



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:54 PM UTC

PDB ID : 7YZM / pdb_00007yzm
Title : MgADPNP-bound DCCP:DCCP-R complex
Authors : Jeoung, J.-H.; Dobbek, H.
Deposited on : 2022-02-21
Resolution : 1.82 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

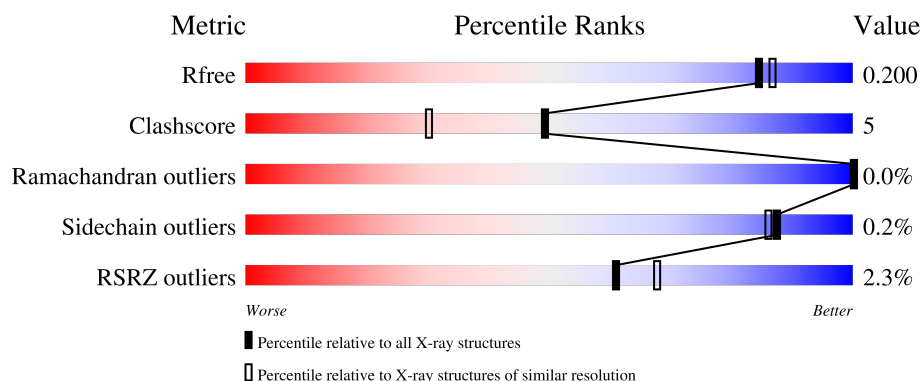
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	422	8% 94% 6%
1	B	422	91% 8%
1	C	422	93% 7%
1	D	422	92% 8%
2	E	243	8% 86% 13% .

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Mol	Chain	Length	Quality of chain
2	F	243	5% 88% 12%
2	G	243	4% 89% 11%
2	H	243	6% 87% 13%

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
4	SO4	A	502	-	-	X	-
6	PEG	D	505	-	-	X	-
8	TAM	B	504	-	X	-	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 46833 atoms, of which 22294 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 Dehydratase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	422	Total	C	H	N	O	S	0	19	0
			7060	2236	3575	600	629	20			
1	B	421	Total	C	H	N	O	S	0	11	0
			6934	2200	3495	591	629	19			
1	C	421	Total	C	H	N	O	S	0	11	0
			6931	2197	3496	594	625	19			
1	D	421	Total	C	H	N	O	S	0	17	0
			6993	2224	3530	586	634	19			

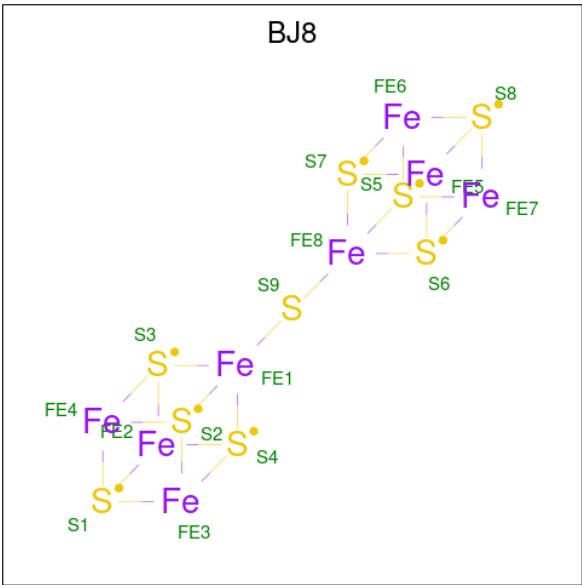
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q3AET9
B	0	GLY	-	expression tag	UNP Q3AET9
C	0	GLY	-	expression tag	UNP Q3AET9
D	0	GLY	-	expression tag	UNP Q3AET9

- Molecule 2 is a protein called Putative CoA-substrate-specific enzyme activase.

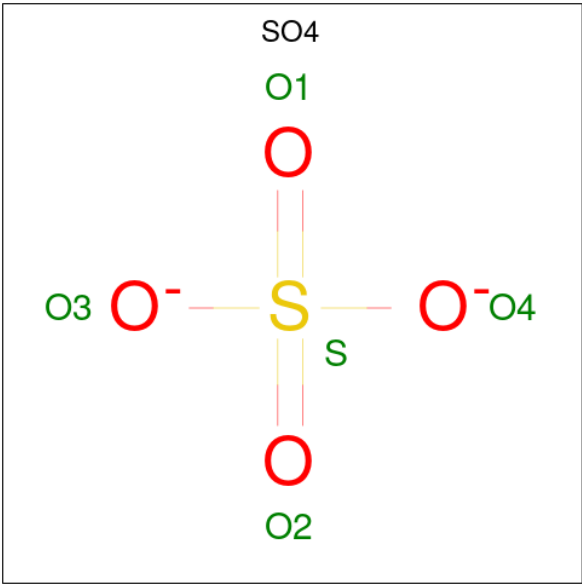
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	G	243	Total	C	H	N	O	S	0	5	0
			3849	1200	1971	323	347	8			
2	H	243	Total	C	H	N	O	S	0	9	0
			3882	1213	1985	322	354	8			
2	E	243	Total	C	H	N	O	S	0	3	0
			3812	1191	1947	319	347	8			
2	F	243	Total	C	H	N	O	S	0	7	0
			3856	1205	1969	324	350	8			

- Molecule 3 is Double cubane cluster (CCD ID: BJ8) (formula: Fe₈S₉) (labeled as "Ligand of Interest" by depositor).



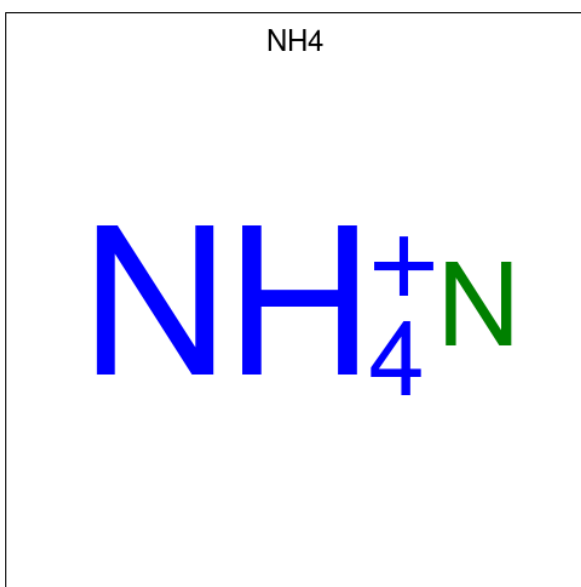
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			17	8	9		
3	B	1	Total	Fe	S	0	0
			17	8	9		
3	C	1	Total	Fe	S	0	0
			17	8	9		
3	D	1	Total	Fe	S	0	0
			17	8	9		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



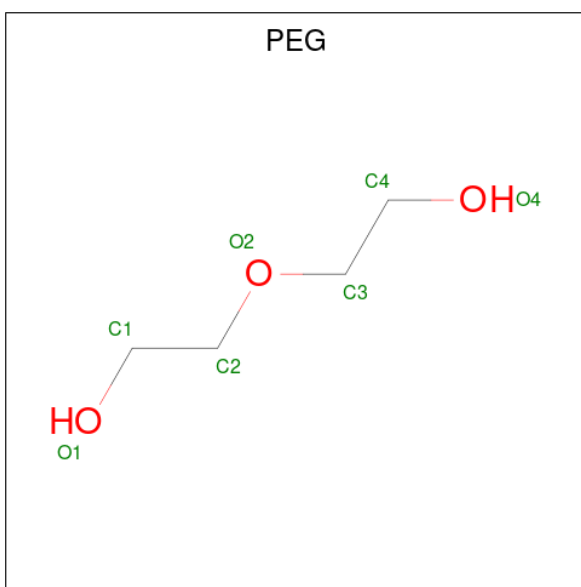
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0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

- Molecule 5 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).



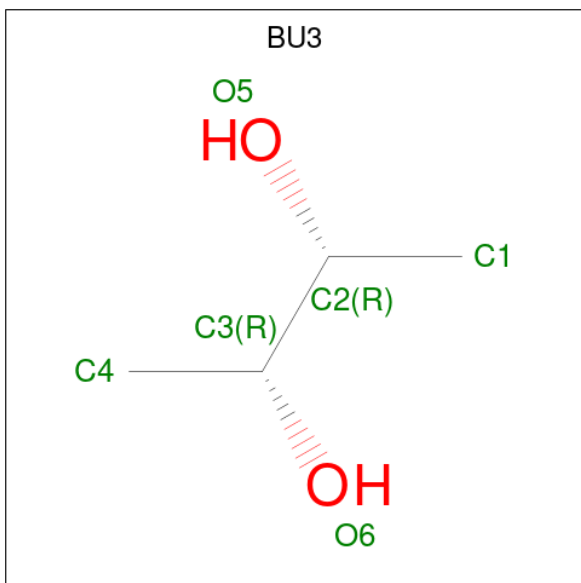
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	H	N	0	0
			5	4	1		
5	A	1	Total	H	N	0	0
			5	4	1		
5	B	1	Total	H	N	0	0
			5	4	1		
5	B	1	Total	H	N	0	0
			5	4	1		
5	G	1	Total	H	N	0	0
			5	4	1		
5	D	1	Total	H	N	0	0
			5	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



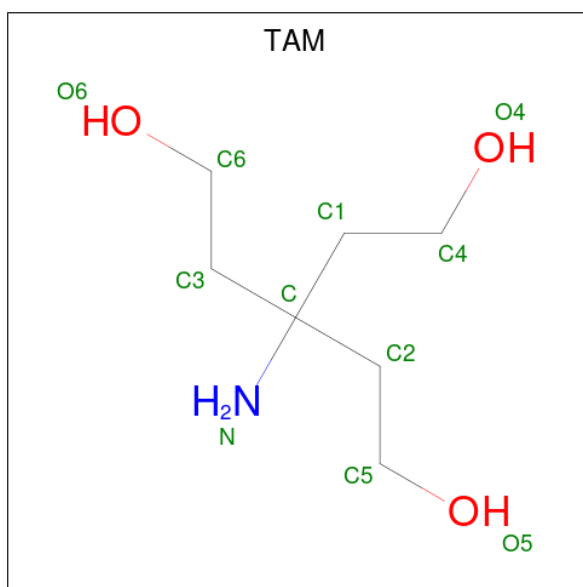
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	A	1	Total	C	H	O	0	0
			17	4	10	3		
6	C	1	Total	C	H	O	0	0
			17	4	10	3		
6	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 7 is (R,R)-2,3-BUTANEDIOL (CCD ID: BU3) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			16	4	10	2		
7	A	1	Total	C	H	O	0	0
			16	4	10	2		
7	B	1	Total	C	H	O	0	0
			16	4	10	2		
7	G	1	Total	C	H	O	0	0
			16	4	10	2		
7	G	1	Total	C	H	O	0	0
			16	4	10	2		
7	G	1	Total	C	H	O	0	0
			16	4	10	2		
7	G	1	Total	C	H	O	0	0
			16	4	10	2		
7	H	1	Total	C	H	O	0	0
			16	4	10	2		
7	H	1	Total	C	H	O	0	0
			16	4	10	2		
7	C	1	Total	C	H	O	0	0
			16	4	10	2		
7	C	1	Total	C	H	O	0	0
			16	4	10	2		
7	C	1	Total	C	H	O	0	0
			16	4	10	2		
7	D	1	Total	C	H	O	0	0
			16	4	10	2		
7	D	1	Total	C	H	O	0	0
			16	4	10	2		
7	E	1	Total	C	H	O	0	0
			16	4	10	2		
7	F	1	Total	C	H	O	0	0
			16	4	10	2		
7	F	1	Total	C	H	O	0	0
			16	4	10	2		
7	F	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 8 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).

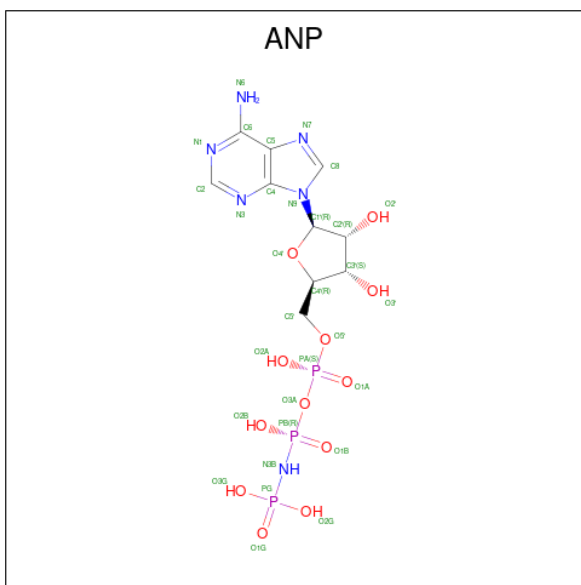


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	0	0
			28	7	17	1	3		
8	D	1	Total	C	H	N	O	0	0
			28	7	17	1	3		

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

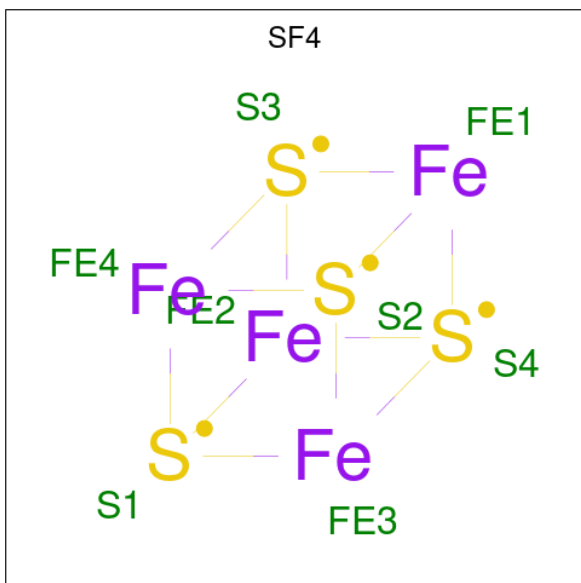
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	G	1	Total	Mg	0	0
			1	1		
9	H	1	Total	Mg	0	0
			1	1		
9	E	1	Total	Mg	0	0
			1	1		
9	F	1	Total	Mg	0	0
			1	1		

- Molecule 10 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	G	1	Total 43	C 10	H 12	N 6	O 12	P 3	0	0
10	H	1	Total 43	C 10	H 12	N 6	O 12	P 3	0	0
10	E	1	Total 43	C 10	H 12	N 6	O 12	P 3	0	0
10	F	1	Total 43	C 10	H 12	N 6	O 12	P 3	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	H	1	Total 8	Fe 4	S 4	0	0
11	E	1	Total 8	Fe 4	S 4	0	0

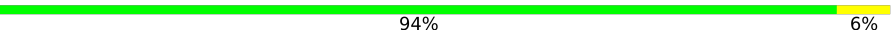
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	551	Total 551	O 551	0	0
12	B	436	Total 436	O 436	0	0
12	G	230	Total 230	O 230	0	0
12	H	160	Total 160	O 160	0	0
12	C	412	Total 412	O 412	0	0
12	D	543	Total 543	O 543	0	0
12	E	160	Total 160	O 160	0	0
12	F	247	Total 247	O 247	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: Dehydratase family protein

Chain A: 



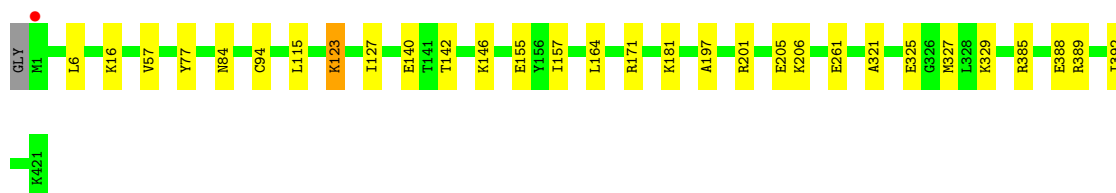
- Molecule 1: Dehydratase family protein

Chain B: 



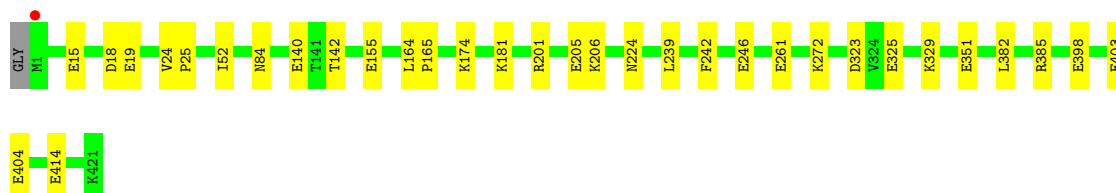
- Molecule 1: Dehydratase family protein

Chain C: 

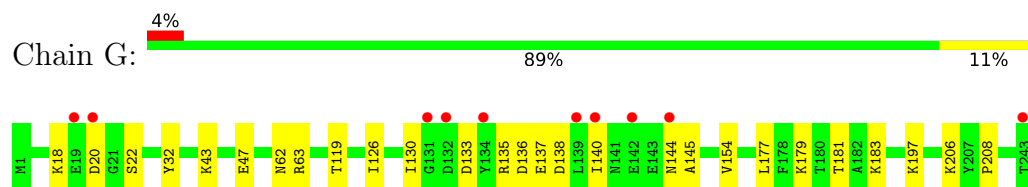


- Molecule 1: Dehydratase family protein

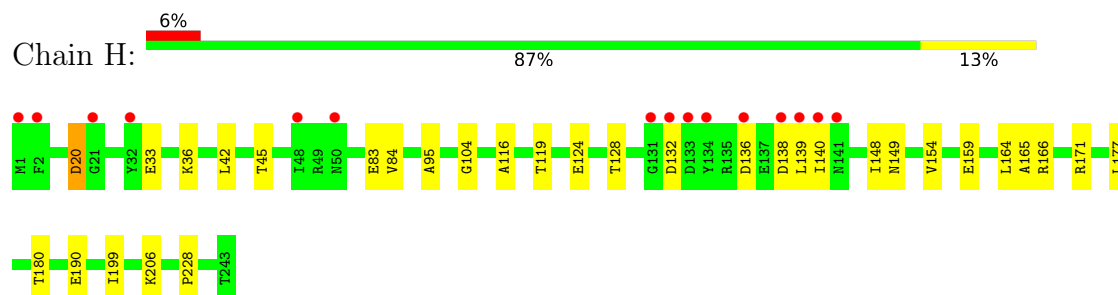
Chain D: 



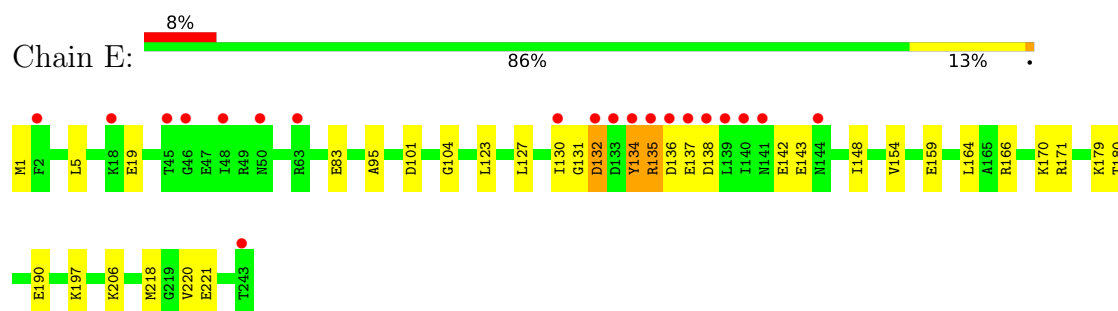
- Molecule 2: Putative CoA-substrate-specific enzyme activase



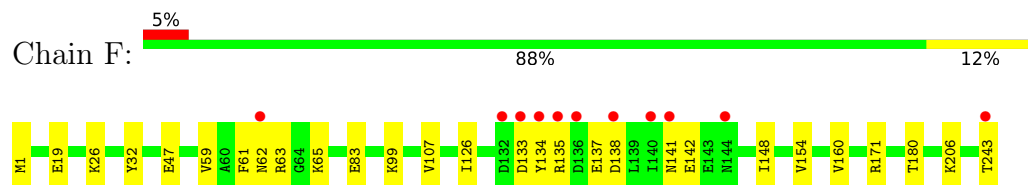
- Molecule 2: Putative CoA-substrate-specific enzyme activase



- Molecule 2: Putative CoA-substrate-specific enzyme activase



- Molecule 2: Putative CoA-substrate-specific enzyme activase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.12Å 81.67Å 121.38Å 100.61° 97.13° 90.00°	Depositor
Resolution (Å)	26.72 – 1.82 26.72 – 1.82	Depositor EDS
% Data completeness (in resolution range)	97.7 (26.72-1.82) 97.9 (26.72-1.82)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.164 , 0.201 0.164 , 0.200	Depositor DCC
R_{free} test set	2100 reflections (0.82%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	46833	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 10.64% 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: BU3, BJ8, SO4, MG, NH4, SF4, PEG, TAM, ANP

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	0.27	1/3612 (0.0%)	0.46	1/4871 (0.0%)
1	B	0.22	0/3544	0.44	0/4782
1	C	0.20	0/3537	0.42	0/4773
1	D	0.24	0/3584	0.47	1/4840 (0.0%)
2	E	0.41	0/1900	0.56	2/2562 (0.1%)
2	F	0.34	0/1930	0.55	0/2604
2	G	0.31	0/1919	0.50	0/2586
2	H	0.19	0/1951	0.43	0/2631
All	All	0.27	1/21977 (0.0%)	0.47	4/29649 (0.0%)

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
2	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	LYS	CE-NZ	-7.77	1.26	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	LYS	CD-CE-NZ	6.77	133.58	111.90
2	E	134	TYR	CA-C-N	5.79	132.60	121.54
2	E	134	TYR	C-N-CA	5.79	132.60	121.54
1	D	181	LYS	CD-CE-NZ	-5.24	95.13	111.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	132	ASP	Mainchain

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	3485	3575	3575	27	0
1	B	3439	3495	3497	38	2
1	C	3435	3496	3498	24	2
1	D	3463	3530	3531	40	0
2	E	1865	1947	1947	32	0
2	F	1887	1969	1965	23	1
2	G	1878	1971	1971	27	0
2	H	1897	1985	1985	26	0
3	A	17	0	0	2	0
3	B	17	0	0	1	0
3	C	17	0	0	0	0
3	D	17	0	0	0	0
4	A	15	0	0	3	0
4	B	10	0	0	2	0
4	C	20	0	0	1	0
4	D	10	0	0	1	0
4	E	5	0	0	0	0
4	F	10	0	0	2	0
4	G	5	0	0	1	0
5	A	2	8	0	2	0
5	B	2	8	0	2	0
5	D	1	4	0	1	0
5	G	1	4	0	1	0
6	A	14	20	20	0	0
6	C	7	10	10	0	0
6	D	7	10	10	4	0
7	A	12	20	20	1	0
7	B	6	10	10	0	0
7	C	18	30	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	12	20	20	2	0
7	E	6	10	10	1	0
7	F	18	30	30	1	0
7	G	24	40	40	3	0
7	H	12	20	20	4	0
8	B	11	17	17	0	0
8	D	11	17	17	1	0
9	E	1	0	0	0	0
9	F	1	0	0	0	0
9	G	1	0	0	0	0
9	H	1	0	0	0	0
10	E	31	12	13	0	0
10	F	31	12	13	0	0
10	G	31	12	13	0	0
10	H	31	12	13	0	0
11	E	8	0	0	0	0
11	H	8	0	0	0	0
12	A	551	0	0	10	3
12	B	436	0	0	17	0
12	C	412	0	0	6	0
12	D	543	0	0	19	2
12	E	160	0	0	12	0
12	F	247	0	0	3	1
12	G	230	0	0	8	1
12	H	160	0	0	5	0
All	All	24539	22294	22275	237	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 5.

All (237) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:135:ARG:NH2	12:E:401:HOH:O	1.87	1.05
1:D:201:ARG:NH2	12:D:603:HOH:O	1.96	0.98
2:E:166:ARG:NH2	12:E:403:HOH:O	1.96	0.97
1:B:212:LYS:NZ	12:B:601:HOH:O	1.96	0.93
1:B:253:ASN:OD1	12:B:601:HOH:O	1.86	0.91
2:F:26:LYS:NZ	12:F:401:HOH:O	2.06	0.88
2:G:43:LYS:NZ	12:G:401:HOH:O	1.91	0.87
2:H:132:ASP:OD1	12:H:401:HOH:O	1.90	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:166:ARG:NH2	12:H:402:HOH:O	2.07	0.86
1:D:261:GLU:OE1	12:D:601:HOH:O	1.91	0.86
1:D:205:GLU:OE1	12:D:602:HOH:O	1.92	0.85
2:E:137:GLU:OE1	12:E:402:HOH:O	1.94	0.85
1:B:358:GLN:NE2	12:B:605:HOH:O	2.11	0.84
2:E:166:ARG:NH1	12:E:405:HOH:O	2.07	0.84
1:A:140:GLU:OE2	1:A:146[A]:LYS:NZ	2.11	0.83
1:B:170:GLU:OE1	12:B:602:HOH:O	1.97	0.82
2:G:144:ASN:ND2	12:G:402:HOH:O	2.13	0.81
1:A:325:GLU:OE1	12:A:601:HOH:O	1.97	0.81
2:E:83:GLU:OE1	12:E:404:HOH:O	1.97	0.81
1:A:170:GLU:OE2	1:A:173[B]:ARG:NH1	2.14	0.80
1:A:173[B]:ARG:NH2	4:A:502:SO4:O1	2.16	0.78
1:C:94:CYS:O	12:C:701:HOH:O	2.03	0.77
1:B:1:MET:N	12:B:611:HOH:O	2.17	0.76
1:D:15:GLU:OE2	12:D:604:HOH:O	2.04	0.74
1:D:15:GLU:OE1	12:D:605:HOH:O	2.06	0.74
2:F:134:TYR:CE2	2:F:171:ARG:HB2	2.23	0.74
2:E:135:ARG:HD3	2:E:136:ASP:H	1.53	0.73
1:A:30:GLU:OE1	12:A:602:HOH:O	2.05	0.73
1:B:2:ASP:OD1	12:B:603:HOH:O	2.07	0.72
4:C:505:SO4:O4	12:C:702:HOH:O	2.07	0.72
2:E:206[A]:LYS:NZ	12:E:410:HOH:O	2.23	0.71
1:C:16:LYS:HB3	1:C:127:ILE:HD11	1.73	0.70
1:D:246[A]:GLU:OE2	12:D:606:HOH:O	2.09	0.70
4:F:301:SO4:O2	12:F:402:HOH:O	2.09	0.70
1:B:123[A]:LYS:NZ	1:B:132:GLN:OE1	2.25	0.69
1:C:155:GLU:OE2	1:D:385[A]:ARG:NH1	2.26	0.69
1:B:94:CYS:O	12:B:604:HOH:O	2.10	0.68
2:H:148:ILE:H	2:H:180[B]:THR:HG21	1.57	0.68
1:B:224:ASN:ND2	12:B:607:HOH:O	2.14	0.68
1:A:14:LEU:HD13	12:A:976:HOH:O	1.94	0.68
1:C:140:GLU:OE2	1:C:146[A]:LYS:NZ	2.20	0.68
1:D:323:ASP:OD1	12:D:607:HOH:O	2.10	0.68
1:A:340[B]:CYS:SG	3:A:501:BJ8:S8	2.91	0.67
1:D:19[A]:GLU:OE2	6:D:505:PEG:O1	2.09	0.66
1:B:374[B]:GLN:OE1	12:B:606:HOH:O	2.12	0.66
1:B:140:GLU:HG2	1:B:142:THR:HG23	1.77	0.66
1:D:414:GLU:OE2	12:D:608:HOH:O	2.12	0.66
2:G:20:ASP:OD1	2:G:22:SER:OG	2.09	0.64
2:F:135:ARG:O	2:F:138:ASP:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:206:LYS:HD3	7:F:307:BU3:H42	1.79	0.64
1:B:205:GLU:OE2	12:B:608:HOH:O	2.15	0.64
1:D:18:ASP:HB2	6:D:505:PEG:H11	1.79	0.64
1:D:201:ARG:NH1	12:D:619:HOH:O	2.31	0.64
1:A:155:GLU:OE2	1:B:385[A]:ARG:NH1	2.31	0.63
1:C:140:GLU:HG2	1:C:142:THR:HG23	1.81	0.63
1:B:403:GLU:OE2	12:B:609:HOH:O	2.16	0.62
1:D:201:ARG:NH1	12:D:618:HOH:O	2.30	0.62
1:C:329:LYS:NZ	12:C:704:HOH:O	2.26	0.61
2:E:127:LEU:O	2:E:131:GLY:N	2.33	0.61
2:E:104:GLY:O	12:E:408:HOH:O	2.16	0.61
1:D:403:GLU:OE2	12:D:609:HOH:O	2.16	0.61
2:H:104:GLY:O	12:H:403:HOH:O	2.16	0.60
2:H:136:ASP:O	2:H:140:ILE:HD12	2.02	0.60
2:G:63[A]:ARG:NH1	12:G:406:HOH:O	2.34	0.60
2:E:134:TYR:HB3	2:E:138:ASP:OD1	2.01	0.60
1:D:325:GLU:O	12:D:610:HOH:O	2.17	0.59
2:H:124:GLU:O	2:H:128:THR:HG23	2.02	0.59
1:B:16:LYS:HB3	1:B:127:ILE:HD11	1.86	0.58
2:F:148:ILE:H	2:F:180[B]:THR:HG21	1.69	0.58
2:E:179:LYS:NZ	12:E:409:HOH:O	2.38	0.57
7:G:308:BU3:O5	2:H:165:ALA:HB2	2.05	0.56
1:B:178:GLU:OE1	12:B:610:HOH:O	2.17	0.56
2:F:1:MET:HE1	2:F:19:GLU:OE1	2.05	0.56
1:A:52:ILE:HD11	1:A:242[B]:PHE:CE2	2.41	0.56
2:G:154:VAL:HG23	2:H:154:VAL:HG23	1.86	0.56
2:G:136:ASP:O	2:G:140:ILE:HD12	2.05	0.56
2:E:142:GLU:CG	2:E:171:ARG:HG2	2.36	0.56
1:D:174:LYS:NZ	12:D:625:HOH:O	2.39	0.55
2:H:83:GLU:OE1	2:H:83:GLU:N	2.30	0.55
1:C:84[B]:ASN:OD1	1:C:206:LYS:HD2	2.07	0.55
2:F:61:PHE:CE2	2:F:63[B]:ARG:HG3	2.41	0.55
1:C:385[A]:ARG:NH2	1:D:155[A]:GLU:OE2	2.39	0.54
2:G:47:GLU:OE1	12:G:403:HOH:O	2.17	0.54
4:B:503:SO4:O2	5:B:506:NH4:N	2.41	0.54
2:E:130:ILE:HB	2:E:170:LYS:HD3	1.90	0.53
2:E:148:ILE:O	2:E:180:THR:HG21	2.08	0.53
1:C:392:ILE:O	12:C:703:HOH:O	2.19	0.53
2:H:84:VAL:HG11	2:H:199:ILE:HG13	1.91	0.53
4:B:502:SO4:O1	5:B:505:NH4:N	2.42	0.53
1:B:212:LYS:HE3	12:B:786:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:133:ASP:OD2	2:F:133:ASP:N	2.40	0.52
1:C:181:LYS:HZ3	1:C:329:LYS:HE3	1.75	0.52
1:D:18:ASP:HB2	6:D:505:PEG:C1	2.39	0.52
1:A:140:GLU:CG	1:A:142:THR:HG23	2.40	0.52
1:B:385[A]:ARG:CZ	1:B:389:ARG:HH12	2.23	0.52
2:F:134:TYR:CD2	2:F:171:ARG:HB2	2.44	0.52
2:E:135:ARG:NH2	12:E:406:HOH:O	2.09	0.52
2:E:154:VAL:HG23	2:F:154:VAL:HG23	1.92	0.51
1:C:197:ALA:HA	1:C:327:MET:HE1	1.92	0.51
1:D:19[A]:GLU:HG2	6:D:505:PEG:O2	2.10	0.51
2:G:63[A]:ARG:NH1	12:G:407:HOH:O	2.36	0.50
2:H:148:ILE:O	2:H:180[A]:THR:HG21	2.11	0.50
1:D:242[A]:PHE:CZ	7:D:507:BU3:H42	2.46	0.50
1:D:398:GLU:OE1	12:D:611:HOH:O	2.19	0.50
2:E:143:GLU:OE2	2:E:143:GLU:HA	2.11	0.50
2:G:63[B]:ARG:HD2	1:D:351:GLU:OE2	2.10	0.50
1:A:212[B]:LYS:NZ	12:A:623:HOH:O	2.44	0.50
1:C:123[B]:LYS:HE2	1:C:157:ILE:HB	1.93	0.50
2:G:18:LYS:HE3	2:G:22:SER:OG	2.12	0.50
1:D:224:ASN:H	8:D:508:TAM:H61	1.77	0.50
1:B:125:GLU:HB2	1:B:127:ILE:HG12	1.92	0.50
4:G:303:SO4:O1	5:G:304:NH4:N	2.45	0.49
1:C:16:LYS:CB	1:C:127:ILE:HD11	2.41	0.49
1:D:84[B]:ASN:HD21	1:D:206:LYS:HD2	1.77	0.49
1:D:201:ARG:HH11	1:D:201:ARG:HG3	1.77	0.49
1:D:52:ILE:HD11	1:D:242[B]:PHE:CE1	2.47	0.49
1:A:140:GLU:HG2	1:A:142:THR:HG23	1.93	0.48
1:A:345:PRO:O	12:A:603:HOH:O	2.19	0.48
1:B:16:LYS:HB3	1:B:127:ILE:CD1	2.43	0.48
1:D:84[B]:ASN:OD1	1:D:206:LYS:HD2	2.13	0.48
2:F:133:ASP:OD1	2:F:134:TYR:CE1	2.66	0.48
2:E:142:GLU:O	12:E:409:HOH:O	2.20	0.48
1:A:239:LEU:HD23	1:A:242[B]:PHE:CZ	2.49	0.48
2:G:62:ASN:OD1	2:G:62:ASN:C	2.57	0.48
2:E:1:MET:HE2	2:E:19:GLU:HG3	1.95	0.48
2:G:197:LYS:HD2	12:G:504:HOH:O	2.14	0.47
2:G:133:ASP:O	2:G:133:ASP:CG	2.57	0.47
1:D:325:GLU:HG3	12:D:610:HOH:O	2.15	0.47
2:F:47:GLU:OE2	12:F:403:HOH:O	2.20	0.47
2:F:65:LYS:HE2	2:F:243:THR:HG21	1.97	0.47
2:E:138:ASP:O	2:E:171:ARG:NH1	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:502:SO4:O3	5:D:503:NH4:N	2.48	0.47
2:E:123:LEU:O	2:E:127:LEU:HG	2.14	0.47
2:F:99:LYS:O	2:F:107[A]:VAL:HG22	2.14	0.47
4:A:502:SO4:O4	5:A:503:NH4:N	2.48	0.47
2:G:126:ILE:HG21	2:G:177:LEU:HD13	1.97	0.47
5:A:510:NH4:N	4:F:304:SO4:O3	2.47	0.47
1:D:272:LYS:NZ	12:D:631:HOH:O	2.42	0.47
1:B:140:GLU:CG	1:B:142:THR:HG23	2.44	0.47
2:H:33:GLU:OE1	2:H:36:LYS:NZ	2.33	0.47
1:B:69:LYS:HG2	12:B:647:HOH:O	2.15	0.46
7:A:509:BU3:H11	12:A:644:HOH:O	2.16	0.46
1:D:164[A]:LEU:HD12	1:D:165:PRO:HD2	1.98	0.46
2:G:43:LYS:HE3	12:G:585:HOH:O	2.15	0.46
2:F:133:ASP:OD1	2:F:134:TYR:CD1	2.68	0.46
2:F:126:ILE:HD11	2:F:160:VAL:HG11	1.98	0.46
1:C:155:GLU:OE1	1:D:385[A]:ARG:NH2	2.48	0.46
1:D:239:LEU:HD23	1:D:242[B]:PHE:CZ	2.51	0.46
1:D:24:VAL:HB	1:D:25:PRO:HD3	1.97	0.46
1:D:84[B]:ASN:ND2	1:D:206:LYS:HD2	2.31	0.46
1:D:140:GLU:HG2	1:D:142:THR:HG23	1.97	0.46
2:H:138:ASP:O	2:H:171:ARG:NH1	2.38	0.45
1:C:77:TYR:CD2	1:C:164:LEU:HD11	2.51	0.45
2:H:206[B]:LYS:HG3	2:H:228:PRO:HG2	1.99	0.45
2:E:95:ALA:HB3	7:E:305:BU3:H43	1.99	0.45
1:A:169:GLU:OE1	4:A:502:SO4:O3	2.34	0.45
1:B:385[B]:ARG:HD3	1:B:389:ARG:HH12	1.82	0.45
1:C:389:ARG:HD3	7:C:509:BU3:H43	1.99	0.45
2:E:218:MET:HB3	2:E:220:VAL:HG22	1.98	0.45
1:B:52:ILE:HD11	1:B:242:PHE:CE1	2.50	0.45
1:C:201:ARG:NH2	1:C:321:ALA:O	2.42	0.45
2:G:183[B]:LYS:NZ	12:G:416:HOH:O	2.49	0.45
1:A:319:GLU:OE2	12:A:604:HOH:O	2.21	0.45
1:B:350:LEU:HD21	1:B:386:GLU:HG2	1.99	0.45
2:H:190[B]:GLU:HG3	12:H:496:HOH:O	2.17	0.45
2:H:148:ILE:HD12	2:H:177:LEU:HG	1.99	0.45
1:A:325:GLU:O	1:A:329:LYS:HG3	2.17	0.45
2:G:119:THR:OG1	7:G:306:BU3:H11	2.17	0.44
1:A:155:GLU:CD	1:B:385[A]:ARG:HH22	2.24	0.44
2:G:181:THR:OG1	7:G:305:BU3:H43	2.17	0.44
7:D:506:BU3:H41	12:D:795:HOH:O	2.17	0.44
1:B:239:LEU:HD23	1:B:242:PHE:CZ	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:126:ILE:O	2:G:130:ILE:HG12	2.17	0.44
1:A:279[B]:ILE:HD12	1:A:292:HIS:CE1	2.53	0.44
2:G:135:ARG:HB2	2:G:138:ASP:OD2	2.17	0.44
2:G:137:GLU:HA	2:G:140:ILE:HD13	2.00	0.44
1:C:77:TYR:CE2	1:C:164:LEU:HD11	2.52	0.44
2:G:43:LYS:HA	2:G:43:LYS:CE	2.48	0.43
2:G:197:LYS:HB3	2:G:197:LYS:HE3	1.77	0.43
7:C:508:BU3:H12	12:C:842:HOH:O	2.18	0.43
2:E:197:LYS:HE3	2:E:221:GLU:CD	2.43	0.43
1:A:75:CYS:HA	3:A:501:BJ8:S5	2.58	0.43
1:A:329:LYS:NZ	12:A:631:HOH:O	2.51	0.43
1:C:388:GLU:HG2	12:C:703:HOH:O	2.19	0.43
1:C:325:GLU:O	1:C:329:LYS:HG2	2.18	0.43
2:E:164:LEU:HD13	2:F:32:TYR:HB3	2.01	0.43
1:C:201:ARG:O	1:C:205:GLU:HG2	2.18	0.43
2:E:131:GLY:O	2:E:132:ASP:HB3	2.19	0.43
2:F:62[B]:ASN:OD1	2:F:62[B]:ASN:C	2.62	0.43
1:B:212:LYS:CE	12:B:786:HOH:O	2.64	0.42
1:D:382:LEU:HG	12:D:780:HOH:O	2.18	0.42
2:H:42:LEU:HA	2:H:45:THR:HG21	2.00	0.42
2:H:159:GLU:OE2	12:H:404:HOH:O	2.21	0.42
2:E:131:GLY:O	2:E:132:ASP:CB	2.67	0.42
1:D:140:GLU:CG	1:D:142:THR:HG23	2.49	0.42
12:E:405:HOH:O	2:F:59:VAL:HG11	2.19	0.42
2:H:149:ASN:O	7:H:305:BU3:H13	2.19	0.42
2:H:119:THR:HG23	7:H:305:BU3:H43	2.02	0.42
1:D:140:GLU:HB2	1:D:164[B]:LEU:HD13	2.01	0.42
2:E:142:GLU:HG2	2:E:171:ARG:HG2	2.01	0.42
2:F:83:GLU:OE1	2:F:83:GLU:N	2.42	0.42
1:B:385[B]:ARG:HG2	12:B:800:HOH:O	2.18	0.42
1:A:206:LYS:HE3	1:A:206:LYS:HB2	1.91	0.42
2:G:206:LYS:O	2:G:208:PRO:HD3	2.20	0.42
2:E:190[B]:GLU:HG3	12:E:413:HOH:O	2.19	0.42
1:B:385[A]:ARG:NH1	1:B:389:ARG:HH12	2.18	0.42
2:G:135:ARG:HA	2:G:135:ARG:HD3	1.98	0.41
1:B:386:GLU:O	1:B:390:ARG:HG3	2.20	0.41
1:B:75:CYS:HA	3:B:501:BJ8:S5	2.60	0.41
1:B:162:MET:HE1	1:B:180:ILE:HD13	2.03	0.41
1:B:163:GLU:O	1:B:179:GLU:HG3	2.20	0.41
2:G:32:TYR:HB3	2:H:164:LEU:HD13	2.02	0.41
2:H:166:ARG:O	2:H:166:ARG:HG2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:GLU:CG	1:C:142:THR:HG23	2.49	0.41
1:D:329:LYS:HG3	12:D:610:HOH:O	2.20	0.41
1:A:403:GLU:O	1:A:406:GLN:HG2	2.20	0.41
1:B:125:GLU:CB	1:B:127:ILE:HG12	2.50	0.41
2:H:95:ALA:HB3	7:H:304:BU3:H12	2.00	0.41
2:H:116:ALA:HB1	7:H:304:BU3:H13	2.03	0.41
2:H:136:ASP:O	2:H:139:LEU:N	2.54	0.41
1:A:267[A]:GLU:OE2	12:A:605:HOH:O	2.22	0.41
1:C:6:LEU:HD21	1:C:57:VAL:HG12	2.03	0.41
2:E:142:GLU:HG2	2:E:171:ARG:NE	2.35	0.41
1:C:115:LEU:C	1:C:115:LEU:HD23	2.45	0.41
2:F:137:GLU:H	2:F:137:GLU:CD	2.25	0.41
1:A:140:GLU:HG3	1:A:142:THR:HG23	2.02	0.41
1:B:77:TYR:CE2	1:B:164:LEU:HD11	2.56	0.41
2:E:101:ASP:OD1	2:E:101:ASP:C	2.64	0.40
1:D:404:GLU:C	2:E:159:GLU:HG2	2.46	0.40
2:F:141:ASN:O	2:F:142:GLU:C	2.63	0.40
1:B:123[A]:LYS:HE3	12:B:744:HOH:O	2.22	0.40
2:G:145:ALA:CB	2:G:179:LYS:HD2	2.51	0.40
1:A:14:LEU:CD1	12:A:976:HOH:O	2.63	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)
1:B:390:ARG:HH22	1:C:261:GLU:OE2[1_566]	1.25	0.35
1:B:390:ARG:NH2	1:C:261:GLU:OE2[1_566]	2.09	0.11
12:A:1014:HOH:O	12:G:597:HOH:O[1_565]	2.15	0.05
12:D:941:HOH:O	12:F:424:HOH:O[1_545]	2.17	0.03
12:A:1072:HOH:O	12:D:1133:HOH:O[1_565]	2.18	0.02
2:F:63[B]:ARG:HH21	12:A:607:HOH:O[1_655]	1.59	0.01

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	439/422 (104%)	433 (99%)	6 (1%)	0	100	100
1	B	431/422 (102%)	422 (98%)	9 (2%)	0	100	100
1	C	430/422 (102%)	421 (98%)	9 (2%)	0	100	100
1	D	436/422 (103%)	428 (98%)	8 (2%)	0	100	100
2	E	244/243 (100%)	235 (96%)	8 (3%)	1 (0%)	30	19
2	F	248/243 (102%)	242 (98%)	6 (2%)	0	100	100
2	G	246/243 (101%)	238 (97%)	8 (3%)	0	100	100
2	H	250/243 (103%)	249 (100%)	1 (0%)	0	100	100
All	All	2724/2660 (102%)	2668 (98%)	55 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	135	ARG

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	382/363 (105%)	382 (100%)	0	100	100
1	B	375/363 (103%)	373 (100%)	2 (0%)	81	77
1	C	374/363 (103%)	370 (99%)	4 (1%)	65	56
1	D	380/363 (105%)	380 (100%)	0	100	100
2	E	199/196 (102%)	197 (99%)	2 (1%)	68	60
2	F	202/196 (103%)	202 (100%)	0	100	100
2	G	201/196 (103%)	201 (100%)	0	100	100
2	H	205/196 (105%)	203 (99%)	2 (1%)	68	60
All	All	2318/2236 (104%)	2308 (100%)	10 (0%)	87	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	385[A]	ARG
1	B	385[B]	ARG
2	H	20[A]	ASP
2	H	20[B]	ASP
1	C	123[A]	LYS
1	C	123[B]	LYS
1	C	171[A]	ARG
1	C	171[B]	ARG
2	E	5[A]	LEU
2	E	5[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	65	GLN
1	A	111	ASN
1	B	111	ASN
2	G	73	GLN
2	G	141	ASN
2	H	44	ASN
2	H	73	GLN
1	C	65	GLN
2	E	215	GLN
2	F	11	ASN
2	F	103	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 59 ligands modelled in this entry, 6 are modelled with single atom and 4 are monoatomic - leaving 49 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
7	BU3	D	507	-	4,5,5	0.34	0	6,6,6	0.48	0
4	SO4	D	504	-	4,4,4	0.26	0	6,6,6	0.06	0
7	BU3	G	308	-	4,5,5	0.30	0	6,6,6	0.68	0
4	SO4	C	502	-	4,4,4	0.23	0	6,6,6	0.17	0
4	SO4	A	504	-	4,4,4	0.24	0	6,6,6	0.11	0
6	PEG	A	507	-	6,6,6	0.47	0	5,5,5	0.52	0
7	BU3	H	305	-	4,5,5	0.22	0	6,6,6	0.46	0
4	SO4	B	502	-	4,4,4	0.20	0	6,6,6	0.12	0
8	TAM	B	504	-	10,10,10	0.58	0	12,12,12	6.37	8 (66%)
4	SO4	A	502	-	4,4,4	0.22	0	6,6,6	0.29	0
11	SF4	E	301	2	0,12,12	-	-	-	-	-
7	BU3	F	306	-	4,5,5	0.35	0	6,6,6	0.50	0
7	BU3	A	509	-	4,5,5	0.26	0	6,6,6	0.47	0
7	BU3	F	307	-	4,5,5	0.27	0	6,6,6	0.32	0
8	TAM	D	508	-	10,10,10	0.48	0	12,12,12	1.49	1 (8%)
10	ANP	H	303	9	33,33,33	1.00	3 (9%)	45,52,52	0.69	1 (2%)
6	PEG	D	505	-	6,6,6	0.44	0	5,5,5	0.49	0
7	BU3	G	307	-	4,5,5	0.37	0	6,6,6	0.36	0
7	BU3	H	304	-	4,5,5	0.31	0	6,6,6	0.34	0
10	ANP	E	303	9	33,33,33	0.92	3 (9%)	45,52,52	0.72	0
3	BJ8	B	501	1	6,26,26	5.66	4 (66%)	-	-	-
4	SO4	F	301	-	4,4,4	0.22	0	6,6,6	0.09	0
4	SO4	G	303	-	4,4,4	0.21	0	6,6,6	0.15	0
10	ANP	F	303	9	33,33,33	0.98	3 (9%)	45,52,52	0.81	1 (2%)
4	SO4	C	503	-	4,4,4	0.23	0	6,6,6	0.16	0
4	SO4	E	304	-	4,4,4	0.23	0	6,6,6	0.12	0
7	BU3	E	305	-	4,5,5	0.27	0	6,6,6	0.27	0
4	SO4	D	502	-	4,4,4	0.27	0	6,6,6	0.15	0
3	BJ8	D	501	1	6,26,26	5.06	5 (83%)	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BU3	G	305	-	4,5,5	0.21	0	6,6,6	0.53	0
4	SO4	F	304	-	4,4,4	0.24	0	6,6,6	0.18	0
4	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.08	0
6	PEG	C	506	-	6,6,6	0.53	0	5,5,5	0.26	0
7	BU3	A	508	-	4,5,5	0.30	0	6,6,6	0.51	0
4	SO4	B	503	-	4,4,4	0.21	0	6,6,6	0.14	0
11	SF4	H	301	2	0,12,12	-	-	-	-	-
7	BU3	C	507	-	4,5,5	0.29	0	6,6,6	0.47	0
3	BJ8	C	501	1	6,26,26	6.31	4 (66%)	-	-	-
7	BU3	D	506	-	4,5,5	0.32	0	6,6,6	0.26	0
7	BU3	G	306	-	4,5,5	0.32	0	6,6,6	0.41	0
4	SO4	A	505	-	4,4,4	0.20	0	6,6,6	0.10	0
7	BU3	C	509	-	4,5,5	0.37	0	6,6,6	0.28	0
10	ANP	G	302	9	33,33,33	0.89	3 (9%)	45,52,52	1.10	2 (4%)
7	BU3	F	305	-	4,5,5	0.23	0	6,6,6	0.53	0
6	PEG	A	506	-	6,6,6	0.47	0	5,5,5	0.20	0
7	BU3	C	508	-	4,5,5	0.40	0	6,6,6	0.26	0
4	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.08	0
7	BU3	B	507	-	4,5,5	0.38	0	6,6,6	0.40	0
3	BJ8	A	501	1	6,26,26	4.82	4 (66%)	-	-	-

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
7	BU3	D	507	-	-	1/4/4/4	-
7	BU3	G	308	-	-	4/4/4/4	-
6	PEG	A	507	-	-	1/4/4/4	-
7	BU3	H	305	-	-	0/4/4/4	-
8	TAM	B	504	-	-	8/12/12/12	-
11	SF4	E	301	2	-	-	0/6/5/5
7	BU3	F	306	-	-	0/4/4/4	-
7	BU3	A	509	-	-	0/4/4/4	-
7	BU3	F	307	-	-	4/4/4/4	-
8	TAM	D	508	-	-	7/12/12/12	-
10	ANP	H	303	9	-	3/18/38/38	0/3/3/3
6	PEG	D	505	-	-	2/4/4/4	-
3	BJ8	A	501	1	-	-	0/12/10/10

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BU3	G	307	-	-	3/4/4/4	-
7	BU3	H	304	-	-	4/4/4/4	-
10	ANP	E	303	9	-	3/18/38/38	0/3/3/3
3	BJ8	B	501	1	-	-	0/12/10/10
10	ANP	F	303	9	-	3/18/38/38	0/3/3/3
7	BU3	E	305	-	-	4/4/4/4	-
3	BJ8	D	501	1	-	-	0/12/10/10
6	PEG	C	506	-	-	3/4/4/4	-
7	BU3	A	508	-	-	3/4/4/4	-
11	SF4	H	301	2	-	-	0/6/5/5
7	BU3	C	507	-	-	0/4/4/4	-
3	BJ8	C	501	1	-	-	0/12/10/10
7	BU3	D	506	-	-	4/4/4/4	-
7	BU3	G	306	-	-	4/4/4/4	-
7	BU3	C	509	-	-	0/4/4/4	-
10	ANP	G	302	9	-	4/18/38/38	0/3/3/3
7	BU3	F	305	-	-	4/4/4/4	-
6	PEG	A	506	-	-	3/4/4/4	-
7	BU3	C	508	-	-	4/4/4/4	-
7	BU3	B	507	-	-	4/4/4/4	-
7	BU3	G	305	-	-	0/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	BJ8	S5-FE8	11.95	2.46	2.28
3	B	501	BJ8	S5-FE8	11.65	2.46	2.28
3	A	501	BJ8	S5-FE8	8.89	2.42	2.28
3	D	501	BJ8	S5-FE8	8.68	2.41	2.28
3	C	501	BJ8	S4-FE1	-7.59	2.16	2.28
3	D	501	BJ8	S2-FE1	5.65	2.37	2.28
3	C	501	BJ8	S2-FE1	5.31	2.36	2.28
3	B	501	BJ8	S4-FE1	-5.20	2.19	2.28
3	D	501	BJ8	S3-FE1	4.94	2.35	2.28
3	A	501	BJ8	S3-FE1	4.63	2.35	2.28
3	B	501	BJ8	S2-FE1	4.32	2.34	2.28
3	A	501	BJ8	S2-FE1	4.29	2.34	2.28
3	A	501	BJ8	S4-FE1	-3.66	2.22	2.28
3	D	501	BJ8	S4-FE1	-3.33	2.22	2.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	303	ANP	PG-O1G	3.32	1.51	1.46
3	D	501	BJ8	S6-FE8	3.22	2.33	2.28
10	H	303	ANP	PG-O1G	3.21	1.51	1.46
3	C	501	BJ8	S3-FE1	2.90	2.32	2.28
10	G	302	ANP	PB-O1B	2.88	1.50	1.46
10	E	303	ANP	PG-O1G	2.87	1.50	1.46
10	H	303	ANP	PB-O1B	2.70	1.50	1.46
10	F	303	ANP	PB-O1B	2.61	1.50	1.46
10	F	303	ANP	PG-N3B	2.56	1.70	1.63
10	E	303	ANP	PB-O1B	2.51	1.50	1.46
10	G	302	ANP	PG-N3B	2.45	1.69	1.63
10	G	302	ANP	PG-O1G	2.40	1.49	1.46
10	H	303	ANP	PG-N3B	2.26	1.69	1.63
10	E	303	ANP	PG-N3B	2.17	1.69	1.63
3	B	501	BJ8	S6-FE8	2.14	2.31	2.28

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	504	TAM	C2-C-C1	-13.15	87.31	110.50
8	B	504	TAM	C3-C-C1	-11.88	89.55	110.50
8	B	504	TAM	C1-C-N	-7.94	88.28	108.22
8	B	504	TAM	C3-C-N	6.43	124.36	108.22
8	B	504	TAM	C5-C2-C	-5.30	109.72	115.97
10	G	302	ANP	O1G-PG-N3B	-4.42	105.26	111.77
8	D	508	TAM	C4-C1-C	-4.40	110.78	115.97
8	B	504	TAM	C2-C-N	4.14	118.61	108.22
10	G	302	ANP	O1B-PB-N3B	-4.03	105.83	111.77
8	B	504	TAM	C3-C-C2	3.57	116.81	110.50
8	B	504	TAM	C6-C3-C	3.02	119.53	115.97
10	F	303	ANP	O3A-PB-N3B	-2.24	100.36	106.59
10	H	303	ANP	O1G-PG-N3B	-2.11	108.66	111.77

There are no chirality outliers.

All (80) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	508	BU3	C1-C2-C3-O6
7	A	508	BU3	O5-C2-C3-C4
7	A	508	BU3	C1-C2-C3-C4
7	B	507	BU3	O5-C2-C3-O6
7	B	507	BU3	C1-C2-C3-O6

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Mol	Chain	Res	Type	Atoms
7	B	507	BU3	O5-C2-C3-C4
7	B	507	BU3	C1-C2-C3-C4
7	G	306	BU3	C1-C2-C3-O6
7	G	306	BU3	O5-C2-C3-C4
7	G	307	BU3	C1-C2-C3-O6
7	G	307	BU3	O5-C2-C3-C4
7	G	307	BU3	C1-C2-C3-C4
7	G	308	BU3	O5-C2-C3-O6
7	H	304	BU3	O5-C2-C3-O6
7	H	304	BU3	C1-C2-C3-C4
7	C	508	BU3	C1-C2-C3-O6
7	C	508	BU3	O5-C2-C3-C4
7	C	508	BU3	C1-C2-C3-C4
7	D	506	BU3	O5-C2-C3-O6
7	D	506	BU3	C1-C2-C3-C4
7	E	305	BU3	O5-C2-C3-O6
7	E	305	BU3	C1-C2-C3-C4
7	F	305	BU3	O5-C2-C3-O6
7	F	305	BU3	C1-C2-C3-O6
7	F	305	BU3	O5-C2-C3-C4
7	F	305	BU3	C1-C2-C3-C4
7	F	307	BU3	O5-C2-C3-O6
7	F	307	BU3	C1-C2-C3-O6
7	F	307	BU3	O5-C2-C3-C4
7	F	307	BU3	C1-C2-C3-C4
8	B	504	TAM	C2-C-C1-C4
8	B	504	TAM	C3-C-C1-C4
8	B	504	TAM	N-C-C1-C4
8	B	504	TAM	C3-C-C2-C5
8	B	504	TAM	N-C-C2-C5
8	B	504	TAM	N-C-C3-C6
8	D	508	TAM	C2-C-C1-C4
8	D	508	TAM	C3-C-C1-C4
8	D	508	TAM	N-C-C1-C4
8	D	508	TAM	C2-C-C3-C6
8	D	508	TAM	N-C-C3-C6
8	D	508	TAM	C-C2-C5-O5
10	G	302	ANP	PB-N3B-PG-O1G
10	G	302	ANP	PG-N3B-PB-O1B
10	H	303	ANP	PB-N3B-PG-O1G
10	E	303	ANP	PB-N3B-PG-O1G
10	F	303	ANP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
6	A	507	PEG	C1-C2-O2-C3
6	A	506	PEG	O1-C1-C2-O2
6	A	506	PEG	O2-C3-C4-O4
6	C	506	PEG	O1-C1-C2-O2
6	C	506	PEG	O2-C3-C4-O4
8	B	504	TAM	C2-C-C3-C6
8	D	508	TAM	C1-C-C3-C6
6	C	506	PEG	C1-C2-O2-C3
7	G	308	BU3	C1-C2-C3-O6
7	G	308	BU3	O5-C2-C3-C4
7	H	304	BU3	C1-C2-C3-O6
7	H	304	BU3	O5-C2-C3-C4
7	D	506	BU3	C1-C2-C3-O6
7	D	506	BU3	O5-C2-C3-C4
7	D	507	BU3	C1-C2-C3-O6
7	E	305	BU3	C1-C2-C3-O6
7	E	305	BU3	O5-C2-C3-C4
7	G	306	BU3	C1-C2-C3-C4
7	G	308	BU3	C1-C2-C3-C4
7	G	306	BU3	O5-C2-C3-O6
7	C	508	BU3	O5-C2-C3-O6
10	G	302	ANP	C5'-O5'-PA-O1A
10	H	303	ANP	C5'-O5'-PA-O1A
6	D	505	PEG	C4-C3-O2-C2
8	B	504	TAM	C-C1-C4-O4
10	E	303	ANP	C3'-C4'-C5'-O5'
6	A	506	PEG	C1-C2-O2-C3
10	E	303	ANP	O4'-C1'-N9-C8
10	G	302	ANP	O4'-C1'-N9-C8
10	H	303	ANP	O4'-C1'-N9-C8
10	F	303	ANP	O4'-C1'-N9-C8
10	F	303	ANP	PA-O3A-PB-O1B
6	D	505	PEG	C1-C2-O2-C3

There are no ring outliers.

24 monomers are involved in 32 short contacts:

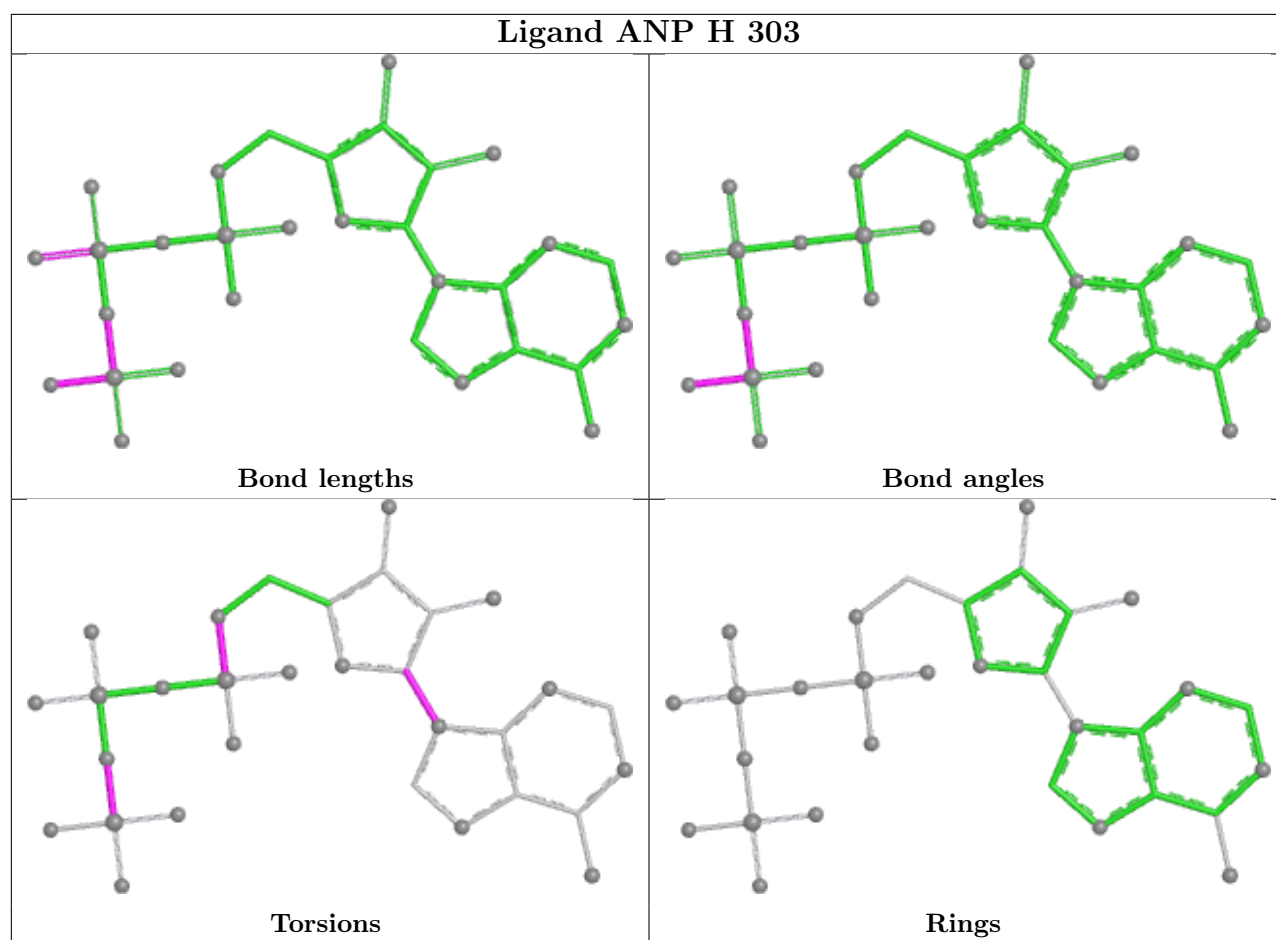
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	507	BU3	1	0
7	G	308	BU3	1	0
7	H	305	BU3	2	0
4	B	502	SO4	1	0

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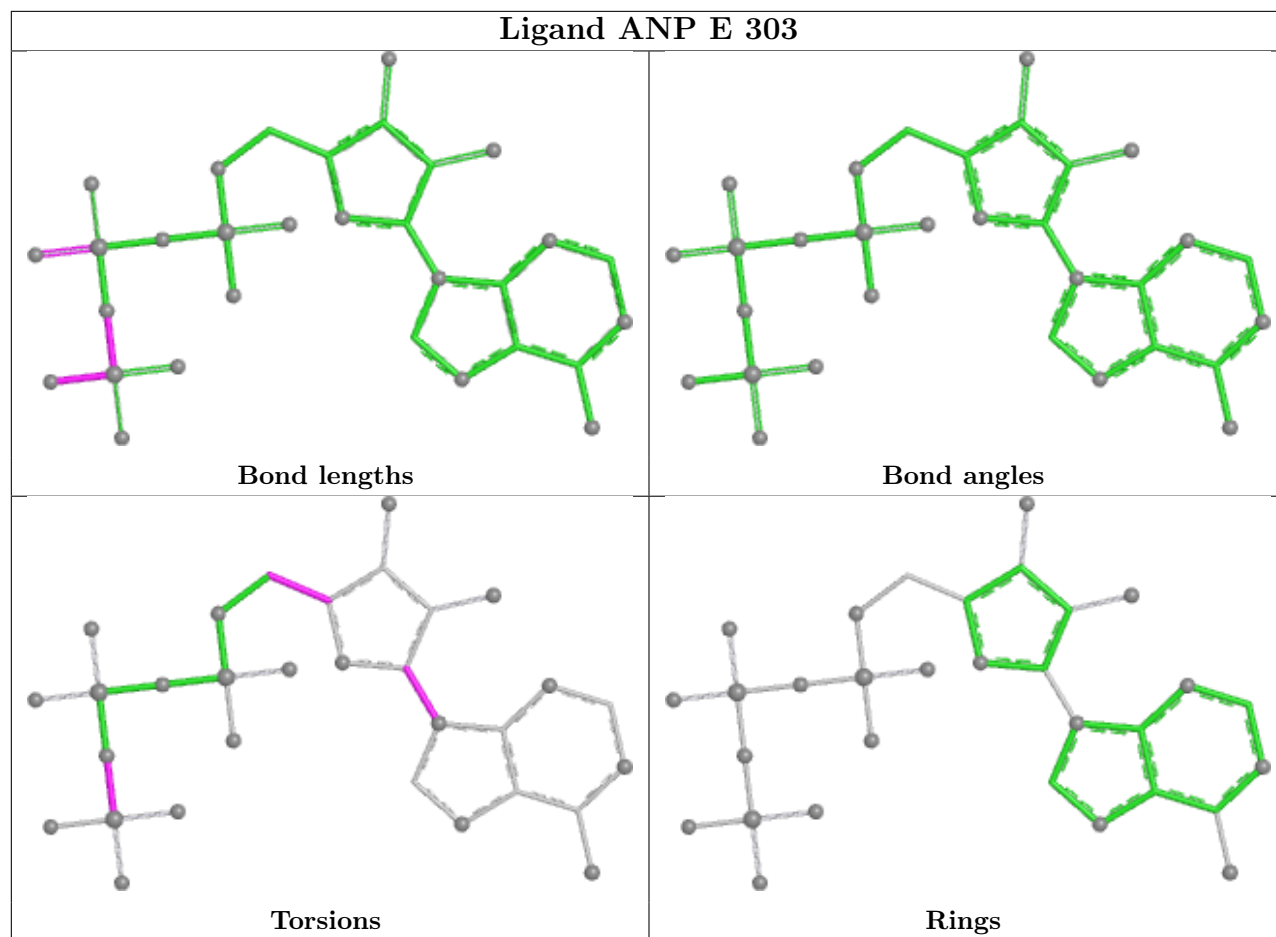
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	SO4	3	0
7	A	509	BU3	1	0
7	F	307	BU3	1	0
8	D	508	TAM	1	0
6	D	505	PEG	4	0
7	H	304	BU3	2	0
3	B	501	BJ8	1	0
4	F	301	SO4	1	0
4	G	303	SO4	1	0
7	E	305	BU3	1	0
4	D	502	SO4	1	0
7	G	305	BU3	1	0
4	F	304	SO4	1	0
4	B	503	SO4	1	0
7	D	506	BU3	1	0
7	G	306	BU3	1	0
7	C	509	BU3	1	0
7	C	508	BU3	1	0
4	C	505	SO4	1	0
3	A	501	BJ8	2	0

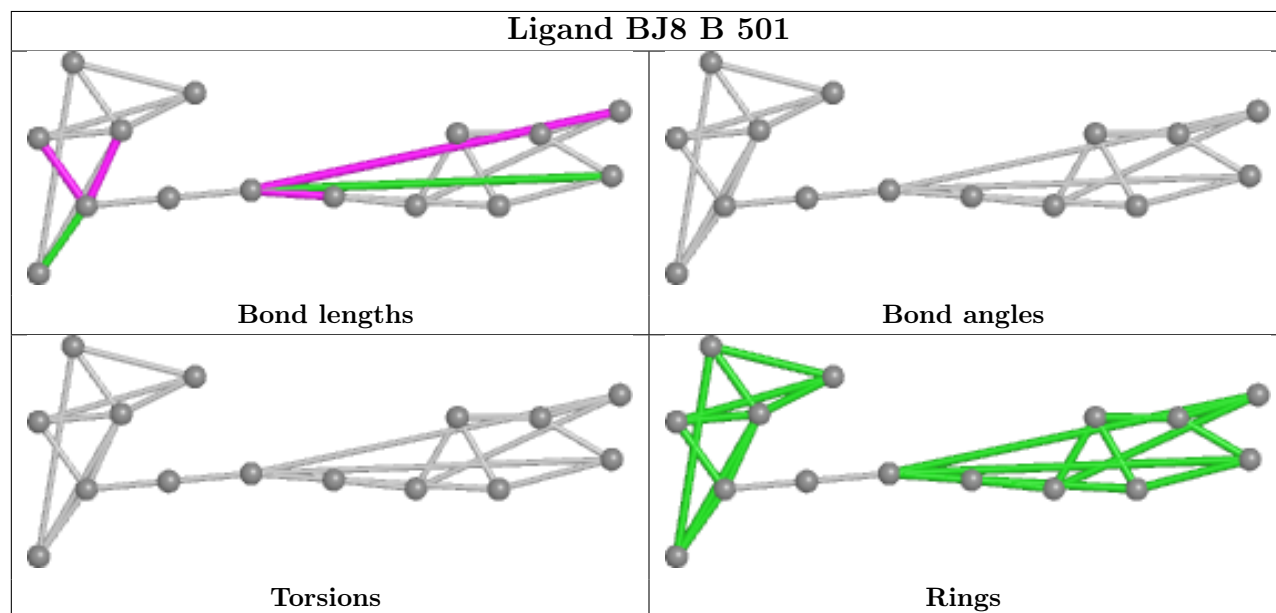
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



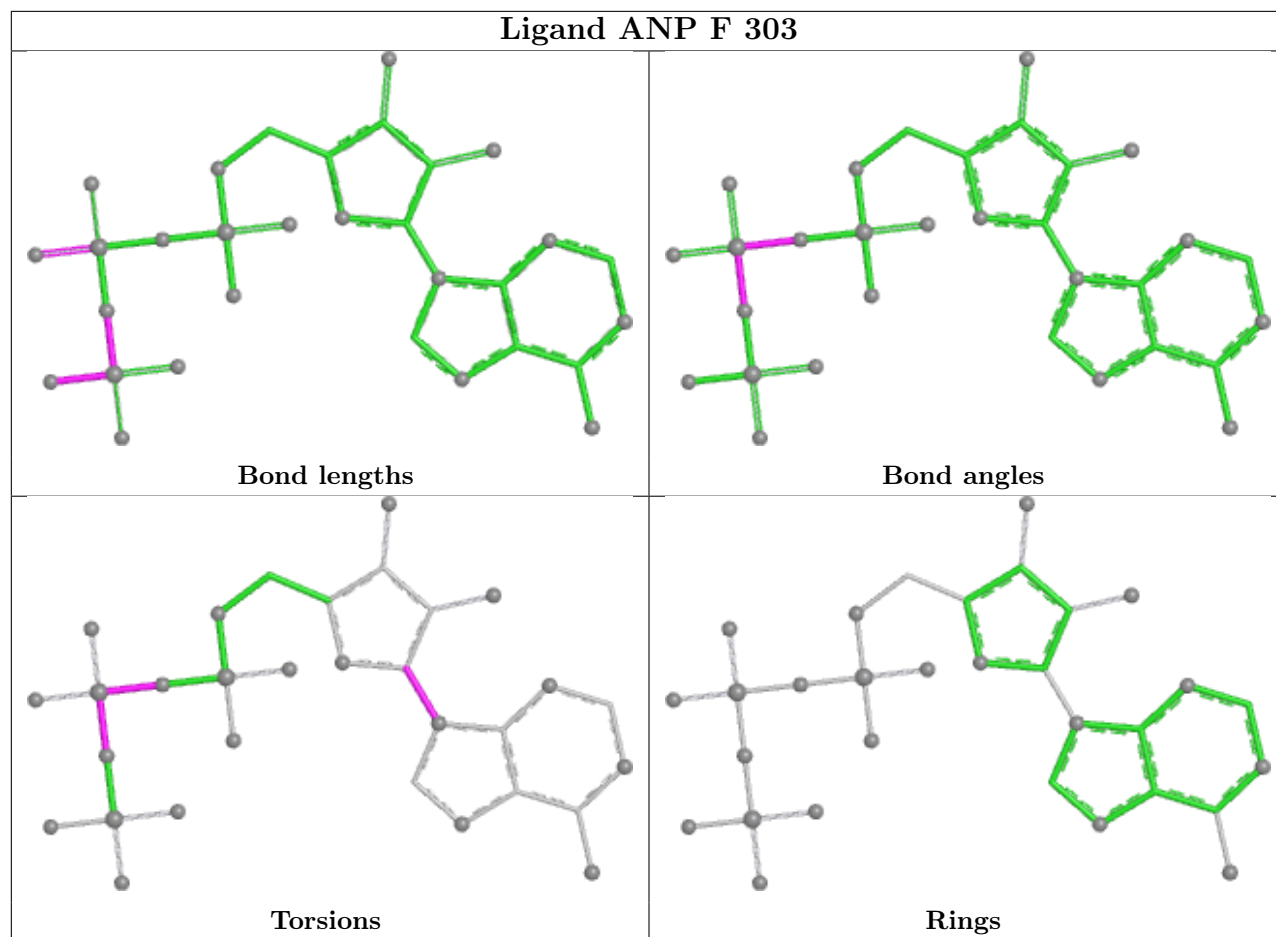
Ligand ANP E 303



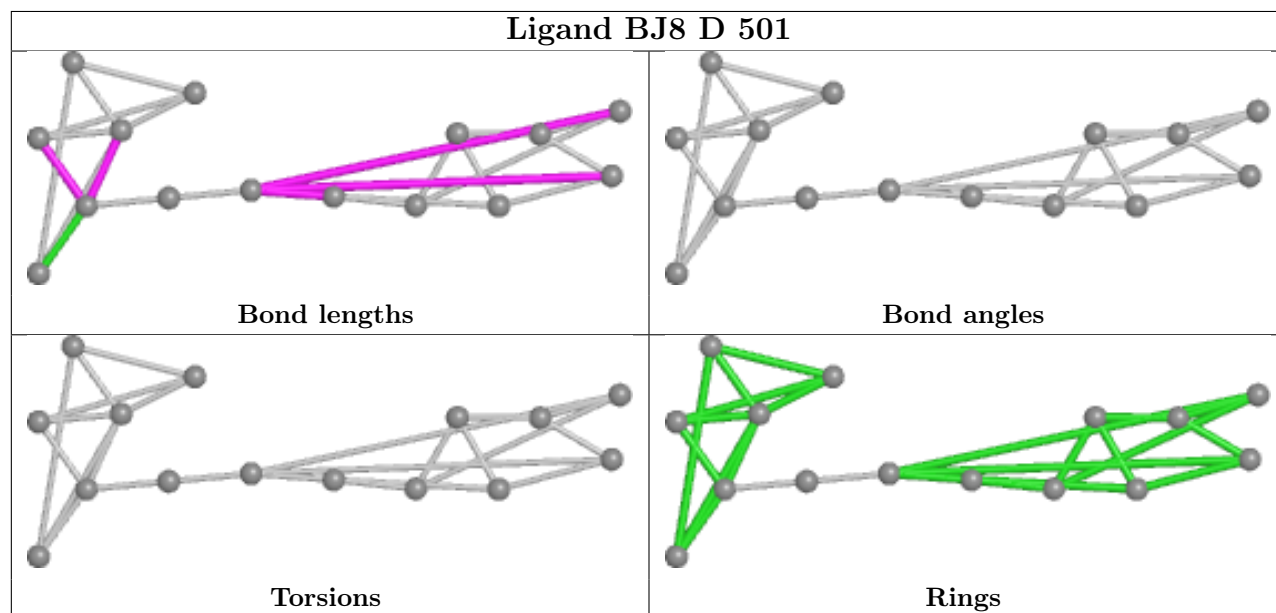
Ligand BJ8 B 501



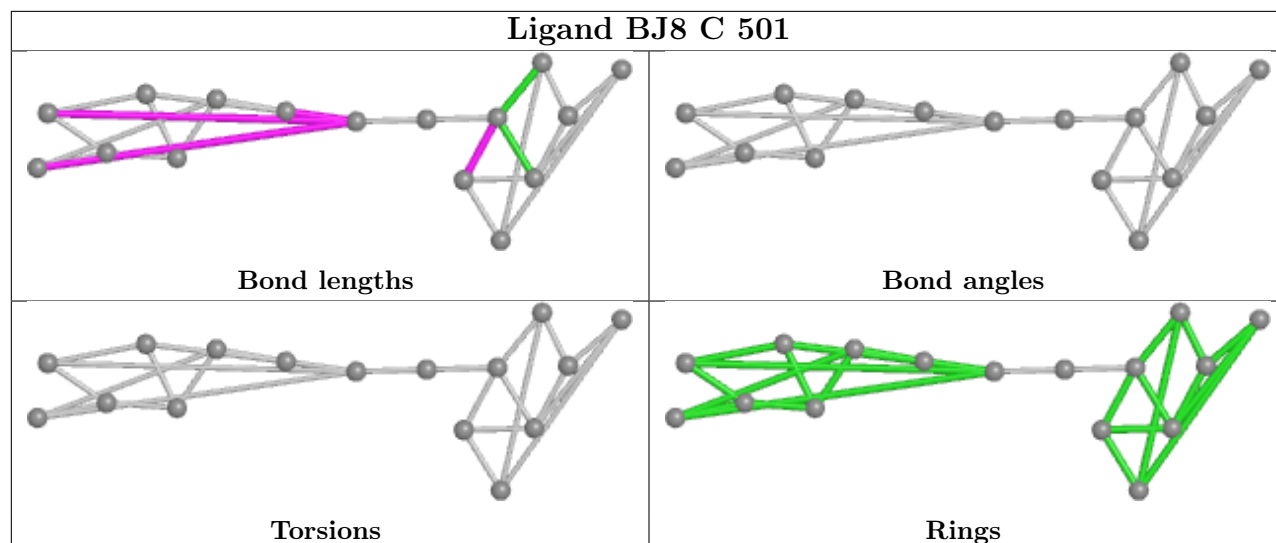
Ligand ANP F 303



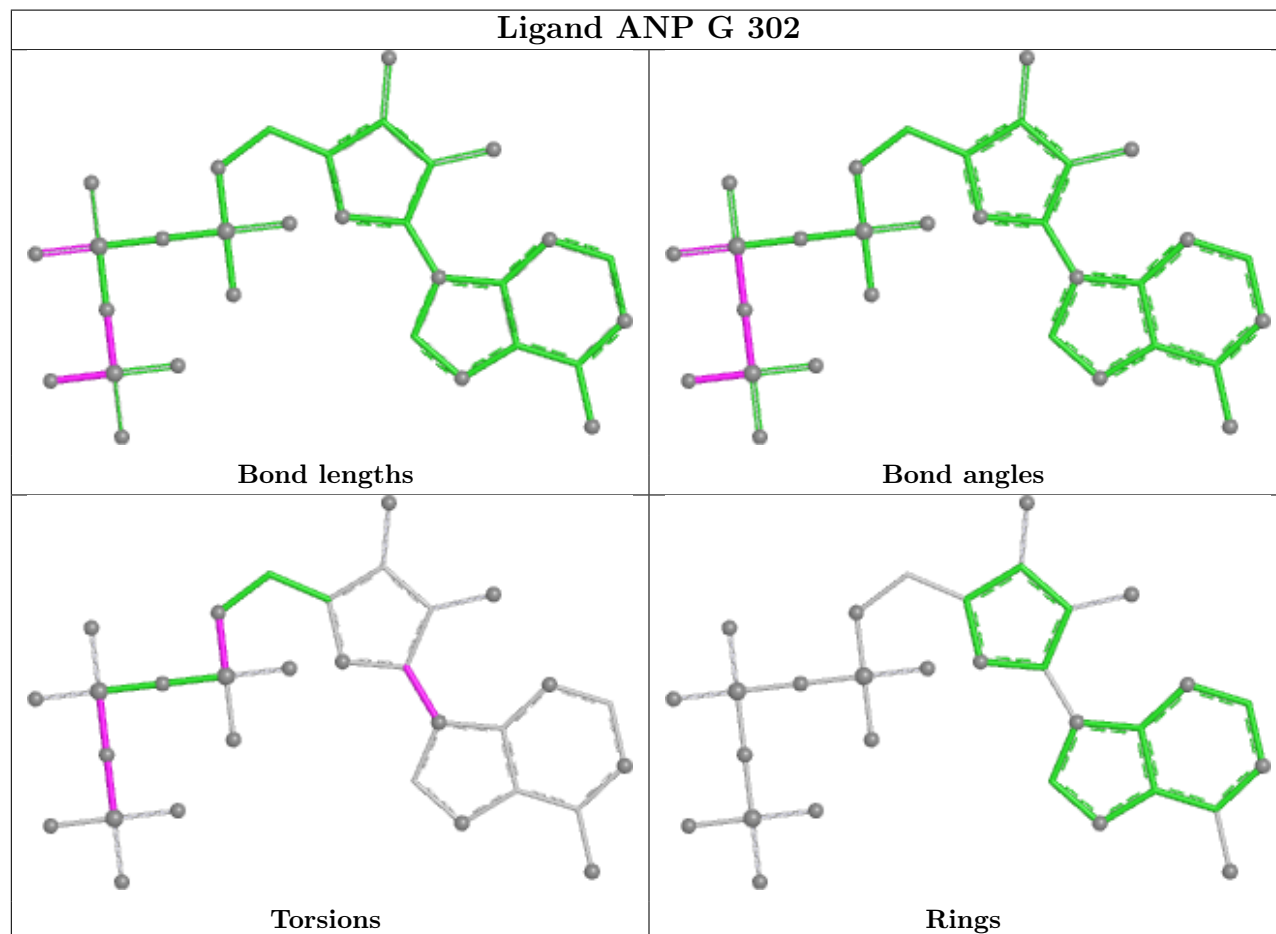
Ligand BJ8 D 501

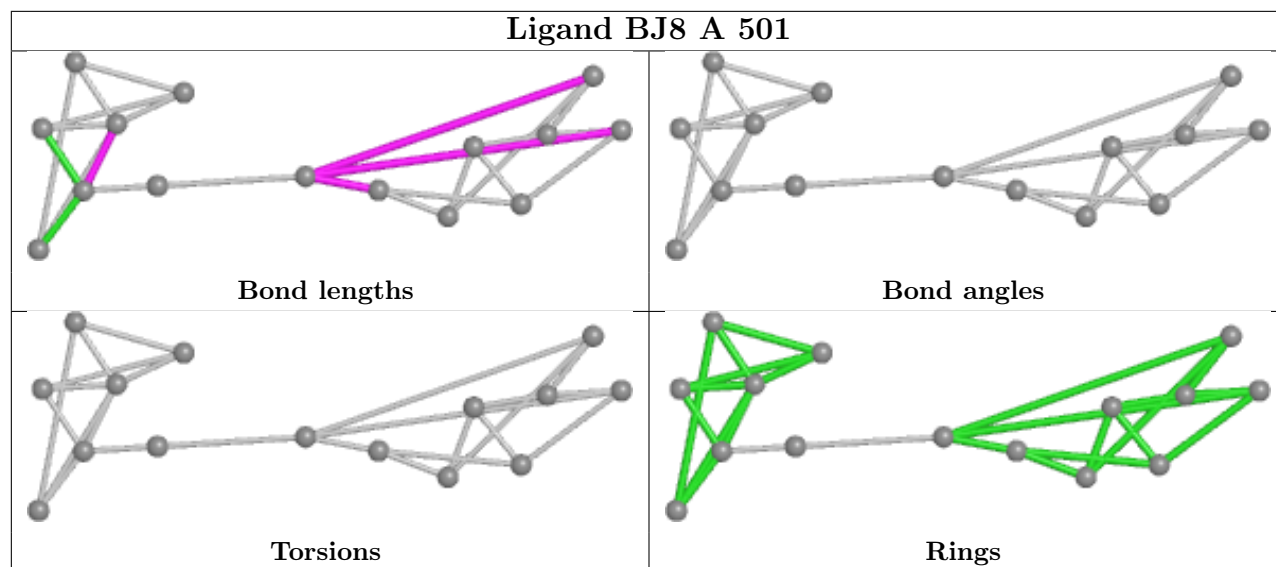


Ligand BJ8 C 501



Ligand ANP G 302





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	422/422 (100%)	-0.57	1 (0%) 91 93	7, 17, 30, 58	19 (4%)
1	B	421/422 (99%)	-0.15	2 (0%) 87 90	8, 25, 41, 78	11 (2%)
1	C	421/422 (99%)	-0.26	1 (0%) 91 93	9, 24, 39, 77	11 (2%)
1	D	421/422 (99%)	-0.56	1 (0%) 91 93	7, 17, 30, 65	17 (4%)
2	E	243/243 (100%)	0.48	20 (8%) 17 20	15, 31, 76, 101	4 (1%)
2	F	243/243 (100%)	-0.08	11 (4%) 38 44	9, 21, 72, 114	7 (2%)
2	G	243/243 (100%)	-0.08	10 (4%) 41 47	8, 21, 66, 101	6 (2%)
2	H	243/243 (100%)	0.31	15 (6%) 26 30	10, 30, 68, 100	10 (4%)
All	All	2657/2660 (99%)	-0.19	61 (2%) 61 68	7, 22, 51, 114	85 (3%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	134	TYR	5.0
2	E	132	ASP	4.6
2	G	134	TYR	4.6
2	F	134	TYR	4.5
2	E	140	ILE	4.2
2	H	134	TYR	4.0
2	H	133	ASP	3.9
1	D	1	MET	3.9
2	E	139	LEU	3.8
2	E	136	ASP	3.6
2	G	144	ASN	3.5
2	E	133	ASP	3.4
2	E	46	GLY	3.3
2	H	140	ILE	3.2
2	E	45	THR	3.1
2	H	21	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	3.1
2	G	132	ASP	3.0
2	G	131	GLY	3.0
2	H	131	GLY	3.0
2	F	133	ASP	2.9
1	B	1	MET	2.9
2	E	48	ILE	2.9
2	H	32	TYR	2.8
1	A	1	MET	2.8
2	F	140	ILE	2.8
1	B	272	LYS	2.8
2	G	19	GLU	2.8
2	F	132	ASP	2.8
2	E	137	GLU	2.8
2	F	243	THR	2.8
2	E	138	ASP	2.8
2	G	243	THR	2.7
2	F	144	ASN	2.7
2	G	139	LEU	2.7
2	G	20	ASP	2.6
2	G	140	ILE	2.6
2	E	18	LYS	2.6
2	H	48	ILE	2.6
2	E	144	ASN	2.6
2	E	130	ILE	2.5
2	F	135	ARG	2.5
2	E	243	THR	2.5
2	H	136	ASP	2.5
2	H	132	ASP	2.4
2	E	63	ARG	2.4
2	E	50	ASN	2.4
2	E	135	ARG	2.3
2	H	1	MET	2.3
2	H	2	PHE	2.3
2	F	141	ASN	2.3
2	H	138	ASP	2.2
2	F	62[A]	ASN	2.2
2	F	138	ASP	2.2
2	H	50	ASN	2.2
2	F	136	ASP	2.2
2	H	139	LEU	2.2
2	E	2	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	142	GLU	2.1
2	E	141	ASN	2.1
2	H	141	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	BU3	C	508	6/6	0.36	0.24	41,53,64,71	16
5	NH4	B	506	1/1	0.57	0.19	41,49,49,49	0
7	BU3	G	308	6/6	0.61	0.34	13,22,31,34	16
6	PEG	A	506	7/7	0.61	0.20	36,52,62,67	0
8	TAM	D	508	11/11	0.62	0.18	31,52,64,69	0
5	NH4	B	505	1/1	0.63	0.16	43,52,52,52	0
5	NH4	A	503	1/1	0.63	0.14	42,50,50,50	0
6	PEG	A	507	7/7	0.66	0.16	30,40,49,58	0
4	SO4	A	502	5/5	0.67	0.14	37,40,43,51	5
8	TAM	B	504	11/11	0.71	0.14	36,48,62,63	0
7	BU3	C	507	6/6	0.71	0.19	34,43,49,51	16
6	PEG	D	505	7/7	0.74	0.20	28,36,51,51	17
4	SO4	B	503	5/5	0.75	0.14	30,35,39,42	5
7	BU3	C	509	6/6	0.76	0.16	34,42,56,57	16
7	BU3	D	507	6/6	0.76	0.18	23,37,44,51	16
6	PEG	C	506	7/7	0.78	0.16	22,30,36,44	17
7	BU3	F	307	6/6	0.78	0.15	26,33,38,44	16
7	BU3	H	305	6/6	0.79	0.16	26,32,41,41	16
4	SO4	F	301	5/5	0.79	0.16	28,29,32,40	5
4	SO4	D	502	5/5	0.80	0.14	30,34,39,48	5

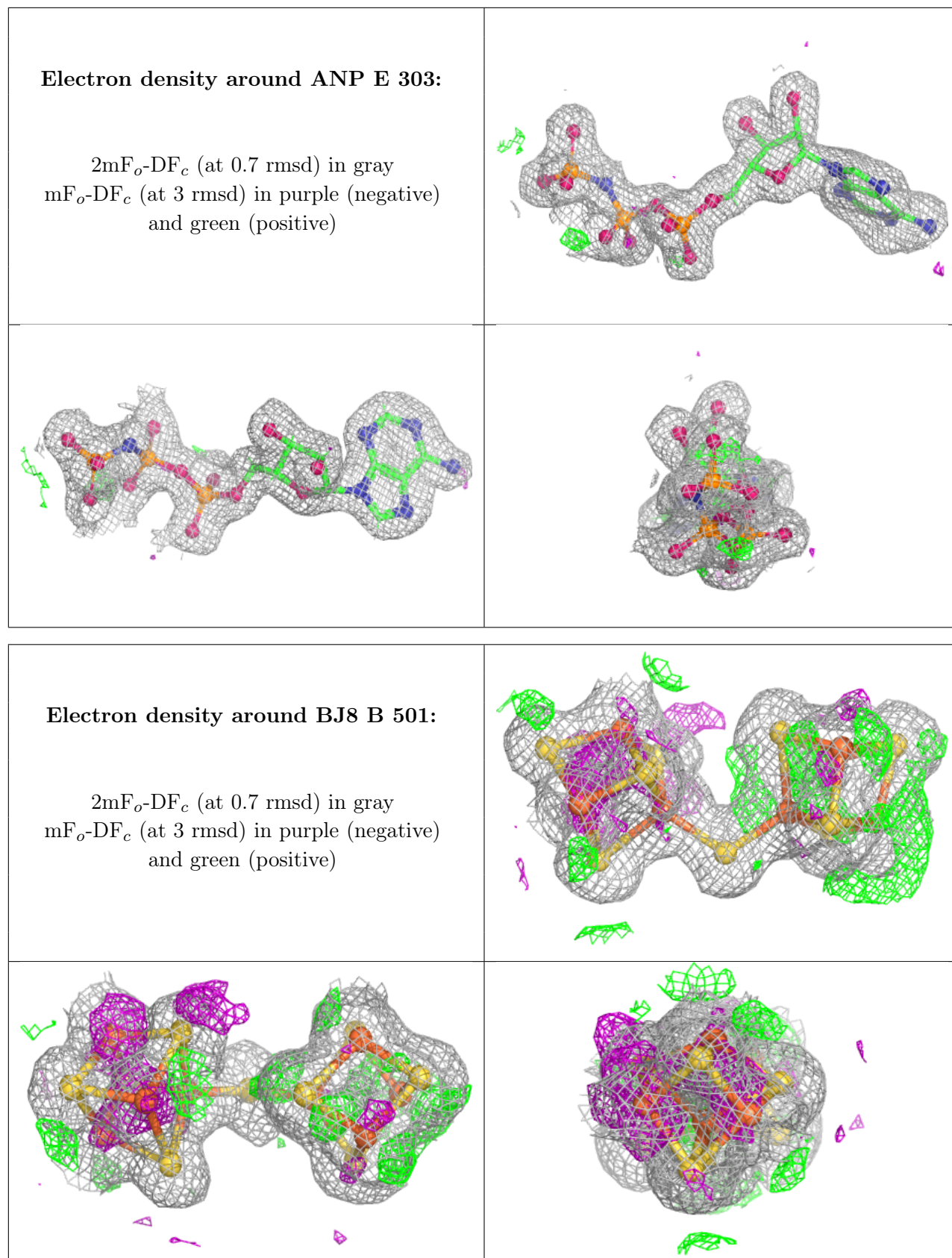
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	504	5/5	0.81	0.14	39,41,49,57	5
7	BU3	A	508	6/6	0.81	0.16	24,37,41,47	16
7	BU3	A	509	6/6	0.81	0.20	16,26,31,33	16
7	BU3	F	305	6/6	0.82	0.17	27,35,38,38	16
4	SO4	E	304	5/5	0.83	0.17	27,29,33,42	5
7	BU3	B	507	6/6	0.83	0.13	31,45,57,57	0
7	BU3	D	506	6/6	0.83	0.15	20,31,40,43	16
7	BU3	G	307	6/6	0.83	0.13	20,33,39,42	16
7	BU3	G	306	6/6	0.85	0.13	14,19,36,38	16
7	BU3	G	305	6/6	0.85	0.17	25,33,40,40	16
7	BU3	F	306	6/6	0.85	0.14	20,30,36,36	16
4	SO4	A	504	5/5	0.86	0.11	38,39,45,56	5
5	NH4	D	503	1/1	0.87	0.12	28,34,34,34	0
7	BU3	E	305	6/6	0.88	0.13	21,29,41,42	16
4	SO4	F	304	5/5	0.88	0.13	32,33,41,41	0
4	SO4	D	504	5/5	0.88	0.11	25,31,37,40	5
5	NH4	A	510	1/1	0.89	0.12	26,31,31,31	0
4	SO4	C	503	5/5	0.89	0.09	44,45,52,62	0
4	SO4	G	303	5/5	0.89	0.12	31,35,39,42	0
7	BU3	H	304	6/6	0.89	0.10	19,32,39,45	0
5	NH4	G	304	1/1	0.90	0.08	19,23,23,23	0
4	SO4	C	505	5/5	0.90	0.09	21,30,41,41	5
4	SO4	C	502	5/5	0.91	0.12	38,44,45,51	0
4	SO4	A	505	5/5	0.91	0.15	26,27,33,38	5
4	SO4	B	502	5/5	0.91	0.10	33,35,38,40	5
9	MG	E	302	1/1	0.96	0.05	17,17,17,17	0
10	ANP	E	303	31/31	0.97	0.06	16,25,39,47	0
3	BJ8	B	501	17/17	0.98	0.04	13,16,21,21	0
10	ANP	H	303	31/31	0.98	0.06	13,23,37,45	0
9	MG	G	301	1/1	0.98	0.02	11,11,11,11	0
9	MG	H	302	1/1	0.99	0.03	15,15,15,15	0
3	BJ8	C	501	17/17	0.99	0.04	14,16,22,23	0
9	MG	F	302	1/1	0.99	0.02	10,10,10,10	0
10	ANP	G	302	31/31	0.99	0.05	9,16,39,48	0
3	BJ8	D	501	17/17	0.99	0.03	10,13,16,16	0
3	BJ8	A	501	17/17	0.99	0.03	10,12,17,17	0
10	ANP	F	303	31/31	0.99	0.05	8,17,36,51	0
11	SF4	H	301	8/8	1.00	0.02	12,13,16,17	0
11	SF4	E	301	8/8	1.00	0.02	12,13,14,16	0

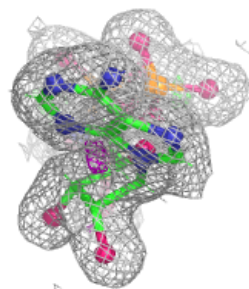
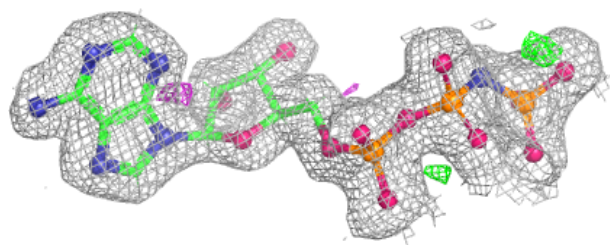
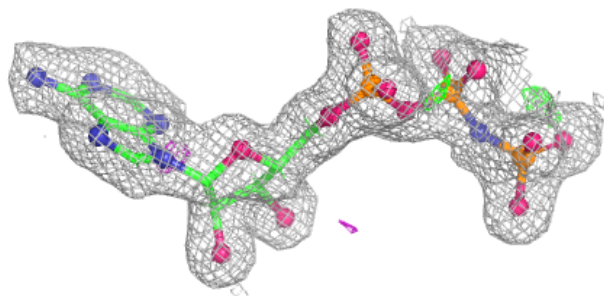
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

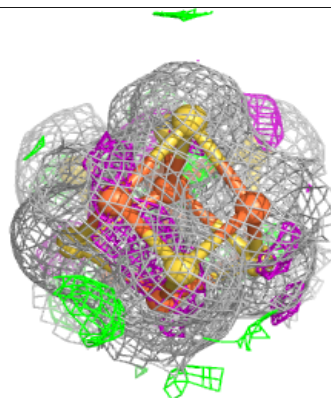
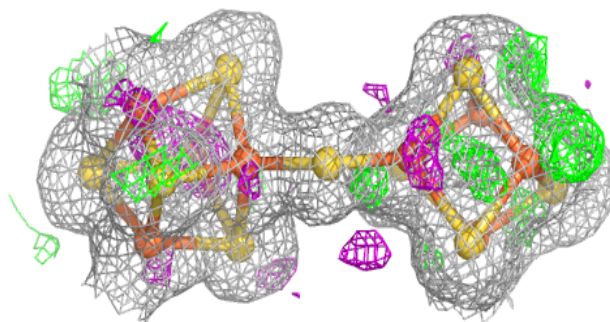
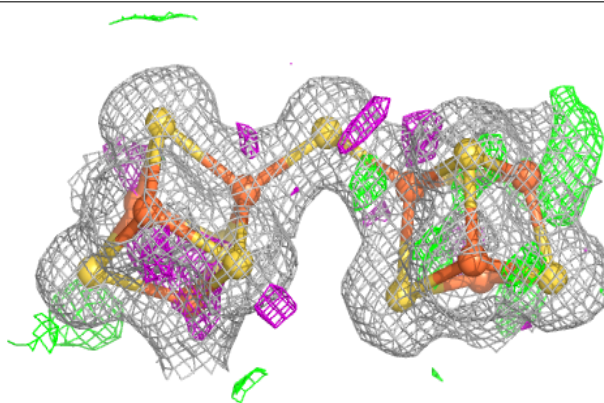


Electron density around ANP H 303:

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

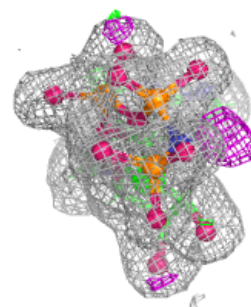
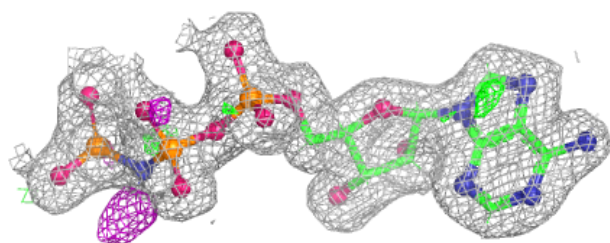
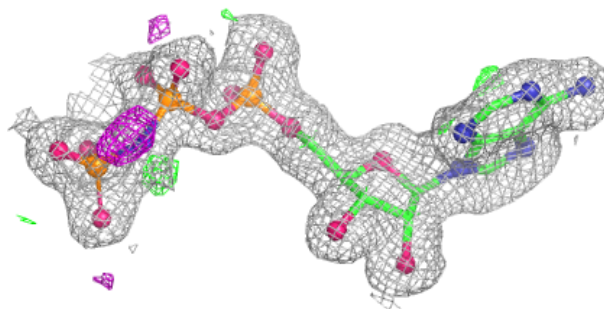
**Electron density around BJ8 C 501:**

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

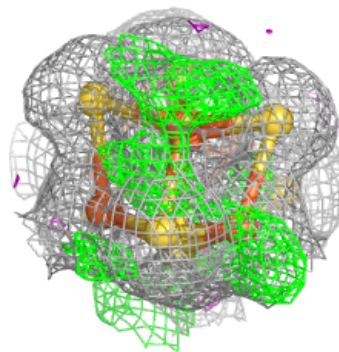
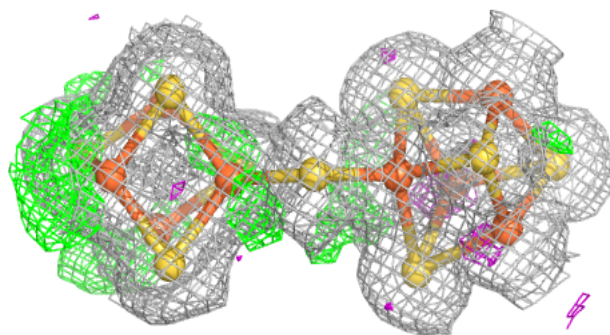
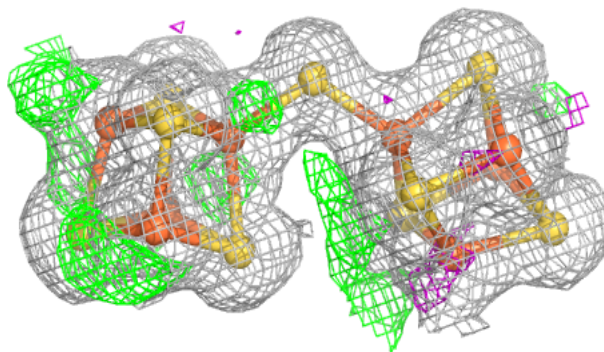


Electron density around ANP G 302:

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

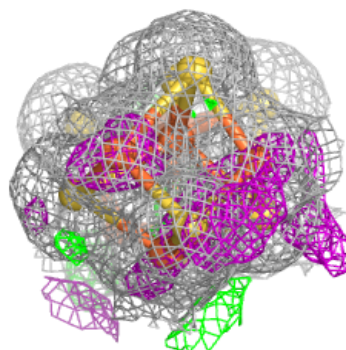
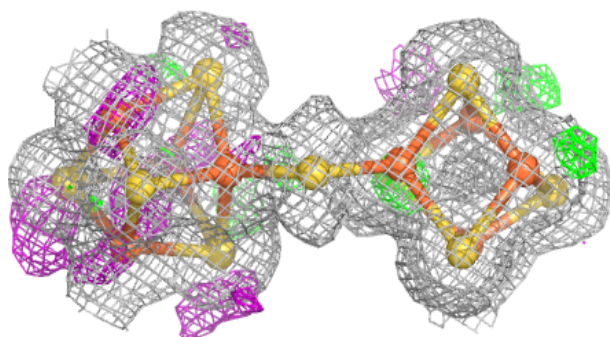
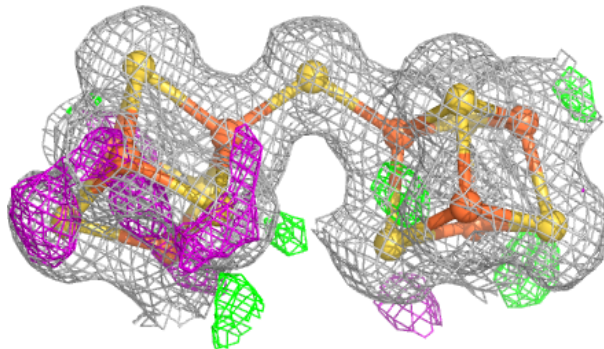
**Electron density around BJ8 D 501:**

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

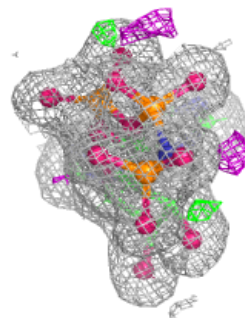
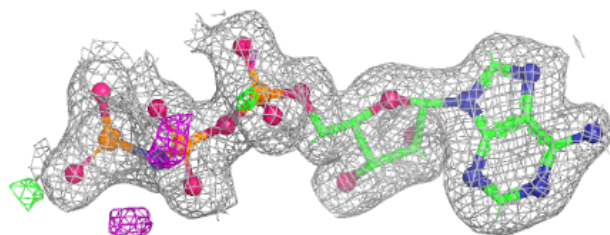
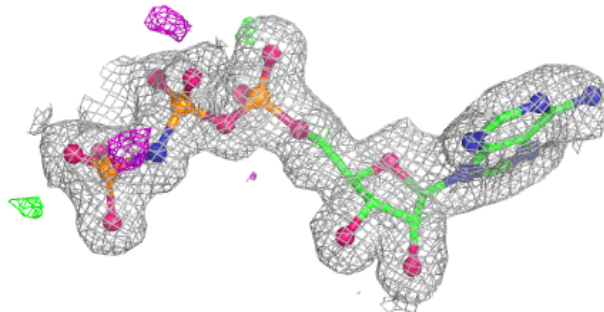


Electron density around BJ8 A 501:

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

**Electron density around ANP F 303:**

$2mF_o-DF_c$ (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.