Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 09:54 PM EDT

PDB ID	:	6BWC
Title	:	X-ray structure of Pen from Bacillus thuringiensis
Authors	:	Delvaux, N.A.; Thoden, J.B.; Holden, H.M.
Deposited on	:	2017-12-14
Resolution	:	2.70 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

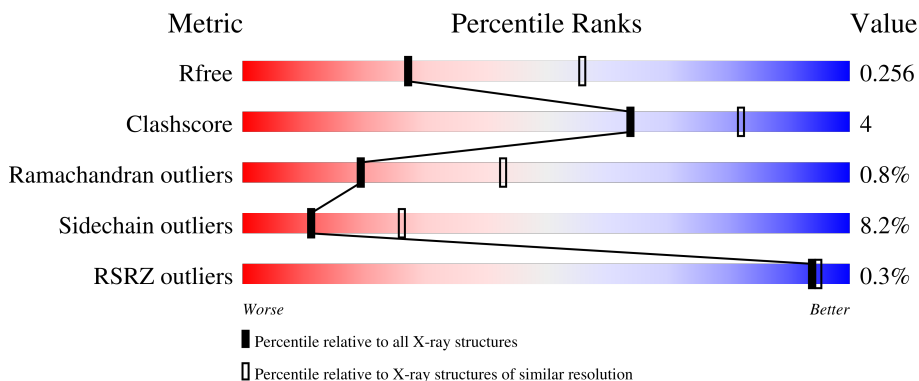|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.70 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	Percentile Ranks	Value
Rfree		0.256
Clashscore		4
Ramachandran outliers		0.8%
Sidechain outliers		8.2%
RSRZ outliers		0.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	343	78% 15% · 6%
1	B	343	80% 10% · 8%
1	C	343	78% 14% · 5%
1	D	343	74% 18% · 6%
1	E	343	80% 13% · 6%

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Mol	Chain	Length	Quality of chain
1	F	343	79% 13% 6%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 16002 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 Polysaccharide biosynthesis protein CapD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2559	1631	427	486	15			
1	B	316	Total	C	N	O	S	0	0	0
			2504	1595	420	474	15			
1	C	327	Total	C	N	O	S	0	0	0
			2590	1650	436	489	15			
1	D	324	Total	C	N	O	S	0	0	0
			2566	1636	431	484	15			
1	E	322	Total	C	N	O	S	0	0	0
			2553	1625	429	484	15			
1	F	323	Total	C	N	O	S	0	0	0
			2549	1624	425	485	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP J3UJH9
A	0	HIS	-	expression tag	UNP J3UJH9
A	128	ASN	ASP	engineered mutation	UNP J3UJH9
A	129	ALA	LYS	engineered mutation	UNP J3UJH9
B	-1	GLY	-	expression tag	UNP J3UJH9
B	0	HIS	-	expression tag	UNP J3UJH9
B	128	ASN	ASP	engineered mutation	UNP J3UJH9
B	129	ALA	LYS	engineered mutation	UNP J3UJH9
C	-1	GLY	-	expression tag	UNP J3UJH9
C	0	HIS	-	expression tag	UNP J3UJH9
C	128	ASN	ASP	engineered mutation	UNP J3UJH9
C	129	ALA	LYS	engineered mutation	UNP J3UJH9
D	-1	GLY	-	expression tag	UNP J3UJH9
D	0	HIS	-	expression tag	UNP J3UJH9
D	128	ASN	ASP	engineered mutation	UNP J3UJH9
D	129	ALA	LYS	engineered mutation	UNP J3UJH9
E	-1	GLY	-	expression tag	UNP J3UJH9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	0	HIS	-	expression tag	UNP J3UJH9
E	128	ASN	ASP	engineered mutation	UNP J3UJH9
E	129	ALA	LYS	engineered mutation	UNP J3UJH9
F	-1	GLY	-	expression tag	UNP J3UJH9
F	0	HIS	-	expression tag	UNP J3UJH9
F	128	ASN	ASP	engineered mutation	UNP J3UJH9
F	129	ALA	LYS	engineered mutation	UNP J3UJH9

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).
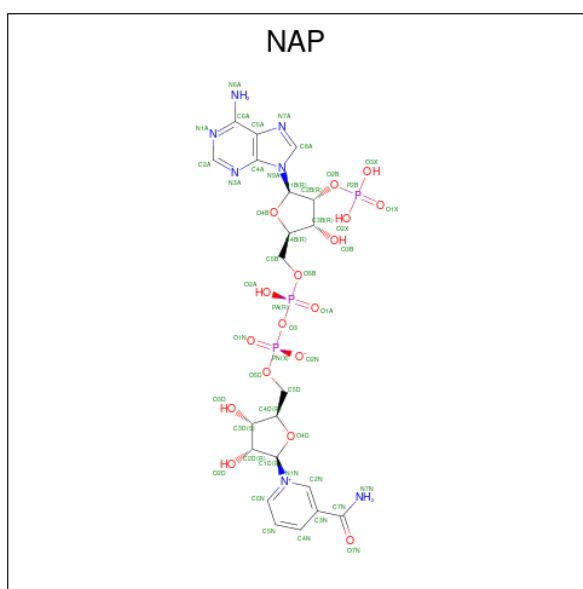
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is URIDINE-DIPHOSPHATE-N-ACETYLGLUCOSAMINE (three-letter code: UD1) (formula: $C_{17}H_{27}N_3O_{17}P_2$).

UD1
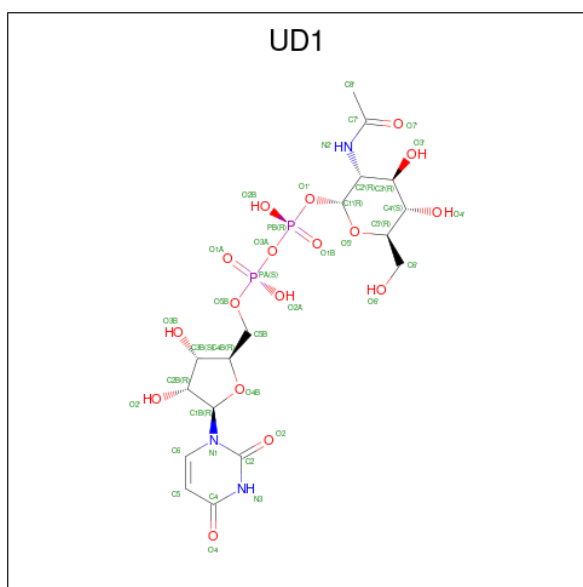
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	C	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	E	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
3	F	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 5	O 4	S 1	0	0
4	A	1	Total 5	O 4	S 1	0	0
4	B	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	34	Total 34	O 34	0	0
5	B	21	Total 21	O 21	0	0
5	C	25	Total 25	O 25	0	0
5	D	21	Total 21	O 21	0	0
5	E	18	Total 18	O 18	0	0
5	F	15	Total 15	O 15	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.
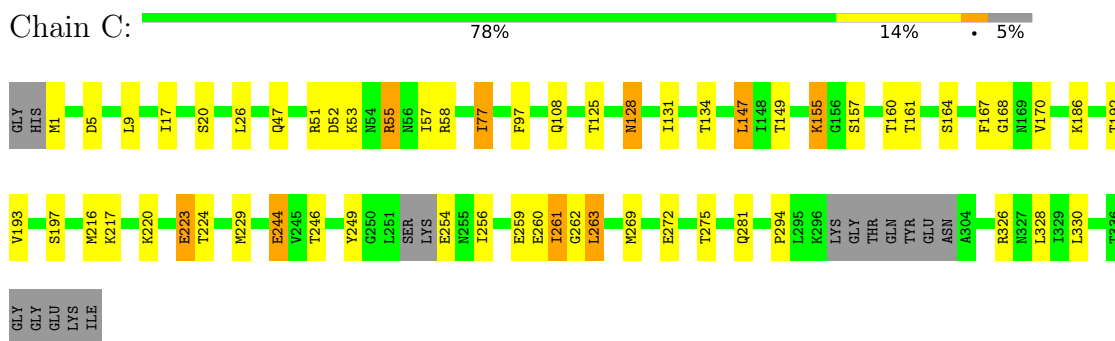
• Molecule 1: Polysaccharide biosynthesis protein CapD
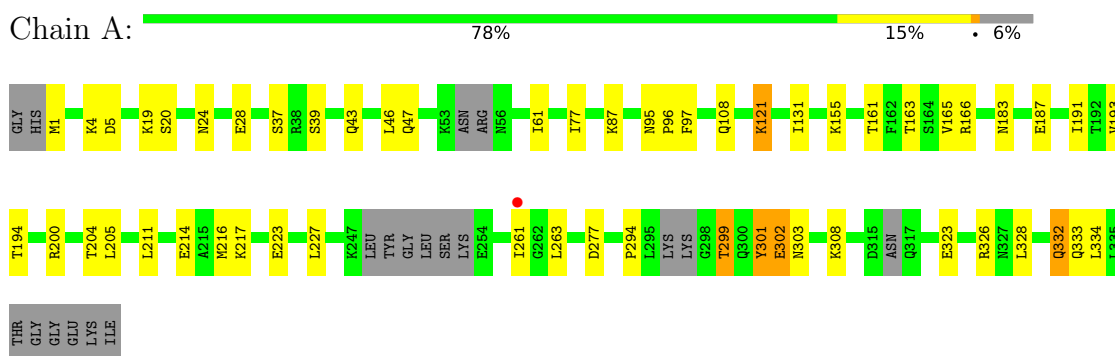
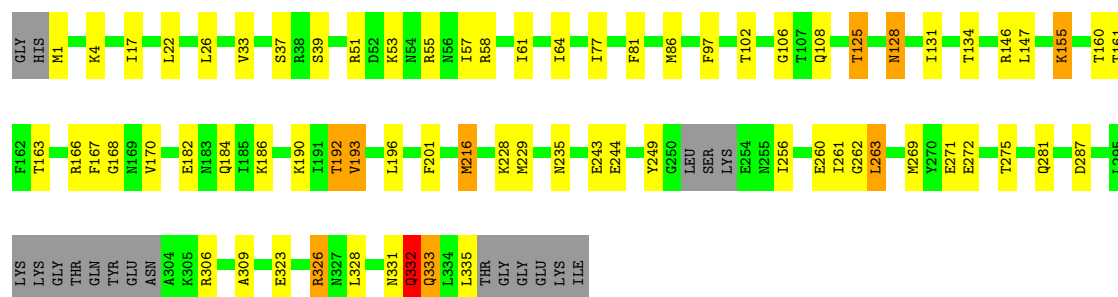• Molecule 1: Polysaccharide biosynthesis protein CapD
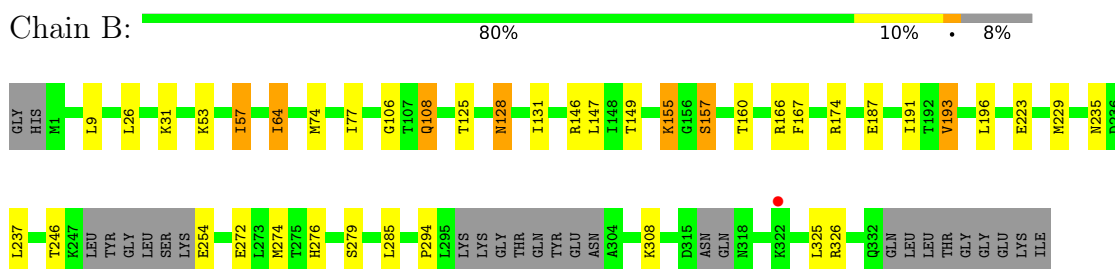
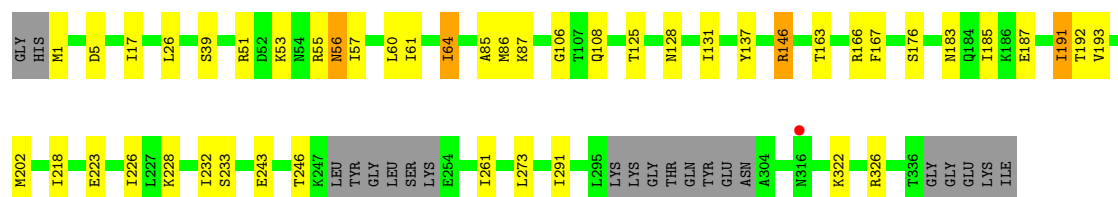• Molecule 1: Polysaccharide biosynthesis protein CapD

• Molecule 1: Polysaccharide biosynthesis protein CapD

Chain D:
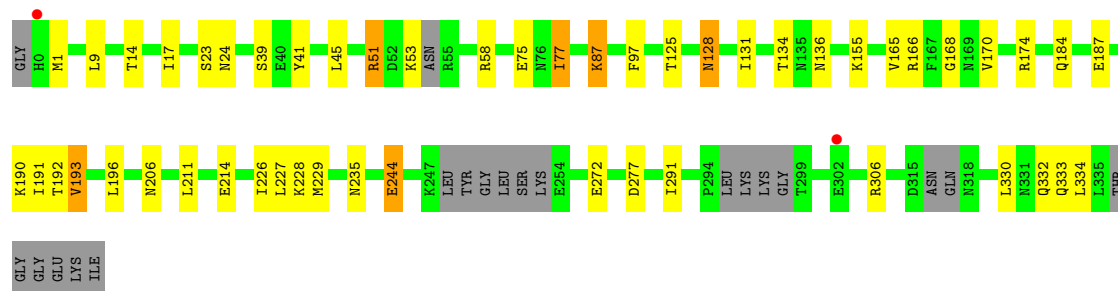

• Molecule 1: Polysaccharide biosynthesis protein CapD

Chain E:

• Molecule 1: Polysaccharide biosynthesis protein CapD

Chain F:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.52Å 141.88Å 93.24Å 90.00° 111.66° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.82 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.7 (30.00-2.70) 88.7 (29.82-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.201 , 0.251 0.206 , 0.256	Depositor DCC
R_{free} test set	2898 reflections (5.21%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , -2.6	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.399 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16002	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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 $< \lvert L \rvert >$, $< L^2 >$ 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: NAP, SO4, UD1

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	0.64	1/2595 (0.0%)	0.82	1/3486 (0.0%)
1	B	0.57	0/2540	0.75	0/3412
1	C	0.59	0/2628	0.80	1/3533 (0.0%)
1	D	0.61	0/2604	0.83	4/3501 (0.1%)
1	E	0.59	0/2590	0.78	0/3482
1	F	0.59	0/2585	0.79	1/3475 (0.0%)
All	All	0.60	1/15542 (0.0%)	0.80	7/20889 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	TYR	CE2-CZ	-5.25	1.31	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	333	GLN	N-CA-C	5.87	126.86	111.00
1	D	58	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	D	326	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	F	174	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	200	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	326	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	326	ARG	NE-CZ-NH1	5.09	122.85	120.30

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	2559	0	2598	20	0
1	B	2504	0	2552	18	0
1	C	2590	0	2642	28	0
1	D	2566	0	2616	38	0
1	E	2553	0	2604	20	0
1	F	2549	0	2576	21	0
2	A	48	0	25	1	0
2	B	48	0	25	0	0
2	C	48	0	25	1	0
2	D	48	0	25	2	0
2	E	48	0	25	0	0
2	F	48	0	25	2	0
3	A	39	0	25	1	0
3	B	39	0	25	0	0
3	C	39	0	25	0	0
3	D	39	0	25	0	0
3	E	39	0	25	0	0
3	F	39	0	25	1	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	F	10	0	0	1	0
5	A	34	0	0	0	0
5	B	21	0	0	1	0
5	C	25	0	0	0	0
5	D	21	0	0	0	0
5	E	18	0	0	0	0
5	F	15	0	0	0	0
All	All	16002	0	15888	133	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (133) 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:182:GLU:OE1	1:D:335:LEU:HD12	1.82	0.79
1:D:17:ILE:HD11	1:D:170:VAL:HG21	1.72	0.72
1:F:17:ILE:HD11	1:F:170:VAL:HG21	1.72	0.71
1:B:31:LYS:NZ	5:B:501:HOH:O	2.18	0.70
1:B:64:ILE:HD13	1:B:106:GLY:HA3	1.74	0.70
1:A:131:ILE:HD11	1:A:166:ARG:CZ	2.23	0.69
1:C:244:GLU:HG2	1:C:330:LEU:HD21	1.76	0.65
1:C:26:LEU:HD11	1:C:57:ILE:HD11	1.79	0.64
1:C:97:PHE:CD1	1:D:108:GLN:HG3	2.32	0.64
1:E:26:LEU:HD11	1:E:57:ILE:HD11	1.80	0.63
1:D:243:GLU:OE1	1:D:326:ARG:NH2	2.32	0.63
1:C:17:ILE:HD11	1:C:170:VAL:HG21	1.81	0.63
1:E:64:ILE:HD13	1:E:106:GLY:HA3	1.80	0.62
1:E:56:ASN:H	1:E:56:ASN:HD22	1.48	0.61
1:A:299:THR:HG22	1:A:301:TYR:CE2	2.36	0.61
1:B:155:LYS:HE2	1:B:160:THR:O	2.01	0.61
1:C:246:THR:HG21	1:C:254:GLU:N	2.16	0.60
1:D:261:ILE:HG22	1:D:262:GLY:O	2.01	0.60
1:C:128:ASN:HB2	1:C:272:GLU:O	2.03	0.58
1:C:108:GLN:HG3	1:D:97:PHE:CD1	2.38	0.58
1:C:108:GLN:HE21	1:C:147:LEU:HG	1.69	0.58
1:C:168:GLY:HA3	1:C:229:MET:HE1	1.85	0.58
1:A:121:LYS:HG3	1:A:161:THR:HB	1.87	0.57
1:F:14:THR:HG1	2:F:401:NAP:HO3A	1.53	0.57
1:E:108:GLN:HG3	1:F:97:PHE:CD1	2.40	0.57
1:F:87:LYS:HD3	3:F:402:UD1:H8'3	1.87	0.56
1:D:64:ILE:HD13	1:D:106:GLY:HA3	1.86	0.56
1:A:4:LYS:HE2	1:A:5:ASP:HB2	1.88	0.55
1:F:58:ARG:NH1	4:F:404:SO4:O2	2.37	0.55
1:B:157:SER:HB2	1:F:75:GLU:OE1	2.08	0.54
1:D:192:THR:HG23	1:D:261:ILE:HD12	1.88	0.54
1:C:261:ILE:HG22	1:C:262:GLY:O	2.07	0.54
1:A:97:PHE:CD1	1:B:108:GLN:HG3	2.43	0.54
1:D:22:LEU:HD13	1:D:33:VAL:HG11	1.90	0.53
1:E:243:GLU:OE1	1:E:326:ARG:NH2	2.37	0.53
1:A:223:GLU:HG2	1:A:301:TYR:OH	2.09	0.53
1:C:55:ARG:O	1:C:58:ARG:NH2	2.42	0.52
1:F:9:LEU:HB2	1:F:77:ILE:HD13	1.91	0.52
1:E:202:MET:HB2	1:E:232:ILE:HD12	1.90	0.52
1:D:193:VAL:HG21	1:D:196:LEU:HD21	1.92	0.52
1:F:41:TYR:CZ	1:F:45:LEU:HD11	2.44	0.52
1:C:125:THR:HG23	1:C:167:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ILE:HD11	1:D:102:THR:HG23	1.91	0.51
1:A:302:GLU:O	1:A:303:ASN:HB2	2.11	0.51
1:F:184:GLN:NE2	1:F:192:THR:OG1	2.40	0.51
1:B:125:THR:HG23	1:B:167:PHE:CE1	2.47	0.50
1:D:201:PHE:HB3	1:D:229:MET:HE2	1.91	0.50
1:E:191:ILE:HG23	1:E:193:VAL:HG23	1.93	0.50
1:D:331:ASN:O	1:D:332:GLN:HG3	2.11	0.50
1:D:168:GLY:HA3	1:D:229:MET:HE1	1.94	0.50
1:C:263:LEU:HD21	1:C:269:MET:HE2	1.93	0.49
1:E:192:THR:HG23	1:E:261:ILE:HG21	1.94	0.49
1:A:131:ILE:HD12	1:A:131:ILE:N	2.27	0.49
1:D:201:PHE:HB3	1:D:229:MET:CE	2.43	0.49
1:A:19:LYS:HD3	1:A:46:LEU:HD13	1.95	0.48
1:A:211:LEU:HD22	1:A:227:LEU:HB2	1.95	0.48
1:C:131:ILE:HD12	1:C:131:ILE:N	2.28	0.48
1:D:128:ASN:HB2	1:D:272:GLU:O	2.13	0.48
1:A:332:GLN:O	1:A:334:LEU:N	2.47	0.48
1:B:128:ASN:HB2	1:B:272:GLU:O	2.14	0.48
1:D:61:ILE:HG21	1:E:86:MET:HE1	1.96	0.48
1:D:128:ASN:ND2	1:D:271:GLU:HB3	2.29	0.47
1:F:131:ILE:HD11	1:F:166:ARG:CZ	2.43	0.47
1:E:17:ILE:HD13	1:E:167:PHE:HE1	1.78	0.47
1:C:108:GLN:NE2	1:C:147:LEU:HG	2.27	0.47
1:D:81:PHE:CZ	1:D:216:MET:HG2	2.49	0.47
1:F:168:GLY:HA3	1:F:229:MET:HE1	1.97	0.47
1:F:128:ASN:HB2	1:F:272:GLU:O	2.14	0.47
1:B:26:LEU:HD11	1:B:57:ILE:HD11	1.97	0.46
1:C:9:LEU:HB2	1:C:77:ILE:HD13	1.97	0.46
1:C:155:LYS:HE3	1:C:160:THR:O	2.16	0.46
1:C:192:THR:HG21	1:C:261:ILE:HD12	1.97	0.46
1:F:332:GLN:HB3	1:F:334:LEU:HG	1.98	0.46
1:D:131:ILE:HD11	1:D:166:ARG:NH1	2.31	0.46
1:F:14:THR:OG1	2:F:401:NAP:O3B	2.28	0.46
1:B:237:LEU:HA	1:B:325:LEU:HD21	1.98	0.46
1:F:211:LEU:HD22	1:F:227:LEU:HB2	1.97	0.45
1:B:246:THR:HG21	1:B:254:GLU:N	2.31	0.45
1:C:275:THR:HG21	1:D:134:THR:HG23	1.96	0.45
1:A:37:SER:O	1:A:61:ILE:HA	2.16	0.45
1:C:167:PHE:HB2	2:C:400:NAP:C5N	2.46	0.45
1:D:155:LYS:CE	1:D:160:THR:O	2.65	0.45
1:E:87:LYS:HA	1:E:137:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:LYS:HE2	1:D:160:THR:O	2.17	0.44
1:A:87:LYS:HE3	2:A:401:NAP:O2N	2.17	0.44
1:D:61:ILE:HG21	1:E:86:MET:CE	2.48	0.44
1:D:186:LYS:HE2	1:D:249:TYR:CZ	2.52	0.44
1:D:86:MET:CE	1:E:61:ILE:HG21	2.48	0.44
1:F:184:GLN:HB3	1:F:190:LYS:O	2.17	0.44
1:F:193:VAL:HG21	1:F:196:LEU:HD21	2.00	0.44
1:B:149:THR:HG21	1:B:294:PRO:HD2	2.00	0.44
1:D:167:PHE:HB2	2:D:400:NAP:C5N	2.47	0.44
1:B:26:LEU:HD11	1:B:57:ILE:CD1	2.47	0.44
1:C:220:LYS:N	1:C:223:GLU:OE1	2.51	0.44
1:D:131:ILE:HG23	1:D:275:THR:HG23	1.99	0.44
1:D:39:SER:HB3	2:D:400:NAP:O1X	2.18	0.43
1:D:131:ILE:HD11	1:D:166:ARG:CZ	2.49	0.43
1:B:276:HIS:O	1:B:279:SER:OG	2.32	0.43
1:D:26:LEU:HD21	1:D:57:ILE:CD1	2.48	0.43
1:D:184:GLN:HB3	1:D:190:LYS:O	2.19	0.43
1:E:125:THR:HG23	1:E:167:PHE:CE1	2.54	0.43
1:A:194:THR:HG23	3:A:402:UD1:C2	2.48	0.43
1:C:155:LYS:CE	1:C:160:THR:O	2.66	0.43
1:A:223:GLU:CG	1:A:301:TYR:OH	2.67	0.43
1:C:168:GLY:HA3	1:C:229:MET:CE	2.47	0.43
1:B:9:LEU:HB2	1:B:77:ILE:HD13	2.01	0.42
1:D:22:LEU:CD1	1:D:33:VAL:HG11	2.49	0.42
1:C:164:SER:O	1:C:224:THR:HA	2.19	0.42
1:A:96:PRO:HB2	1:B:147:LEU:HD12	2.02	0.42
1:A:28:GLU:OE2	1:A:217:LYS:NZ	2.52	0.42
1:B:193:VAL:HG11	1:B:196:LEU:HG	2.01	0.42
1:A:43:GLN:O	1:A:47:GLN:HB2	2.20	0.41
1:E:17:ILE:HD13	1:E:167:PHE:CE1	2.55	0.41
1:C:186:LYS:CE	1:C:249:TYR:CZ	3.04	0.41
1:E:146:ARG:HG2	1:F:136:ASN:HB2	2.02	0.41
1:F:191:ILE:HG23	1:F:193:VAL:HG23	2.02	0.41
1:C:149:THR:HG21	1:C:294:PRO:HD2	2.02	0.41
1:E:226:ILE:HG21	1:E:273:LEU:HB3	2.03	0.41
1:E:131:ILE:HD11	1:E:166:ARG:NH1	2.35	0.41
1:A:20:SER:HB2	1:A:205:LEU:HD11	2.01	0.41
1:B:74:MET:HA	1:B:77:ILE:HD12	2.02	0.41
1:C:125:THR:O	1:C:125:THR:HG22	2.21	0.41
1:F:244:GLU:HG2	1:F:330:LEU:HD21	2.01	0.41
1:D:86:MET:HE2	1:E:61:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:LEU:HD21	1:D:269:MET:CE	2.51	0.41
1:A:204:THR:HG22	1:A:332:GLN:OE1	2.21	0.41
1:D:125:THR:O	1:D:125:THR:HG22	2.20	0.41
1:D:184:GLN:HE22	1:D:192:THR:HG22	1.85	0.41
1:F:226:ILE:HD11	1:F:291:ILE:HD12	2.03	0.41
1:E:226:ILE:HD11	1:E:291:ILE:HD12	2.03	0.41
1:C:263:LEU:HD11	1:C:269:MET:CE	2.51	0.40
1:B:131:ILE:HD11	1:B:166:ARG:CZ	2.50	0.40
1:D:128:ASN:HD22	1:D:128:ASN:C	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/343 (92%)	294 (94%)	17 (5%)	3 (1%)	15	37
1	B	308/343 (90%)	297 (96%)	10 (3%)	1 (0%)	41	66
1	C	321/343 (94%)	300 (94%)	19 (6%)	2 (1%)	25	50
1	D	318/343 (93%)	300 (94%)	15 (5%)	3 (1%)	17	40
1	E	316/343 (92%)	296 (94%)	16 (5%)	4 (1%)	12	30
1	F	313/343 (91%)	292 (93%)	19 (6%)	2 (1%)	25	50
All	All	1890/2058 (92%)	1779 (94%)	96 (5%)	15 (1%)	19	43

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	155	LYS
1	E	322	LYS
1	F	51	ARG

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Mol	Chain	Res	Type
1	F	155	LYS
1	A	155	LYS
1	E	51	ARG
1	C	55	ARG
1	D	155	LYS
1	B	155	LYS
1	E	185	ILE
1	A	333	GLN
1	D	309	ALA
1	A	294	PRO
1	D	332	GLN
1	E	85	ALA

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	284/302 (94%)	259 (91%)	25 (9%)	10	23
1	B	279/302 (92%)	261 (94%)	18 (6%)	17	38
1	C	288/302 (95%)	262 (91%)	26 (9%)	9	22
1	D	285/302 (94%)	256 (90%)	29 (10%)	7	17
1	E	285/302 (94%)	265 (93%)	20 (7%)	15	35
1	F	282/302 (93%)	260 (92%)	22 (8%)	12	29
All	All	1703/1812 (94%)	1563 (92%)	140 (8%)	11	26

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	24	ASN
1	A	39	SER
1	A	77	ILE
1	A	95	ASN
1	A	108	GLN

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Mol	Chain	Res	Type
1	A	121	LYS
1	A	163	THR
1	A	165	VAL
1	A	183	ASN
1	A	187	GLU
1	A	191	ILE
1	A	193	VAL
1	A	214	GLU
1	A	216	MET
1	A	261	ILE
1	A	263	LEU
1	A	277	ASP
1	A	299	THR
1	A	302	GLU
1	A	308	LYS
1	A	323	GLU
1	A	326	ARG
1	A	328	LEU
1	A	332	GLN
1	B	53	LYS
1	B	57	ILE
1	B	64	ILE
1	B	108	GLN
1	B	128	ASN
1	B	146	ARG
1	B	157	SER
1	B	174	ARG
1	B	187	GLU
1	B	191	ILE
1	B	193	VAL
1	B	223	GLU
1	B	229	MET
1	B	235	ASN
1	B	274	MET
1	B	285	LEU
1	B	308	LYS
1	B	326	ARG
1	C	1	MET
1	C	5	ASP
1	C	20	SER
1	C	47	GLN
1	C	51	ARG

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Mol	Chain	Res	Type
1	C	52	ASP
1	C	53	LYS
1	C	77	ILE
1	C	128	ASN
1	C	134	THR
1	C	147	LEU
1	C	157	SER
1	C	161	THR
1	C	193	VAL
1	C	197	SER
1	C	216	MET
1	C	217	LYS
1	C	223	GLU
1	C	244	GLU
1	C	256	ILE
1	C	259	GLU
1	C	260	GLU
1	C	261	ILE
1	C	263	LEU
1	C	281	GLN
1	C	328	LEU
1	D	1	MET
1	D	4	LYS
1	D	37	SER
1	D	51	ARG
1	D	53	LYS
1	D	55	ARG
1	D	77	ILE
1	D	125	THR
1	D	128	ASN
1	D	146	ARG
1	D	147	LEU
1	D	161	THR
1	D	163	THR
1	D	192	THR
1	D	193	VAL
1	D	216	MET
1	D	228	LYS
1	D	235	ASN
1	D	244	GLU
1	D	256	ILE
1	D	260	GLU

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Mol	Chain	Res	Type
1	D	263	LEU
1	D	281	GLN
1	D	287	ASP
1	D	306	ARG
1	D	323	GLU
1	D	328	LEU
1	D	332	GLN
1	D	333	GLN
1	E	1	MET
1	E	5	ASP
1	E	39	SER
1	E	53	LYS
1	E	55	ARG
1	E	56	ASN
1	E	60	LEU
1	E	64	ILE
1	E	128	ASN
1	E	146	ARG
1	E	163	THR
1	E	176	SER
1	E	183	ASN
1	E	187	GLU
1	E	191	ILE
1	E	218	ILE
1	E	223	GLU
1	E	228	LYS
1	E	233	SER
1	E	246	THR
1	F	1	MET
1	F	23	SER
1	F	24	ASN
1	F	39	SER
1	F	51	ARG
1	F	53	LYS
1	F	77	ILE
1	F	87	LYS
1	F	125	THR
1	F	128	ASN
1	F	134	THR
1	F	165	VAL
1	F	187	GLU
1	F	193	VAL

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Mol	Chain	Res	Type
1	F	206	ASN
1	F	214	GLU
1	F	228	LYS
1	F	235	ASN
1	F	244	GLU
1	F	277	ASP
1	F	306	ARG
1	F	333	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	128	ASN
1	A	183	ASN
1	A	300	GLN
1	B	108	GLN
1	B	128	ASN
1	B	184	GLN
1	C	108	GLN
1	C	128	ASN
1	C	189	GLN
1	D	47	GLN
1	D	108	GLN
1	D	128	ASN
1	D	327	ASN
1	E	56	ASN
1	E	188	ASN
1	F	24	ASN
1	F	47	GLN
1	F	183	ASN
1	F	235	ASN

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　ⓘ

17 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	UD1	D	401	-	38,41,41	0.86	1 (2%)	57,62,62	1.54	9 (15%)
2	NAP	E	400	-	45,52,52	1.52	5 (11%)	56,80,80	1.69	9 (16%)
2	NAP	B	401	-	45,52,52	1.45	3 (6%)	56,80,80	1.91	12 (21%)
3	UD1	A	402	-	38,41,41	0.96	3 (7%)	57,62,62	1.37	6 (10%)
4	SO4	F	403	-	4,4,4	0.34	0	6,6,6	0.25	0
4	SO4	F	404	-	4,4,4	0.33	0	6,6,6	0.60	0
4	SO4	A	404	-	4,4,4	0.44	0	6,6,6	0.41	0
2	NAP	D	400	-	45,52,52	1.56	5 (11%)	56,80,80	1.56	8 (14%)
3	UD1	E	401	-	38,41,41	1.05	2 (5%)	57,62,62	1.43	7 (12%)
4	SO4	B	403	-	4,4,4	0.38	0	6,6,6	0.65	0
2	NAP	F	401	-	45,52,52	1.47	4 (8%)	56,80,80	1.65	9 (16%)
3	UD1	B	402	-	38,41,41	1.05	2 (5%)	57,62,62	1.49	10 (17%)
3	UD1	C	401	-	38,41,41	0.95	2 (5%)	57,62,62	1.47	8 (14%)
4	SO4	A	403	-	4,4,4	0.36	0	6,6,6	0.39	0
2	NAP	A	401	-	45,52,52	1.62	4 (8%)	56,80,80	1.48	6 (10%)
3	UD1	F	402	-	38,41,41	1.01	2 (5%)	57,62,62	1.70	12 (21%)
2	NAP	C	400	-	45,52,52	1.38	3 (6%)	56,80,80	1.59	10 (17%)

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	UD1	D	401	-	-	4/26/63/63	0/3/3/3
2	NAP	E	400	-	-	10/31/67/67	0/5/5/5
2	NAP	B	401	-	-	4/31/67/67	0/5/5/5
3	UD1	A	402	-	-	2/26/63/63	0/3/3/3
2	NAP	D	400	-	-	4/31/67/67	0/5/5/5
3	UD1	E	401	-	-	5/26/63/63	0/3/3/3
2	NAP	F	401	-	-	9/31/67/67	0/5/5/5
3	UD1	B	402	-	-	1/26/63/63	0/3/3/3
3	UD1	C	401	-	-	5/26/63/63	0/3/3/3
2	NAP	A	401	-	-	9/31/67/67	0/5/5/5
3	UD1	F	402	-	-	7/26/63/63	0/3/3/3
2	NAP	C	400	-	-	5/31/67/67	0/5/5/5

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NAP	C4N-C3N	7.51	1.52	1.39
2	E	400	NAP	C4N-C3N	7.44	1.52	1.39
2	A	401	NAP	C4N-C3N	7.37	1.51	1.39
2	F	401	NAP	C4N-C3N	6.83	1.51	1.39
2	D	400	NAP	C4N-C3N	6.21	1.49	1.39
2	C	400	NAP	C4N-C3N	5.64	1.49	1.39
3	E	401	UD1	C2-N1	4.34	1.45	1.38
2	D	400	NAP	C5N-C4N	4.30	1.48	1.38
2	A	401	NAP	C5N-C4N	4.29	1.48	1.38
2	C	400	NAP	C5N-C4N	3.91	1.47	1.38
3	B	402	UD1	C2-N1	3.76	1.44	1.38
2	F	401	NAP	C5N-C4N	3.58	1.46	1.38
2	E	400	NAP	C5N-C4N	3.45	1.46	1.38
2	A	401	NAP	O4B-C1B	3.00	1.45	1.41
3	C	401	UD1	C2-N1	2.96	1.43	1.38
2	D	400	NAP	C5A-C4A	2.89	1.48	1.40
2	C	400	NAP	C5A-C4A	2.87	1.48	1.40
2	B	401	NAP	C5N-C4N	2.84	1.44	1.38
3	A	402	UD1	C4-N3	-2.71	1.33	1.38
3	C	401	UD1	C5-C4	-2.68	1.37	1.43
3	F	402	UD1	C2-N3	-2.64	1.33	1.38
3	F	402	UD1	C4-N3	-2.55	1.34	1.38
2	D	400	NAP	C2A-N3A	2.49	1.36	1.32
2	F	401	NAP	C5A-C4A	2.44	1.47	1.40
3	B	402	UD1	C6-C5	2.40	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	NAP	C5A-C4A	2.34	1.47	1.40
3	D	401	UD1	C2-N1	2.30	1.42	1.38
2	E	400	NAP	O4D-C1D	2.29	1.44	1.41
2	D	400	NAP	O4D-C1D	2.28	1.44	1.41
2	F	401	NAP	O4D-C1D	2.27	1.44	1.41
2	A	401	NAP	C5A-C4A	2.27	1.46	1.40
3	A	402	UD1	C5-C4	-2.18	1.38	1.43
3	E	401	UD1	O2-C2	2.18	1.27	1.23
2	B	401	NAP	C5A-C4A	2.16	1.46	1.40
3	A	402	UD1	C2-N3	-2.14	1.34	1.38
2	E	400	NAP	C5A-N7A	-2.05	1.32	1.39

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	401	NAP	C5N-C4N-C3N	-7.21	111.81	120.34
2	D	400	NAP	C5N-C4N-C3N	-6.70	112.41	120.34
2	B	401	NAP	C5N-C4N-C3N	-6.67	112.45	120.34
2	E	400	NAP	C5N-C4N-C3N	-6.21	112.99	120.34
2	C	400	NAP	C5N-C4N-C3N	-5.91	113.35	120.34
2	B	401	NAP	C3N-C7N-N7N	5.63	124.51	117.75
2	A	401	NAP	C5N-C4N-C3N	-5.33	114.03	120.34
3	F	402	UD1	C4-N3-C2	-4.74	120.33	126.58
3	D	401	UD1	C4-N3-C2	-4.64	120.46	126.58
3	F	402	UD1	C5-C4-N3	4.42	121.45	114.84
3	D	401	UD1	N3-C2-N1	4.40	120.72	114.89
3	A	402	UD1	C4-N3-C2	-4.29	120.92	126.58
3	A	402	UD1	C5-C4-N3	4.23	121.16	114.84
3	D	401	UD1	O4-C4-C5	-4.04	118.06	125.16
3	C	401	UD1	O4-C4-C5	-4.00	118.12	125.16
2	A	401	NAP	C3N-C7N-N7N	3.99	122.54	117.75
3	E	401	UD1	C4-N3-C2	-3.95	121.37	126.58
3	E	401	UD1	C5-C4-N3	3.92	120.71	114.84
3	E	401	UD1	O4-C4-C5	-3.92	118.27	125.16
2	E	400	NAP	C3N-C7N-N7N	3.89	122.42	117.75
2	C	400	NAP	N3A-C2A-N1A	-3.88	122.62	128.68
3	C	401	UD1	C5-C4-N3	3.77	120.48	114.84
2	B	401	NAP	N3A-C2A-N1A	-3.76	122.80	128.68
3	C	401	UD1	C4-N3-C2	-3.72	121.68	126.58
2	E	400	NAP	N3A-C2A-N1A	-3.71	122.87	128.68
3	F	402	UD1	O5'-C1'-C2'	-3.70	103.35	110.58
3	D	401	UD1	C5-C4-N3	3.67	120.33	114.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	UD1	N3-C2-N1	3.60	119.67	114.89
3	F	402	UD1	C4'-C3'-C2'	3.58	115.59	110.34
2	E	400	NAP	O4B-C1B-C2B	-3.56	100.41	106.59
3	B	402	UD1	N3-C2-N1	3.45	119.47	114.89
2	B	401	NAP	C4A-C5A-N7A	-3.45	105.81	109.40
3	F	402	UD1	O1'-C1'-C2'	3.45	114.64	108.40
3	B	402	UD1	C3'-C4'-C5'	3.40	116.30	110.24
2	D	400	NAP	N3A-C2A-N1A	-3.35	123.44	128.68
2	C	400	NAP	C3N-C7N-N7N	3.33	121.75	117.75
3	B	402	UD1	C5-C4-N3	3.29	119.77	114.84
3	C	401	UD1	O5'-C1'-O1'	-3.28	107.07	111.36
2	A	401	NAP	C4A-C5A-N7A	-3.22	106.05	109.40
3	F	402	UD1	N3-C2-N1	3.22	119.16	114.89
3	B	402	UD1	C4-N3-C2	-3.20	122.37	126.58
3	B	402	UD1	O4-C4-C5	-3.13	119.65	125.16
2	F	401	NAP	C3N-C7N-N7N	3.10	121.47	117.75
2	A	401	NAP	N3A-C2A-N1A	-3.08	123.86	128.68
2	D	400	NAP	C3N-C2N-N1N	3.06	123.42	120.43
3	A	402	UD1	O4-C4-C5	-3.06	119.78	125.16
2	F	401	NAP	N3A-C2A-N1A	-3.05	123.92	128.68
2	B	401	NAP	O7N-C7N-N7N	-3.02	118.29	122.58
2	D	400	NAP	O2B-P2B-O1X	-3.01	97.77	109.39
2	C	400	NAP	C3N-C2N-N1N	3.00	123.36	120.43
3	A	402	UD1	N3-C2-N1	2.98	118.85	114.89
2	E	400	NAP	O7N-C7N-N7N	-2.98	118.35	122.58
3	E	401	UD1	N3-C2-N1	2.98	118.84	114.89
3	F	402	UD1	O4-C4-C5	-2.89	120.07	125.16
2	F	401	NAP	O7N-C7N-C3N	-2.81	116.27	119.63
2	F	401	NAP	C1B-N9A-C4A	-2.75	121.80	126.64
2	B	401	NAP	C2N-C3N-C4N	2.74	121.37	118.26
2	C	400	NAP	O2B-P2B-O1X	-2.65	99.15	109.39
2	D	400	NAP	C6N-C5N-C4N	2.62	123.24	119.44
3	F	402	UD1	C3'-C4'-C5'	2.61	114.90	110.24
2	D	400	NAP	C4A-C5A-N7A	-2.58	106.70	109.40
2	E	400	NAP	O2B-P2B-O1X	-2.58	99.44	109.39
3	B	402	UD1	C6-N1-C2	-2.56	117.72	120.99
2	A	401	NAP	O7N-C7N-C3N	-2.55	116.58	119.63
2	B	401	NAP	O2X-P2B-O1X	2.55	120.67	110.68
2	B	401	NAP	C1B-N9A-C4A	-2.55	122.17	126.64
3	F	402	UD1	C3'-C2'-N2'	2.51	115.35	110.62
2	B	401	NAP	O2B-P2B-O1X	-2.50	99.73	109.39
3	F	402	UD1	C1'-C2'-N2'	-2.49	106.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	401	NAP	PN-O3-PA	-2.47	124.35	132.83
2	E	400	NAP	C4A-C5A-N7A	-2.46	106.83	109.40
3	C	401	UD1	C6-N1-C2	-2.46	117.85	120.99
2	F	401	NAP	C3N-C2N-N1N	2.44	122.81	120.43
2	C	400	NAP	C4A-C5A-N7A	-2.40	106.90	109.40
2	B	401	NAP	C2A-N1A-C6A	2.38	122.82	118.75
2	F	401	NAP	C6N-C5N-C4N	2.35	122.86	119.44
3	D	401	UD1	PB-O1'-C1'	2.35	128.82	119.74
3	A	402	UD1	C1'-C2'-N2'	-2.35	106.96	111.00
2	C	400	NAP	C1B-N9A-C4A	-2.33	122.55	126.64
3	B	402	UD1	O4B-C1B-N1	2.32	113.67	108.36
3	B	402	UD1	O2A-PA-O1A	2.31	123.65	112.24
3	B	402	UD1	O5'-C5'-C6'	2.30	112.14	106.44
3	C	401	UD1	PB-O1'-C1'	2.29	128.60	119.74
2	D	400	NAP	O2N-PN-O1N	2.29	123.57	112.24
3	B	402	UD1	O4'-C4'-C5'	-2.28	103.63	109.30
3	E	401	UD1	O2'-C2B-C1B	2.23	117.49	110.02
2	C	400	NAP	O3B-C3B-C4B	-2.22	104.62	111.05
2	E	400	NAP	N6A-C6A-N1A	2.21	123.16	118.57
2	A	401	NAP	O3X-P2B-O2X	2.20	116.03	107.64
3	D	401	UD1	O7'-C7'-N2'	2.18	125.97	121.95
2	F	401	NAP	C4A-C5A-N7A	-2.17	107.14	109.40
2	C	400	NAP	C6N-C5N-C4N	2.16	122.58	119.44
3	E	401	UD1	C1'-C2'-N2'	-2.15	107.31	111.00
3	F	402	UD1	C5-C6-N1	-2.12	118.25	121.81
2	C	400	NAP	C2A-N1A-C6A	2.12	122.38	118.75
3	A	402	UD1	C3'-C4'-C5'	2.11	114.01	110.24
3	C	401	UD1	C1B-N1-C2	2.10	121.38	117.57
3	D	401	UD1	O2-C2-N1	-2.08	120.02	122.79
2	B	401	NAP	O7N-C7N-C3N	-2.08	117.14	119.63
2	E	400	NAP	C2A-N1A-C6A	2.07	122.30	118.75
3	E	401	UD1	O2A-PA-O1A	2.06	122.44	112.24
3	F	402	UD1	O4B-C4B-C3B	2.04	109.15	105.11
2	B	401	NAP	O2X-P2B-O2B	-2.04	96.87	105.99
3	D	401	UD1	O7'-C7'-C8'	-2.03	118.28	122.06
3	D	401	UD1	C3'-C4'-C5'	2.02	113.83	110.24
2	D	400	NAP	C1B-N9A-C4A	-2.01	123.11	126.64

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NAP	C5B-O5B-PA-O1A
2	A	401	NAP	C5B-O5B-PA-O2A
2	A	401	NAP	C2B-O2B-P2B-O1X
2	A	401	NAP	C5D-O5D-PN-O1N
2	C	400	NAP	C5B-O5B-PA-O2A
2	C	400	NAP	C2B-O2B-P2B-O2X
2	D	400	NAP	O4D-C4D-C5D-O5D
2	E	400	NAP	C5B-O5B-PA-O2A
2	E	400	NAP	C2B-O2B-P2B-O1X
2	E	400	NAP	C5D-O5D-PN-O1N
2	F	401	NAP	C5B-O5B-PA-O2A
2	F	401	NAP	O4B-C4B-C5B-O5B
2	F	401	NAP	C2B-O2B-P2B-O1X
2	F	401	NAP	C5D-O5D-PN-O1N
3	A	402	UD1	PB-O3A-PA-O5B
3	B	402	UD1	C1'-O1'-PB-O3A
3	C	401	UD1	C1'-O1'-PB-O3A
3	D	401	UD1	C5B-O5B-PA-O2A
3	E	401	UD1	C1'-O1'-PB-O3A
3	F	402	UD1	C5B-O5B-PA-O2A
2	A	401	NAP	O4B-C4B-C5B-O5B
2	A	401	NAP	C3B-C4B-C5B-O5B
2	D	400	NAP	C3D-C4D-C5D-O5D
2	E	400	NAP	O4B-C4B-C5B-O5B
3	C	401	UD1	C4'-C5'-C6'-O6'
2	E	400	NAP	C3B-C4B-C5B-O5B
2	F	401	NAP	C3B-C4B-C5B-O5B
3	E	401	UD1	C4'-C5'-C6'-O6'
3	C	401	UD1	O5'-C5'-C6'-O6'
3	F	402	UD1	C4'-C5'-C6'-O6'
3	D	401	UD1	PB-O3A-PA-O1A
3	A	402	UD1	C1'-O1'-PB-O3A
3	E	401	UD1	O5'-C5'-C6'-O6'
3	C	401	UD1	PB-O3A-PA-O5B
3	D	401	UD1	PB-O3A-PA-O5B
3	E	401	UD1	PB-O3A-PA-O5B
3	F	402	UD1	PB-O3A-PA-O5B
2	A	401	NAP	C5D-O5D-PN-O3
2	B	401	NAP	C5D-O5D-PN-O3
2	E	400	NAP	C5B-O5B-PA-O3
2	E	400	NAP	C5D-O5D-PN-O3
2	F	401	NAP	C5B-O5B-PA-O3
3	F	402	UD1	C5B-O5B-PA-O3A

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Mol	Chain	Res	Type	Atoms
3	C	401	UD1	C1'-O1'-PB-O1B
2	B	401	NAP	C5D-O5D-PN-O1N
2	E	400	NAP	C5B-O5B-PA-O1A
2	E	400	NAP	C5D-O5D-PN-O2N
2	F	401	NAP	C5B-O5B-PA-O1A
2	F	401	NAP	C5D-O5D-PN-O2N
3	F	402	UD1	O5'-C5'-C6'-O6'
2	B	401	NAP	O4B-C4B-C5B-O5B
3	F	402	UD1	C1'-O1'-PB-O3A
3	E	401	UD1	O4B-C1B-N1-C6
2	A	401	NAP	C5B-O5B-PA-O3
2	A	401	NAP	C2B-O2B-P2B-O3X
2	C	400	NAP	C5B-O5B-PA-O3
2	D	400	NAP	C5B-O5B-PA-O3
2	E	400	NAP	C2B-O2B-P2B-O3X
2	F	401	NAP	C5D-O5D-PN-O3
2	C	400	NAP	C5B-O5B-PA-O1A
3	D	401	UD1	C5B-O5B-PA-O1A
3	F	402	UD1	C5B-O5B-PA-O1A
2	B	401	NAP	C3D-C4D-C5D-O5D
2	C	400	NAP	O4B-C4B-C5B-O5B
2	D	400	NAP	O4B-C4B-C5B-O5B

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	UD1	1	0
4	F	404	SO4	1	0
2	D	400	NAP	2	0
2	F	401	NAP	2	0
2	A	401	NAP	1	0
3	F	402	UD1	1	0
2	C	400	NAP	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 UD1 D 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP E 400

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand UD1 A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 400

Bond lengths

Bond angles

Torsions

Rings

Ligand UD1 E 401

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report

Ligand NAP F 401

Bond lengths

Bond angles

Torsions

Rings

Ligand UD1 B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand UD1 C 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP A 401

Bond lengths

Bond angles

Torsions

Rings

Ligand UD1 F 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 400

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	324/343 (94%)	-0.42	1 (0%)	94	95	10, 23, 45, 61	0
1	B	316/343 (92%)	-0.34	1 (0%)	94	95	9, 26, 53, 74	0
1	C	327/343 (95%)	-0.43	0	100	100	10, 22, 40, 68	0
1	D	324/343 (94%)	-0.43	0	100	100	9, 21, 43, 60	0
1	E	322/343 (93%)	-0.31	1 (0%)	94	95	10, 28, 57, 75	0
1	F	323/343 (94%)	-0.39	2 (0%)	89	91	10, 24, 49, 77	0
All	All	1936/2058 (94%)	-0.39	5 (0%)	94	95	9, 24, 49, 77	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	316	ASN	2.8
1	A	261	ILE	2.7
1	F	0	HIS	2.3
1	B	322	LYS	2.3
1	F	302	GLU	2.2

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	SO4	F	404	5/5	0.89	0.21	66,68,72,73	0
4	SO4	A	403	5/5	0.93	0.16	60,62,64,65	0
4	SO4	F	403	5/5	0.95	0.10	57,58,62,66	0
4	SO4	B	403	5/5	0.96	0.14	49,50,52,53	0
2	NAP	F	401	48/48	0.97	0.11	13,14,24,26	0
3	UD1	A	402	39/39	0.97	0.12	17,20,25,25	0
3	UD1	B	402	39/39	0.97	0.14	19,20,31,32	0
3	UD1	C	401	39/39	0.97	0.13	12,15,19,20	0
3	UD1	D	401	39/39	0.97	0.12	13,16,18,18	0
3	UD1	E	401	39/39	0.97	0.13	23,25,30,31	0
3	UD1	F	402	39/39	0.97	0.13	16,19,26,27	0
2	NAP	A	401	48/48	0.97	0.12	10,12,23,25	0
4	SO4	A	404	5/5	0.97	0.13	57,58,61,63	0
2	NAP	B	401	48/48	0.97	0.12	14,19,30,34	0
2	NAP	D	400	48/48	0.97	0.12	11,14,24,27	0
2	NAP	E	400	48/48	0.97	0.12	14,17,27,29	0
2	NAP	C	400	48/48	0.98	0.10	11,14,19,20	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 NAP F 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
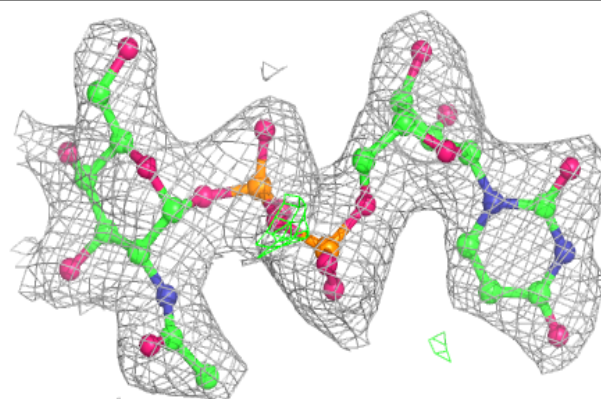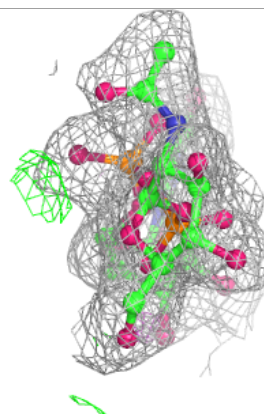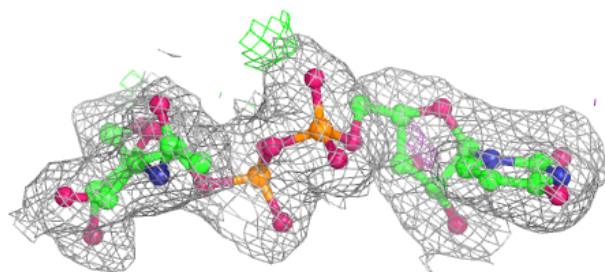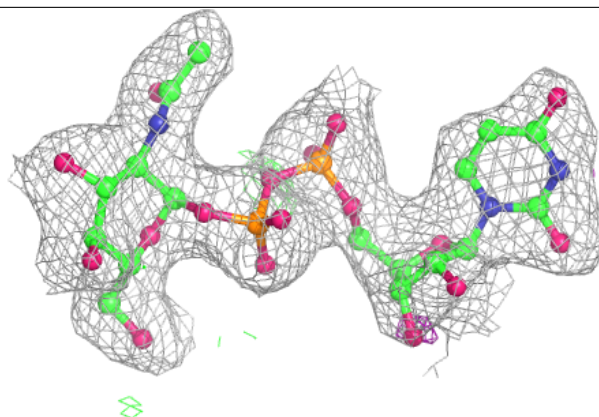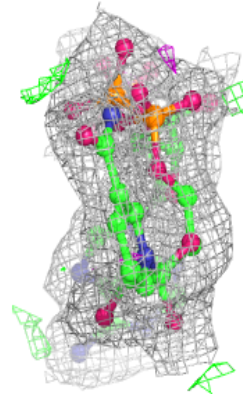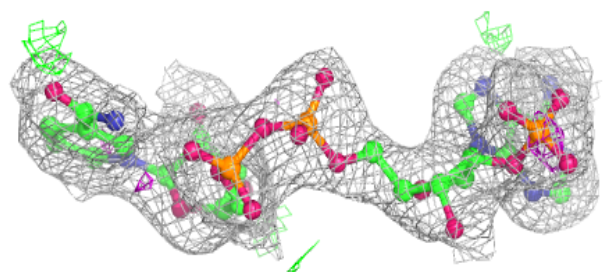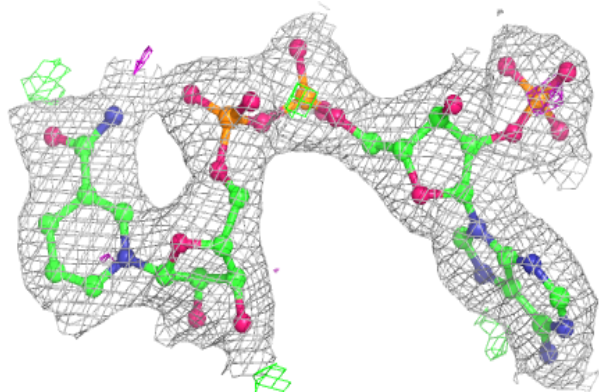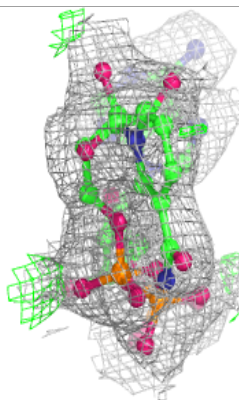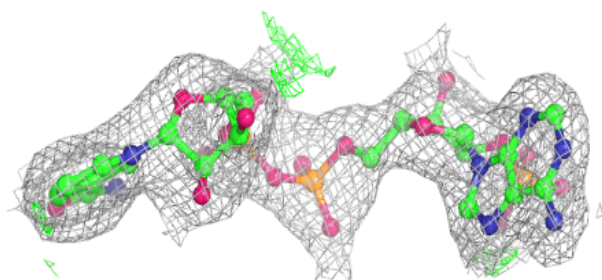mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
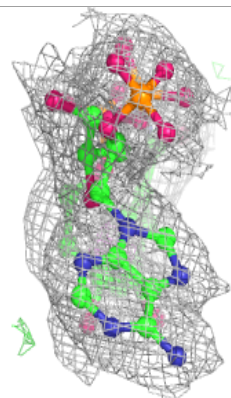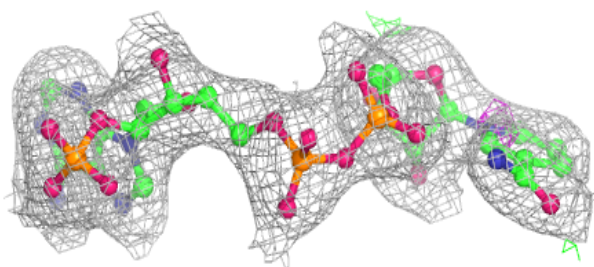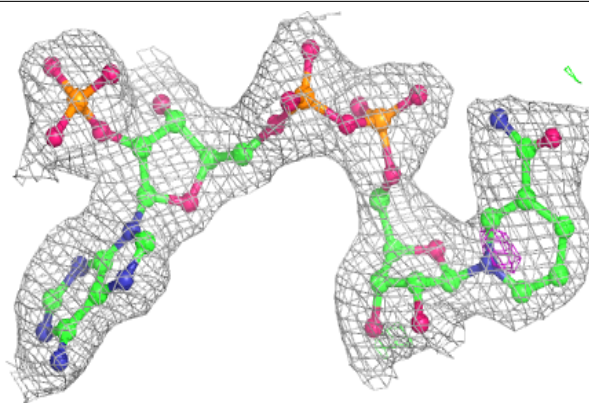
Electron density around UD1 A 402:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
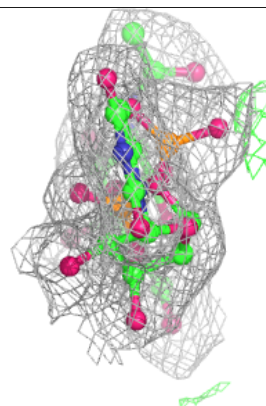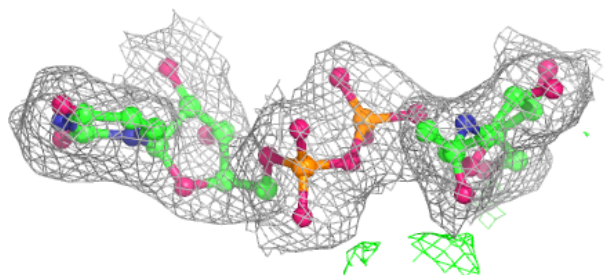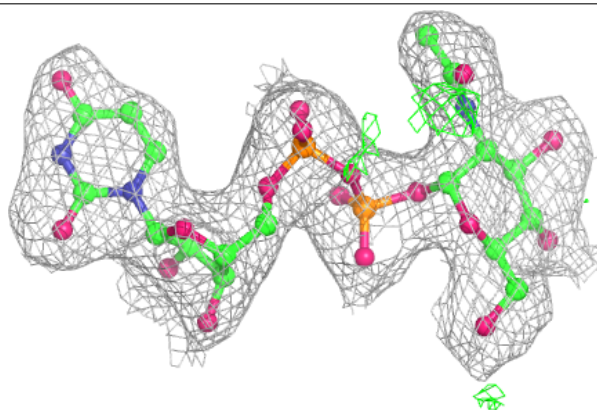
Electron density around UD1 B 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
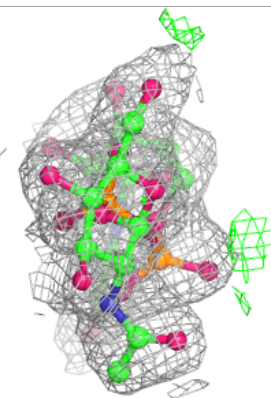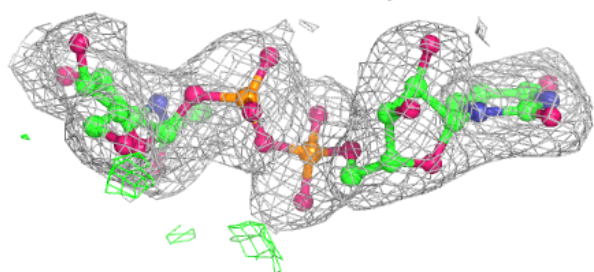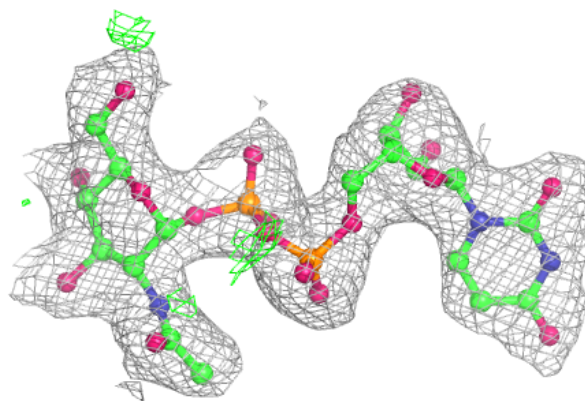
Electron density around UD1 C 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
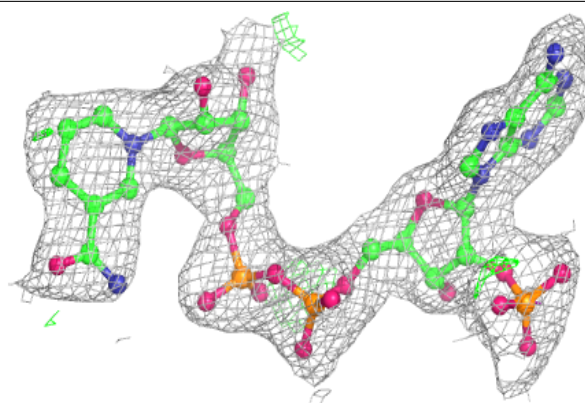$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
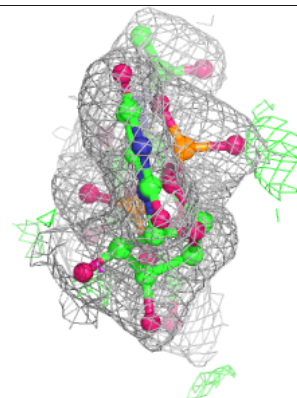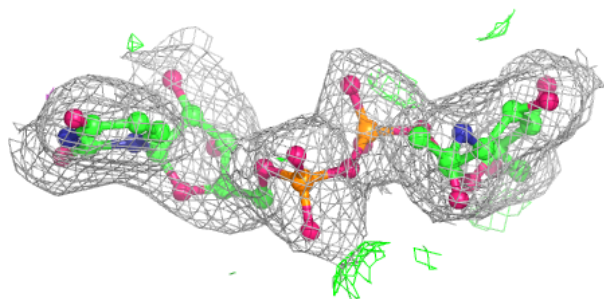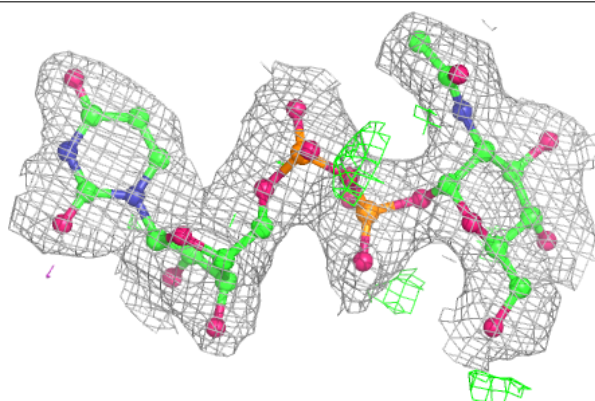
Electron density around UD1 D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
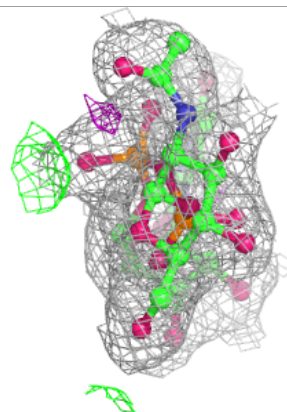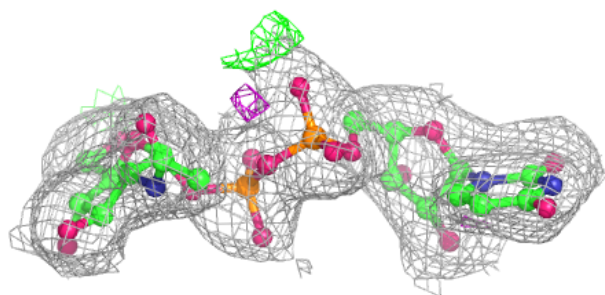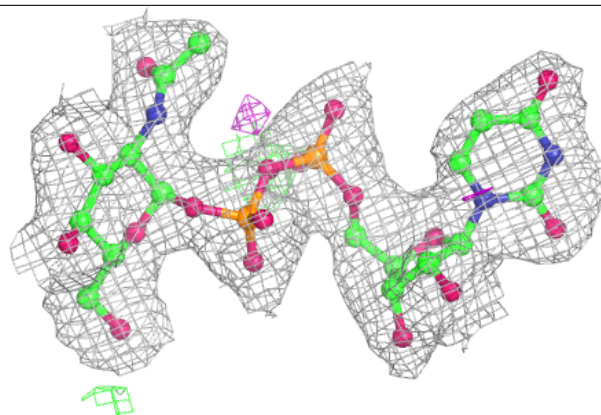
Electron density around UD1 E 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
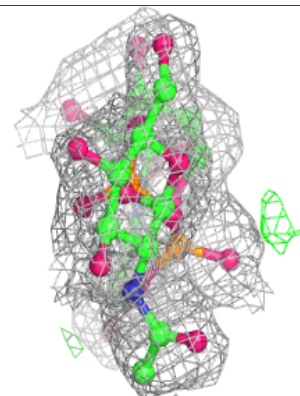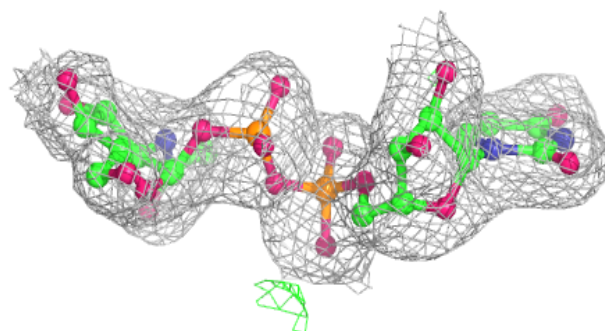
**Electron density around UD1 F 402:**

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 NAP A 401:

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 NAP B 401:

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

Electron density around NAP D 400:

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

Electron density around NAP E 400:

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

Electron density around NAP C 400:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
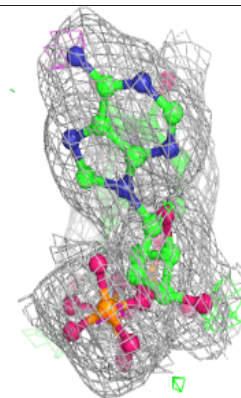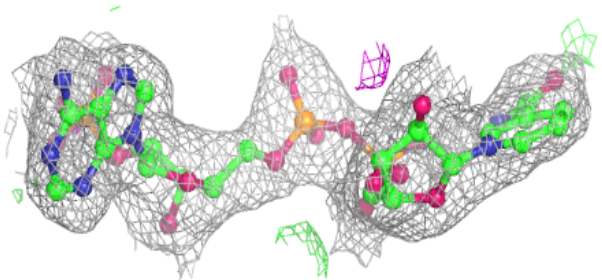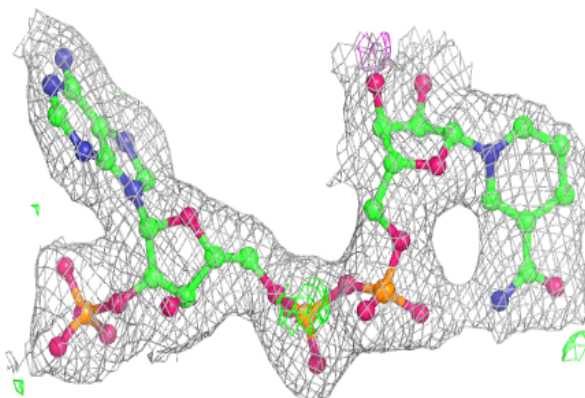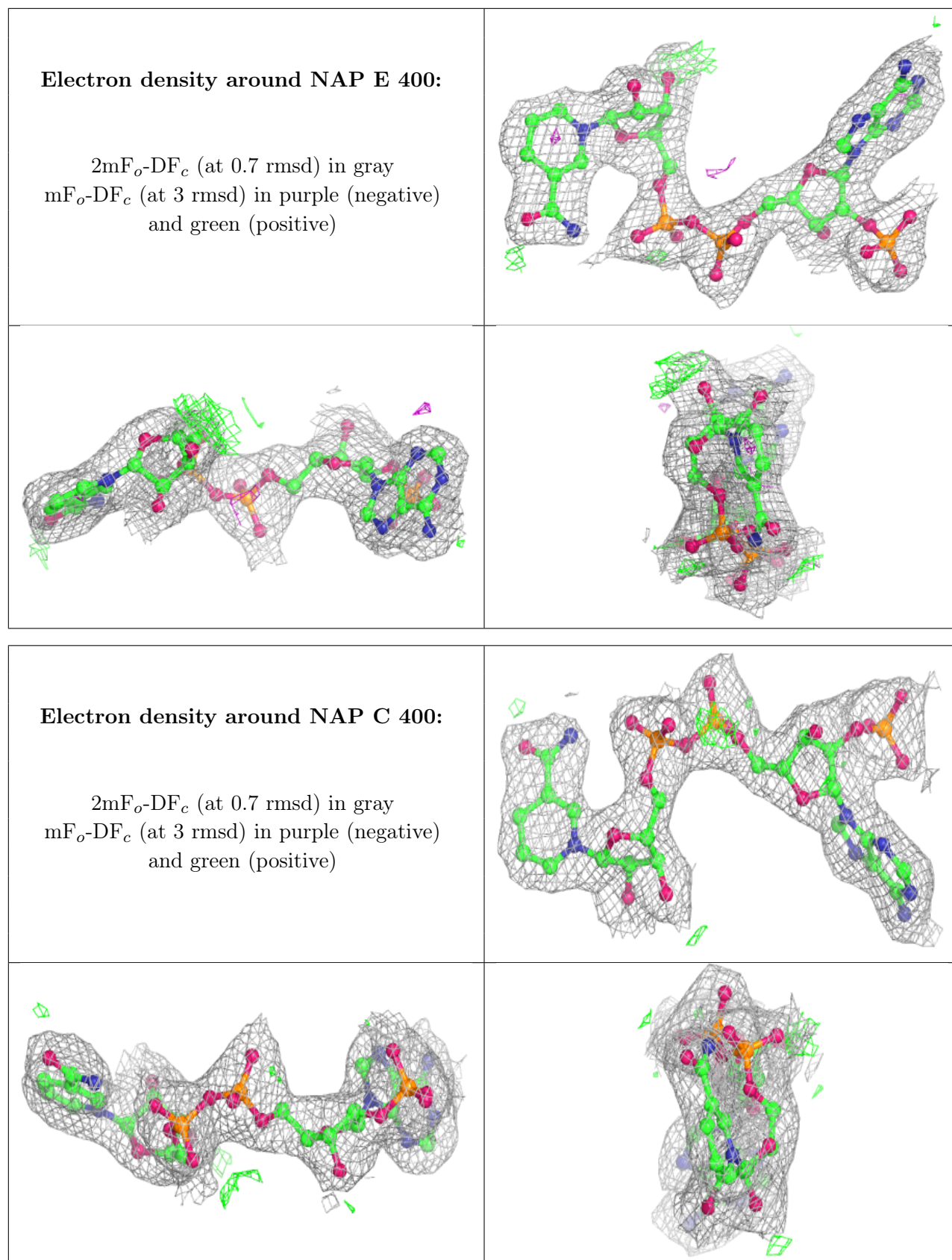
6.5 Other polymers (i)

There are no such residues in this entry.