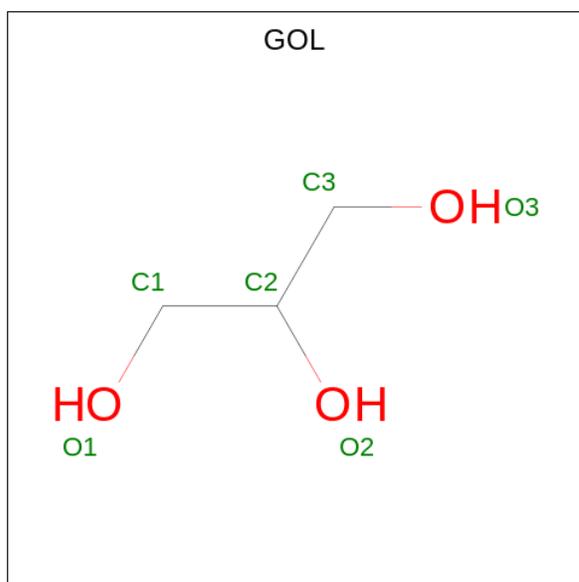
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 14	C 3	H 8	O 3	0	0
5	E	1	Total 14	C 3	H 8	O 3	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG
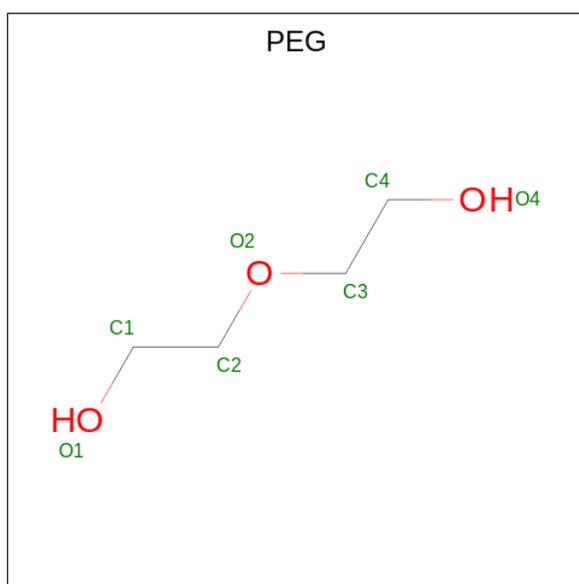
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	K	1	Total 17	C 4	H 10	O 3	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

PG4

C8 OH O5

O4

C7

C5 C6

C4 O3

O2 C3

C1

C2

HO

O1
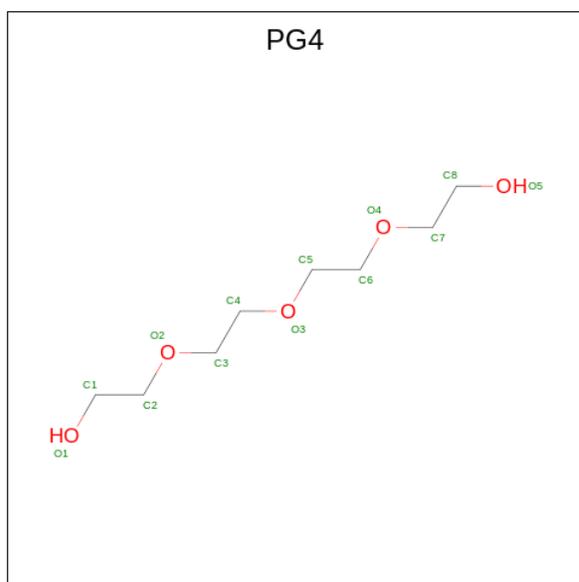
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	F	1	31	8	18	5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	155	Total 155	O 155	0	0
8	D	215	Total 215	O 215	0	0
8	B	185	Total 185	O 185	0	0
8	C	245	Total 245	O 245	0	0
8	E	185	Total 185	O 185	0	0
8	J	274	Total 274	O 274	0	0
8	H	118	Total 118	O 118	0	0
8	K	297	Total 297	O 297	0	0
8	I	265	Total 265	O 265	0	0
8	F	189	Total 189	O 189	0	0
8	G	94	Total 94	O 94	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	294	Total 294	O 294	0	0

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: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain A:

- Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain D:

- Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain B:

- Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain C:

- Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain E:

A234 L238 E239 H240 HIS HIS HIS HIS

• Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain J:

MET G2 T5 N32 T36 K41 K45 V56 G89 E90 E93 K104 E123 G142 R158 R167 G168 L238 H241 H242 H243 HIS HIS

• Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain H:

MET G2 K7 R34 F35 T36 S40 K41 D42 K45 R46 L47 A48 Q49 V56 V66 V69 S73 L76 I85 G86 V87 F88 G89 E90 A91 L92 E93 D100 R101 L102 F103 K104 M121 L128 S132 V133 N134 G135 D136 R137 M138 P139 V140 A141 G142

A148 S149 K150 S151 A152 G155 M156 A157 R158 V173 D182 A183 N184 P185 A186 N187 G188 P189 M190 R191 D192 M193 A199 V213 S222 T225 G226 A227 I231 A234 H240 HIS HIS HIS HIS

• Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain K:

MET G2 T8 V9 L10 R34 F35 T36 K45 V56 S73 G89 G131 N134 R137 M138 P139 G142 M143 R158 R167 F235 H240 H243 H244 H245

• Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain I:

MET G2 T8 R34 F35 T36 D42 K45 Q49 V56 S73 V81 R101 I107 P110 I129 I130 G131 M138 S149 R167 A186 R191 E239 H240 H241 H242 HIS HIS HIS

• Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain F:

MET G2 G6 T36 K41 V56 D64 S73 L76 F88 G89 E90 A91 L92 E93 D98 L102 I107 S132 M138 P139 V140 M143 S149 K150 S151 A152 R158 R162 M187 M190 R191 D192 I231 A234 L238 E239 H240

HIS HIS HIS HIS

• Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain G:

• Molecule 1: Cyclic-di-GMP-binding biofilm dispersal mediator protein

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.83Å 72.28Å 172.32Å 99.22° 86.78° 107.70°	Depositor
Resolution (Å)	43.73 – 1.70 43.73 – 1.70	Depositor EDS
% Data completeness (in resolution range)	92.3 (43.73-1.70) 92.3 (43.73-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.99 (at 1.70Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.151 , 0.179 0.151 , 0.178	Depositor DCC
R_{free} test set	2009 reflections (0.66%)	wwPDB-VP
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,k+l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	25111	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, EDO, PG0, PG4, PEG, NDP

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	0.36	0/1862	0.55	0/2516
1	B	0.36	0/1918	0.53	0/2590
1	C	0.44	0/1936	0.63	0/2614
1	D	0.40	0/1847	0.57	0/2496
1	E	0.37	0/1841	0.56	0/2487
1	F	0.36	0/1840	0.57	0/2486
1	G	0.31	0/1847	0.51	0/2498
1	H	0.33	0/1814	0.52	0/2453
1	I	0.44	0/1867	0.60	0/2526
1	J	0.46	0/1911	0.60	0/2583
1	K	0.49	0/1990	0.66	0/2688
1	L	0.50	0/1869	0.65	0/2525
All	All	0.41	0/22542	0.58	0/30462

There are no bond length outliers.

There are no bond angle outliers.

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	A	1784	0	1796	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1823	0	1815	22	0
1	C	1842	0	1835	40	0
1	D	1776	0	1768	19	0
1	E	1772	0	1778	24	0
1	F	1768	0	1780	25	0
1	G	1769	0	1769	47	0
1	H	1757	0	1755	31	0
1	I	1786	0	1778	20	0
1	J	1815	0	1801	17	0
1	K	1882	0	1865	22	0
1	L	1777	0	1765	19	0
2	A	8	12	12	0	0
3	A	48	26	26	0	0
3	B	48	26	26	0	0
3	C	48	26	26	1	0
3	D	48	26	26	1	0
3	E	48	26	26	1	0
3	F	48	26	26	0	0
3	G	48	26	26	1	0
3	H	48	26	26	0	0
3	I	48	26	26	1	0
3	J	48	26	26	0	0
3	K	48	26	26	1	0
3	L	48	26	26	1	0
4	B	4	6	6	2	0
4	C	8	12	12	2	0
4	E	4	6	6	0	0
4	G	4	6	6	0	0
4	I	4	6	6	0	0
5	C	6	8	8	0	0
5	E	6	8	8	0	0
6	K	7	10	10	0	0
7	F	13	18	18	0	0
8	A	155	0	0	2	1
8	B	185	0	0	2	0
8	C	245	0	0	11	2
8	D	215	0	0	6	2
8	E	185	0	0	3	0
8	F	189	0	0	5	0
8	G	94	0	0	7	0
8	H	118	0	0	3	1
8	I	265	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	274	0	0	6	1
8	K	297	0	0	5	4
8	L	294	0	0	7	1
All	All	24707	404	21909	270	6

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 6.

All (270) 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:E:45:LYS:NZ	8:E:401:HOH:O	1.82	1.13
1:D:95:ASN:ND2	8:D:401:HOH:O	1.96	0.97
1:A:167:ARG:NH1	8:A:401:HOH:O	1.98	0.94
1:I:81:VAL:HB	1:I:129[B]:ILE:HD13	1.51	0.90
4:C:303:EDO:O2	8:C:401:HOH:O	1.91	0.88
1:D:46:ARG:NH1	8:D:402:HOH:O	2.07	0.87
1:K:89:GLY:O	1:K:142[A]:GLY:HA2	1.78	0.82
1:G:41:LYS:HD2	8:G:492:HOH:O	1.79	0.82
1:I:42:ASP:OD2	8:I:401:HOH:O	1.98	0.82
1:D:89:GLY:HA2	1:B:243:HIS:HB2	1.60	0.82
1:L:97:ASP:OD1	8:L:401:HOH:O	2.00	0.78
1:J:93[A]:GLU:OE1	8:J:402:HOH:O	2.00	0.78
1:G:42[A]:ASP:OD1	8:G:401:HOH:O	2.02	0.78
1:H:100:ASP:OD2	8:H:401:HOH:O	2.03	0.77
1:G:15:SER:O	8:G:402:HOH:O	2.03	0.76
1:I:110:PRO:HB3	1:I:129[B]:ILE:HD12	1.67	0.76
1:F:143[B]:MET:HE1	8:F:468:HOH:O	1.86	0.76
1:F:238:LEU:O	8:F:402:HOH:O	2.04	0.75
8:D:423:HOH:O	1:C:141[A]:ALA:HA	1.88	0.74
1:G:37:TYR:CE2	1:G:41:LYS:HG3	2.23	0.73
1:B:71[B]:ARG:NH1	1:B:116:GLU:OE2	2.21	0.73
1:K:245:HIS:NE2	8:K:401:HOH:O	2.13	0.72
1:L:90[B]:GLU:OE2	8:L:402:HOH:O	2.08	0.72
1:J:167[B]:ARG:NH1	8:J:401:HOH:O	1.86	0.72
1:I:186:ALA:O	1:I:191:ARG:HG3	1.90	0.72
1:A:128[B]:LEU:HD13	1:A:213:VAL:HG13	1.72	0.72
1:D:158[A]:ARG:HD3	8:D:420:HOH:O	1.89	0.71
1:E:238:LEU:HD22	1:G:197[A]:LEU:HD21	1.71	0.71
1:K:36:THR:HG22	1:K:56[B]:VAL:HG13	1.69	0.71
1:E:34:ARG:HG2	1:E:54:THR:HB	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:34[B]:ARG:NH1	1:K:73:SER:OG	2.23	0.70
1:E:40:SER:OG	8:E:402:HOH:O	2.10	0.70
1:C:89:GLY:O	1:C:142[A]:GLY:HA2	1.92	0.69
1:C:64:ASP:H	4:C:303:EDO:H21	1.57	0.69
1:K:10:LEU:HD13	1:K:34[B]:ARG:HD3	1.75	0.69
1:H:128:LEU:HD13	1:H:213:VAL:HG13	1.74	0.69
1:D:101[B]:ARG:NE	8:D:403:HOH:O	2.23	0.69
1:F:90:GLU:OE1	1:F:92:LEU:N	2.27	0.68
1:C:139[B]:PRO:HB2	1:C:235:PHE:CE2	2.29	0.68
1:I:101:ARG:NH2	8:I:402:HOH:O	2.12	0.68
1:C:241:HIS:NE2	8:C:405:HOH:O	2.27	0.68
1:C:154:GLN:HA	1:C:228[B]:MET:HE1	1.76	0.67
1:C:90[A]:GLU:OE1	1:C:92:LEU:HB2	1.94	0.67
1:I:239:GLU:HB2	8:I:550:HOH:O	1.94	0.66
1:G:128:LEU:HD13	1:G:213:VAL:HG13	1.78	0.66
1:C:207[A]:GLU:OE2	8:C:403:HOH:O	2.12	0.66
1:C:139[B]:PRO:HB2	1:C:235:PHE:HE2	1.61	0.66
1:H:89:GLY:O	1:H:142:GLY:HA2	1.96	0.65
1:G:42[A]:ASP:OD1	1:G:43:ALA:N	2.30	0.65
1:E:238:LEU:HD23	1:G:193:MET:HG3	1.79	0.65
1:J:2:GLY:N	1:J:5:THR:HG1	1.95	0.64
1:G:8:THR:HG22	1:G:76:LEU:HD23	1.78	0.64
1:A:101:ARG:NH2	8:A:402:HOH:O	2.18	0.63
1:C:228[B]:MET:SD	8:C:508:HOH:O	2.55	0.63
1:E:101[A]:ARG:NH1	8:E:403:HOH:O	2.12	0.63
1:D:158[A]:ARG:HD2	1:C:138[A]:MET:SD	2.39	0.63
1:C:134:ASN:HD22	1:C:138[B]:MET:HA	1.63	0.63
1:A:240:HIS:HB3	8:C:408:HOH:O	1.98	0.62
1:J:90[B]:GLU:CG	1:J:93[B]:GLU:HG3	2.29	0.62
1:G:167:ARG:NE	8:G:403:HOH:O	2.17	0.62
1:C:134:ASN:HA	1:C:137[B]:ARG:O	1.98	0.62
1:E:207:GLU:CD	1:E:207:GLU:H	2.03	0.62
1:G:140:VAL:HG22	1:G:143[A]:MET:CE	2.30	0.62
1:B:89:GLY:O	1:B:142:GLY:HA2	2.01	0.61
1:G:68:ASP:OD1	1:G:72:LYS:HE3	2.01	0.61
1:K:158[A]:ARG:HD2	1:L:138[A]:MET:SD	2.41	0.61
1:C:138[B]:MET:HG3	1:C:143[B]:MET:SD	2.41	0.61
1:I:81:VAL:CB	1:I:129[B]:ILE:HD13	2.29	0.61
1:F:140:VAL:HG22	1:F:143[B]:MET:CE	2.31	0.61
1:A:237:ALA:HA	1:C:139[B]:PRO:HA	1.82	0.61
1:L:89:GLY:O	1:L:142:GLY:HA2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:LYS:NZ	8:C:404:HOH:O	2.18	0.60
1:L:34:ARG:HG2	1:L:54:THR:HB	1.84	0.60
1:C:134:ASN:ND2	1:C:138[B]:MET:HA	2.17	0.59
1:F:98:ASP:OD1	8:F:403:HOH:O	2.16	0.59
1:H:34:ARG:HE	1:H:56:VAL:HG21	1.66	0.59
1:I:167:ARG:NH1	8:I:404:HOH:O	2.34	0.59
1:I:34:ARG:HH11	1:I:73:SER:HG	1.51	0.58
1:B:186:ALA:O	1:B:191[B]:ARG:HD2	2.04	0.58
1:I:101:ARG:NE	8:I:402:HOH:O	2.33	0.58
1:E:128:LEU:HD13	1:E:213:VAL:HG13	1.86	0.58
1:F:138[B]:MET:HG3	8:F:443:HOH:O	2.04	0.57
1:K:138[B]:MET:SD	1:K:143[B]:MET:HG3	2.45	0.57
1:G:101[B]:ARG:NH2	8:G:407:HOH:O	2.38	0.57
1:K:134:ASN:HA	1:K:137[B]:ARG:O	2.04	0.57
1:H:132:SER:HB3	1:H:150:LYS:HG3	1.87	0.56
1:G:132:SER:HB3	1:G:150:LYS:HG3	1.87	0.56
1:F:64:ASP:OD1	8:F:404:HOH:O	2.18	0.56
1:H:138[A]:MET:HG3	8:G:428:HOH:O	2.06	0.56
1:K:167:ARG:NH2	8:K:402:HOH:O	2.39	0.56
1:L:90[A]:GLU:HG2	1:L:93:GLU:HG3	1.87	0.56
1:C:8[A]:THR:HG23	8:C:544:HOH:O	2.06	0.56
1:H:85:ILE:HD11	1:H:102:LEU:HA	1.87	0.55
1:D:2:GLY:N	8:D:408:HOH:O	2.39	0.55
1:G:9:VAL:HG22	1:G:78:ILE:HB	1.88	0.55
1:L:45:LYS:HD3	8:L:570:HOH:O	2.05	0.55
1:B:36:THR:HA	1:B:56:VAL:O	2.07	0.55
1:H:92:LEU:HD23	1:G:115:VAL:HG13	1.88	0.55
1:D:239:GLU:O	1:D:240:HIS:CB	2.55	0.55
1:D:187:ASN:OD1	1:D:191[B]:ARG:NH2	2.39	0.55
1:D:239:GLU:O	1:D:240:HIS:HB2	2.07	0.54
1:I:36:THR:HG22	1:I:56[B]:VAL:HG23	1.90	0.54
1:B:207:GLU:OE2	8:B:401:HOH:O	2.18	0.54
1:C:154:GLN:HG2	1:C:228[B]:MET:HE2	1.89	0.54
1:J:158[A]:ARG:HD2	1:I:138[A]:MET:SD	2.48	0.54
1:J:90[B]:GLU:HG3	1:J:93[B]:GLU:HG3	1.89	0.54
1:H:41:LYS:O	1:H:45:LYS:HG2	2.08	0.53
1:H:152:ALA:HB2	1:G:152:ALA:HB2	1.90	0.53
8:K:477:HOH:O	1:L:138[B]:MET:HG3	2.09	0.53
1:E:89:GLY:O	1:E:142:GLY:HA2	2.09	0.53
1:A:193[B]:MET:HG3	1:C:238:LEU:HD23	1.91	0.53
1:G:36:THR:HA	1:G:56:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34[B]:ARG:NH2	1:C:73:SER:OG	2.40	0.53
1:E:36:THR:HA	1:E:56:VAL:O	2.09	0.53
1:A:127:ILE:C	1:A:128[A]:LEU:HD22	2.29	0.53
1:I:34:ARG:NH1	1:I:73:SER:OG	2.24	0.52
1:F:88:PHE:CD1	1:F:143[B]:MET:HG2	2.45	0.52
1:K:138[A]:MET:HG3	8:L:509:HOH:O	2.09	0.52
1:I:81:VAL:HB	1:I:129[B]:ILE:CD1	2.33	0.52
1:G:37:TYR:HE2	1:G:41:LYS:HG3	1.69	0.52
1:K:10:LEU:HD13	1:K:34[B]:ARG:CD	2.40	0.52
1:G:66:VAL:O	1:G:69:VAL:HG12	2.10	0.52
1:F:73:SER:HB3	1:F:76[A]:LEU:HD21	1.93	0.51
1:H:187:ASN:HA	1:H:191:ARG:HH11	1.75	0.51
1:G:89:GLY:O	1:G:142:GLY:HA2	2.11	0.51
1:D:238:LEU:HD23	1:B:193[B]:MET:HG3	1.93	0.51
1:A:36:THR:HA	1:A:56:VAL:O	2.11	0.50
1:J:36:THR:HA	1:J:56:VAL:O	2.11	0.50
1:A:128[B]:LEU:CD1	1:A:213:VAL:HG13	2.41	0.50
1:J:104:LYS:NZ	8:J:403:HOH:O	2.25	0.50
1:G:88:PHE:CD1	1:G:143[A]:MET:HG2	2.46	0.50
1:B:41[B]:LYS:HE2	8:B:472:HOH:O	2.12	0.50
1:G:23:VAL:HG11	1:G:47:LEU:HD11	1.93	0.50
1:F:73:SER:HB3	1:F:76[A]:LEU:CD2	2.41	0.50
1:G:45:LYS:O	1:G:49[B]:GLN:HG3	2.11	0.50
1:C:139[B]:PRO:HG2	1:C:235:PHE:CD2	2.47	0.50
1:J:41:LYS:NZ	8:J:404:HOH:O	2.27	0.50
1:J:41:LYS:O	1:J:45:LYS:HG2	2.11	0.50
1:E:167[B]:ARG:CZ	1:F:92:LEU:HD22	2.42	0.49
1:F:90:GLU:OE1	1:F:92:LEU:HB2	2.11	0.49
1:L:36:THR:HG22	1:L:56[B]:VAL:HG13	1.94	0.49
1:G:8:THR:CG2	1:G:76:LEU:HD23	2.43	0.49
1:D:36:THR:HA	1:D:56:VAL:O	2.12	0.49
1:D:138[B]:MET:HG3	8:C:503:HOH:O	2.12	0.49
1:H:34:ARG:NH1	1:H:73:SER:OG	2.45	0.49
1:A:45:LYS:O	1:A:49:GLN:HG3	2.13	0.49
1:A:2:GLY:HA3	1:A:5:THR:OG1	2.12	0.49
1:A:193[A]:MET:HG2	1:C:238:LEU:HD23	1.95	0.48
1:E:238:LEU:CD2	1:G:197[A]:LEU:HD21	2.40	0.48
1:K:139[B]:PRO:HG2	1:K:235:PHE:CE2	2.48	0.48
1:L:45:LYS:CD	8:L:570:HOH:O	2.61	0.48
1:K:45:LYS:HE2	8:K:463:HOH:O	2.13	0.48
1:L:2:GLY:HA3	1:L:5:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138[B]:MET:HG3	8:I:500:HOH:O	2.14	0.48
1:E:98:ASP:OD1	1:E:101[C]:ARG:NH2	2.45	0.47
1:G:8:THR:HG22	1:G:76:LEU:CD2	2.43	0.47
1:G:137:ARG:O	1:G:139:PRO:HD3	2.14	0.47
1:K:8[A]:THR:HG23	8:K:550:HOH:O	2.13	0.47
1:H:139:PRO:HD2	1:G:158:ARG:HB3	1.97	0.47
1:G:118:ALA:O	1:G:167:ARG:NH1	2.47	0.47
1:L:123:GLU:OE2	8:L:403:HOH:O	2.21	0.47
1:C:139[B]:PRO:HG2	1:C:235:PHE:CE2	2.51	0.46
1:E:200:ILE:HD13	1:H:222:SER:O	2.15	0.46
1:K:139[B]:PRO:HG2	1:K:235:PHE:CD2	2.49	0.46
1:H:152:ALA:HA	1:G:151[B]:SER:OG	2.15	0.46
1:B:102:LEU:HD23	1:B:102:LEU:C	2.36	0.46
1:E:132:SER:HB3	1:E:150:LYS:HG3	1.95	0.46
1:I:8[A]:THR:HG23	8:I:512:HOH:O	2.15	0.46
1:B:235:PHE:HZ	4:B:301:EDO:H12	1.79	0.46
1:J:104:LYS:CE	8:J:403:HOH:O	2.63	0.46
1:C:36:THR:HA	1:C:56:VAL:O	2.15	0.46
1:G:193:MET:O	1:G:197[A]:LEU:HD23	2.15	0.46
1:H:193[B]:MET:HG2	1:F:238:LEU:HD23	1.98	0.46
1:B:88:PHE:HA	1:B:142:GLY:O	2.15	0.46
1:H:92:LEU:CD2	1:G:115:VAL:HG13	2.45	0.46
1:B:240:HIS:O	1:B:241:HIS:ND1	2.49	0.46
1:K:10:LEU:CD1	1:K:34[B]:ARG:HD3	2.45	0.46
1:C:140[A]:VAL:HG22	1:C:143[A]:MET:CE	2.47	0.45
1:J:90[B]:GLU:HG2	1:J:93[B]:GLU:HG3	1.96	0.45
1:B:140:VAL:HG21	4:B:301:EDO:H22	1.98	0.45
1:H:141:ALA:HB2	1:G:162:ARG:HG3	1.99	0.45
1:G:140:VAL:HG22	1:G:143[A]:MET:HE1	1.97	0.45
1:C:139[B]:PRO:CB	1:C:235:PHE:HE2	2.26	0.45
1:H:137:ARG:O	1:H:139:PRO:HD3	2.17	0.45
1:H:36:THR:HA	1:H:56:VAL:O	2.17	0.45
1:G:231:ILE:HG23	1:G:231:ILE:O	2.17	0.45
1:L:131:GLY:O	3:L:301:NDP:H6N	2.17	0.45
1:E:138:MET:SD	1:F:158:ARG:HD2	2.57	0.45
1:E:225:THR:HG23	1:H:234:ALA:HB2	1.99	0.44
1:D:132:SER:HB3	1:D:150:LYS:HG3	1.99	0.44
1:C:101:ARG:NH2	8:C:402:HOH:O	2.08	0.44
1:B:68:ASP:OD2	1:B:72:LYS:HE3	2.18	0.44
1:B:85:ILE:HD11	1:B:102:LEU:HA	1.99	0.44
1:C:18:ILE:HA	1:C:206:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:36:THR:HG22	1:K:56[B]:VAL:CG1	2.41	0.44
1:C:132:SER:HB3	1:C:150:LYS:HG3	2.00	0.44
1:G:131:GLY:O	3:G:302:NDP:H6N	2.18	0.44
1:C:128:LEU:HD13	1:C:213:VAL:HG13	1.99	0.44
1:F:132:SER:HB3	1:F:150:LYS:HG3	2.00	0.44
1:E:141:ALA:HB2	1:F:162:ARG:HG3	2.00	0.43
1:J:123[A]:GLU:CD	1:J:168:GLY:HA3	2.39	0.43
1:H:66:VAL:O	1:H:69:VAL:HG12	2.18	0.43
1:I:107:ILE:HD11	1:I:149:SER:HA	2.01	0.43
1:F:73:SER:CB	1:F:76[A]:LEU:HG	2.48	0.43
1:D:190:MET:HB3	1:D:193[B]:MET:HE3	2.01	0.43
1:D:238:LEU:HD23	1:B:193[A]:MET:HG2	2.00	0.43
1:G:60:SER:HA	1:G:66:VAL:CG2	2.48	0.43
1:B:109:ALA:HB3	1:B:110:PRO:HD3	2.00	0.43
1:F:36:THR:HA	1:F:56:VAL:O	2.19	0.43
1:L:90[A]:GLU:HG2	1:L:93:GLU:CG	2.48	0.43
1:D:73:SER:HB3	1:D:76:LEU:HD21	2.00	0.43
1:J:32[A]:ASN:ND2	8:J:409:HOH:O	2.43	0.43
1:B:61:ALA:O	1:B:104:LYS:HE2	2.19	0.43
1:A:89:GLY:O	1:A:142:GLY:HA2	2.19	0.42
1:F:140:VAL:HG22	1:F:143[B]:MET:HE1	2.01	0.42
1:C:131:GLY:O	3:C:304:NDP:H6N	2.19	0.42
1:H:199:ALA:HB3	1:H:234:ALA:HB3	2.01	0.42
1:G:109:ALA:HB3	1:G:110:PRO:HD3	2.00	0.42
1:L:158[A]:ARG:HD3	8:L:514:HOH:O	2.19	0.42
1:C:34[A]:ARG:HG3	8:C:544:HOH:O	2.18	0.42
1:C:137[B]:ARG:C	1:C:139[B]:PRO:HD3	2.39	0.42
1:E:109:ALA:HB3	1:E:110:PRO:HD3	2.02	0.42
1:F:234:ALA:HB2	1:G:225:THR:HG23	2.02	0.42
1:D:131:GLY:O	3:D:301:NDP:H6N	2.20	0.42
1:E:234:ALA:HB2	1:H:225:THR:HG23	2.02	0.42
1:F:102:LEU:C	1:F:102:LEU:HD23	2.40	0.42
1:E:8[A]:THR:HG22	1:E:76:LEU:HD23	2.01	0.41
1:I:45:LYS:O	1:I:49:GLN:HG3	2.20	0.41
1:G:167:ARG:CD	8:G:403:HOH:O	2.63	0.41
1:G:196:SER:OG	1:G:197[A]:LEU:HD22	2.20	0.41
1:G:197[A]:LEU:HD13	1:G:238:LEU:HA	2.01	0.41
1:J:238:LEU:HD23	1:L:193[B]:MET:HG2	2.02	0.41
1:J:238:LEU:HD23	1:L:193[A]:MET:HG3	2.02	0.41
1:C:138[B]:MET:SD	1:C:143[B]:MET:HG3	2.59	0.41
1:C:139[B]:PRO:CG	1:C:235:PHE:HE2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228[B]:MET:HG2	8:C:537:HOH:O	2.20	0.41
1:F:231:ILE:O	1:F:231:ILE:HG23	2.20	0.41
1:H:76:LEU:O	1:H:121:MET:HG3	2.21	0.41
1:H:158:ARG:HD2	1:G:138[A]:MET:SD	2.60	0.41
1:K:131:GLY:O	3:K:302:NDP:H6N	2.21	0.41
1:F:107:ILE:HD11	1:F:149:SER:HA	2.03	0.41
1:K:137[B]:ARG:O	1:K:139[B]:PRO:HD3	2.21	0.41
1:D:159:GLY:HA2	1:C:138[B]:MET:CE	2.51	0.41
8:H:463:HOH:O	1:G:138[B]:MET:HG3	2.19	0.41
1:E:131:GLY:O	3:E:303:NDP:H6N	2.20	0.41
1:J:89:GLY:O	1:J:142:GLY:HA2	2.20	0.41
1:H:100:ASP:CG	8:H:401:HOH:O	2.54	0.41
1:H:102:LEU:C	1:H:102:LEU:HD23	2.41	0.41
1:K:158[A]:ARG:CD	1:L:138[A]:MET:SD	3.08	0.40
1:C:139[B]:PRO:CB	1:C:235:PHE:CE2	3.02	0.40
1:H:7:LYS:HD3	1:H:7:LYS:HA	1.86	0.40
1:H:231:ILE:HG23	1:H:231:ILE:O	2.22	0.40
1:K:240:HIS:HE1	1:K:243[A]:HIS:CG	2.39	0.40
1:H:100:ASP:OD2	1:G:63:ARG:HD3	2.22	0.40
1:I:131:GLY:O	3:I:302:NDP:H6N	2.22	0.40
1:C:139[B]:PRO:CG	1:C:235:PHE:CE2	3.05	0.40
1:E:152:ALA:HB2	1:F:152:ALA:HB2	2.04	0.40
1:G:140:VAL:HG22	1:G:143[A]:MET:HE2	2.01	0.40

All (6) 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)
8:C:606:HOH:O	8:K:542:HOH:O[1_445]	1.90	0.30
8:K:634:HOH:O	8:L:630:HOH:O[1_655]	1.90	0.30
8:D:402:HOH:O	8:C:587:HOH:O[1_455]	1.99	0.21
8:D:587:HOH:O	8:K:575:HOH:O[1_445]	2.11	0.09
8:A:546:HOH:O	8:H:495:HOH:O[1_455]	2.12	0.08
8:J:673:HOH:O	8:K:697:HOH:O[1_545]	2.18	0.02

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	247/245 (101%)	241 (98%)	6 (2%)	0	100	100
1	B	252/245 (103%)	247 (98%)	5 (2%)	0	100	100
1	C	256/245 (104%)	245 (96%)	9 (4%)	2 (1%)	19	6
1	D	245/245 (100%)	237 (97%)	7 (3%)	1 (0%)	34	18
1	E	244/245 (100%)	238 (98%)	6 (2%)	0	100	100
1	F	245/245 (100%)	239 (98%)	6 (2%)	0	100	100
1	G	246/245 (100%)	238 (97%)	8 (3%)	0	100	100
1	H	242/245 (99%)	233 (96%)	9 (4%)	0	100	100
1	I	248/245 (101%)	243 (98%)	5 (2%)	0	100	100
1	J	252/245 (103%)	244 (97%)	8 (3%)	0	100	100
1	K	261/245 (106%)	252 (97%)	9 (3%)	0	100	100
1	L	248/245 (101%)	240 (97%)	8 (3%)	0	100	100
All	All	2986/2940 (102%)	2897 (97%)	86 (3%)	3 (0%)	51	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	143[A]	MET
1	C	143[B]	MET
1	D	240	HIS

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	181/177 (102%)	176 (97%)	5 (3%)	43	25
1	B	186/177 (105%)	186 (100%)	0	100	100
1	C	188/177 (106%)	187 (100%)	1 (0%)	88	83
1	D	179/177 (101%)	179 (100%)	0	100	100
1	E	178/177 (101%)	178 (100%)	0	100	100
1	F	179/177 (101%)	179 (100%)	0	100	100
1	G	180/177 (102%)	178 (99%)	2 (1%)	73	63
1	H	176/177 (99%)	174 (99%)	2 (1%)	73	63
1	I	182/177 (103%)	182 (100%)	0	100	100
1	J	186/177 (105%)	185 (100%)	1 (0%)	88	83
1	K	193/177 (109%)	193 (100%)	0	100	100
1	L	182/177 (103%)	180 (99%)	2 (1%)	73	63
All	All	2190/2124 (103%)	2177 (99%)	13 (1%)	91	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46[A]	ARG
1	A	46[B]	ARG
1	A	123[A]	GLU
1	A	123[B]	GLU
1	A	163	ASP
1	C	241	HIS
1	J	241	HIS
1	H	92	LEU
1	H	104	LYS
1	G	101[A]	ARG
1	G	101[B]	ARG
1	L	90[A]	GLU
1	L	90[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

23 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	#$|Z| > 2$
3	NDP	F	302	-	45,52,52	0.92	2 (4%)	53,80,80	1.26	6 (11%)
4	EDO	E	302	-	3,3,3	0.52	0	2,2,2	0.22	0
3	NDP	J	301	-	45,52,52	1.10	4 (8%)	53,80,80	1.23	6 (11%)
6	PEG	K	301	-	6,6,6	0.44	0	5,5,5	0.29	0
3	NDP	B	302	-	45,52,52	1.03	3 (6%)	53,80,80	1.23	6 (11%)
3	NDP	C	304	-	45,52,52	0.94	1 (2%)	53,80,80	1.32	8 (15%)
3	NDP	I	302	-	45,52,52	1.04	4 (8%)	53,80,80	1.29	7 (13%)
5	GOL	E	301	-	5,5,5	0.32	0	5,5,5	0.30	0
3	NDP	A	302	-	45,52,52	0.96	3 (6%)	53,80,80	1.25	5 (9%)
7	PG4	F	301	-	12,12,12	0.50	0	11,11,11	0.32	0
4	EDO	C	303	-	3,3,3	0.38	0	2,2,2	0.37	0
2	PG0	A	301	-	7,7,7	0.49	0	6,6,6	0.25	0
3	NDP	D	301	-	45,52,52	0.97	3 (6%)	53,80,80	1.17	5 (9%)
4	EDO	B	301	-	3,3,3	0.42	0	2,2,2	0.39	0
4	EDO	C	302	-	3,3,3	0.48	0	2,2,2	0.27	0
3	NDP	E	303	-	45,52,52	1.00	3 (6%)	53,80,80	1.26	5 (9%)
4	EDO	I	301	-	3,3,3	0.48	0	2,2,2	0.26	0
3	NDP	H	301	-	45,52,52	0.95	3 (6%)	53,80,80	1.20	5 (9%)
4	EDO	G	301	-	3,3,3	0.45	0	2,2,2	0.40	0
5	GOL	C	301	-	5,5,5	0.36	0	5,5,5	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	NDP	K	302	-	45,52,52	1.00	2 (4%)	53,80,80	1.35	8 (15%)
3	NDP	G	302	-	45,52,52	0.95	2 (4%)	53,80,80	1.18	4 (7%)
3	NDP	L	301	-	45,52,52	0.96	2 (4%)	53,80,80	1.28	6 (11%)

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
3	NDP	F	302	-	-	6/30/77/77	0/5/5/5
4	EDO	E	302	-	-	0/1/1/1	-
3	NDP	J	301	-	-	6/30/77/77	0/5/5/5
6	PEG	K	301	-	-	2/4/4/4	-
3	NDP	B	302	-	-	4/30/77/77	0/5/5/5
3	NDP	C	304	-	-	4/30/77/77	0/5/5/5
3	NDP	I	302	-	-	4/30/77/77	0/5/5/5
5	GOL	E	301	-	-	2/4/4/4	-
3	NDP	A	302	-	-	3/30/77/77	0/5/5/5
7	PG4	F	301	-	-	3/10/10/10	-
4	EDO	C	303	-	-	0/1/1/1	-
2	PG0	A	301	-	-	3/5/5/5	-
3	NDP	D	301	-	-	4/30/77/77	0/5/5/5
4	EDO	B	301	-	-	0/1/1/1	-
4	EDO	C	302	-	-	0/1/1/1	-
3	NDP	E	303	-	-	5/30/77/77	0/5/5/5
4	EDO	I	301	-	-	0/1/1/1	-
3	NDP	H	301	-	-	6/30/77/77	0/5/5/5
4	EDO	G	301	-	-	0/1/1/1	-
5	GOL	C	301	-	-	0/4/4/4	-
3	NDP	K	302	-	-	5/30/77/77	0/5/5/5
3	NDP	G	302	-	-	3/30/77/77	0/5/5/5
3	NDP	L	301	-	-	6/30/77/77	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	303	NDP	C6N-C5N	3.36	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	NDP	C6N-C5N	3.14	1.38	1.33
3	I	302	NDP	C6N-C5N	3.07	1.38	1.33
3	C	304	NDP	C6N-C5N	2.97	1.38	1.33
3	G	302	NDP	C6N-C5N	2.91	1.38	1.33
3	K	302	NDP	C6N-C5N	2.87	1.38	1.33
3	D	301	NDP	C6N-C5N	2.77	1.38	1.33
3	L	301	NDP	C6N-C5N	2.75	1.38	1.33
3	A	302	NDP	C6N-C5N	2.73	1.38	1.33
3	H	301	NDP	C6N-C5N	2.72	1.38	1.33
3	F	302	NDP	C6N-C5N	2.58	1.37	1.33
3	J	301	NDP	P2B-O2B	2.55	1.64	1.59
3	B	302	NDP	P2B-O2B	2.51	1.64	1.59
3	I	302	NDP	P2B-O2B	2.49	1.64	1.59
3	E	303	NDP	C5A-C4A	2.45	1.47	1.40
3	J	301	NDP	O4B-C1B	2.40	1.44	1.41
3	I	302	NDP	C2A-N3A	2.39	1.35	1.32
3	J	301	NDP	C2A-N3A	2.37	1.35	1.32
3	D	301	NDP	C5A-C4A	2.37	1.47	1.40
3	G	302	NDP	C5A-C4A	2.28	1.47	1.40
3	K	302	NDP	P2B-O2B	2.24	1.63	1.59
3	J	301	NDP	C6N-C5N	2.16	1.37	1.33
3	A	302	NDP	C5A-C4A	2.16	1.46	1.40
3	B	302	NDP	C5A-C4A	2.16	1.46	1.40
3	E	303	NDP	C2N-C3N	2.16	1.41	1.34
3	H	301	NDP	O4B-C1B	2.10	1.44	1.41
3	F	302	NDP	C2A-N3A	2.09	1.35	1.32
3	L	301	NDP	C5A-C4A	2.08	1.46	1.40
3	I	302	NDP	C5A-C4A	2.08	1.46	1.40
3	H	301	NDP	C5A-C4A	2.07	1.46	1.40
3	A	302	NDP	P2B-O2B	2.06	1.63	1.59
3	D	301	NDP	C2N-C3N	2.06	1.40	1.34

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	301	NDP	N3A-C2A-N1A	-4.35	121.88	128.68
3	D	301	NDP	N3A-C2A-N1A	-4.16	122.18	128.68
3	F	302	NDP	N3A-C2A-N1A	-4.11	122.25	128.68
3	K	302	NDP	N3A-C2A-N1A	-4.06	122.33	128.68
3	E	303	NDP	N3A-C2A-N1A	-3.86	122.64	128.68
3	G	302	NDP	N3A-C2A-N1A	-3.82	122.71	128.68
3	I	302	NDP	N3A-C2A-N1A	-3.78	122.77	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	NDP	N3A-C2A-N1A	-3.74	122.84	128.68
3	J	301	NDP	N3A-C2A-N1A	-3.64	122.99	128.68
3	B	302	NDP	N3A-C2A-N1A	-3.64	122.99	128.68
3	H	301	NDP	N3A-C2A-N1A	-3.46	123.28	128.68
3	C	304	NDP	C1D-N1N-C6N	-3.09	114.18	120.83
3	C	304	NDP	N3A-C2A-N1A	-3.06	123.89	128.68
3	I	302	NDP	O2B-P2B-O1X	-3.02	97.73	109.39
3	E	303	NDP	O2N-PN-O1N	2.99	127.04	112.24
3	K	302	NDP	C1B-N9A-C4A	-2.98	121.41	126.64
3	L	301	NDP	C1B-N9A-C4A	-2.98	121.41	126.64
3	B	302	NDP	O2B-P2B-O1X	-2.96	97.96	109.39
3	E	303	NDP	C1B-N9A-C4A	-2.92	121.50	126.64
3	J	301	NDP	O2B-P2B-O1X	-2.88	98.29	109.39
3	A	302	NDP	C4A-C5A-N7A	-2.86	106.42	109.40
3	I	302	NDP	C1B-N9A-C4A	-2.81	121.70	126.64
3	J	301	NDP	O3X-P2B-O2X	2.78	118.25	107.64
3	K	302	NDP	O2B-P2B-O1X	-2.76	98.74	109.39
3	J	301	NDP	O2A-PA-O1A	2.74	125.80	112.24
3	A	302	NDP	C3N-C7N-N7N	2.70	122.45	117.67
3	K	302	NDP	N6A-C6A-N1A	2.62	124.01	118.57
3	I	302	NDP	C1D-N1N-C6N	-2.57	115.29	120.83
3	C	304	NDP	N6A-C6A-N1A	2.53	123.82	118.57
3	C	304	NDP	C1B-N9A-C4A	-2.52	122.21	126.64
3	C	304	NDP	O2B-P2B-O1X	-2.50	99.76	109.39
3	H	301	NDP	C3N-C7N-N7N	2.49	122.08	117.67
3	H	301	NDP	O2B-P2B-O1X	-2.40	100.14	109.39
3	G	302	NDP	C3N-C7N-N7N	2.38	121.89	117.67
3	I	302	NDP	O2A-PA-O1A	2.37	123.96	112.24
3	L	301	NDP	C1D-N1N-C6N	-2.35	115.78	120.83
3	C	304	NDP	O3X-P2B-O2X	2.34	116.58	107.64
3	D	301	NDP	C4A-C5A-N7A	-2.34	106.96	109.40
3	B	302	NDP	N6A-C6A-N1A	2.33	123.41	118.57
3	D	301	NDP	C3N-C2N-N1N	-2.33	119.77	123.10
3	C	304	NDP	C3N-C2N-N1N	-2.32	119.78	123.10
3	L	301	NDP	O2A-PA-O1A	2.32	123.69	112.24
3	J	301	NDP	C1D-N1N-C6N	-2.31	115.85	120.83
3	G	302	NDP	C4A-C5A-N7A	-2.29	107.02	109.40
3	F	302	NDP	O2N-PN-O1N	2.28	123.49	112.24
3	K	302	NDP	O2A-PA-O1A	2.27	123.48	112.24
3	L	301	NDP	C2A-N1A-C6A	2.26	122.63	118.75
3	C	304	NDP	O2A-PA-O1A	2.25	123.37	112.24
3	L	301	NDP	C3N-C2N-N1N	-2.25	119.89	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	302	NDP	O2N-PN-O1N	2.23	123.27	112.24
3	H	301	NDP	PN-O3-PA	-2.22	125.22	132.83
3	F	302	NDP	O2B-P2B-O1X	-2.19	100.93	109.39
3	F	302	NDP	C1B-N9A-C4A	-2.19	122.79	126.64
3	J	301	NDP	C4A-C5A-N7A	-2.19	107.12	109.40
3	D	301	NDP	C1D-N1N-C6N	-2.15	116.19	120.83
3	B	302	NDP	O2A-PA-O1A	2.15	122.86	112.24
3	G	302	NDP	O7N-C7N-C3N	-2.14	116.86	120.90
3	A	302	NDP	C1D-N1N-C6N	-2.12	116.25	120.83
3	B	302	NDP	C2A-N1A-C6A	2.11	122.37	118.75
3	E	303	NDP	C2A-N1A-C6A	2.11	122.36	118.75
3	F	302	NDP	C1D-N1N-C6N	-2.10	116.31	120.83
3	H	301	NDP	O2A-PA-O1A	2.09	122.56	112.24
3	A	302	NDP	O2A-PA-O1A	2.08	122.52	112.24
3	K	302	NDP	C1D-N1N-C6N	-2.07	116.37	120.83
3	K	302	NDP	C4A-C5A-N7A	-2.07	107.24	109.40
3	B	302	NDP	O3X-P2B-O2X	2.06	115.51	107.64
3	E	303	NDP	O2A-PA-O1A	2.05	122.40	112.24
3	I	302	NDP	C2A-N1A-C6A	2.05	122.26	118.75
3	I	302	NDP	O2N-PN-O1N	2.04	122.33	112.24
3	D	301	NDP	O2A-PA-O1A	2.02	122.25	112.24
3	F	302	NDP	O2A-PA-O1A	2.01	122.19	112.24

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	304	NDP	C2B-O2B-P2B-O2X
3	E	303	NDP	C5D-O5D-PN-O2N
3	J	301	NDP	C5D-O5D-PN-O2N
3	H	301	NDP	C5D-O5D-PN-O2N
3	K	302	NDP	C5D-O5D-PN-O2N
3	F	302	NDP	C5D-O5D-PN-O2N
3	L	301	NDP	C5D-O5D-PN-O2N
5	E	301	GOL	O1-C1-C2-C3
2	A	301	PG0	O1-C3-C4-O2
6	K	301	PEG	O1-C1-C2-O2
2	A	301	PG0	OTT-C1-C2-O1
5	E	301	GOL	O1-C1-C2-O2
7	F	301	PG4	O1-C1-C2-O2
3	G	302	NDP	O4D-C1D-N1N-C6N
3	A	302	NDP	O4D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
3	H	301	NDP	O4D-C1D-N1N-C6N
3	B	302	NDP	O4D-C1D-N1N-C6N
3	K	302	NDP	O4D-C1D-N1N-C6N
6	K	301	PEG	C1-C2-O2-C3
7	F	301	PG4	C5-C6-O4-C7
2	A	301	PG0	C1-C2-O1-C3
3	D	301	NDP	C2B-O2B-P2B-O2X
3	E	303	NDP	C2B-O2B-P2B-O2X
3	J	301	NDP	C2B-O2B-P2B-O2X
3	J	301	NDP	C5D-O5D-PN-O3
3	H	301	NDP	C5D-O5D-PN-O3
3	K	302	NDP	C2B-O2B-P2B-O2X
3	K	302	NDP	C5D-O5D-PN-O3
3	I	302	NDP	C5D-O5D-PN-O3
3	F	302	NDP	C2B-O2B-P2B-O2X
3	F	302	NDP	C5D-O5D-PN-O3
3	G	302	NDP	C2B-O2B-P2B-O2X
3	L	301	NDP	C2B-O2B-P2B-O2X
3	L	301	NDP	C5D-O5D-PN-O3
3	D	301	NDP	O4D-C1D-N1N-C6N
3	C	304	NDP	O4D-C1D-N1N-C6N
3	E	303	NDP	O4D-C1D-N1N-C6N
3	J	301	NDP	O4D-C1D-N1N-C6N
3	I	302	NDP	O4D-C1D-N1N-C6N
3	F	302	NDP	O4D-C1D-N1N-C6N
3	L	301	NDP	O4D-C1D-N1N-C6N
3	J	301	NDP	C5D-O5D-PN-O1N
3	H	301	NDP	C5D-O5D-PN-O1N
7	F	301	PG4	C6-C5-O3-C4
3	F	302	NDP	O4B-C4B-C5B-O5B
3	A	302	NDP	O4B-C4B-C5B-O5B
3	G	302	NDP	O4B-C4B-C5B-O5B
3	I	302	NDP	O4B-C4B-C5B-O5B
3	A	302	NDP	C5D-O5D-PN-O3
3	D	301	NDP	C5D-O5D-PN-O3
3	B	302	NDP	C5D-O5D-PN-O3
3	C	304	NDP	C5D-O5D-PN-O3
3	E	303	NDP	C5D-O5D-PN-O3
3	H	301	NDP	C2B-O2B-P2B-O2X
3	D	301	NDP	O4B-C4B-C5B-O5B
3	B	302	NDP	O4B-C4B-C5B-O5B
3	E	303	NDP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	J	301	NDP	O4B-C4B-C5B-O5B
3	H	301	NDP	O4B-C4B-C5B-O5B
3	B	302	NDP	C5D-O5D-PN-O2N
3	I	302	NDP	C5D-O5D-PN-O2N
3	F	302	NDP	C5D-O5D-PN-O1N
3	L	301	NDP	C5D-O5D-PN-O1N
3	C	304	NDP	O4B-C4B-C5B-O5B
3	K	302	NDP	O4B-C4B-C5B-O5B
3	L	301	NDP	O4B-C4B-C5B-O5B

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	304	NDP	1	0
3	I	302	NDP	1	0
4	C	303	EDO	2	0
3	D	301	NDP	1	0
4	B	301	EDO	2	0
3	E	303	NDP	1	0
3	K	302	NDP	1	0
3	G	302	NDP	1	0
3	L	301	NDP	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 then 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.

Ligand NDP F 302

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP J 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP C 304

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP I 302

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report

Ligand NDP A 302

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP E 303

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP H 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP K 302

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP G 302

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP L 301

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	239/245 (97%)	0.08	8 (3%)	46	51	21, 33, 50, 59	0
1	B	243/245 (99%)	-0.14	7 (2%)	51	56	18, 30, 46, 66	0
1	C	241/245 (98%)	-0.37	4 (1%)	70	74	14, 20, 34, 64	0
1	D	240/245 (97%)	-0.24	2 (0%)	86	88	13, 24, 37, 63	0
1	E	239/245 (97%)	0.00	7 (2%)	51	56	21, 29, 43, 63	0
1	F	239/245 (97%)	0.02	9 (3%)	40	45	21, 32, 49, 79	0
1	G	239/245 (97%)	0.88	38 (15%)	1	2	36, 54, 68, 73	0
1	H	239/245 (97%)	0.55	32 (13%)	3	3	26, 42, 64, 77	0
1	I	241/245 (98%)	-0.33	2 (0%)	86	88	13, 20, 34, 60	0
1	J	242/245 (98%)	-0.27	3 (1%)	79	82	13, 20, 34, 62	0
1	K	244/245 (99%)	-0.24	3 (1%)	79	82	10, 17, 30, 64	0
1	L	239/245 (97%)	-0.41	0	100	100	11, 17, 29, 45	0
All	All	2885/2940 (98%)	-0.04	115 (3%)	38	42	10, 26, 56, 79	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	241	HIS	6.0
1	D	241	HIS	5.8
1	H	89	GLY	5.8
1	F	240	HIS	5.6
1	J	242	HIS	5.2
1	C	241	HIS	5.1
1	H	240	HIS	5.1
1	G	240	HIS	4.7
1	G	75	ALA	4.4
1	C	139[A]	PRO	4.4
1	G	68	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	I	241	HIS	3.9
1	G	153	LEU	3.8
1	B	241	HIS	3.7
1	H	49	GLN	3.6
1	B	244	HIS	3.5
1	K	245	HIS	3.5
1	G	133	VAL	3.5
1	G	187[A]	ASN	3.4
1	B	189	PRO	3.3
1	H	183	ALA	3.3
1	J	243	HIS	3.2
1	H	189	PRO	3.2
1	G	72	LYS	3.2
1	G	56	VAL	3.2
1	D	240	HIS	3.2
1	G	74	GLY	3.2
1	H	41	LYS	3.1
1	K	138[A]	MET	3.1
1	H	173	VAL	3.1
1	G	64	ASP	3.1
1	K	139[A]	PRO	3.1
1	G	76	LEU	3.1
1	E	240	HIS	3.0
1	G	23	VAL	3.0
1	B	242	HIS	3.0
1	F	190	MET	3.0
1	H	48	ALA	3.0
1	G	73	SER	2.9
1	H	186	ALA	2.9
1	I	240	HIS	2.9
1	F	187	ASN	2.9
1	G	57	PHE	2.9
1	H	133	VAL	2.9
1	H	90	GLU	2.9
1	H	185	PRO	2.8
1	H	86	GLY	2.8
1	G	151[A]	SER	2.8
1	H	188	GLY	2.8
1	G	188	GLY	2.8
1	F	2	GLY	2.7
1	C	242	HIS	2.7
1	E	133	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	239	GLU	2.6
1	G	40	SER	2.6
1	H	47	LEU	2.6
1	G	47	LEU	2.6
1	G	34	ARG	2.6
1	G	152	ALA	2.6
1	H	46	ARG	2.6
1	H	88	PHE	2.5
1	E	187	ASN	2.5
1	H	152	ALA	2.5
1	A	189	PRO	2.5
1	A	227	ALA	2.5
1	F	192	ASP	2.5
1	G	148	ALA	2.5
1	G	190	MET	2.5
1	G	189	PRO	2.5
1	G	78	ILE	2.5
1	H	42	ASP	2.5
1	G	37	TYR	2.5
1	G	138[A]	MET	2.5
1	G	191	ARG	2.5
1	A	46[A]	ARG	2.4
1	B	190	MET	2.4
1	H	190	MET	2.4
1	G	54	THR	2.4
1	H	187	ASN	2.4
1	G	71	ARG	2.4
1	B	187	ASN	2.4
1	G	227	ALA	2.4
1	A	72	LYS	2.4
1	E	151[A]	SER	2.4
1	H	151[A]	SER	2.4
1	A	240	HIS	2.4
1	F	191	ARG	2.3
1	H	227	ALA	2.3
1	G	43	ALA	2.3
1	H	182	ASP	2.3
1	G	192	ASP	2.3
1	A	42	ASP	2.2
1	G	136	ASP	2.2
1	B	74	GLY	2.2
1	E	191	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	93	GLU	2.2
1	H	191	ARG	2.2
1	G	135	GLY	2.2
1	E	132	SER	2.2
1	H	40	SER	2.2
1	C	138[A]	MET	2.2
1	H	135	GLY	2.2
1	A	230	THR	2.1
1	H	148	ALA	2.1
1	H	192	ASP	2.1
1	H	155	GLY	2.1
1	F	6	GLY	2.1
1	G	90	GLU	2.1
1	H	93	GLU	2.1
1	H	157	ALA	2.1
1	A	152	ALA	2.0
1	E	227	ALA	2.0
1	G	123	GLU	2.0
1	G	39	GLY	2.0
1	G	155	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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
4	EDO	E	302	4/4	0.34	0.25	67,80,82,82	0
4	EDO	C	302	4/4	0.40	0.30	79,94,96,97	0
7	PG4	F	301	13/13	0.51	0.44	99,119,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	E	301	6/6	0.70	0.19	61,73,80,81	0
2	PG0	A	301	8/8	0.74	0.15	73,88,91,93	0
4	EDO	G	301	4/4	0.74	0.28	72,87,88,90	0
4	EDO	I	301	4/4	0.79	0.25	55,66,71,71	10
4	EDO	C	303	4/4	0.79	0.33	34,41,47,49	10
5	GOL	C	301	6/6	0.80	0.18	41,49,56,59	14
6	PEG	K	301	7/7	0.86	0.10	34,49,65,65	17
3	NDP	G	302	48/48	0.89	0.11	29,48,68,71	0
4	EDO	B	301	4/4	0.93	0.30	59,71,74,75	10
3	NDP	H	301	48/48	0.94	0.13	30,39,48,49	0
3	NDP	A	302	48/48	0.96	0.06	22,31,38,41	0
3	NDP	F	302	48/48	0.97	0.09	18,26,34,39	0
3	NDP	E	303	48/48	0.97	0.06	19,24,32,37	0
3	NDP	B	302	48/48	0.97	0.07	22,29,36,39	0
3	NDP	C	304	48/48	0.98	0.06	14,19,25,26	0
3	NDP	K	302	48/48	0.98	0.06	11,15,19,22	0
3	NDP	I	302	48/48	0.98	0.05	15,20,26,31	0
3	NDP	D	301	48/48	0.98	0.05	18,24,30,34	0
3	NDP	J	301	48/48	0.98	0.05	16,20,24,30	0
3	NDP	L	301	48/48	0.99	0.05	11,17,21,23	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 NDP G 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
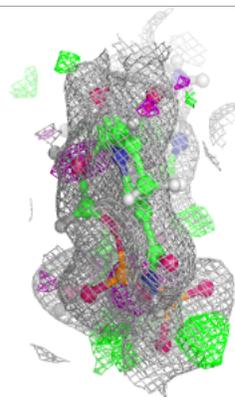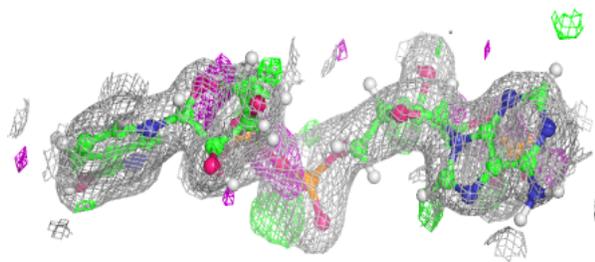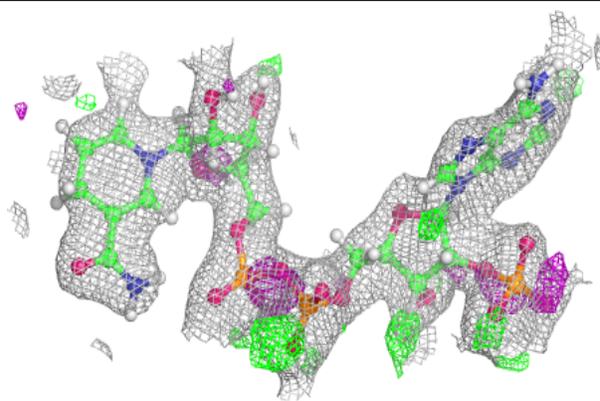
Electron density around NDP H 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
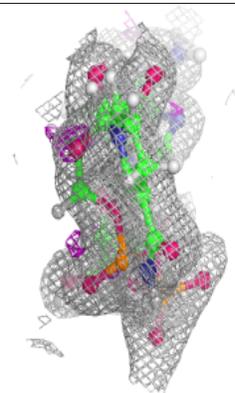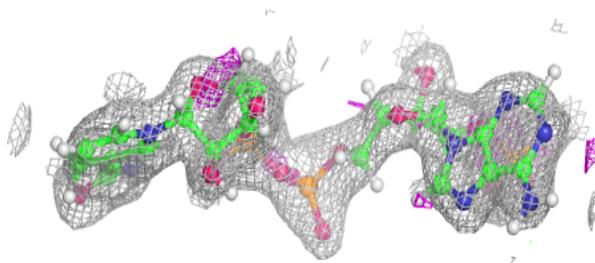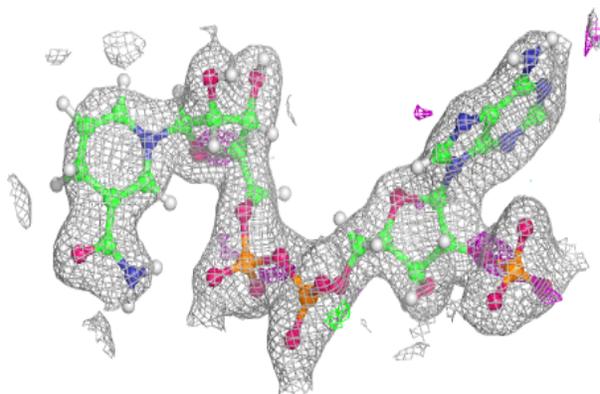
Electron density around NDP A 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
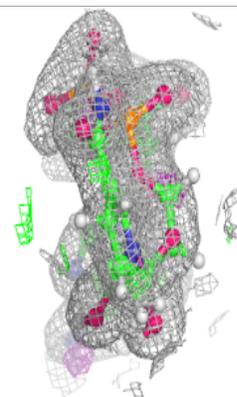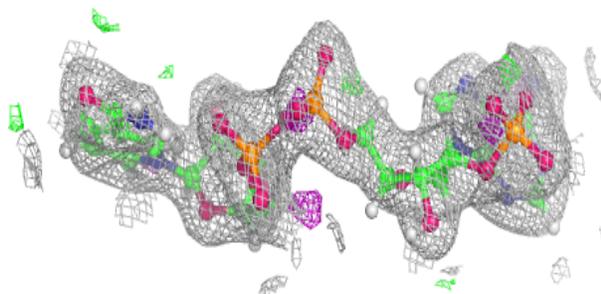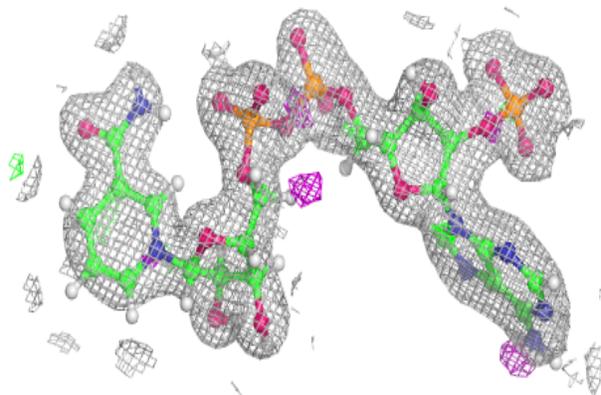
Electron density around NDP F 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
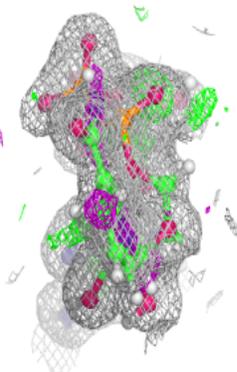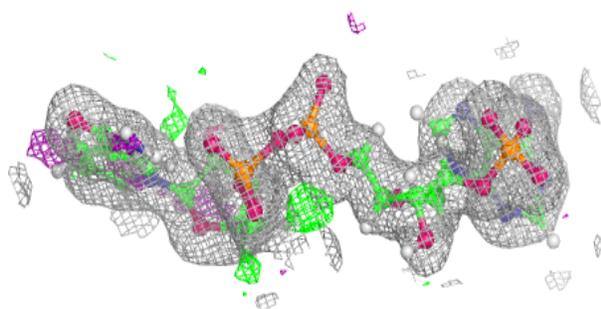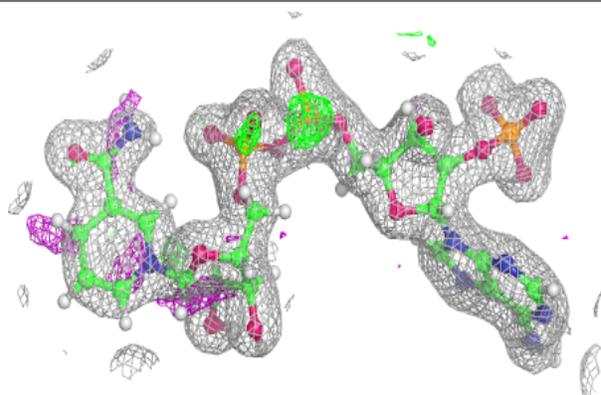
Electron density around NDP E 303:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
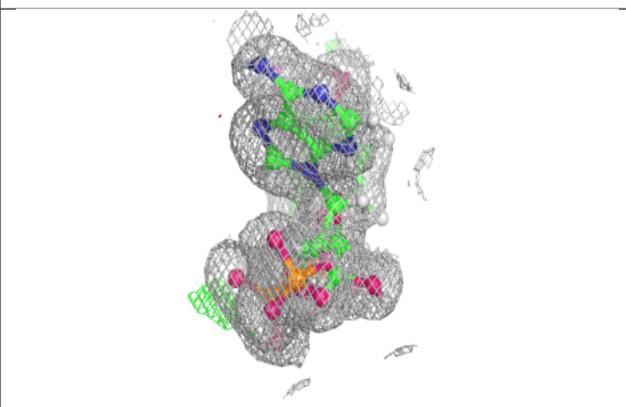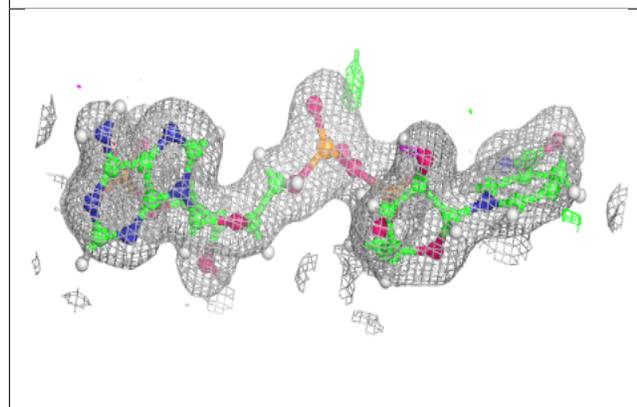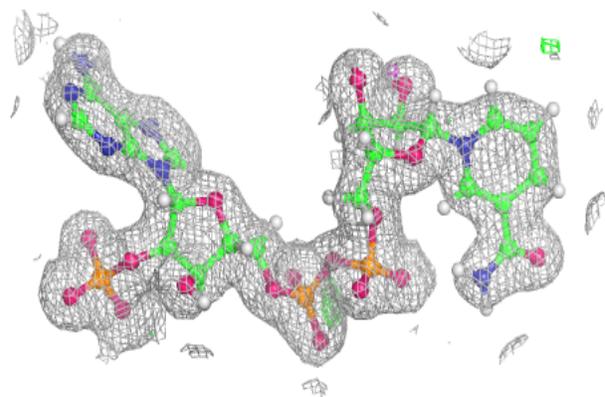
Electron density around NDP B 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
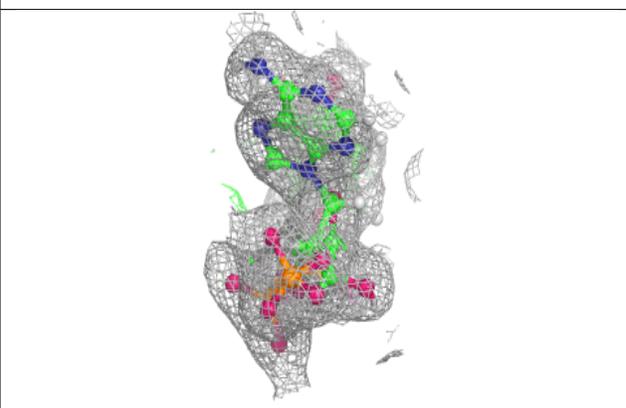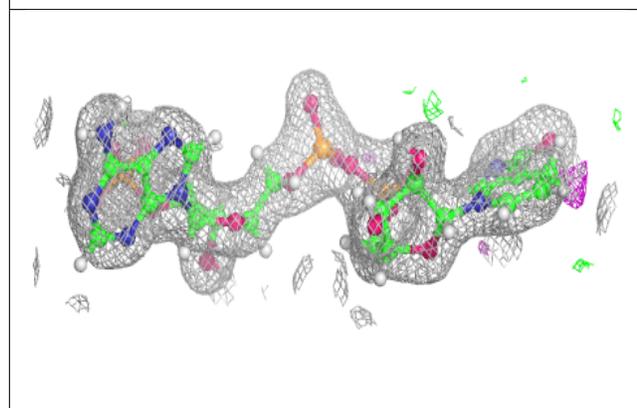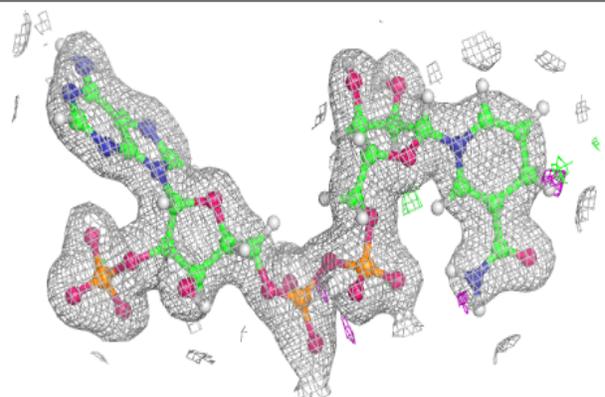
Electron density around NDP C 304:

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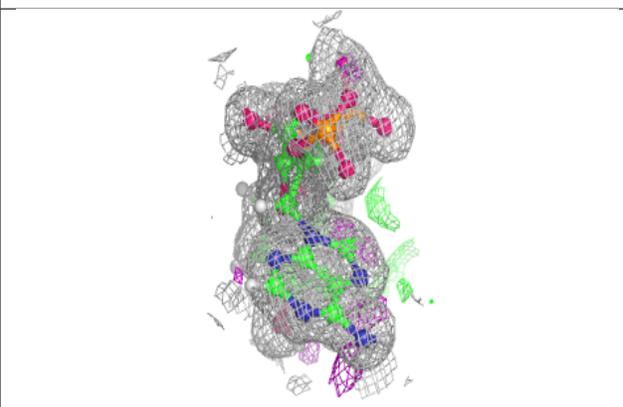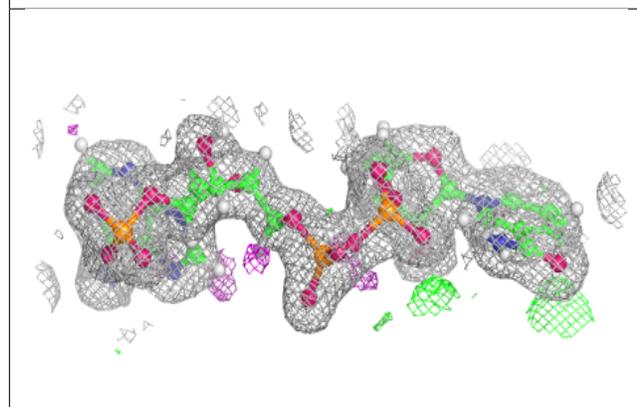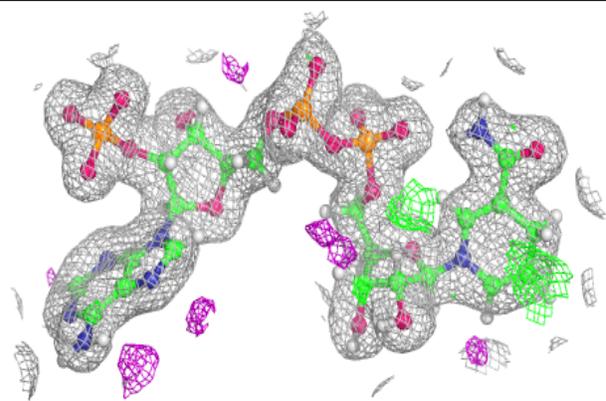

Electron density around NDP K 302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
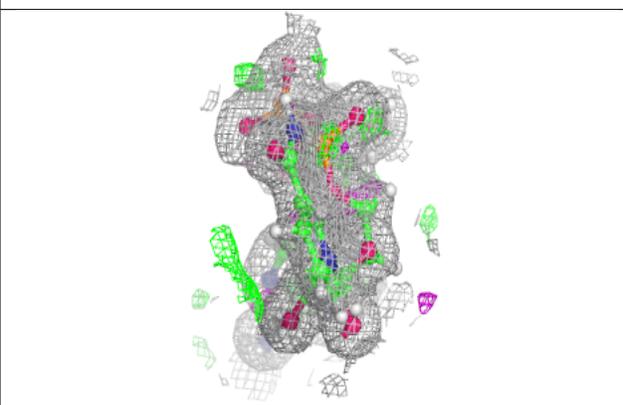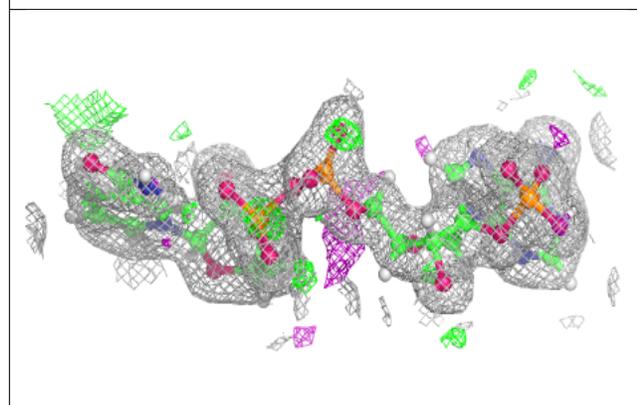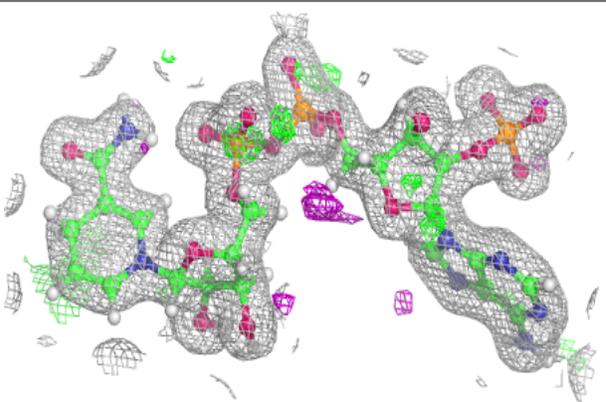
Electron density around NDP I 302:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
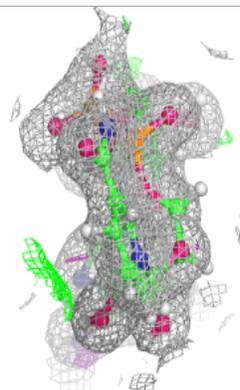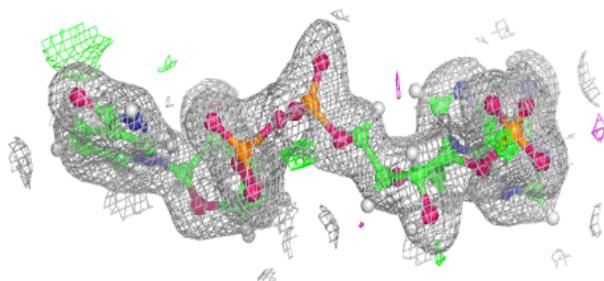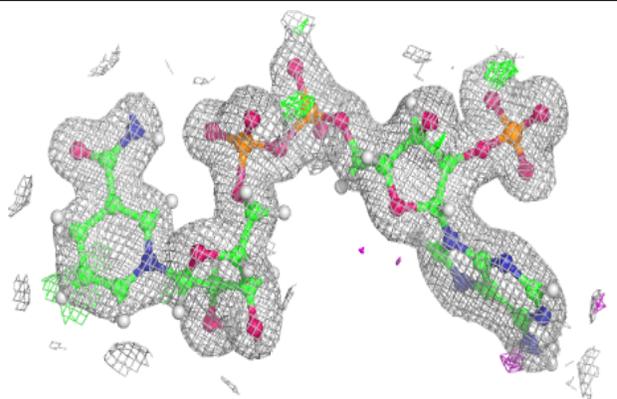
Electron density around NDP D 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
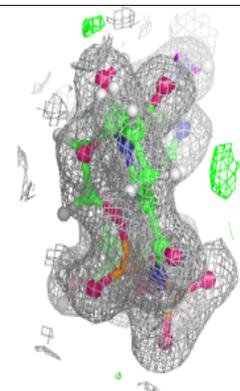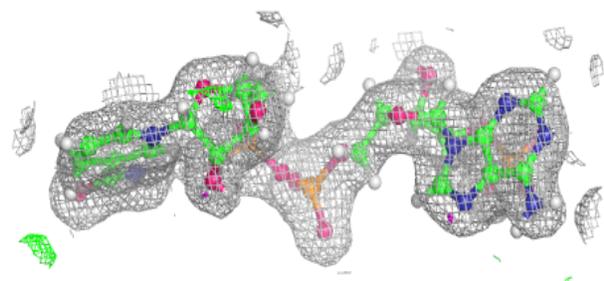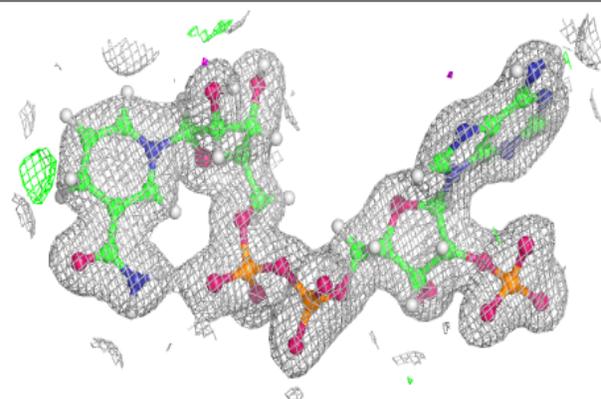
Electron density around NDP J 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
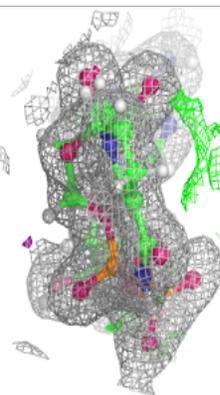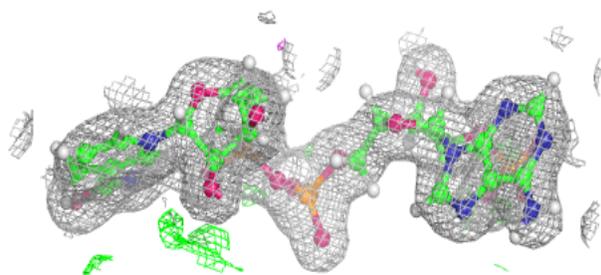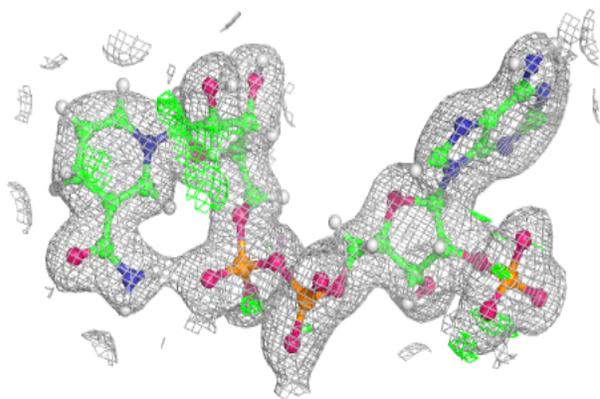
Electron density around NDP L 301:

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 ⓘ

There are no such residues in this entry.