



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:58 AM UTC

PDB ID : 8RPL / pdb_00008rpl
Title : AMP-forming acetyl-CoA synthetase from Chloroflexota bacterium with bound acetyl AMP
Authors : Striska, K.; Palm, G.J.; Lammers, M.
Deposited on : 2024-01-16
Resolution : 2.37 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

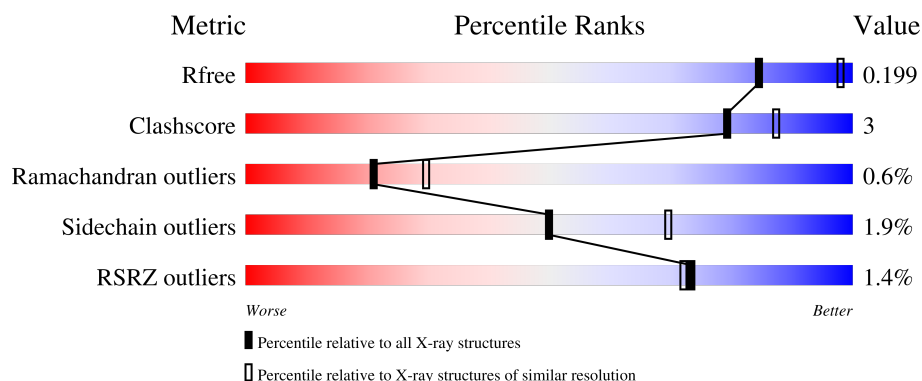
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	657	% 85% 9% • 5%
1	B	657	2% 87% 8% •
1	C	657	% 88% 7% 5%
1	D	657	2% 84% 11% • 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 40647 atoms, of which 20104 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 Acetate–CoA ligase.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	627	Total	C	H	N	O	P	S		126	9	0
			10030	3250	4986	844	921	1	28				
1	B	630	Total	C	H	N	O	P	S		127	9	0
			10071	3263	5007	846	926	1	28				
1	C	627	Total	C	H	N	O	P	S		127	10	0
			10036	3252	4991	843	921	1	28				
1	D	626	Total	C	H	N	O	P	S		127	10	0
			10029	3250	4988	842	920	1	28				

There are 44 discrepancies between the modelled and reference sequences:

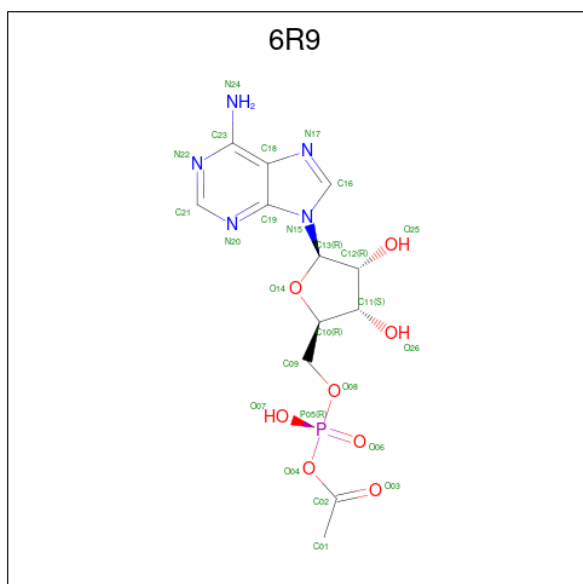
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	initiating methionine	UNP A0A535FEC2
A	-8	ALA	-	expression tag	UNP A0A535FEC2
A	-7	HIS	-	expression tag	UNP A0A535FEC2
A	-6	HIS	-	expression tag	UNP A0A535FEC2
A	-5	HIS	-	expression tag	UNP A0A535FEC2
A	-4	HIS	-	expression tag	UNP A0A535FEC2
A	-3	HIS	-	expression tag	UNP A0A535FEC2
A	-2	HIS	-	expression tag	UNP A0A535FEC2
A	-1	VAL	-	expression tag	UNP A0A535FEC2
A	0	GLY	-	expression tag	UNP A0A535FEC2
A	1	THR	-	expression tag	UNP A0A535FEC2
B	-9	MET	-	initiating methionine	UNP A0A535FEC2
B	-8	ALA	-	expression tag	UNP A0A535FEC2
B	-7	HIS	-	expression tag	UNP A0A535FEC2
B	-6	HIS	-	expression tag	UNP A0A535FEC2
B	-5	HIS	-	expression tag	UNP A0A535FEC2
B	-4	HIS	-	expression tag	UNP A0A535FEC2
B	-3	HIS	-	expression tag	UNP A0A535FEC2
B	-2	HIS	-	expression tag	UNP A0A535FEC2
B	-1	VAL	-	expression tag	UNP A0A535FEC2
B	0	GLY	-	expression tag	UNP A0A535FEC2

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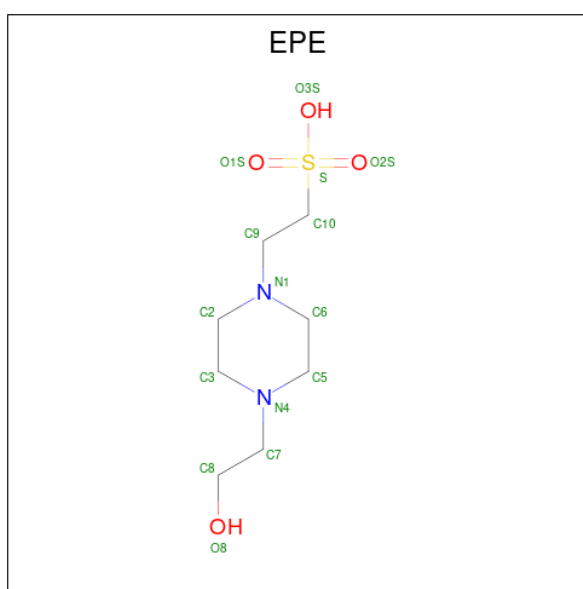
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	THR	-	expression tag	UNP A0A535FEC2
C	-9	MET	-	initiating methionine	UNP A0A535FEC2
C	-8	ALA	-	expression tag	UNP A0A535FEC2
C	-7	HIS	-	expression tag	UNP A0A535FEC2
C	-6	HIS	-	expression tag	UNP A0A535FEC2
C	-5	HIS	-	expression tag	UNP A0A535FEC2
C	-4	HIS	-	expression tag	UNP A0A535FEC2
C	-3	HIS	-	expression tag	UNP A0A535FEC2
C	-2	HIS	-	expression tag	UNP A0A535FEC2
C	-1	VAL	-	expression tag	UNP A0A535FEC2
C	0	GLY	-	expression tag	UNP A0A535FEC2
C	1	THR	-	expression tag	UNP A0A535FEC2
D	-9	MET	-	initiating methionine	UNP A0A535FEC2
D	-8	ALA	-	expression tag	UNP A0A535FEC2
D	-7	HIS	-	expression tag	UNP A0A535FEC2
D	-6	HIS	-	expression tag	UNP A0A535FEC2
D	-5	HIS	-	expression tag	UNP A0A535FEC2
D	-4	HIS	-	expression tag	UNP A0A535FEC2
D	-3	HIS	-	expression tag	UNP A0A535FEC2
D	-2	HIS	-	expression tag	UNP A0A535FEC2
D	-1	VAL	-	expression tag	UNP A0A535FEC2
D	0	GLY	-	expression tag	UNP A0A535FEC2
D	1	THR	-	expression tag	UNP A0A535FEC2

- Molecule 2 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] ethanoate (CCD ID: 6R9) (formula: C₁₂H₁₆N₅O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	
			41	12	15	5	8	1	
2	B	1	Total	C	H	N	O	P	
			41	12	15	5	8	1	
2	C	1	Total	C	H	N	O	P	
			41	12	15	5	8	1	
2	D	1	Total	C	H	N	O	P	
			41	12	15	5	8	1	

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	
			33	8	18	2	4	1	
3	B	1	Total	C	H	N	O	S	
			33	8	18	2	4	1	
3	C	1	Total	C	H	N	O	S	
			33	8	18	2	4	1	
3	D	1	Total	C	H	N	O	S	
			33	8	18	2	4	1	

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg		
			1	1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	Na 1	0	0

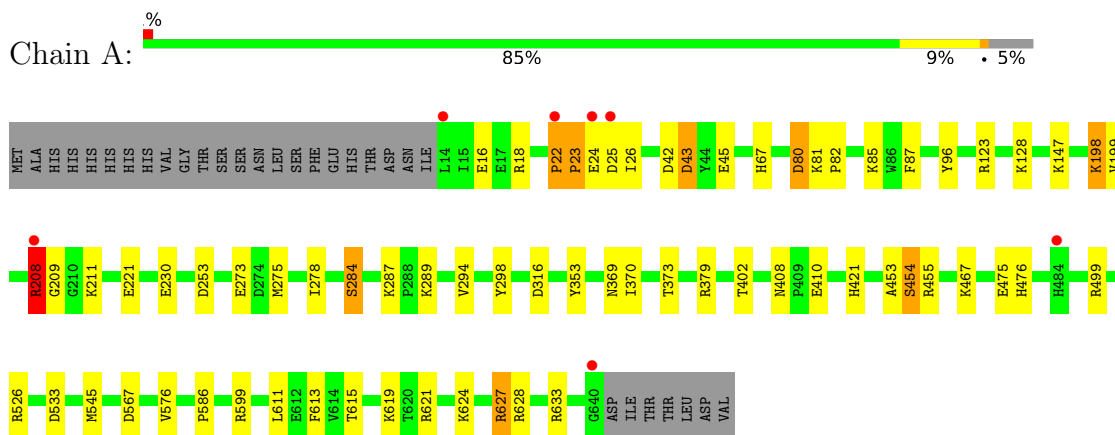
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	66	Total 66	O 66	0	0
6	B	44	Total 44	O 44	0	0
6	C	42	Total 42	O 42	0	0
6	D	29	Total 29	O 29	0	0

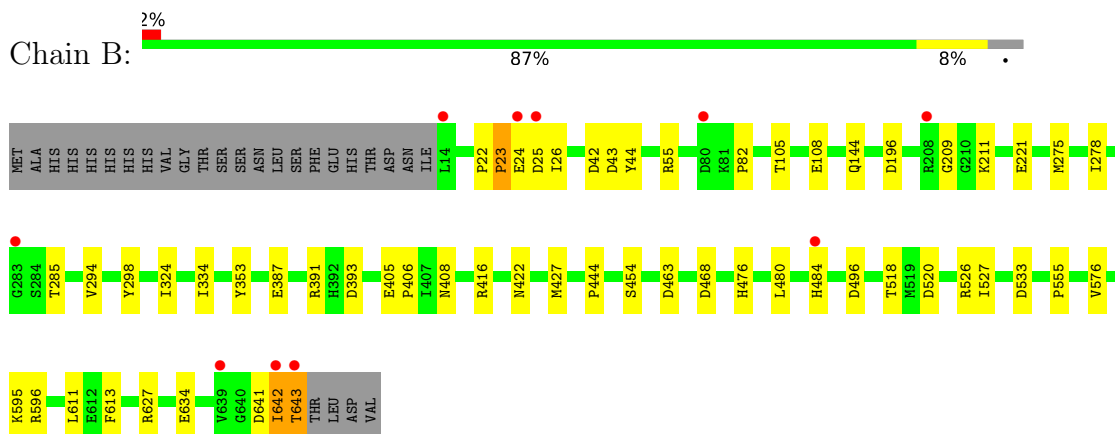
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

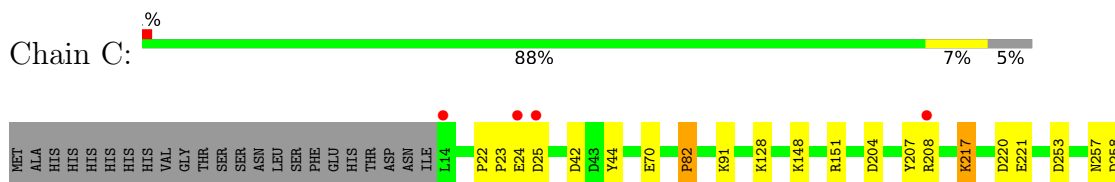
- Molecule 1: Acetate–CoA ligase

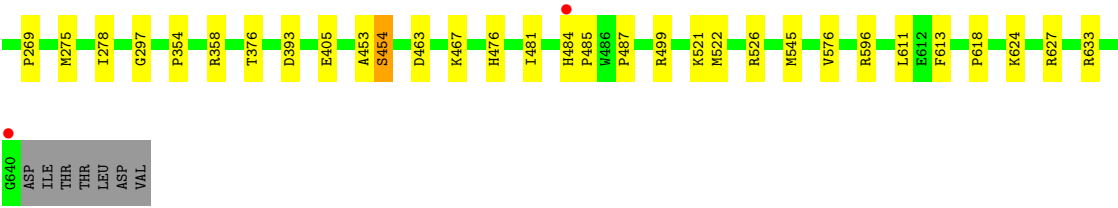


- Molecule 1: Acetate–CoA ligase

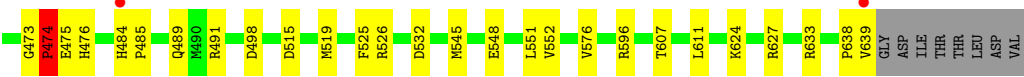
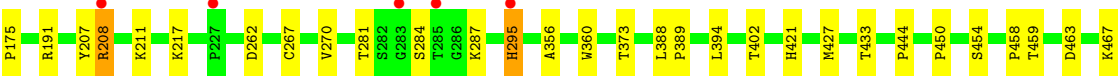
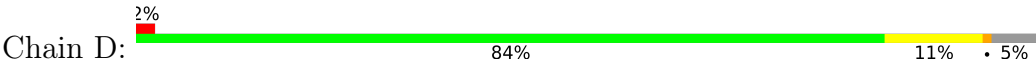


- Molecule 1: Acetate–CoA ligase





● Molecule 1: Acetate-CoA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	161.91Å 161.91Å 817.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.30 – 2.37 48.30 – 2.37	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.30-2.37) 92.0 (48.30-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.77 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.161 , 0.201 0.160 , 0.199	Depositor DCC
R_{free} test set	8378 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	61.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	40647	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, EPE, NA, NEP, 6R9

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	0.65	0/5182	1.13	16/7046 (0.2%)
1	B	0.61	0/5205	1.11	17/7078 (0.2%)
1	C	0.60	0/5189	1.12	15/7056 (0.2%)
1	D	0.58	0/5185	1.10	10/7051 (0.1%)
All	All	0.61	0/20761	1.11	58/28231 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
1	B	0	3
1	C	0	2
1	D	0	4
All	All	0	17

There are no bond length outliers.

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	295	HIS	CA-CB-CG	7.22	121.02	113.80
1	C	253	ASP	CA-CB-CG	7.08	119.67	112.60
1	A	253	ASP	CA-CB-CG	7.06	119.66	112.60
1	C	376	THR	CA-CB-OG1	-6.94	99.19	109.60
1	B	42	ASP	CB-CA-C	-6.65	97.19	109.29
1	A	42	ASP	CA-CB-CG	6.39	118.99	112.60
1	C	44	TYR	N-CA-CB	6.33	119.53	110.16
1	C	220	ASP	CA-CB-CG	6.26	118.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	421	HIS	CA-CB-CG	6.08	119.88	113.80
1	B	520	ASP	CA-CB-CG	6.08	118.67	112.60
1	A	410	GLU	N-CA-CB	-6.02	101.25	110.16
1	D	150	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	43	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	230	GLU	CB-CA-C	-5.86	98.63	109.29
1	A	627	ARG	CG-CD-NE	-5.85	99.12	112.00
1	C	82	PRO	N-CA-CB	-5.85	96.16	102.60
1	A	567	ASP	CA-CB-CG	5.84	118.44	112.60
1	D	211	LYS	CB-CA-C	-5.81	98.74	109.37
1	C	258	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	634	GLU	CB-CA-C	-5.72	101.86	110.90
1	A	221	GLU	CB-CA-C	5.69	120.24	110.79
1	D	75	THR	CA-CB-OG1	-5.68	101.07	109.60
1	A	80	ASP	CA-CB-CG	5.67	118.27	112.60
1	D	463	ASP	CA-CB-CG	5.67	118.27	112.60
1	B	285	THR	CA-CB-OG1	-5.64	101.14	109.60
1	B	463	ASP	CA-CB-CG	5.63	118.23	112.60
1	B	496	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	393	ASP	CA-CB-CG	5.50	118.11	112.60
1	B	196	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	533	ASP	CA-CB-CG	5.46	118.06	112.60
1	C	221	GLU	N-CA-CB	-5.43	102.12	110.16
1	A	42	ASP	CB-CA-C	-5.39	99.96	109.02
1	A	43	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	408	ASN	CB-CA-C	5.35	119.41	109.51
1	C	269	PRO	N-CA-CB	5.35	105.92	102.92
1	B	393	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	42	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	463	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	217	LYS	CB-CA-C	5.29	120.83	110.67
1	A	316	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	221	GLU	CB-CA-C	5.26	119.52	110.79
1	B	468	ASP	CA-CB-CG	5.25	117.84	112.60
1	A	615	THR	CA-CB-OG1	-5.24	101.75	109.60
1	A	87	PHE	N-CA-CB	-5.22	103.78	111.71
1	B	555	PRO	N-CA-C	5.17	120.56	113.84
1	C	204	ASP	CA-CB-CG	5.15	117.75	112.60
1	B	408	ASN	CB-CA-C	5.13	117.87	109.46
1	C	521	LYS	CB-CA-C	-5.13	99.50	110.32
1	D	607	THR	CA-CB-OG1	-5.12	101.92	109.60
1	A	633	ARG	N-CA-CB	5.10	117.61	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	LYS	CB-CA-C	-5.09	100.05	109.37
1	B	422	ASN	CB-CA-C	-5.09	104.37	111.80
1	D	624	LYS	CB-CA-C	5.08	118.12	109.53
1	C	405	GLU	CB-CG-CD	5.08	121.23	112.60
1	B	44	TYR	N-CA-CB	5.07	117.36	110.01
1	D	118	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	267	CYS	CB-CA-C	-5.03	102.72	110.26
1	D	532	ASP	CB-CA-C	5.03	120.43	110.42

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ARG	Sidechain
1	A	18	ARG	Sidechain
1	A	208[A]	ARG	Sidechain
1	A	208[B]	ARG	Sidechain
1	A	379	ARG	Sidechain
1	A	526	ARG	Sidechain
1	A	599	ARG	Sidechain
1	A	628	ARG	Sidechain
1	B	526	ARG	Sidechain
1	B	596	ARG	Sidechain
1	B	627	ARG	Sidechain
1	C	526	ARG	Sidechain
1	C	596	ARG	Sidechain
1	D	208[A]	ARG	Sidechain
1	D	208[B]	ARG	Sidechain
1	D	596	ARG	Sidechain
1	D	627	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5044	4986	4974	31	0
1	B	5064	5007	4996	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5045	4991	4981	24	0
1	D	5041	4988	4978	33	0
2	A	26	15	0	0	0
2	B	26	15	0	0	0
2	C	26	15	0	0	0
2	D	26	15	0	1	0
3	A	15	18	18	1	0
3	B	15	18	18	1	0
3	C	15	18	18	2	0
3	D	15	18	18	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	66	0	0	0	0
6	B	44	0	0	0	0
6	C	42	0	0	0	0
6	D	29	0	0	0	0
All	All	20543	20104	20001	110	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 3.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23[A]:PRO:O	1:A:25[A]:ASP:N	1.86	1.07
1:B:24[A]:GLU:O	1:B:24[A]:GLU:HG2	1.52	1.06
1:A:23[A]:PRO:HB2	1:A:26[A]:ILE:HG22	1.54	0.89
1:A:23[A]:PRO:C	1:A:25[A]:ASP:H	1.80	0.88
1:B:23[A]:PRO:C	1:B:25[A]:ASP:H	1.87	0.83
1:B:23[A]:PRO:O	1:B:25[A]:ASP:N	2.20	0.74
1:C:208[A]:ARG:HH11	1:C:208[A]:ARG:HG2	1.54	0.70
1:A:45:GLU:OE1	1:A:455:ARG:HD3	1.92	0.69
1:B:416:ARG:HH11	1:B:416:ARG:HG3	1.59	0.65
1:B:642:ILE:O	1:B:643:THR:C	2.41	0.64
1:D:551:LEU:CD1	1:D:576[A]:VAL:HG11	2.29	0.62
1:A:586:PRO:O	3:A:702:EPE:H81	2.02	0.60
1:B:105:THR:O	1:B:108:GLU:HG2	2.02	0.59
1:B:23[A]:PRO:C	1:B:25[A]:ASP:N	2.52	0.58
1:B:611[B]:LEU:HD21	1:B:613:PHE:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611[B]:LEU:HD21	1:A:613:PHE:CE1	2.40	0.56
1:D:23[A]:PRO:O	1:D:26[A]:ILE:HG22	2.05	0.56
1:D:270:VAL:HG21	1:D:295:HIS:CD2	2.39	0.56
1:D:427:MET:HE1	1:D:444:PRO:HA	1.87	0.56
1:C:207:TYR:O	1:C:208[B]:ARG:HG3	2.06	0.56
1:C:611[B]:LEU:HD21	1:C:613:PHE:CE1	2.41	0.55
1:B:24[A]:GLU:O	1:B:24[A]:GLU:CG	2.38	0.55
1:C:70:GLU:HB2	1:C:91:LYS:HB2	1.89	0.55
1:C:208[A]:ARG:HG2	1:C:208[A]:ARG:NH1	2.22	0.55
1:D:24[B]:GLU:O	1:D:25[B]:ASP:HB2	2.06	0.54
1:D:281[A]:THR:CG2	1:D:433:THR:HG21	2.38	0.54
1:A:22[A]:PRO:O	1:A:24[A]:GLU:N	2.41	0.53
1:C:484[B]:HIS:CD2	1:C:485:PRO:HD2	2.44	0.53
1:D:23[A]:PRO:HB2	1:D:26[A]:ILE:HG22	1.88	0.53
1:A:23[A]:PRO:C	1:A:25[A]:ASP:N	2.45	0.53
1:D:281[A]:THR:HG21	1:D:433:THR:HG21	1.92	0.52
1:D:576[A]:VAL:HB	1:D:611[A]:LEU:HD23	1.90	0.52
1:A:284:SER:HA	1:A:533:ASP:OD1	2.09	0.52
1:B:275:MET:HE1	1:B:278:ILE:HD11	1.90	0.52
1:A:576[A]:VAL:HB	1:A:611[A]:LEU:CD2	2.40	0.51
1:D:450:PRO:O	1:D:526:ARG:NH2	2.44	0.51
1:A:198:LYS:HG2	1:A:199:VAL:HG13	1.92	0.51
1:A:23[A]:PRO:CB	1:A:26[A]:ILE:HG22	2.36	0.51
1:B:55:ARG:HD2	1:B:484[B]:HIS:CE1	2.48	0.49
1:A:208[A]:ARG:HH11	1:A:208[A]:ARG:HG3	1.77	0.49
1:A:85:LYS:HD2	1:A:273:GLU:HG3	1.95	0.49
1:A:453:ALA:O	1:A:454:SER:CB	2.59	0.49
1:A:576[A]:VAL:HB	1:A:611[A]:LEU:HD23	1.93	0.49
1:C:522:MET:CE	1:D:639:VAL:HG13	2.42	0.49
1:D:576[A]:VAL:HB	1:D:611[A]:LEU:CD2	2.43	0.49
1:B:294:VAL:O	1:B:298:TYR:HB3	2.13	0.48
1:C:22[B]:PRO:O	1:D:633:ARG:NH2	2.46	0.48
1:D:191:ARG:HG3	1:D:191:ARG:HH11	1.79	0.48
1:B:595:LYS:NZ	3:B:702:EPE:O1S	2.35	0.48
1:C:208[A]:ARG:NH1	1:C:208[A]:ARG:CG	2.76	0.47
1:A:545:MET:CE	1:A:627:ARG:HH22	2.27	0.47
1:A:45:GLU:OE1	1:A:455:ARG:CD	2.62	0.47
1:B:416:ARG:HH11	1:B:416:ARG:CG	2.24	0.47
1:C:576[A]:VAL:HB	1:C:611[A]:LEU:HD23	1.97	0.46
1:A:373:THR:O	1:A:402:THR:HA	2.16	0.46
1:B:427:MET:HE1	1:B:444:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:GLN:O	1:D:491:ARG:NH1	2.49	0.46
1:A:294:VAL:O	1:A:298:TYR:HB3	2.16	0.46
1:A:619:LYS:HA	1:A:624:LYS:O	2.16	0.45
1:D:638:PRO:O	1:D:639:VAL:C	2.59	0.45
1:D:150:ASP:O	1:D:175:PRO:HD2	2.17	0.45
1:C:275:MET:HE1	1:C:278:ILE:HD11	1.98	0.45
1:D:519:MET:HE2	1:D:525:PHE:CZ	2.51	0.45
1:C:208[B]:ARG:HH11	1:C:208[B]:ARG:CG	2.30	0.45
1:A:81:LYS:HA	1:A:82:PRO:HA	1.82	0.44
1:B:209:GLY:HA2	1:B:353:TYR:CG	2.53	0.44
1:C:297:GLY:HA3	1:C:487:PRO:O	2.18	0.44
1:C:453:ALA:O	1:C:454:SER:CB	2.65	0.44
1:D:458:PRO:C	1:D:459:THR:HG23	2.42	0.44
1:B:427:MET:HE3	1:B:444:PRO:HG3	1.98	0.44
1:D:112:ALA:HB2	1:D:127:TYR:CD1	2.52	0.44
1:D:284:SER:O	1:D:545:MET:HE3	2.17	0.44
1:C:522:MET:HE3	1:D:639:VAL:HG13	2.00	0.43
1:D:388:LEU:HB2	1:D:389:PRO:HD3	2.00	0.43
1:C:545:MET:HE2	1:C:627:ARG:HH12	1.83	0.43
1:A:209:GLY:HA2	1:A:353:TYR:CG	2.54	0.43
1:C:618:PRO:HD3	1:C:633:ARG:HH12	1.83	0.43
1:C:481:ILE:C	1:C:481:ILE:HD12	2.42	0.43
1:D:548:GLU:O	1:D:552:VAL:HG23	2.18	0.43
1:D:81:LYS:HA	1:D:82:PRO:HA	1.89	0.42
1:D:515:ASP:OD2	2:D:701:6R9:O26	2.37	0.42
1:A:289:LYS:HE3	1:A:499:ARG:HG3	2.01	0.42
1:C:24[B]:GLU:O	1:C:24[B]:GLU:OE1	2.38	0.42
1:D:473:GLY:O	1:D:474:PRO:C	2.62	0.42
1:D:551:LEU:HD12	1:D:576[A]:VAL:HG11	2.01	0.42
1:C:354:PRO:HD2	1:C:358:ARG:HD3	2.02	0.42
1:A:275:MET:HE1	1:A:278:ILE:HD11	2.02	0.42
1:B:387:GLU:O	1:B:391:ARG:HG3	2.19	0.42
1:C:24[B]:GLU:O	1:C:25[B]:ASP:HB2	2.18	0.42
1:A:67:HIS:CD2	1:A:96:TYR:CD1	3.08	0.42
1:A:275:MET:HB3	1:A:275:MET:HE2	1.76	0.42
1:B:480:LEU:HD22	1:B:527:ILE:HD12	2.02	0.42
1:D:373:THR:O	1:D:402:THR:HA	2.20	0.42
1:D:207:TYR:O	1:D:208[A]:ARG:HG2	2.19	0.42
1:B:324:ILE:HD13	1:B:334:ILE:HD11	2.02	0.41
1:C:208[B]:ARG:HG2	1:C:208[B]:ARG:NH1	2.34	0.41
1:A:23[A]:PRO:HB2	1:A:26[A]:ILE:CG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASN:C	1:A:370:ILE:HG13	2.45	0.41
1:C:453:ALA:O	1:C:454:SER:HB3	2.21	0.41
1:B:144:GLN:O	1:B:144:GLN:HG3	2.20	0.41
1:B:405:GLU:HB2	1:B:406:PRO:HD2	2.02	0.41
1:C:208[A]:ARG:HH11	1:C:208[A]:ARG:CG	2.21	0.41
1:A:80:ASP:O	1:A:81:LYS:C	2.63	0.41
1:A:453:ALA:O	1:A:454:SER:HB3	2.21	0.41
1:D:360:TRP:HB3	1:D:394:LEU:HD21	2.02	0.41
1:D:356:ALA:HB3	1:D:388:LEU:CD1	2.51	0.41
1:B:576[A]:VAL:HB	1:B:611[A]:LEU:CD2	2.51	0.40
1:D:484[A]:HIS:HA	1:D:485:PRO:HD3	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	633/657 (96%)	615 (97%)	15 (2%)	3 (0%)	24	34
1	B	636/657 (97%)	610 (96%)	21 (3%)	5 (1%)	16	23
1	C	634/657 (96%)	613 (97%)	18 (3%)	3 (0%)	24	34
1	D	633/657 (96%)	606 (96%)	20 (3%)	7 (1%)	11	16
All	All	2536/2628 (96%)	2444 (96%)	74 (3%)	18 (1%)	21	26

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	SER
1	C	23[A]	PRO
1	C	23[B]	PRO
1	C	454	SER

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Mol	Chain	Res	Type
1	D	25[A]	ASP
1	D	25[B]	ASP
1	D	80	ASP
1	D	421	HIS
1	D	475	GLU
1	B	454	SER
1	B	642	ILE
1	D	454	SER
1	B	641	ASP
1	D	474	PRO
1	A	23[A]	PRO
1	A	23[B]	PRO
1	B	23[A]	PRO
1	B	23[B]	PRO

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	538/557 (97%)	523 (97%)	15 (3%)	38	58
1	B	541/557 (97%)	534 (99%)	7 (1%)	61	78
1	C	539/557 (97%)	530 (98%)	9 (2%)	53	72
1	D	539/557 (97%)	522 (97%)	17 (3%)	34	53
All	All	2157/2228 (97%)	2109 (98%)	48 (2%)	50	65

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	22[A]	PRO
1	A	22[B]	PRO
1	A	43	ASP
1	A	128	LYS
1	A	147	LYS
1	A	198	LYS

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Mol	Chain	Res	Type
1	A	208[A]	ARG
1	A	208[B]	ARG
1	A	211	LYS
1	A	284	SER
1	A	287	LYS
1	A	467	LYS
1	A	475	GLU
1	A	621	ARG
1	B	22[A]	PRO
1	B	22[B]	PRO
1	B	26[A]	ILE
1	B	26[B]	ILE
1	B	82	PRO
1	B	518	THR
1	B	643	THR
1	C	82	PRO
1	C	128	LYS
1	C	148	LYS
1	C	151	ARG
1	C	217	LYS
1	C	257	ASN
1	C	467	LYS
1	C	499	ARG
1	C	624	LYS
1	D	18	ARG
1	D	22[A]	PRO
1	D	22[B]	PRO
1	D	25[A]	ASP
1	D	25[B]	ASP
1	D	26[A]	ILE
1	D	26[B]	ILE
1	D	42	ASP
1	D	43	ASP
1	D	73	LYS
1	D	85	LYS
1	D	217	LYS
1	D	262	ASP
1	D	287	LYS
1	D	467	LYS
1	D	474	PRO
1	D	498	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	67	HIS
1	A	257	ASN
1	A	528	GLN
1	B	54	ASN
1	B	582	ASN
1	C	29	ASN
1	C	54	ASN
1	D	67	HIS
1	D	422	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	NEP	B	476	1	11,14,15	1.50	1 (9%)	8,20,22	0.58	0
1	NEP	A	476	1	11,14,15	1.46	1 (9%)	8,20,22	0.81	1 (12%)
1	NEP	D	476	1	11,14,15	1.40	1 (9%)	8,20,22	0.72	0
1	NEP	C	476	1	11,14,15	1.48	1 (9%)	8,20,22	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NEP	B	476	1	-	2/5/12/14	0/1/1/1
1	NEP	A	476	1	-	2/5/12/14	0/1/1/1
1	NEP	D	476	1	-	2/5/12/14	0/1/1/1
1	NEP	C	476	1	-	2/5/12/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	476	NEP	P-O3P	4.20	1.52	1.46
1	A	476	NEP	P-O3P	4.04	1.52	1.46
1	C	476	NEP	P-O3P	3.99	1.52	1.46
1	D	476	NEP	P-O3P	3.60	1.51	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	NEP	O1P-P-O3P	-2.18	107.58	112.95

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	476	NEP	CA-CB-CG-CD2
1	D	476	NEP	CA-CB-CG-CD2
1	A	476	NEP	CA-CB-CG-ND1
1	B	476	NEP	CA-CB-CG-ND1
1	C	476	NEP	CA-CB-CG-ND1
1	D	476	NEP	CA-CB-CG-ND1
1	B	476	NEP	CA-CB-CG-CD2
1	C	476	NEP	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	6R9	D	701	-	27,28,28	0.69	1 (3%)	39,42,42	0.55	0
2	6R9	A	701	-	27,28,28	0.77	1 (3%)	39,42,42	0.69	0
3	EPE	D	702	-	15,15,15	0.63	1 (6%)	19,20,20	1.05	1 (5%)
2	6R9	C	701	-	27,28,28	0.64	1 (3%)	39,42,42	0.63	1 (2%)
2	6R9	B	701	-	27,28,28	0.68	1 (3%)	39,42,42	0.64	0
3	EPE	C	702	-	15,15,15	0.63	0	19,20,20	0.84	1 (5%)
3	EPE	A	702	-	15,15,15	0.69	1 (6%)	19,20,20	0.68	0
3	EPE	B	702	-	15,15,15	0.53	0	19,20,20	0.90	2 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6R9	D	701	-	-	1/13/31/31	0/3/3/3
2	6R9	A	701	-	-	1/13/31/31	0/3/3/3
3	EPE	D	702	-	-	2/9/19/19	0/1/1/1
2	6R9	C	701	-	-	1/13/31/31	0/3/3/3
2	6R9	B	701	-	-	1/13/31/31	0/3/3/3
3	EPE	C	702	-	-	3/9/19/19	0/1/1/1
3	EPE	A	702	-	-	1/9/19/19	0/1/1/1
3	EPE	B	702	-	-	6/9/19/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	6R9	P05-O08	2.87	1.70	1.59
2	D	701	6R9	P05-O08	2.35	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	6R9	P05-O04	2.34	1.64	1.60
3	D	702	EPE	O3S-S	2.19	1.55	1.47
3	A	702	EPE	O3S-S	2.13	1.55	1.47
2	C	701	6R9	P05-O08	2.09	1.67	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	702	EPE	O3S-S-C10	-4.12	97.94	106.00
3	B	702	EPE	O3S-S-O2S	-2.83	104.32	111.40
2	C	701	6R9	O07-P05-O04	2.36	112.57	104.94
3	B	702	EPE	O2S-S-O1S	2.27	121.22	113.82
3	C	702	EPE	O3S-S-C10	-2.07	101.95	106.00

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	EPE	C10-C9-N1-C2
3	B	702	EPE	C10-C9-N1-C6
3	B	702	EPE	C9-C10-S-O1S
3	B	702	EPE	C9-C10-S-O2S
3	B	702	EPE	C9-C10-S-O3S
3	C	702	EPE	C10-C9-N1-C2
3	C	702	EPE	C10-C9-N1-C6
3	C	702	EPE	C8-C7-N4-C5
3	B	702	EPE	N4-C7-C8-O8
3	A	702	EPE	N4-C7-C8-O8
3	D	702	EPE	N4-C7-C8-O8
3	D	702	EPE	C8-C7-N4-C5
2	B	701	6R9	C02-O04-P05-O08
2	C	701	6R9	C02-O04-P05-O08
2	D	701	6R9	C02-O04-P05-O08
2	A	701	6R9	C02-O04-P05-O08

There are no ring outliers.

4 monomers are involved in 5 short contacts:

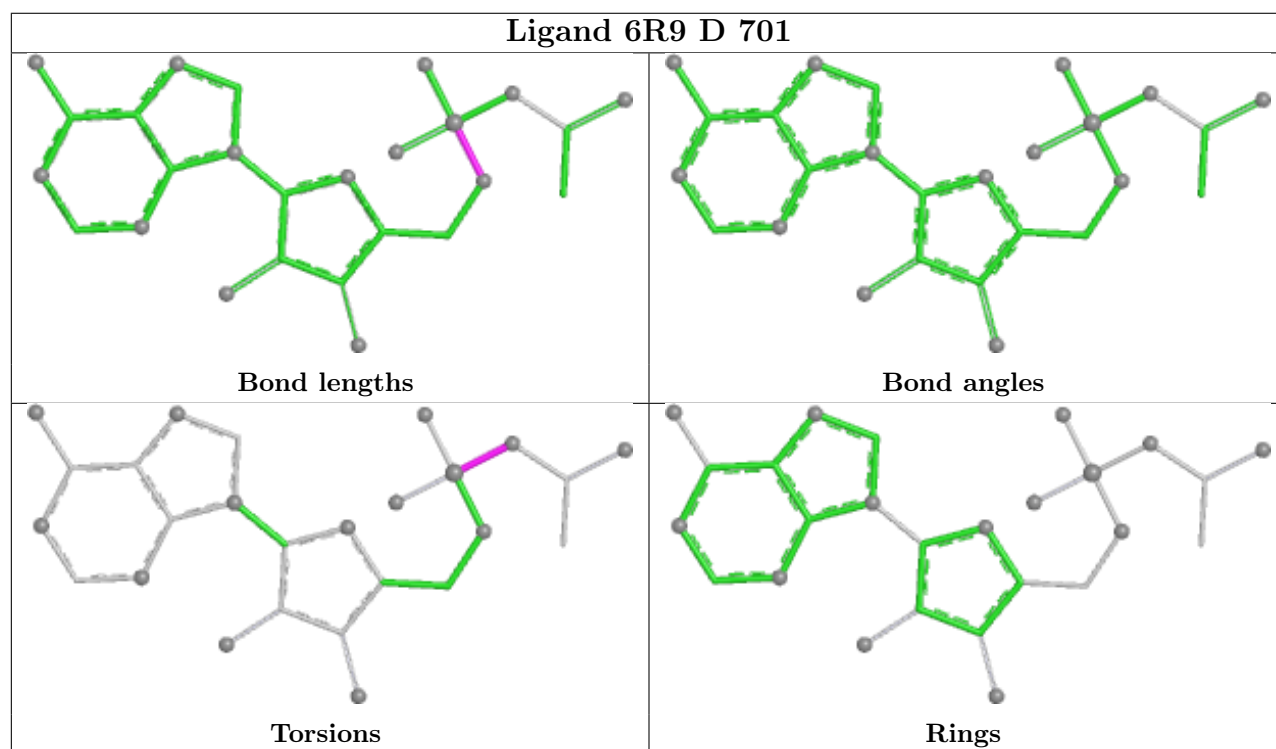
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	6R9	1	0
3	C	702	EPE	2	0

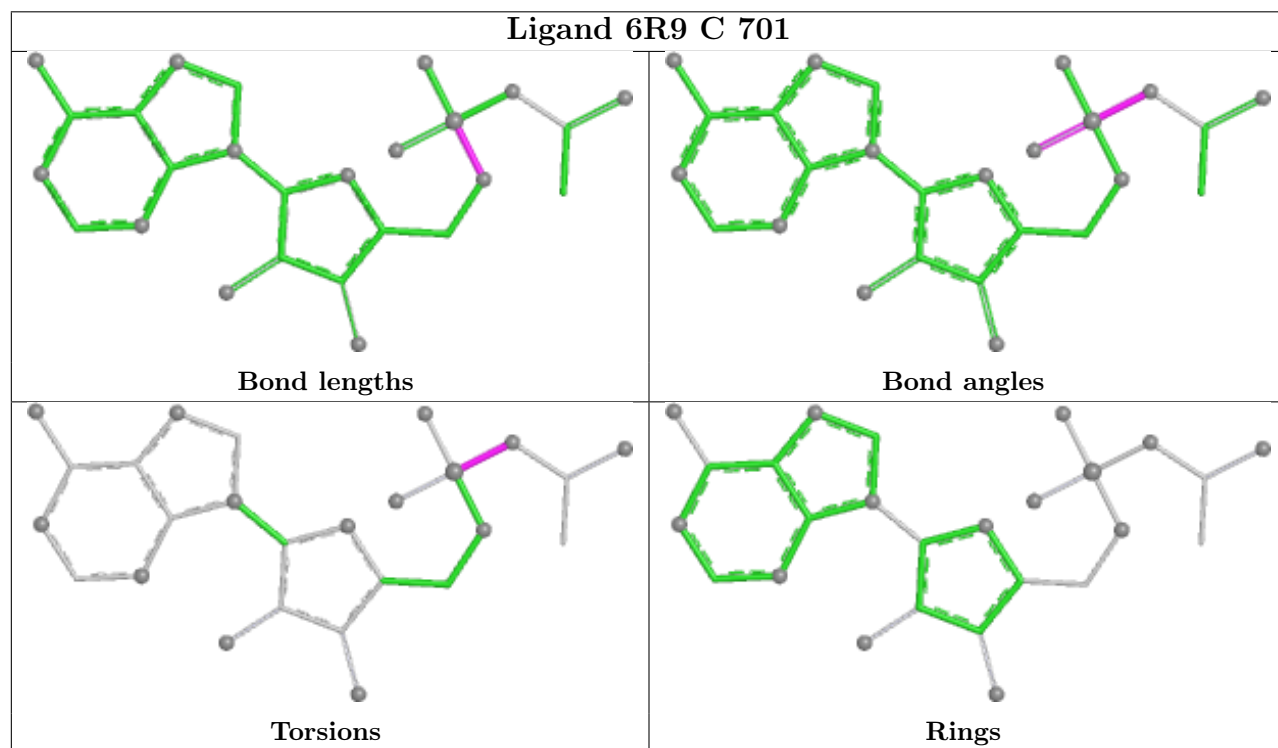
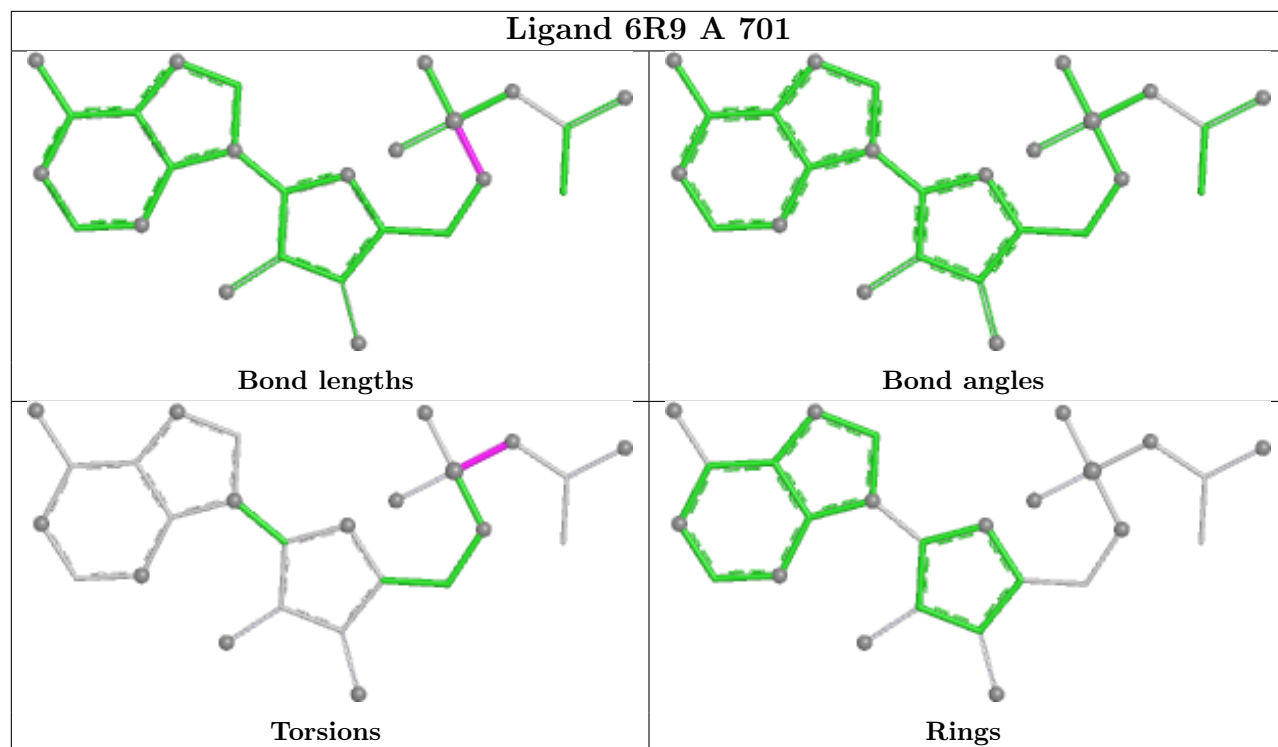
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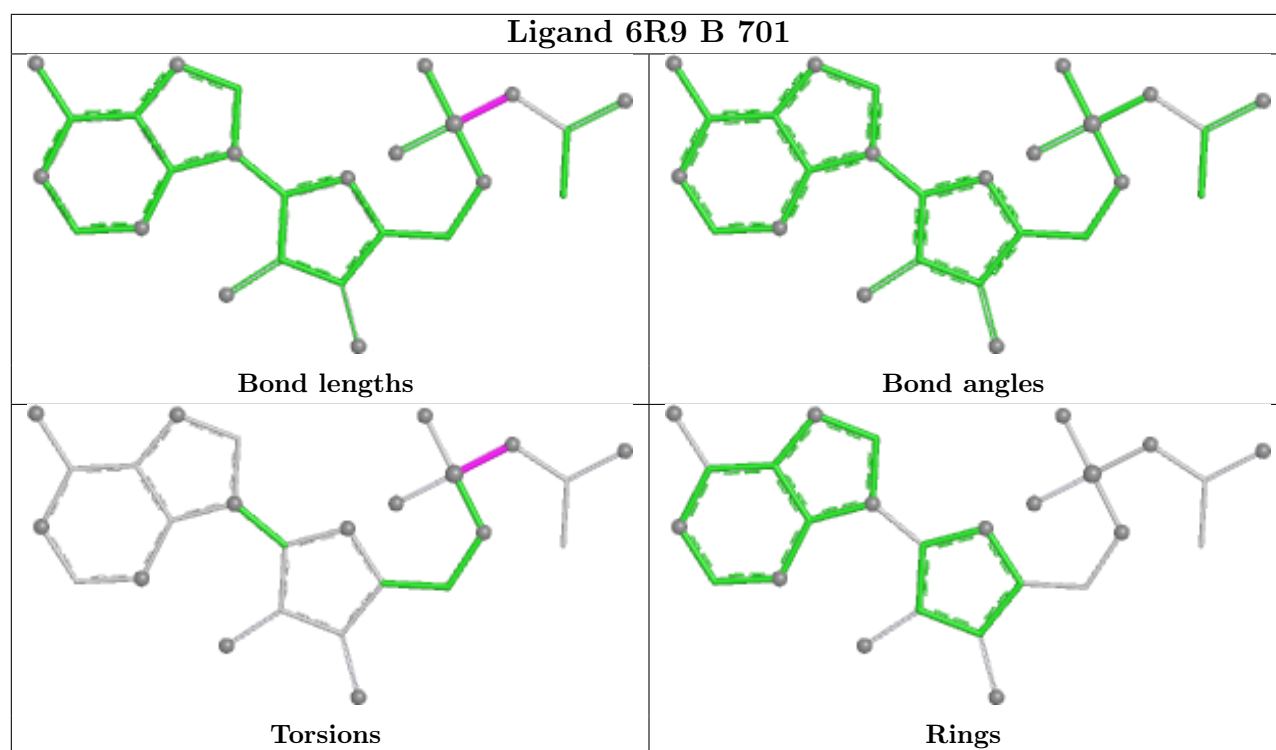
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	EPE	1	0
3	B	702	EPE	1	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	626/657 (95%)	-0.55	7 (1%) 78 77	26, 61, 93, 146	9 (1%)
1	B	629/657 (95%)	-0.40	10 (1%) 70 69	35, 71, 104, 168	9 (1%)
1	C	626/657 (95%)	-0.40	6 (0%) 79 78	33, 71, 104, 142	10 (1%)
1	D	625/657 (95%)	-0.12	13 (2%) 63 62	38, 86, 123, 145	10 (1%)
All	All	2506/2628 (95%)	-0.37	36 (1%) 73 72	26, 72, 112, 168	38 (1%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24[A]	GLU	20.7
1	B	24[A]	GLU	19.4
1	D	24[A]	GLU	17.1
1	C	24[A]	GLU	8.6
1	A	25[A]	ASP	8.6
1	D	25[A]	ASP	7.1
1	B	25[A]	ASP	6.1
1	A	14	LEU	5.2
1	C	25[A]	ASP	5.0
1	A	640	GLY	4.5
1	B	642	ILE	4.4
1	D	639	VAL	4.4
1	D	283	GLY	4.3
1	C	640	GLY	4.1
1	A	22[A]	PRO	4.1
1	B	14	LEU	4.0
1	C	14	LEU	3.3
1	D	295	HIS	3.1
1	B	283	GLY	2.8
1	A	208[A]	ARG	2.7
1	B	208[A]	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	14	LEU	2.7
1	D	87	PHE	2.6
1	D	227	PRO	2.6
1	D	484[A]	HIS	2.5
1	B	639	VAL	2.4
1	A	484[A]	HIS	2.4
1	B	80	ASP	2.4
1	D	285	THR	2.4
1	C	208[A]	ARG	2.4
1	D	56	PHE	2.4
1	D	58	PHE	2.3
1	D	208[A]	ARG	2.3
1	B	643	THR	2.3
1	B	484[A]	HIS	2.2
1	C	484[A]	HIS	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	NEP	A	476	14/15	0.88	0.09	70,111,143,148	0
1	NEP	D	476	14/15	0.88	0.08	102,136,164,164	0
1	NEP	C	476	14/15	0.89	0.08	77,116,146,151	0
1	NEP	B	476	14/15	0.93	0.07	73,107,139,149	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

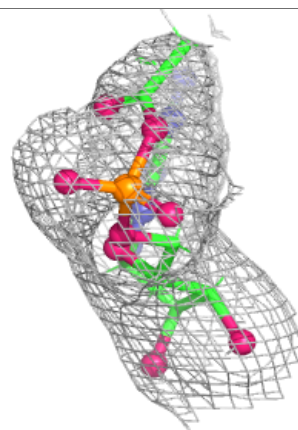
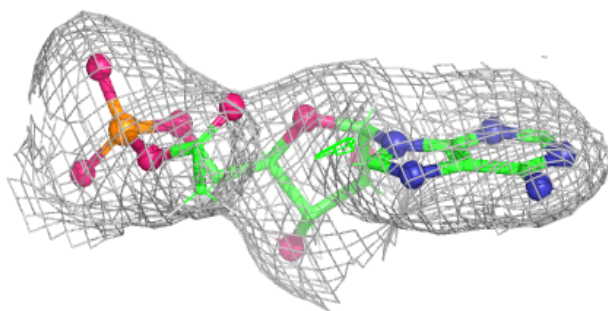
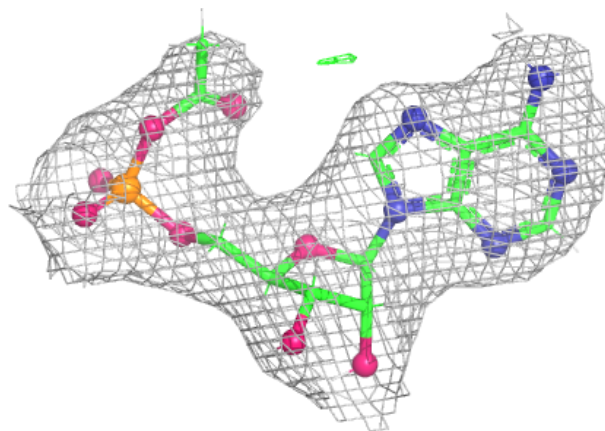
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EPE	C	702	15/15	0.79	0.23	30,130,143,145	2
3	EPE	A	702	15/15	0.84	0.23	30,113,124,125	33
3	EPE	D	702	15/15	0.85	0.21	30,125,142,142	33
3	EPE	B	702	15/15	0.90	0.25	30,99,119,124	33
4	MG	B	703	1/1	0.97	0.08	83,83,83,83	0
5	NA	D	703	1/1	0.97	0.05	76,76,76,76	0
2	6R9	D	701	26/26	0.98	0.06	30,76,91,96	2
2	6R9	B	701	26/26	0.99	0.04	30,59,73,77	2
4	MG	A	703	1/1	0.99	0.07	69,69,69,69	0
2	6R9	C	701	26/26	0.99	0.05	30,56,77,86	2
4	MG	C	703	1/1	0.99	0.04	70,70,70,70	0
2	6R9	A	701	26/26	0.99	0.04	30,52,68,74	2

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.

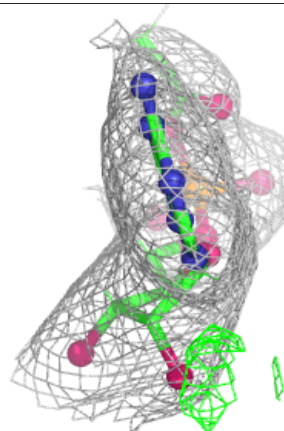
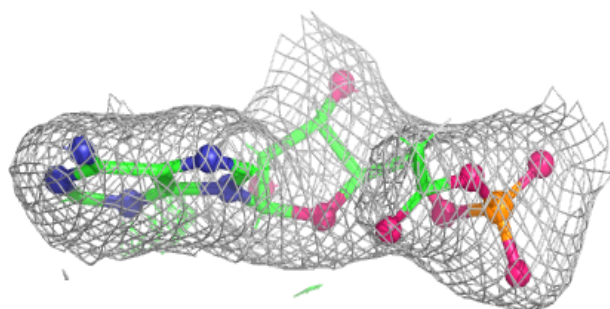
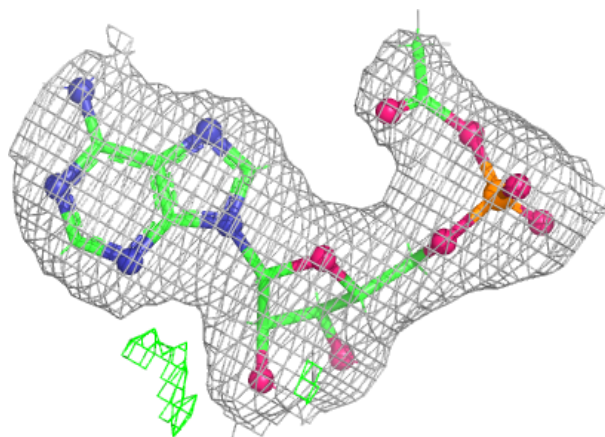
Electron density around 6R9 D 701:

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

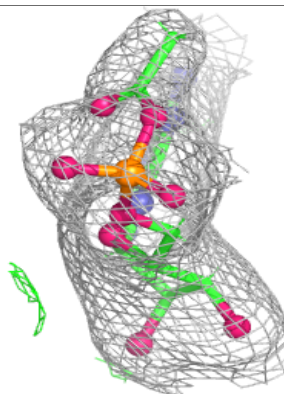
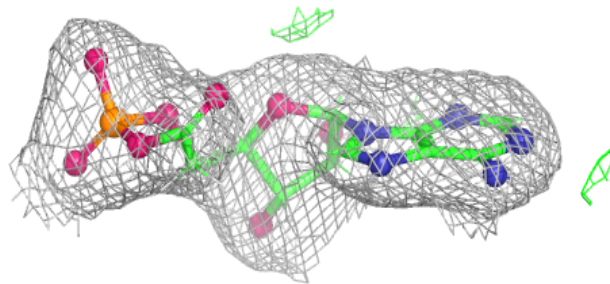
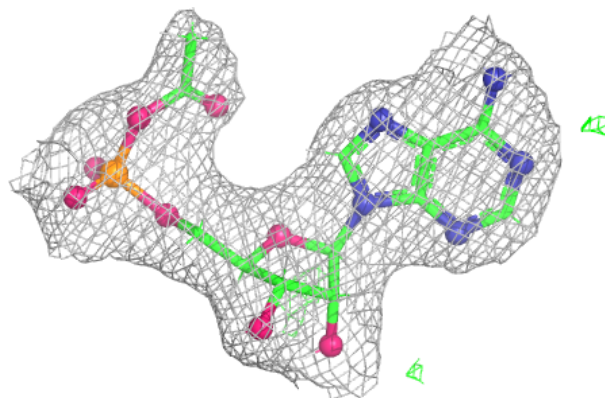


Electron density around 6R9 B 701:

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

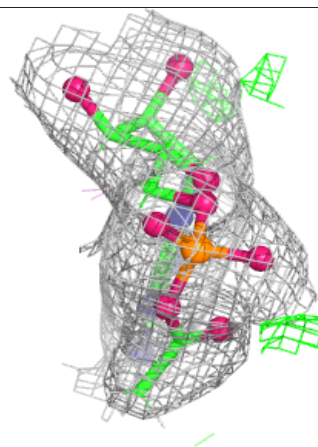
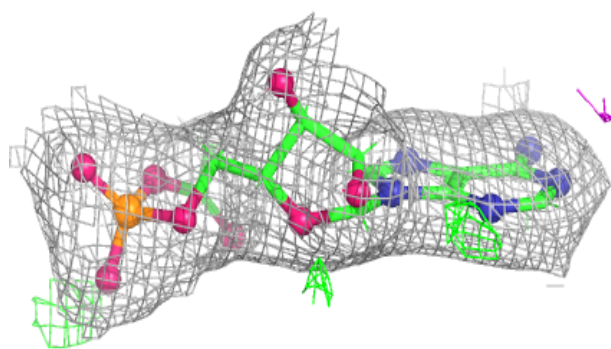
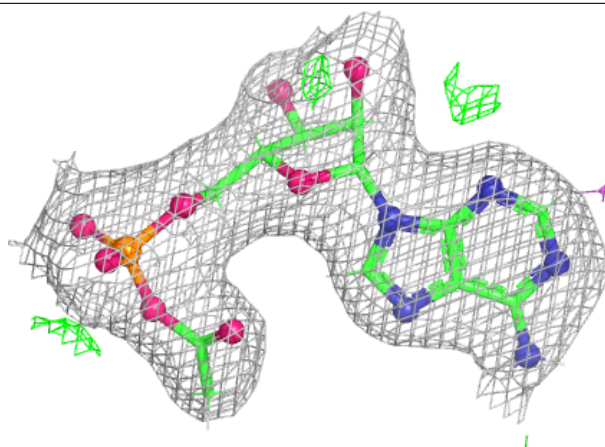
**Electron density around 6R9 C 701:**

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



Electron density around 6R9 A 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.