wwPDB X-ray Structure Validation Summary Report (i)

Dec 20, 2022 – 09:33 am GMT

PDB ID	:	7YZQ
Title	:	MgADP-AlF4-bound DCCP:DCCP-R complex
Authors	:	Jeoung, J.-H.; Dobbek, H.
Deposited on	:	2022-02-21
Resolution	:	1.96 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

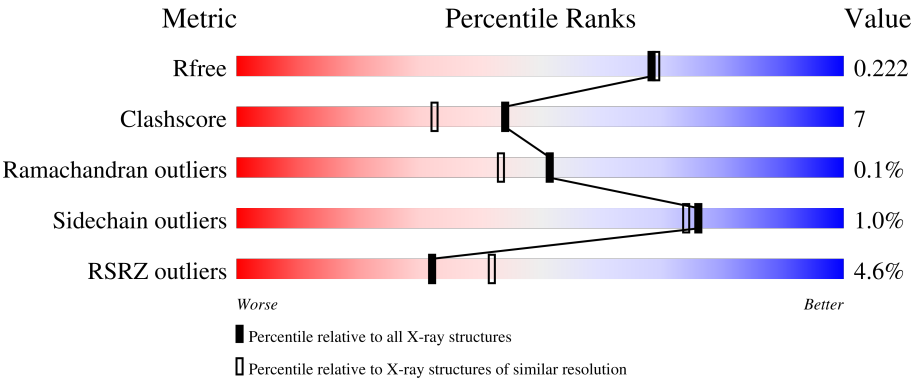
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	422	92% 8%
1	B	422	3% 89% 11%
1	C	422	90% 10%
1	D	422	3% 89% 10%
2	E	243	6% 87% 12%

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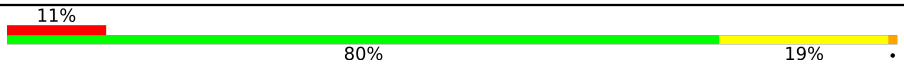
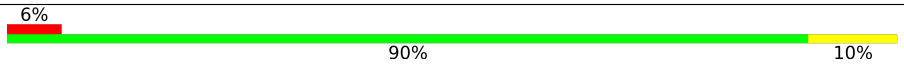
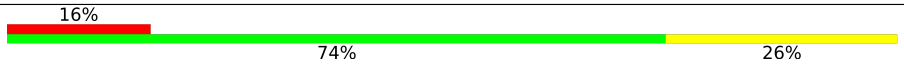
Mol	Chain	Length	Quality of chain
2	F	243	
2	G	243	
2	H	243	

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 46029 atoms, of which 21708 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	C	420	Total	C	H	N	O	S	0	3	0
			6776	2157	3402	579	621	17			
1	D	421	Total	C	H	N	O	S	0	6	0
			6886	2184	3471	592	621	18			
1	A	421	Total	C	H	N	O	S	0	6	0
			6828	2172	3429	582	626	19			
1	B	422	Total	C	H	N	O	S	0	10	0
			6900	2189	3472	593	628	18			

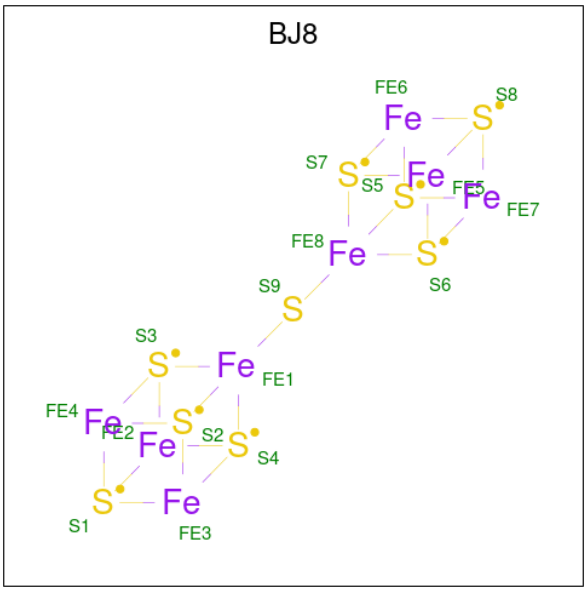
There are 4 discrepancies between the modelled and reference sequences:

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

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

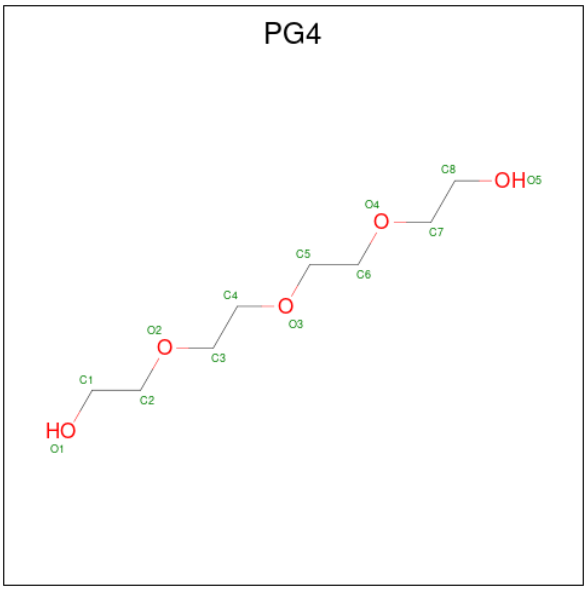
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	243	Total	C	H	N	O	S	0	4	0
			3823	1193	1955	321	346	8			
2	F	243	Total	C	H	N	O	S	0	2	0
			3803	1187	1943	320	345	8			
2	G	243	Total	C	H	N	O	S	0	0	0
			3765	1177	1917	318	345	8			
2	H	243	Total	C	H	N	O	S	0	1	0
			3777	1181	1923	318	347	8			

- Molecule 3 is Double cubane cluster (three-letter code: BJ8) (formula: Fe_8S_9) (labeled as "Ligand of Interest" by depositor).



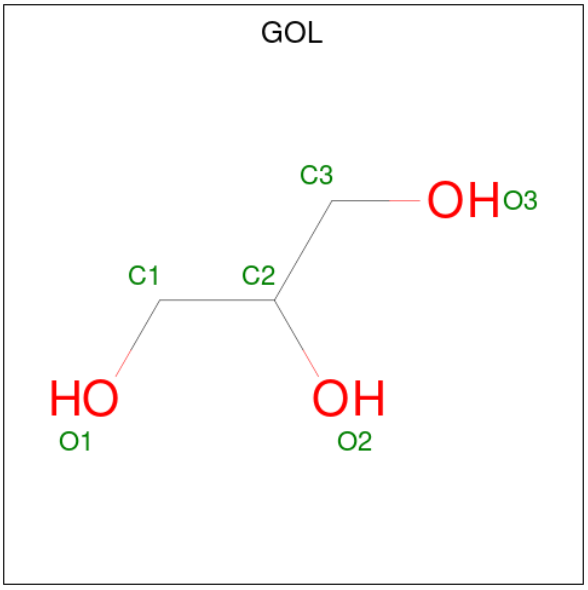
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Fe S 17 8 9	0	0
3	D	1	Total Fe S 17 8 9	0	0
3	A	1	Total Fe S 17 8 9	0	0
3	B	1	Total Fe S 17 8 9	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



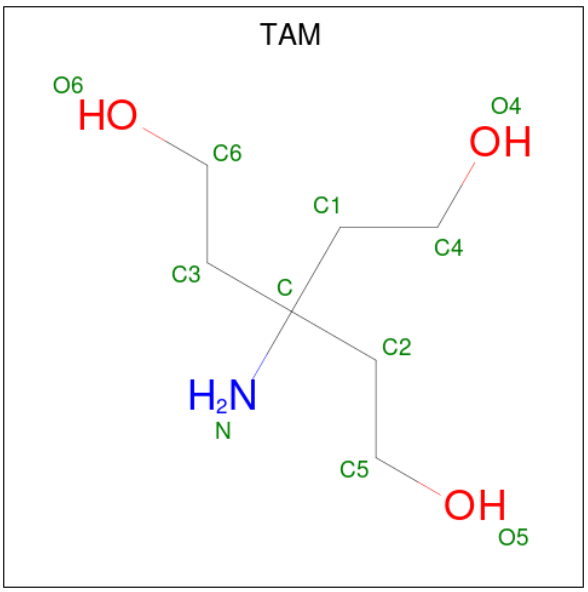
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	H	O	0	1
			62	16	36	10		

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



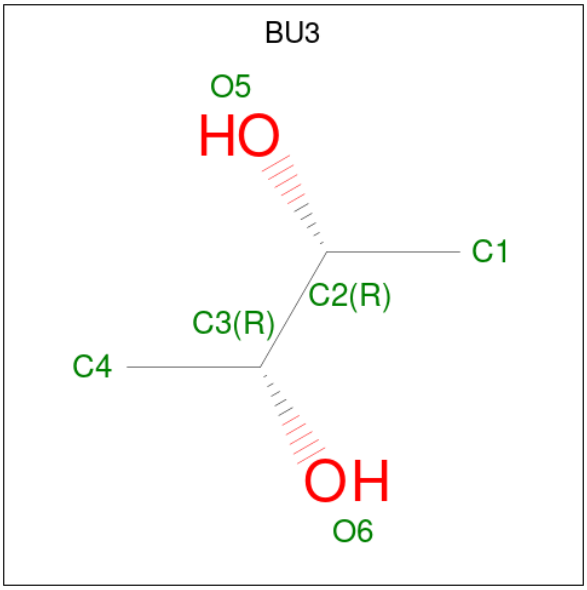
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is TRIS(HYDROXYETHYL)AMINOMETHANE (three-letter code: TAM) (formula: $C_7H_{17}NO_3$).



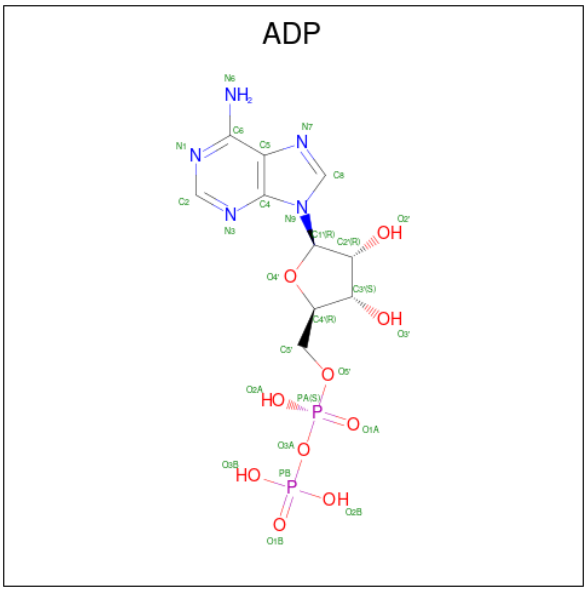
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	D	1	Total	C	H	N	O	0	0
			28	7	17	1	3		
6	E	1	Total	C	H	N	O	0	0
			28	7	17	1	3		
6	B	1	Total	C	H	N	O	0	0
			28	7	17	1	3		
6	G	1	Total	C	H	N	O	0	0
			28	7	17	1	3		

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	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	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		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

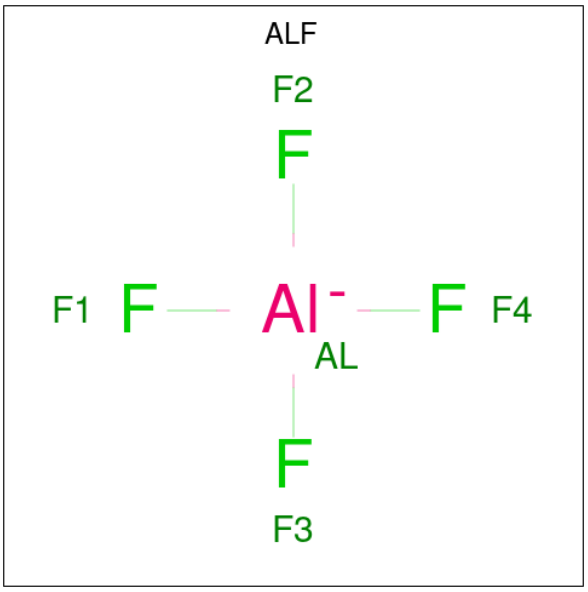


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	E	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
8	F	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
8	G	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		
8	H	1	Total	C	H	N	O	P	0	0
			38	10	11	5	10	2		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

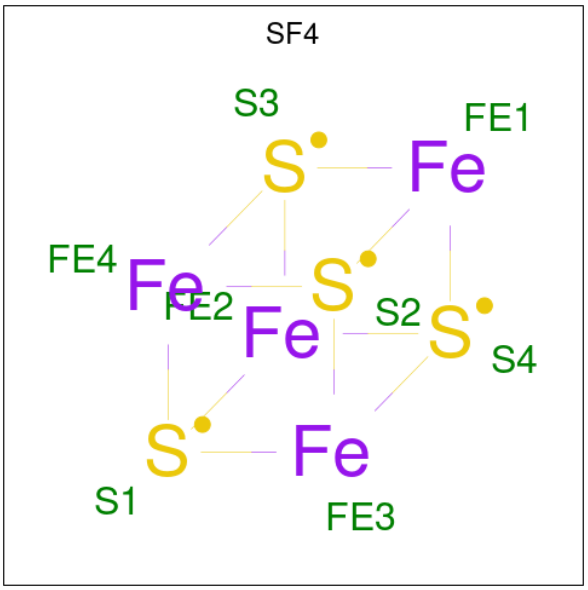
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	1	Total	Mg	0	0
			1	1		
9	F	1	Total	Mg	0	0
			1	1		
9	G	1	Total	Mg	0	0
			1	1		
9	H	1	Total	Mg	0	0
			1	1		

- Molecule 10 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



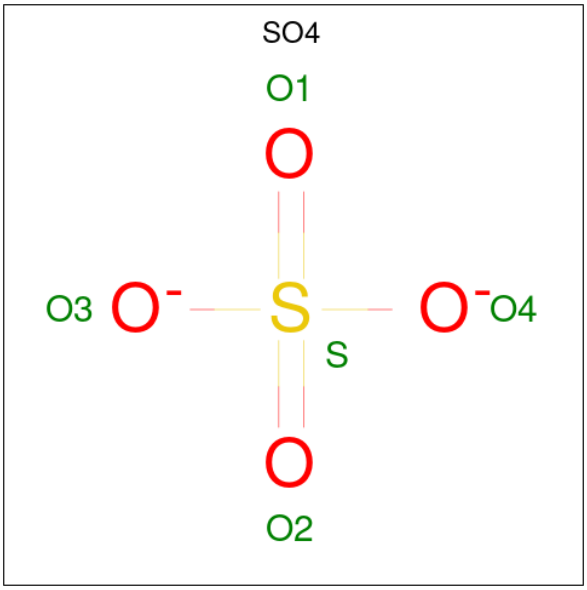
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	E	1	Total Al F 5 1 4	0	0
10	F	1	Total Al F 5 1 4	0	0
10	G	1	Total Al F 5 1 4	0	0
10	H	1	Total Al F 5 1 4	0	0

- Molecule 11 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



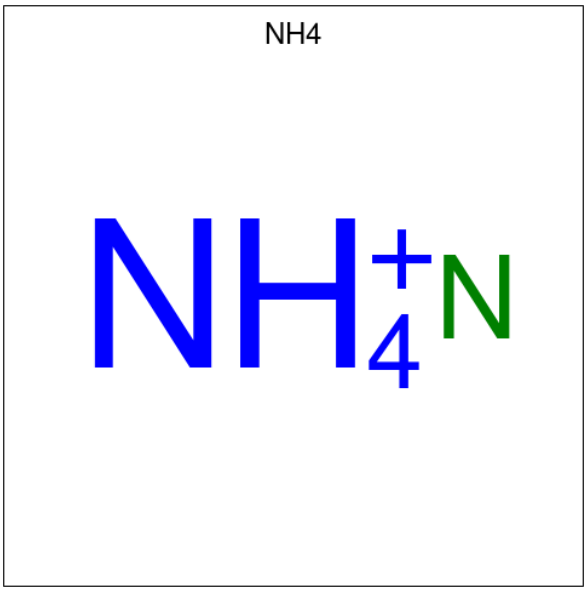
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	F	1	Total Fe S 8 4 4	0	0
11	G	1	Total Fe S 8 4 4	0	0

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 13 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total N 1 1	0	0
13	G	1	Total N 1 1	0	0

- Molecule 14 is water.

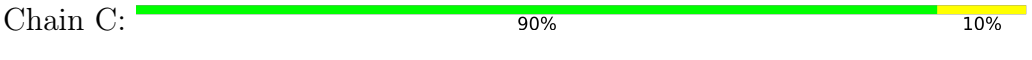
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	584	Total O 584 584	0	0
14	D	435	Total O 435 435	0	0
14	E	256	Total O 256 256	0	0
14	F	154	Total O 154 154	0	0
14	A	632	Total O 632 632	0	0
14	B	441	Total O 441 441	0	0
14	G	271	Total O 271 271	0	0
14	H	159	Total O 159 159	0	0

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.

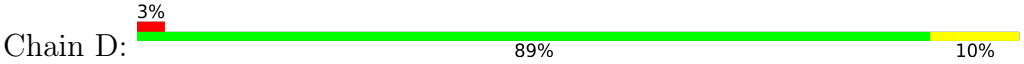
• Molecule 1: Dehydratase family protein

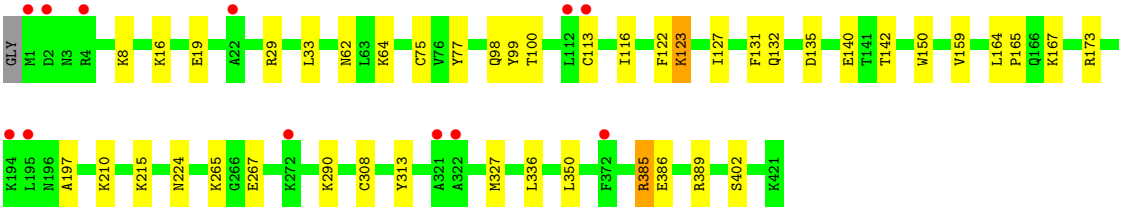
Chain C:



• Molecule 1: Dehydratase family protein

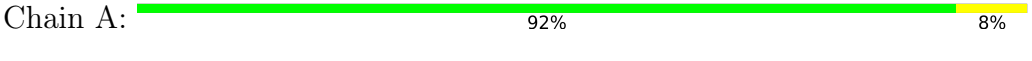
Chain D:

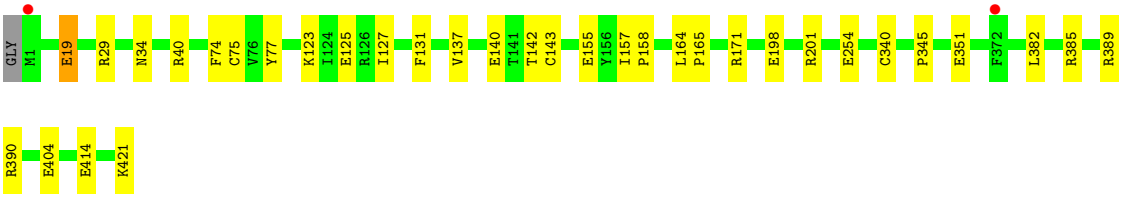




• Molecule 1: Dehydratase family protein

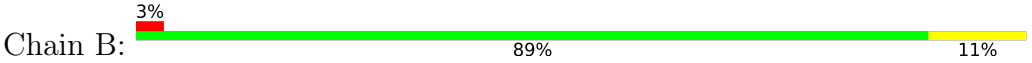
Chain A:

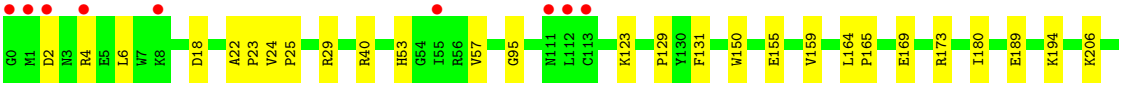




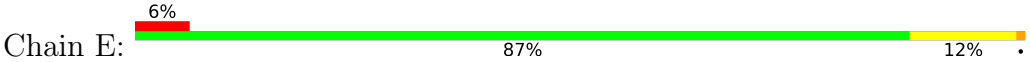
• Molecule 1: Dehydratase family protein

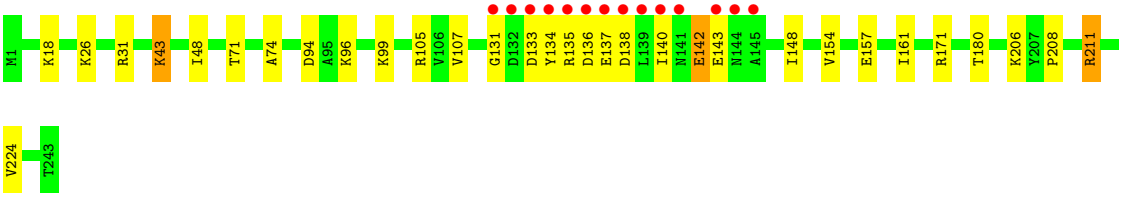
Chain B:



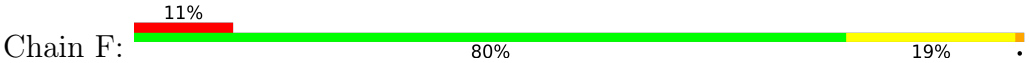


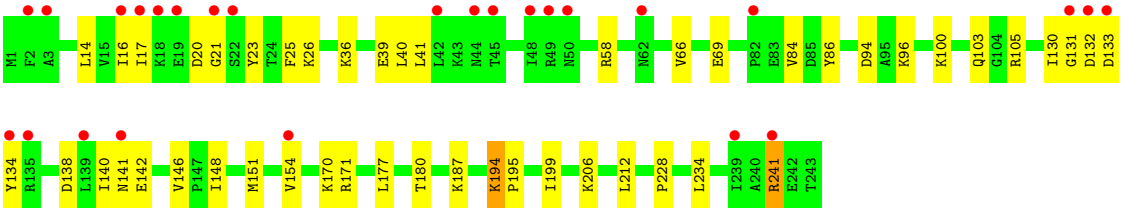
• Molecule 2: Putative CoA-substrate-specific enzyme activase



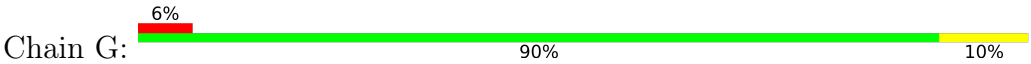


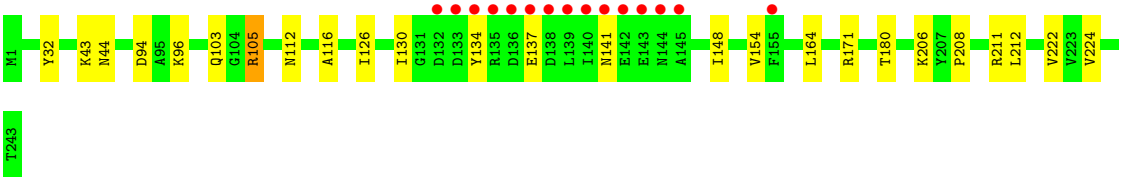
• Molecule 2: Putative CoA-substrate-specific enzyme activase



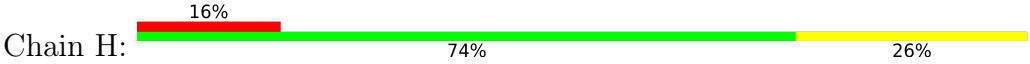


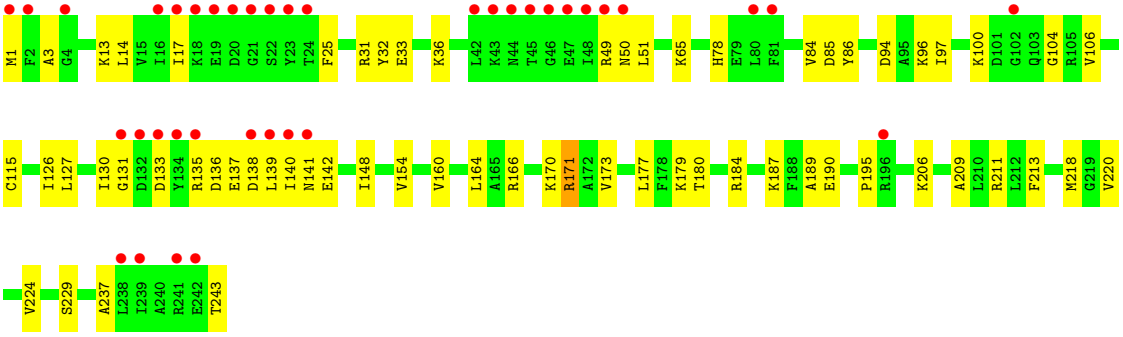
• Molecule 2: Putative CoA-substrate-specific enzyme activase





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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	78.03Å 81.59Å 121.48Å 100.83° 96.92° 90.17°	Depositor
Resolution (Å)	46.16 – 1.96 46.16 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.16-1.96) 96.0 (46.16-1.96)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.178 , 0.223 0.178 , 0.222	Depositor DCC
R_{free} test set	2128 reflections (1.05%)	wwPDB-VP
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	46029	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NH4, SO4, BU3, ALF, PG4, ADP, GOL, SF4, MG, TAM, BJ8

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	0.78	2/3486 (0.1%)	0.69	1/4707 (0.0%)
1	B	0.58	0/3532	0.58	0/4766
1	C	0.71	0/3452	0.69	3/4663 (0.1%)
1	D	0.58	1/3505 (0.0%)	0.61	0/4728
2	E	0.65	0/1906	0.71	0/2572
2	F	0.50	0/1892	0.60	0/2551
2	G	0.63	0/1874	0.66	0/2528
2	H	0.55	1/1883 (0.1%)	0.65	0/2540
All	All	0.64	4/21530 (0.0%)	0.65	4/29055 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	CYS	CB-SG	-18.08	1.51	1.82
1	D	308	CYS	CB-SG	-6.67	1.71	1.82
1	A	340	CYS	CB-SG	-5.28	1.73	1.81
2	H	115	CYS	CB-SG	-5.28	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	276	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	143	CYS	CA-CB-SG	5.84	124.52	114.00
1	C	349	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	323	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3399	3429	3431	25	0
1	B	3428	3472	3453	37	0
1	C	3374	3402	3402	37	1
1	D	3415	3471	3473	33	0
2	E	1868	1955	1955	31	0
2	F	1860	1943	1943	43	0
2	G	1848	1917	1917	21	0
2	H	1854	1923	1923	66	0
3	A	17	0	0	0	0
3	B	17	0	0	0	0
3	C	17	0	0	1	0
3	D	17	0	0	0	0
4	C	26	36	36	5	0
5	D	6	8	8	0	0
6	B	11	17	17	1	0
6	D	11	17	17	0	0
6	E	11	17	17	0	0
6	G	11	17	17	0	0
7	B	12	20	20	3	0
7	D	6	10	10	0	0
7	G	6	10	10	0	0
8	E	27	11	12	0	0
8	F	27	11	12	0	0
8	G	27	11	12	0	0
8	H	27	11	12	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	5	0	0	0	0
10	F	5	0	0	0	0
10	G	5	0	0	0	0
10	H	5	0	0	0	0
11	F	8	0	0	0	0
11	G	8	0	0	0	0
12	A	15	0	0	1	0
12	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	G	5	0	0	1	0
13	A	1	0	0	1	0
13	G	1	0	0	1	0
14	A	632	0	0	15	4
14	B	441	0	0	10	0
14	C	584	0	0	17	3
14	D	435	0	0	4	0
14	E	256	0	0	12	2
14	F	154	0	0	5	0
14	G	271	0	0	5	4
14	H	159	0	0	9	0
All	All	24321	21708	21697	286	7

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 7.

The worst 5 of 286 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:H:138:ASP:HB3	2:H:171:ARG:NH1	1.64	1.12
2:F:206:LYS:NZ	14:F:402:HOH:O	1.84	1.10
2:H:179:LYS:NZ	14:H:401:HOH:O	1.90	1.04
2:G:105:ARG:NH2	14:G:401:HOH:O	1.93	1.00
1:B:4:ARG:NH2	1:B:18:ASP:OD2	1.99	0.94

The worst 5 of 7 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)
14:C:655:HOH:O	14:E:438:HOH:O[1_565]	1.95	0.25
14:A:975:HOH:O	14:G:428:HOH:O[1_545]	2.02	0.18
14:C:1170:HOH:O	14:A:1105:HOH:O[1_565]	2.06	0.14
14:A:605:HOH:O	14:G:413:HOH:O[1_545]	2.07	0.13
1:C:66:GLU:O	14:E:401:HOH:O[1_565]	2.15	0.05

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	425/422 (101%)	415 (98%)	10 (2%)	0	100 100
1	B	430/422 (102%)	420 (98%)	10 (2%)	0	100 100
1	C	421/422 (100%)	410 (97%)	11 (3%)	0	100 100
1	D	426/422 (101%)	416 (98%)	10 (2%)	0	100 100
2	E	245/243 (101%)	240 (98%)	3 (1%)	2 (1%)	19 9
2	F	243/243 (100%)	238 (98%)	4 (2%)	1 (0%)	34 22
2	G	241/243 (99%)	233 (97%)	8 (3%)	0	100 100
2	H	242/243 (100%)	240 (99%)	2 (1%)	0	100 100
All	All	2673/2660 (100%)	2612 (98%)	58 (2%)	3 (0%)	51 43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	136	ASP
2	E	131	GLY
2	F	131	GLY

5.3.2 Protein sidechains (i)

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	369/363 (102%)	365 (99%)	4 (1%)	73 71
1	B	373/363 (103%)	368 (99%)	5 (1%)	69 65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	365/363 (101%)	364 (100%)	1 (0%)	92	92
1	D	370/363 (102%)	364 (98%)	6 (2%)	62	58
2	E	200/196 (102%)	194 (97%)	6 (3%)	41	30
2	F	198/196 (101%)	194 (98%)	4 (2%)	55	48
2	G	196/196 (100%)	193 (98%)	3 (2%)	65	60
2	H	197/196 (100%)	196 (100%)	1 (0%)	88	88
All	All	2268/2236 (101%)	2238 (99%)	30 (1%)	76	65

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	194[A]	LYS
2	G	137	GLU
1	A	19[A]	GLU
2	H	171	ARG
1	B	406[A]	GLN

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

Mol	Chain	Res	Type
1	D	62	ASN
1	A	361	GLN
1	B	11	ASN
2	G	44	ASN
2	H	141	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 36 ligands modelled in this entry, 4 are monoatomic and 2 are modelled with single atom - leaving 30 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	B	502	-	4,5,5	0.79	0	6,6,6	0.35	0
12	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.19	0
12	SO4	G	304	-	4,4,4	0.28	0	6,6,6	0.26	0
11	SF4	G	308	2	0,12,12	-	-	-		
6	TAM	E	304	-	7,10,10	0.49	0	9,12,12	0.52	0
12	SO4	A	505	-	4,4,4	0.16	0	6,6,6	0.22	0
12	SO4	A	501	-	4,4,4	0.19	0	6,6,6	0.27	0
3	BJ8	B	501	1	0,26,26	-	-	-		
4	PG4	C	502[B]	-	12,12,12	0.54	0	11,11,11	0.50	0
8	ADP	F	302	9	24,29,29	1.11	3 (12%)	29,45,45	1.70	8 (27%)
7	BU3	G	307	-	4,5,5	0.49	0	6,6,6	0.66	0
10	ALF	F	304	-	0,4,4	-	-	-		
10	ALF	H	303	-	0,4,4	-	-	-		
7	BU3	D	504	-	4,5,5	0.66	0	6,6,6	0.43	0
10	ALF	E	303	-	0,4,4	-	-	-		
8	ADP	E	301	9	24,29,29	1.22	3 (12%)	29,45,45	1.60	5 (17%)
6	TAM	D	503	-	7,10,10	0.61	0	9,12,12	1.27	1 (11%)
10	ALF	G	303	-	0,4,4	-	-	-		
3	BJ8	D	501	1	0,26,26	-	-	-		
7	BU3	B	503	-	4,5,5	0.64	0	6,6,6	0.80	0
8	ADP	H	301	9	24,29,29	1.18	2 (8%)	29,45,45	1.74	4 (13%)
4	PG4	C	502[A]	-	12,12,12	0.64	0	11,11,11	0.71	0
5	GOL	D	502	-	5,5,5	0.97	0	5,5,5	0.82	0
6	TAM	B	504	-	7,10,10	0.49	0	9,12,12	1.68	3 (33%)
3	BJ8	A	504	1	0,26,26	-	-	-		
12	SO4	F	305	-	4,4,4	0.14	0	6,6,6	0.29	0
8	ADP	G	301	9	24,29,29	1.34	3 (12%)	29,45,45	1.63	7 (24%)
11	SF4	F	301	2	0,12,12	-	-	-		
3	BJ8	C	501	1	0,26,26	-	-	-		
6	TAM	G	306	-	7,10,10	0.63	0	9,12,12	0.66	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
7	BU3	B	502	-	-	0/4/4/4	-
11	SF4	G	308	2	-	-	0/6/5/5
6	TAM	E	304	-	-	6/12/12/12	-
3	BJ8	B	501	1	-	-	0/12/10/10
4	PG4	C	502[B]	-	-	4/10/10/10	-
8	ADP	F	302	9	-	1/12/32/32	0/3/3/3
7	BU3	G	307	-	-	4/4/4/4	-
7	BU3	D	504	-	-	0/4/4/4	-
8	ADP	E	301	9	-	0/12/32/32	0/3/3/3
6	TAM	D	503	-	-	9/12/12/12	-
3	BJ8	D	501	1	-	-	0/12/10/10
7	BU3	B	503	-	-	2/4/4/4	-
8	ADP	H	301	9	-	1/12/32/32	0/3/3/3
4	PG4	C	502[A]	-	-	3/10/10/10	-
5	GOL	D	502	-	-	4/4/4/4	-
6	TAM	B	504	-	-	8/12/12/12	-
3	BJ8	A	504	1	-	-	0/12/10/10
8	ADP	G	301	9	-	0/12/32/32	0/3/3/3
11	SF4	F	301	2	-	-	0/6/5/5
3	BJ8	C	501	1	-	-	0/12/10/10
6	TAM	G	306	-	-	3/12/12/12	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	301	ADP	C2-N3	3.59	1.37	1.32
8	G	301	ADP	C2-N3	3.26	1.37	1.32
8	G	301	ADP	O4'-C1'	3.25	1.45	1.41
8	E	301	ADP	O4'-C1'	3.20	1.45	1.41
8	H	301	ADP	C5-C4	3.00	1.48	1.40

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	302	ADP	C3'-C2'-C1'	5.13	108.71	100.98
8	H	301	ADP	C3'-C2'-C1'	4.84	108.27	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	301	ADP	N3-C2-N1	-4.33	121.91	128.68
8	E	301	ADP	C3'-C2'-C1'	4.33	107.50	100.98
8	E	301	ADP	N3-C2-N1	-4.24	122.05	128.68

There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	502	GOL	O1-C1-C2-C3
5	D	502	GOL	O2-C2-C3-O3
6	D	503	TAM	C2-C-C1-C4
6	D	503	TAM	C3-C-C1-C4
6	D	503	TAM	N-C-C1-C4

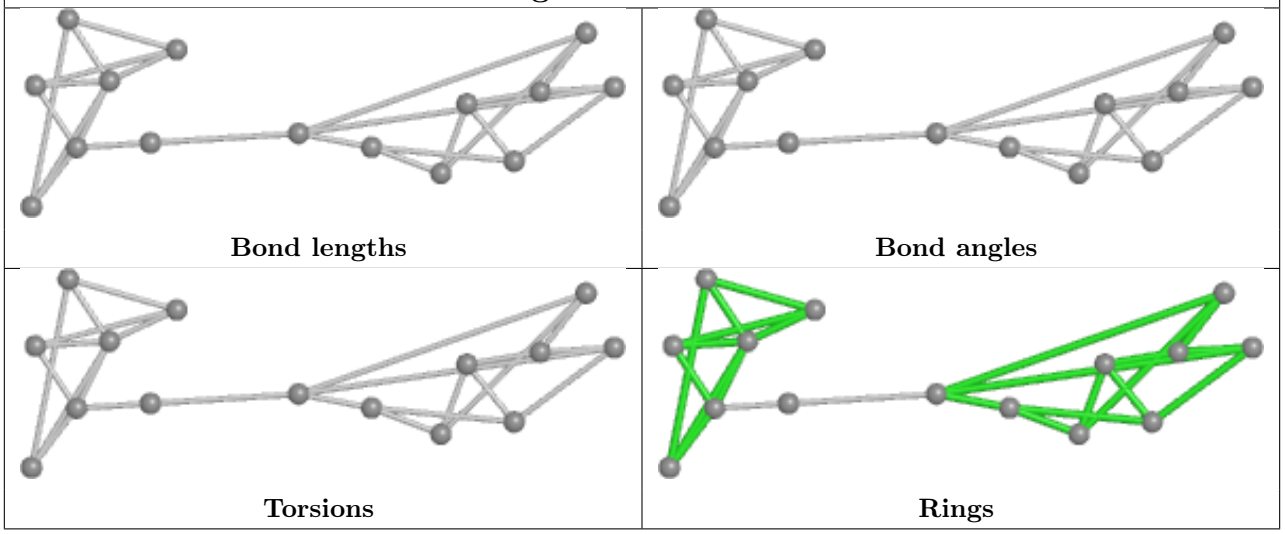
There are no ring outliers.

8 monomers are involved in 13 short contacts:

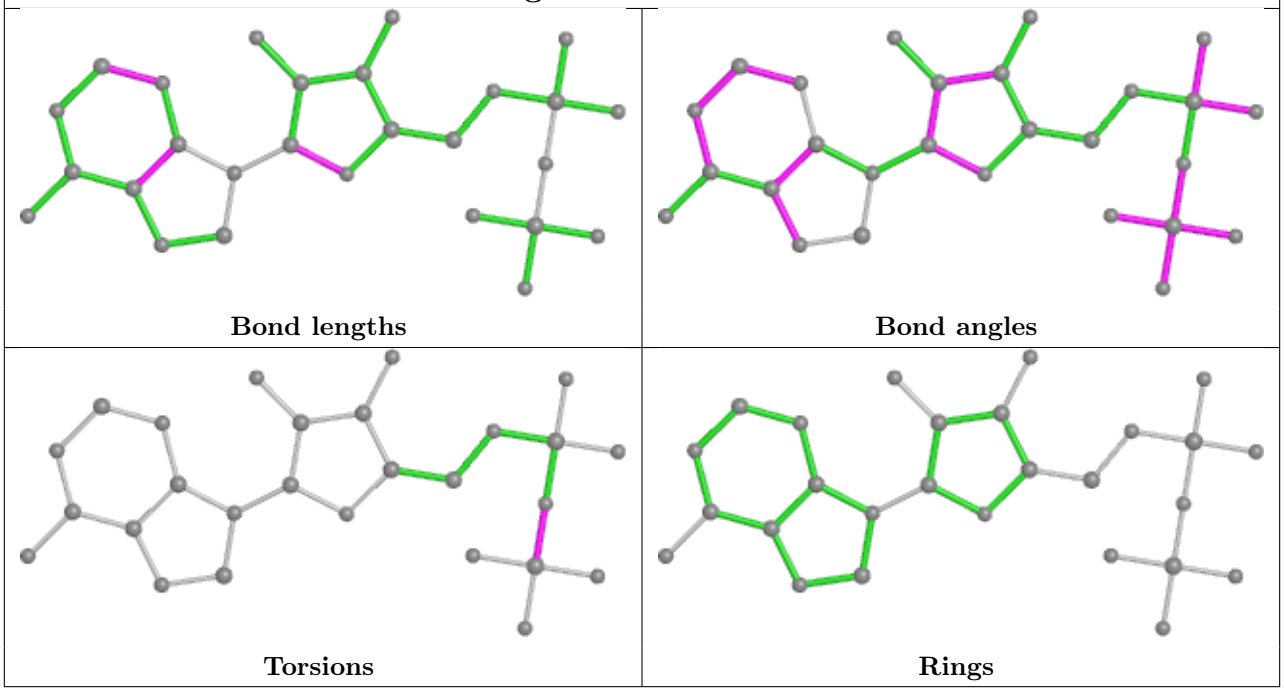
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	304	SO4	1	0
12	A	501	SO4	1	0
4	C	502[B]	PG4	1	0
7	B	503	BU3	3	0
8	H	301	ADP	1	0
4	C	502[A]	PG4	4	0
6	B	504	TAM	1	0
3	C	501	BJ8	1	0

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.

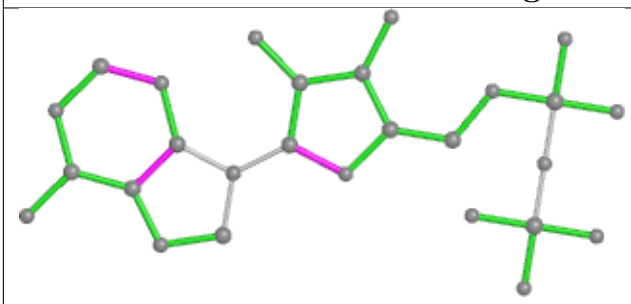
Ligand BJ8 B 501



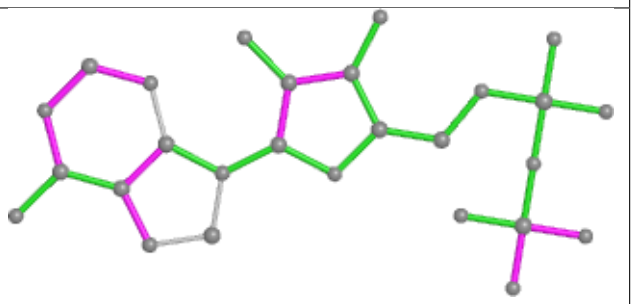
Ligand ADP F 302



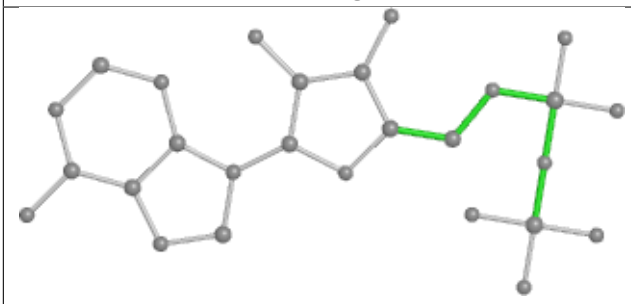
Ligand ADP E 301



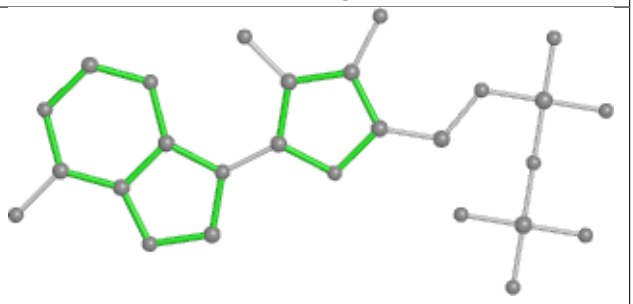
Bond lengths



Bond angles

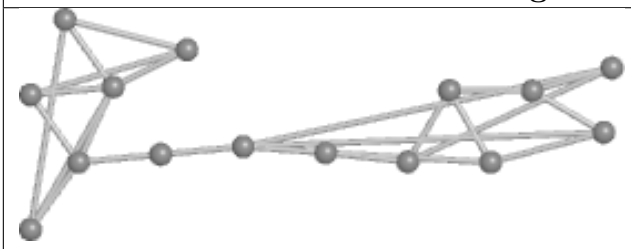


Torsions

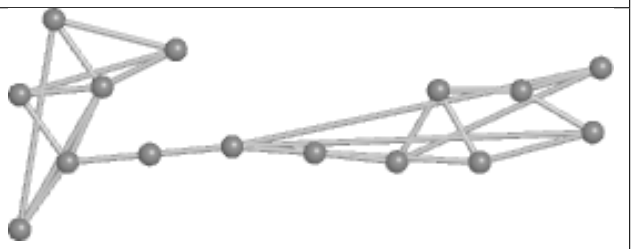


Rings

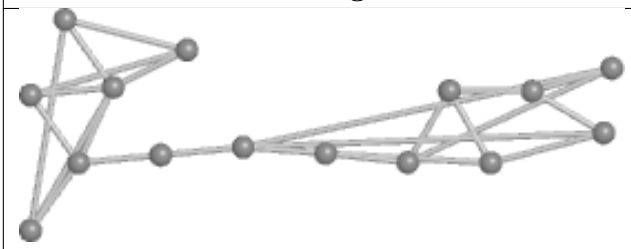
Ligand BJ8 D 501



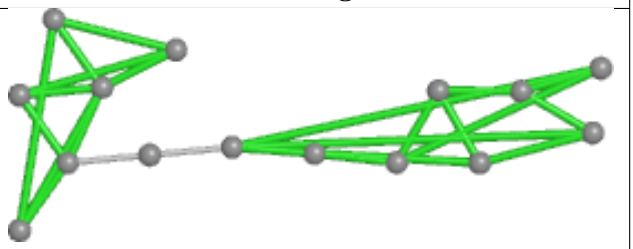
Bond lengths



Bond angles

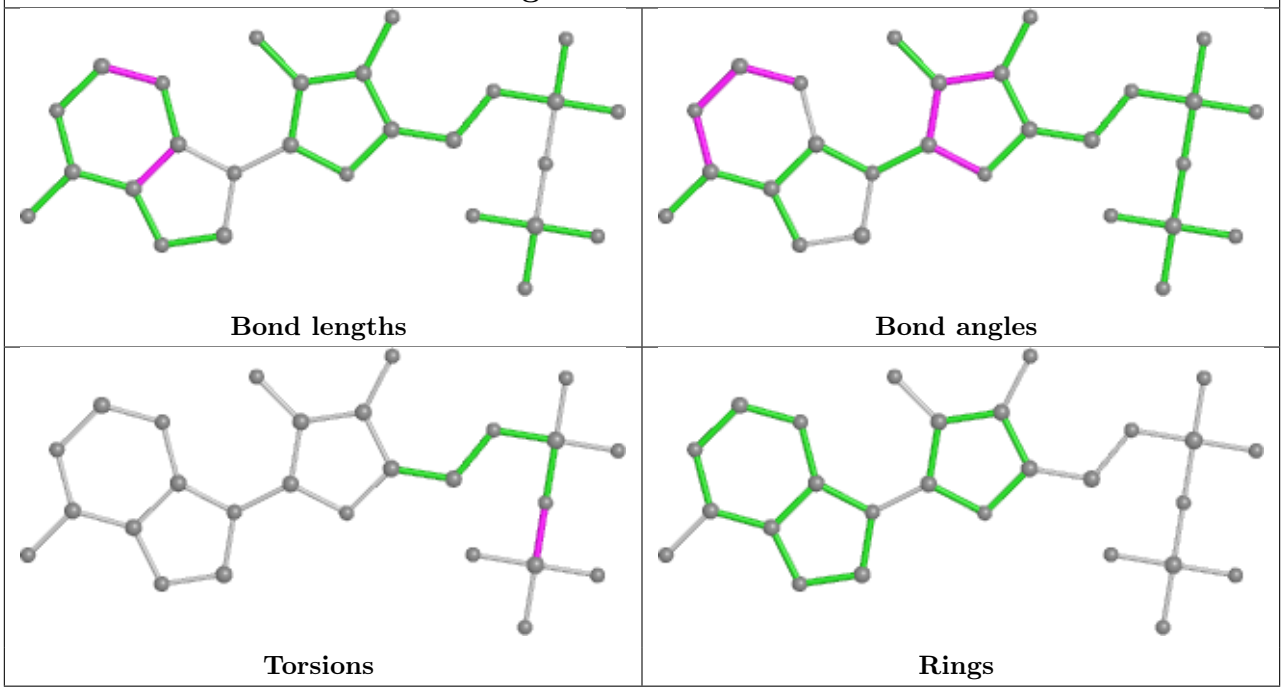


Torsions

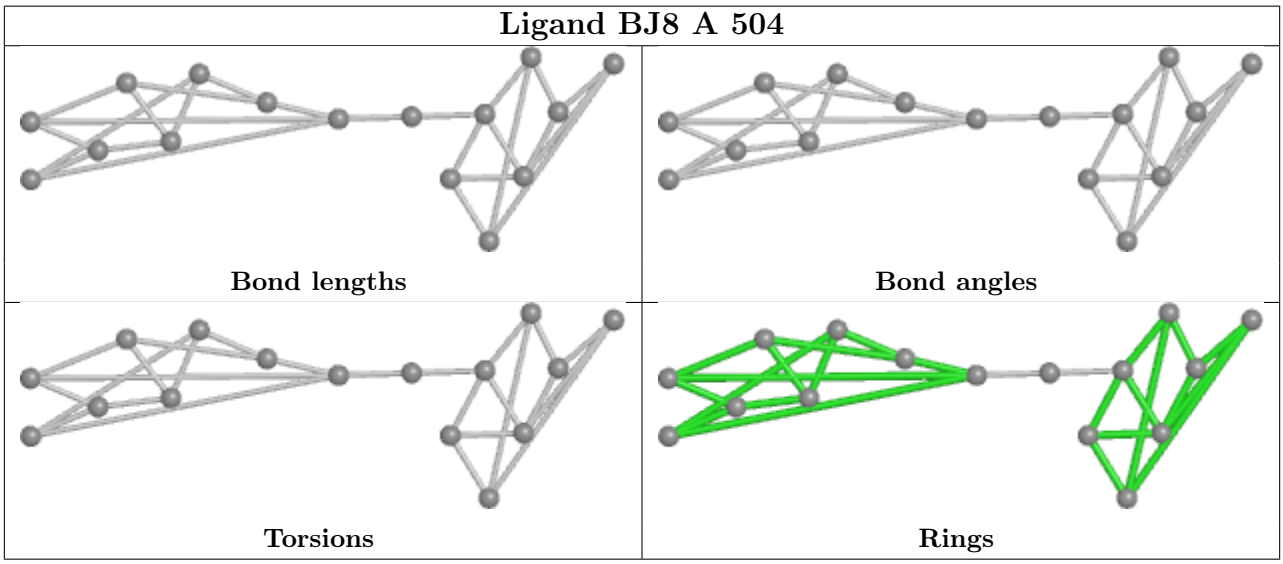


Rings

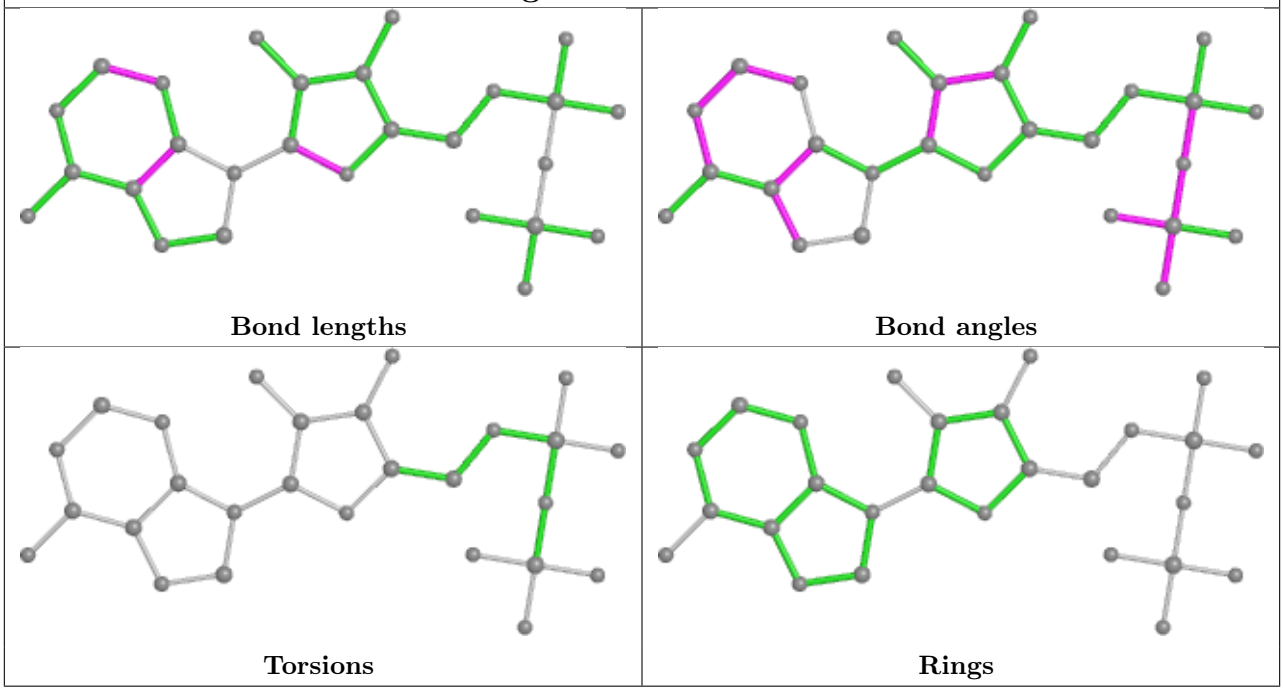
Ligand ADP H 301



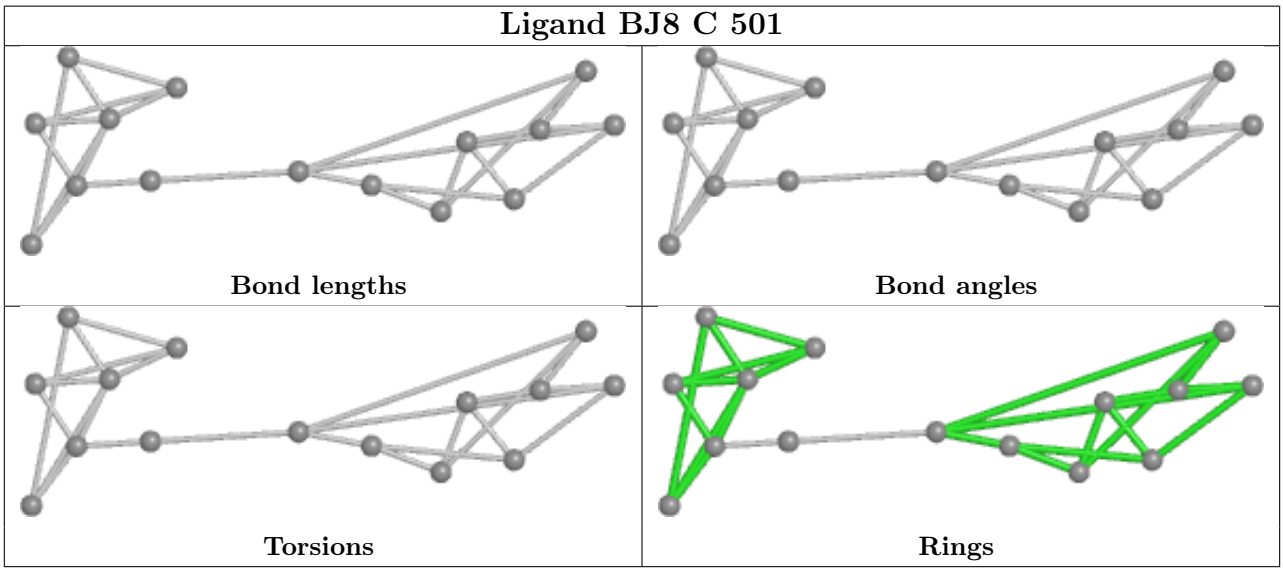
Ligand BJ8 A 504



Ligand ADP G 301



Ligand BJ8 C 501



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, 95^{th} 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	421/422 (99%)	-0.33	2 (0%) 91 94	11, 18, 29, 75	0
1	B	422/422 (100%)	0.06	13 (3%) 49 58	15, 26, 40, 85	0
1	C	420/422 (99%)	-0.38	1 (0%) 95 97	11, 17, 30, 42	1 (0%)
1	D	421/422 (99%)	0.00	12 (2%) 51 60	14, 27, 40, 79	0
2	E	243/243 (100%)	-0.01	14 (5%) 23 31	11, 21, 60, 107	9 (3%)
2	F	243/243 (100%)	0.54	26 (10%) 6 9	14, 33, 60, 75	13 (5%)
2	G	243/243 (100%)	0.02	15 (6%) 20 29	11, 21, 65, 102	9 (3%)
2	H	243/243 (100%)	0.78	38 (15%) 2 3	14, 36, 71, 88	10 (4%)
All	All	2656/2660 (99%)	0.02	121 (4%) 32 42	11, 24, 50, 107	42 (1%)

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	134	TYR	8.1
2	E	140	ILE	7.2
2	E	134	TYR	6.9
2	G	140	ILE	6.7
1	D	1	MET	6.4

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 (i)

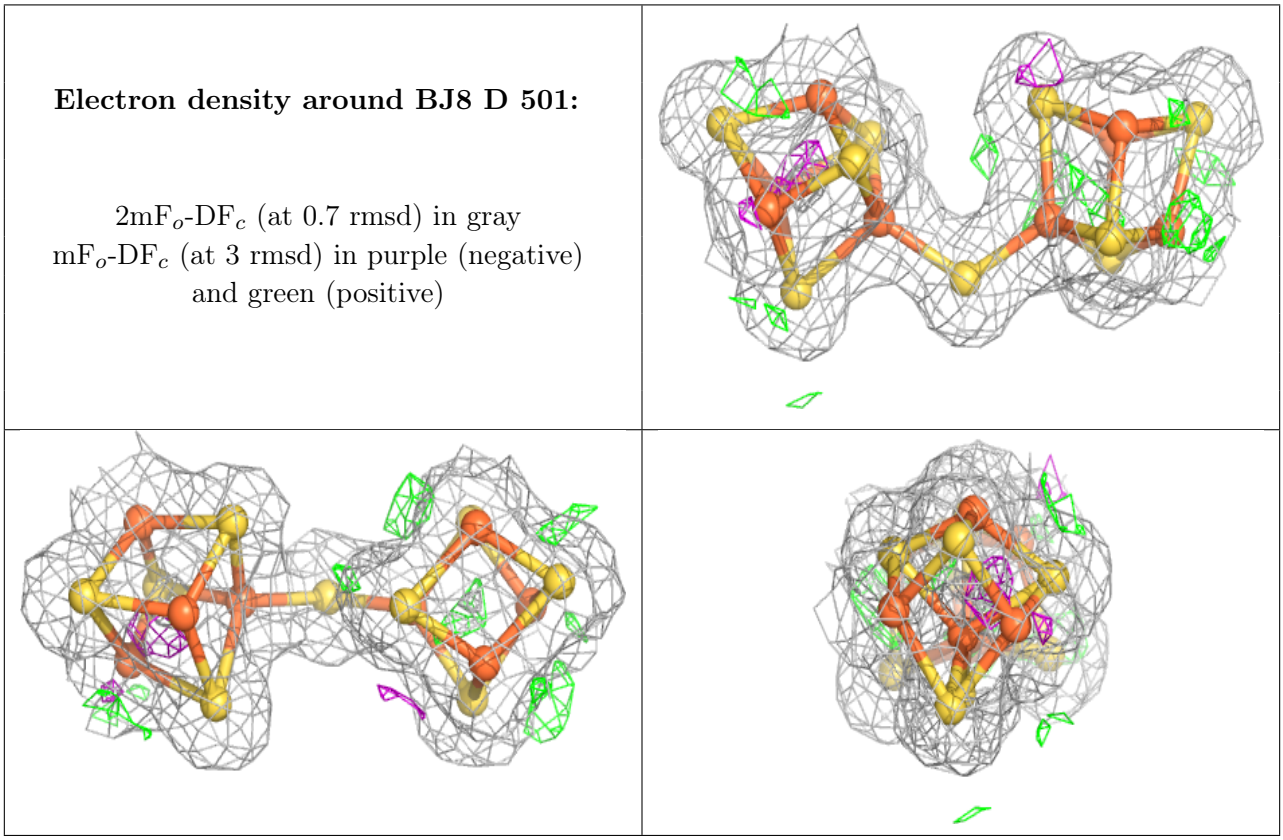
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	TAM	E	304	11/11	0.46	0.28	59,75,82,83	0
6	TAM	B	504	11/11	0.62	0.23	42,56,67,68	28
6	TAM	G	306	11/11	0.68	0.28	31,42,52,54	28
7	BU3	B	502	6/6	0.69	0.22	29,44,50,51	0
7	BU3	D	504	6/6	0.70	0.21	48,64,77,78	0
7	BU3	B	503	6/6	0.77	0.26	35,55,61,62	16
6	TAM	D	503	11/11	0.81	0.17	30,39,56,59	0
4	PG4	C	502[B]	13/13	0.82	0.24	26,32,39,42	31
4	PG4	C	502[A]	13/13	0.82	0.24	27,33,40,44	31
12	SO4	A	503	5/5	0.84	0.23	33,34,41,44	5
7	BU3	G	307	6/6	0.85	0.30	34,49,65,65	16
5	GOL	D	502	6/6	0.86	0.19	29,37,53,64	14
12	SO4	A	505	5/5	0.87	0.29	26,33,35,46	5
12	SO4	F	305	5/5	0.90	0.23	27,34,41,44	5
13	NH4	G	305	1/1	0.93	0.19	27,27,27,27	0
13	NH4	A	502	1/1	0.94	0.15	21,21,21,21	0
12	SO4	A	501	5/5	0.96	0.11	33,36,42,45	0
10	ALF	F	304	5/5	0.97	0.09	20,21,25,25	0
10	ALF	H	303	5/5	0.98	0.07	21,23,29,30	0
3	BJ8	D	501	17/17	0.98	0.07	16,19,26,26	0
8	ADP	E	301	27/27	0.98	0.10	10,19,38,46	0
8	ADP	F	302	27/27	0.98	0.09	17,27,38,45	0
8	ADP	H	301	27/27	0.98	0.08	20,27,38,44	0
12	SO4	G	304	5/5	0.98	0.07	36,36,43,44	0
3	BJ8	B	501	17/17	0.98	0.08	18,20,27,29	0
10	ALF	G	303	5/5	0.98	0.10	11,12,15,16	0
9	MG	F	303	1/1	0.99	0.07	21,21,21,21	0
9	MG	G	302	1/1	0.99	0.07	10,10,10,10	0
9	MG	H	302	1/1	0.99	0.08	25,25,25,25	0
10	ALF	E	303	5/5	0.99	0.09	8,12,14,15	0
3	BJ8	A	504	17/17	0.99	0.08	12,15,18,19	0
8	ADP	G	301	27/27	0.99	0.07	10,19,38,40	0
3	BJ8	C	501	17/17	0.99	0.07	11,14,18,18	0
11	SF4	F	301	8/8	1.00	0.10	13,15,17,18	0
11	SF4	G	308	8/8	1.00	0.10	13,16,18,18	0
9	MG	E	302	1/1	1.00	0.05	12,12,12,12	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.

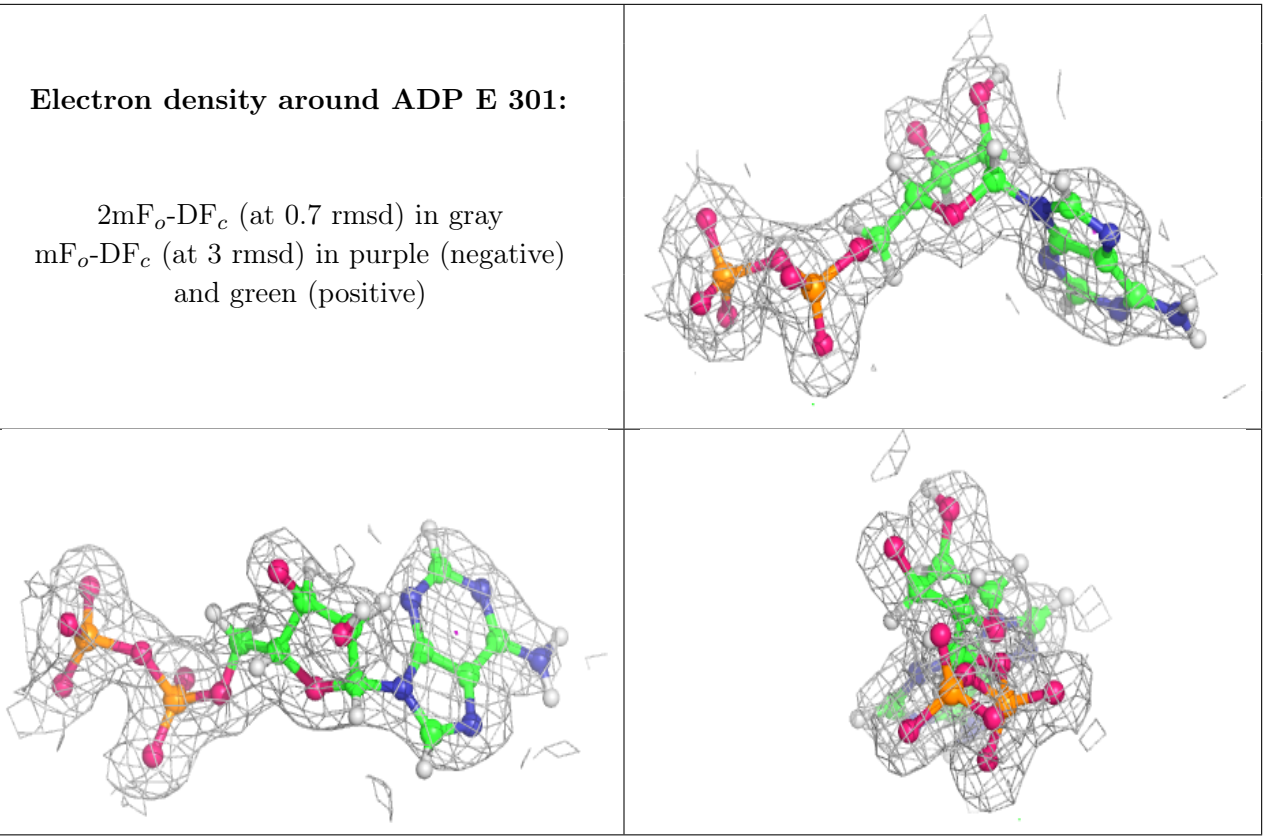
Electron density around BJ8 D 501:

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



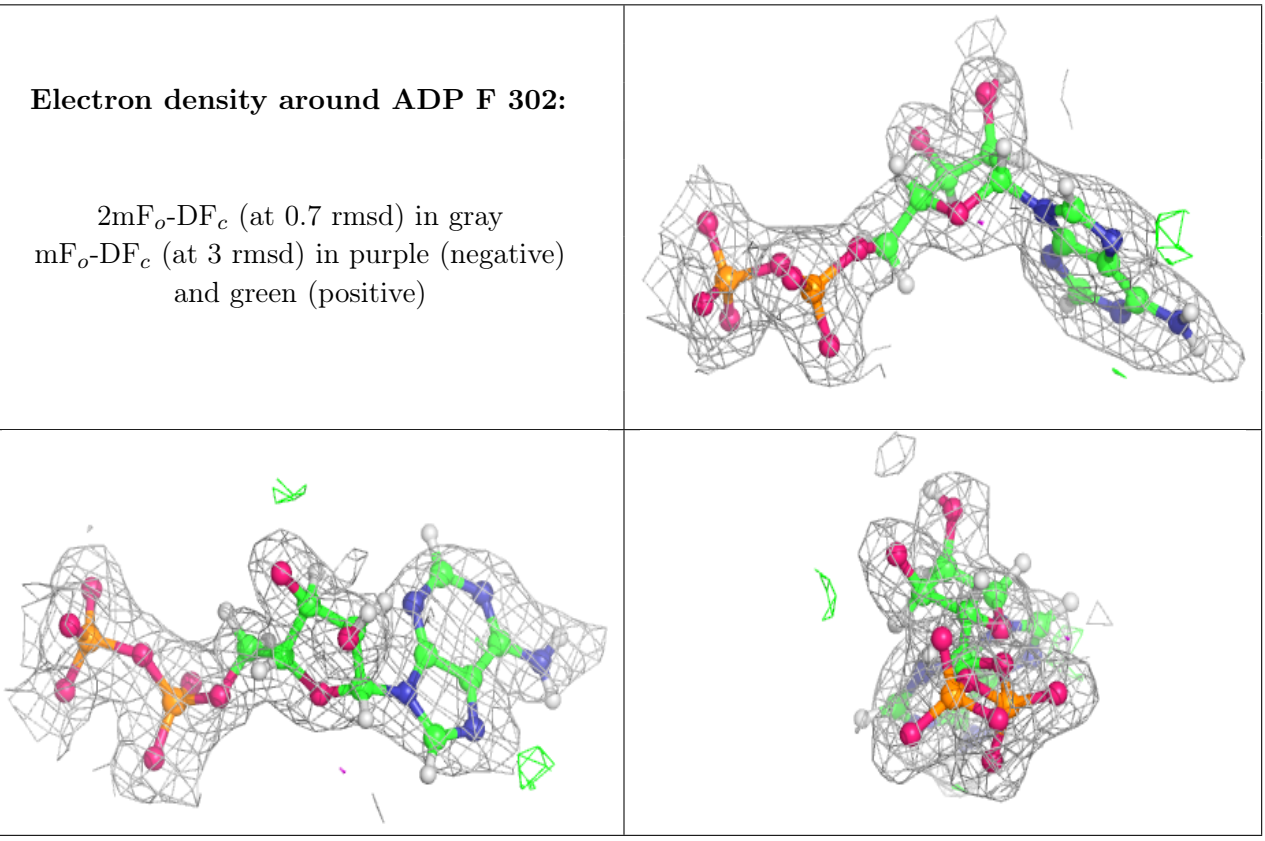
Electron density around ADP E 301:

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



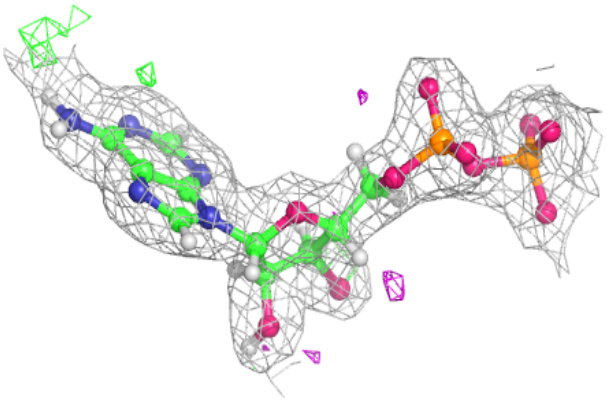
Electron density around ADP F 302:

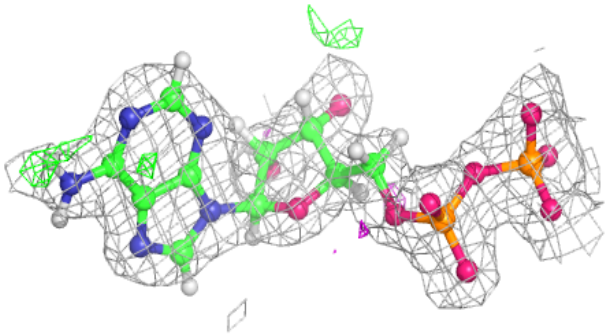
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

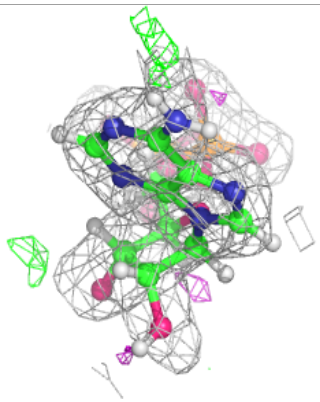


Electron density around ADP H 301:

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

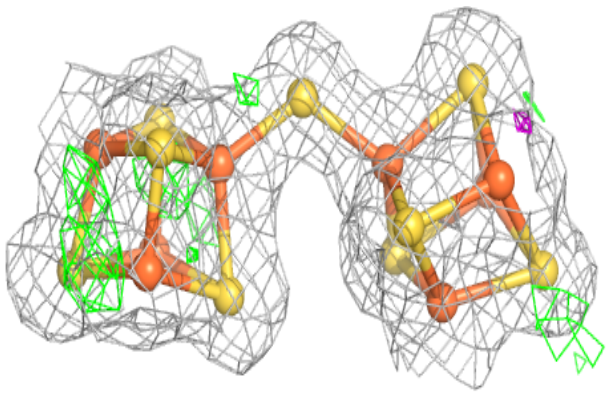


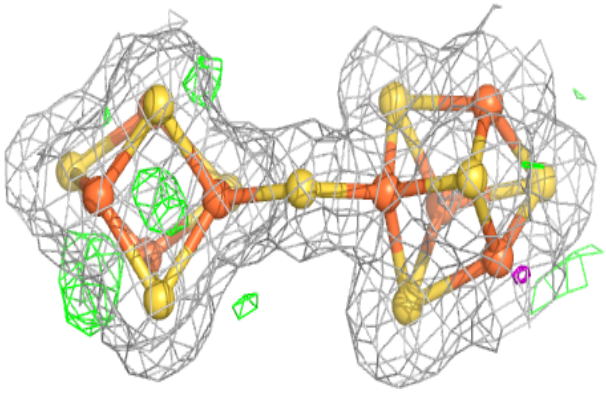


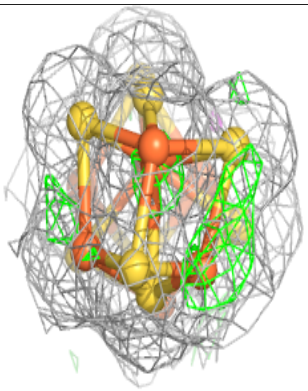


Electron density around BJ8 B 501:

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

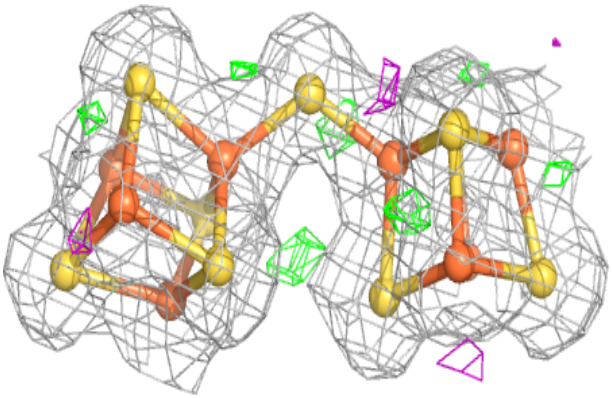


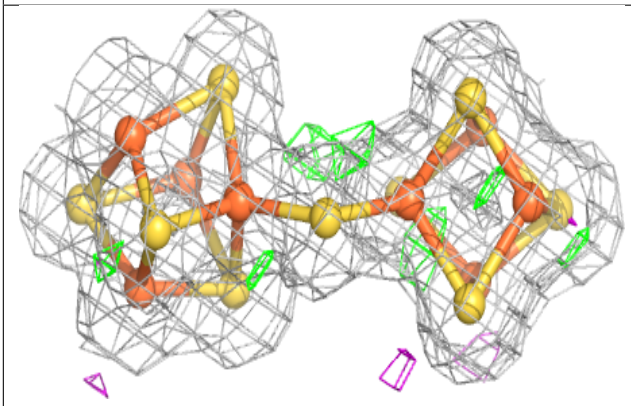


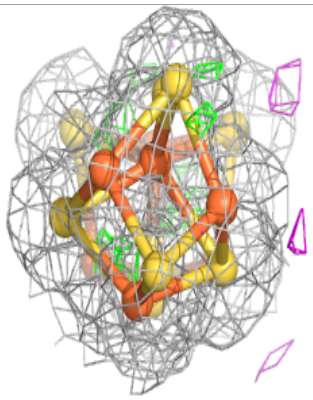


Electron density around BJ8 A 504:

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

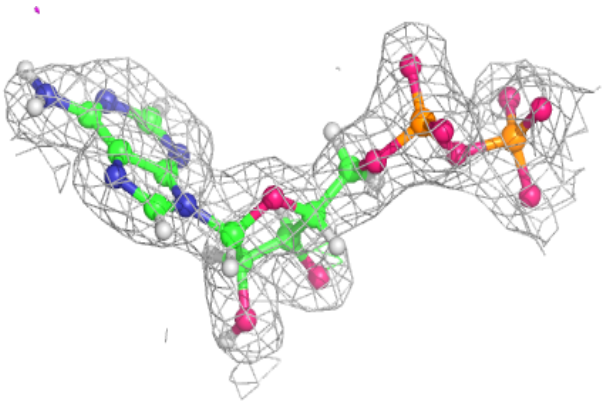


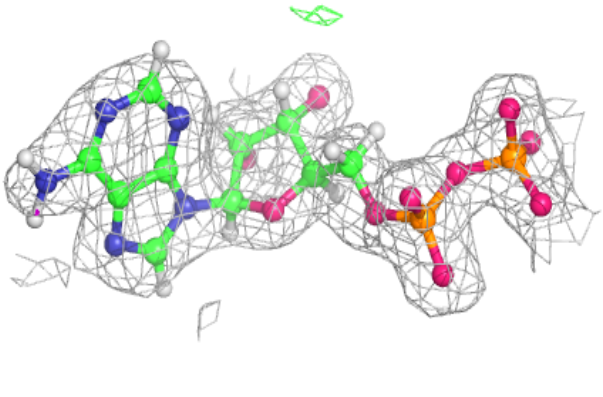


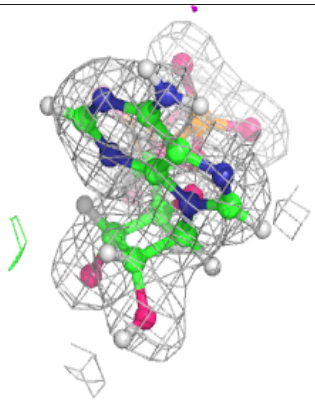


Electron density around ADP G 301:

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

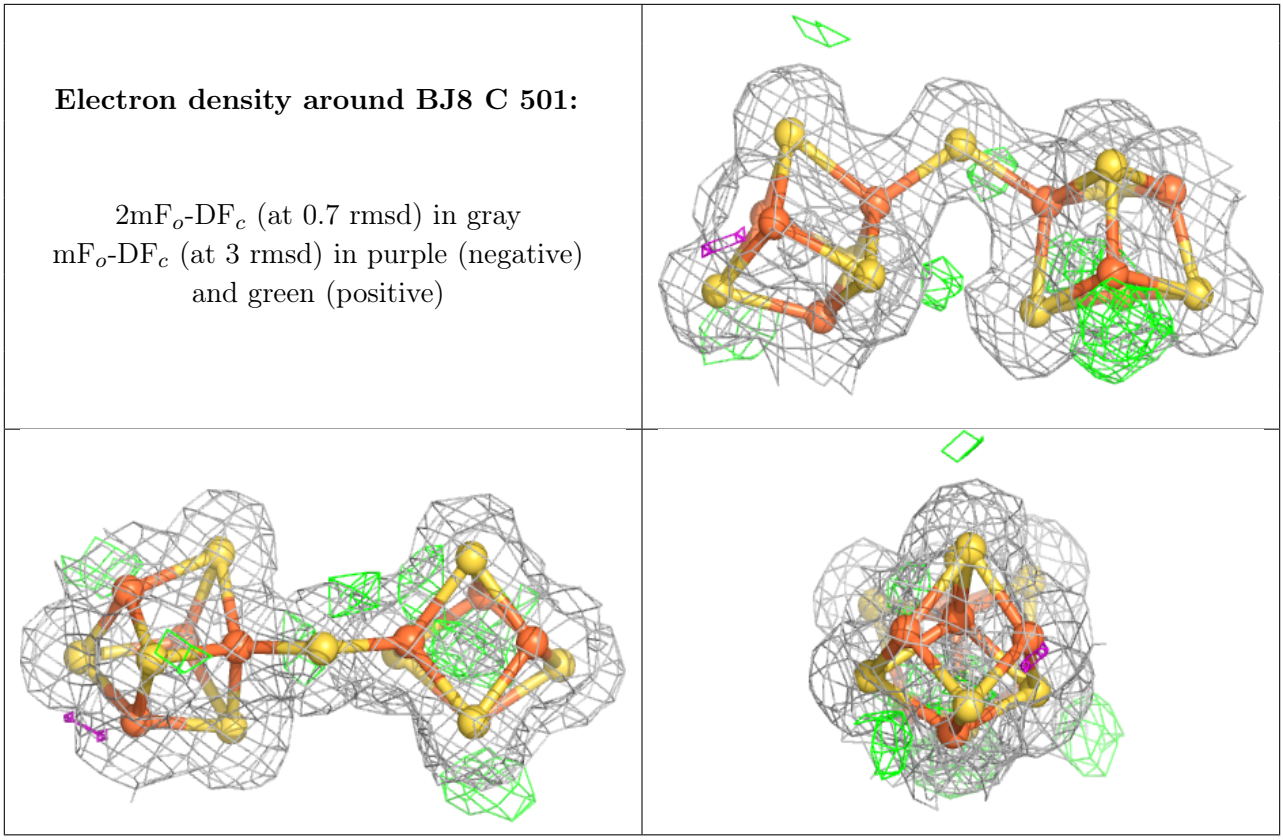






Electron density around BJ8 C 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.