Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 11:26 AM EDT

PDB ID	:	6X9N
Title	:	Pseudomonas aeruginosa MurC with AZ5595
Authors	:	Horanyi, P.S.; Mayclin, S.J.; Durand-Reville, T.F.; Lorimer, D.D.; Edwards, T.E.; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2020-06-03
Resolution	:	2.25 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:

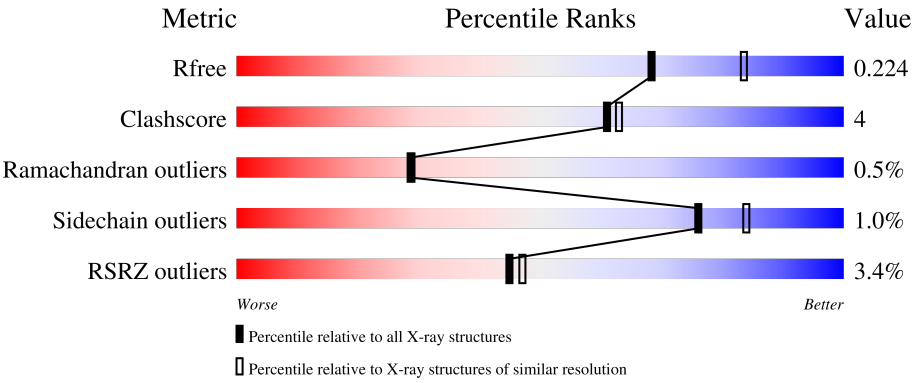
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	466	3% 56% 9% 35%
1	B	466	3% 58% 7% 35%
1	C	466	3% 58% 8% 35%
1	D	466	2% 59% 7% 35%
1	E	466	% 58% 7% 35%

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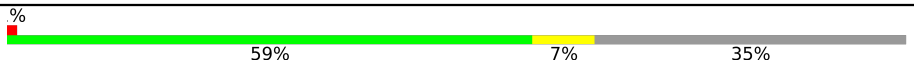
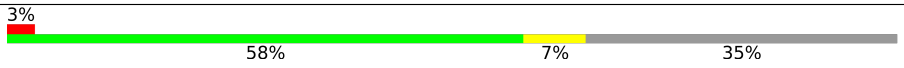
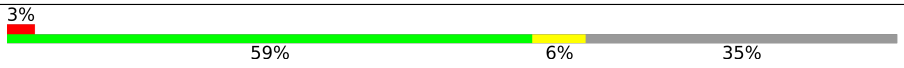
Mol	Chain	Length	Quality of chain
1	F	466	
1	G	466	
1	H	466	

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
3	EDO	F	502	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19389 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

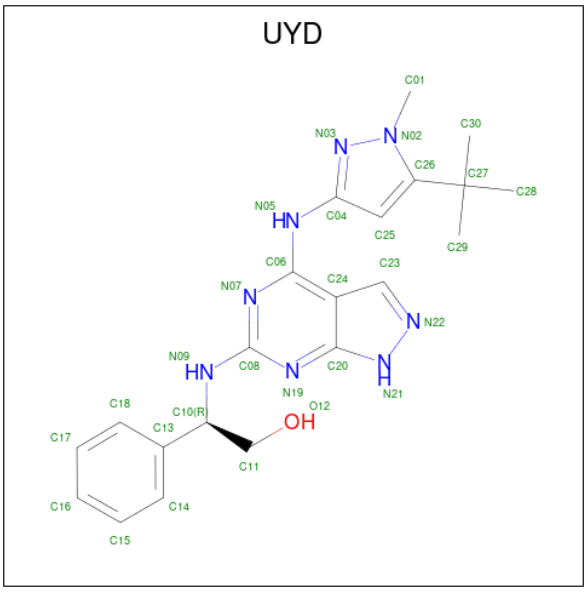
- Molecule 1 is a protein called UDP-N-acetylmuramate--L-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	3	0
			2240	1416	393	422	9			
1	B	305	Total	C	N	O	S	0	4	0
			2273	1433	399	431	10			
1	C	305	Total	C	N	O	S	0	2	0
			2235	1411	394	421	9			
1	D	305	Total	C	N	O	S	0	2	0
			2246	1417	396	424	9			
1	E	305	Total	C	N	O	S	0	4	0
			2287	1441	406	431	9			
1	F	305	Total	C	N	O	S	0	2	0
			2260	1425	398	428	9			
1	G	305	Total	C	N	O	S	0	3	0
			2260	1428	399	424	9			
1	H	305	Total	C	N	O	S	0	2	0
			2261	1426	397	429	9			

There are 8 discrepancies between the modelled and reference sequences:

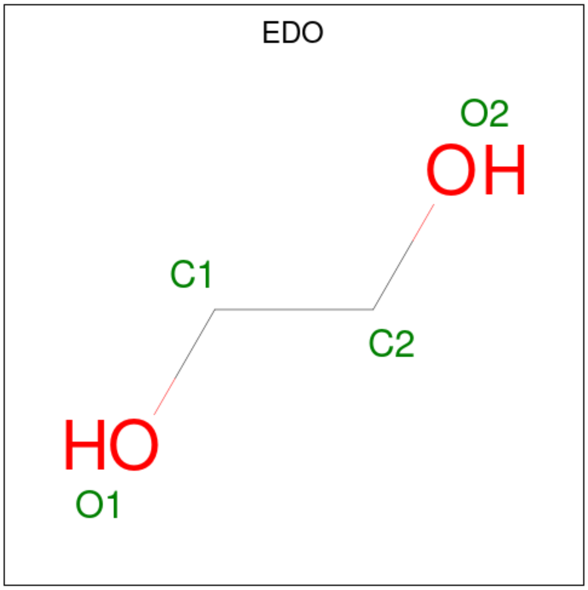
Chain	Residue	Modelled	Actual	Comment	Reference
A	15	HIS	-	expression tag	UNP Q9HW02
B	15	HIS	-	expression tag	UNP Q9HW02
C	15	HIS	-	expression tag	UNP Q9HW02
D	15	HIS	-	expression tag	UNP Q9HW02
E	15	HIS	-	expression tag	UNP Q9HW02
F	15	HIS	-	expression tag	UNP Q9HW02
G	15	HIS	-	expression tag	UNP Q9HW02
H	15	HIS	-	expression tag	UNP Q9HW02

- Molecule 2 is (2R)-2-({4-[(5-tert-butyl-1-methyl-1H-pyrazol-3-yl)amino]-1H-pyrazolo[3,4-d]pyrimidin-6-yl}amino)-2-phenylethan-1-ol (three-letter code: UYD) (formula: $C_{21}H_{26}N_8O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	21	8	1		
2	B	1	Total	C	N	O	0	0
			30	21	8	1		
2	C	1	Total	C	N	O	0	0
			30	21	8	1		
2	D	1	Total	C	N	O	0	0
			30	21	8	1		
2	E	1	Total	C	N	O	0	0
			30	21	8	1		
2	F	1	Total	C	N	O	0	0
			30	21	8	1		
2	G	1	Total	C	N	O	0	0
			30	21	8	1		
2	H	1	Total	C	N	O	0	0
			30	21	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

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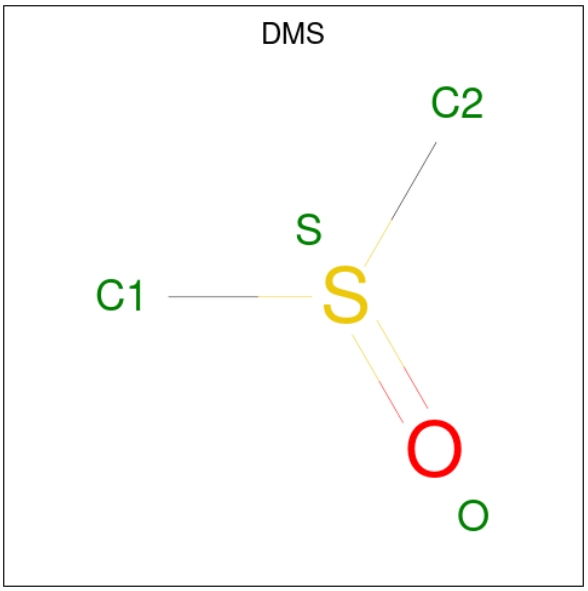
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).

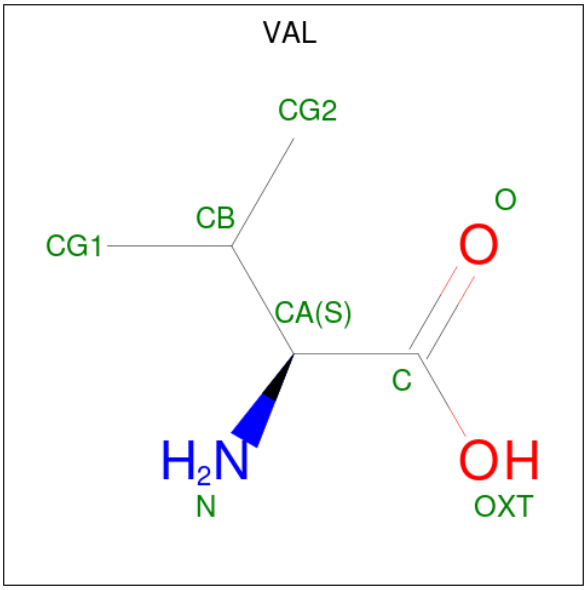


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	E	1	Total C O S 4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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	F	1	Total Cl 1 1	0	0
5	G	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0

- Molecule 6 is VALINE (three-letter code: VAL) (formula: $C_5H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C N O 7 5 1 1	0	0

- Molecule 7 is water.

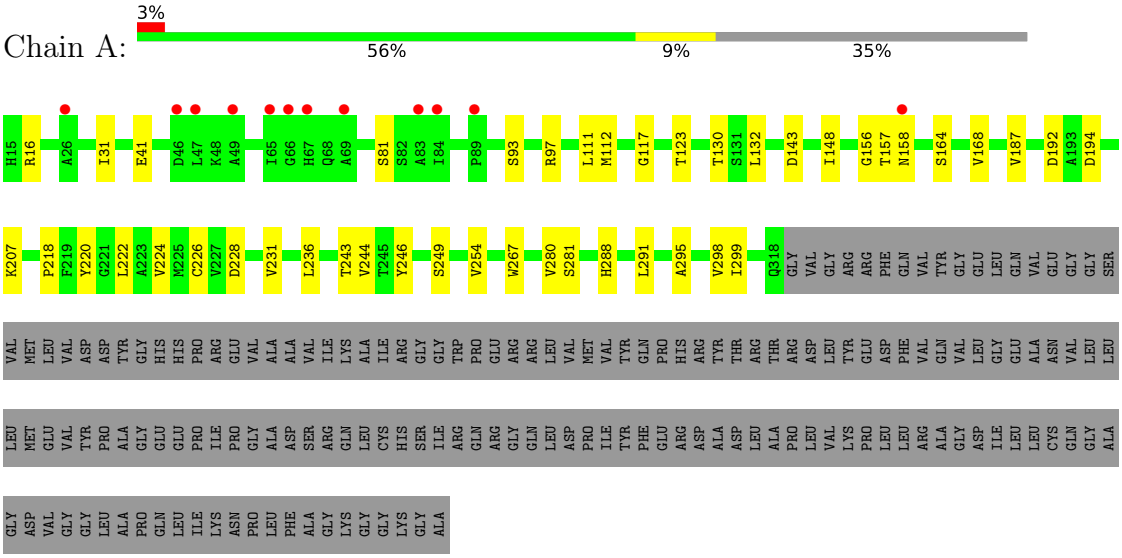
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	108	Total O 108 108	0	0
7	B	113	Total O 113 113	0	0
7	C	100	Total O 100 100	0	0
7	D	109	Total O 109 109	0	0
7	E	110	Total O 110 110	0	0
7	F	111	Total O 111 111	0	0
7	G	102	Total O 102 102	0	0
7	H	127	Total O 127 127	0	0

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.

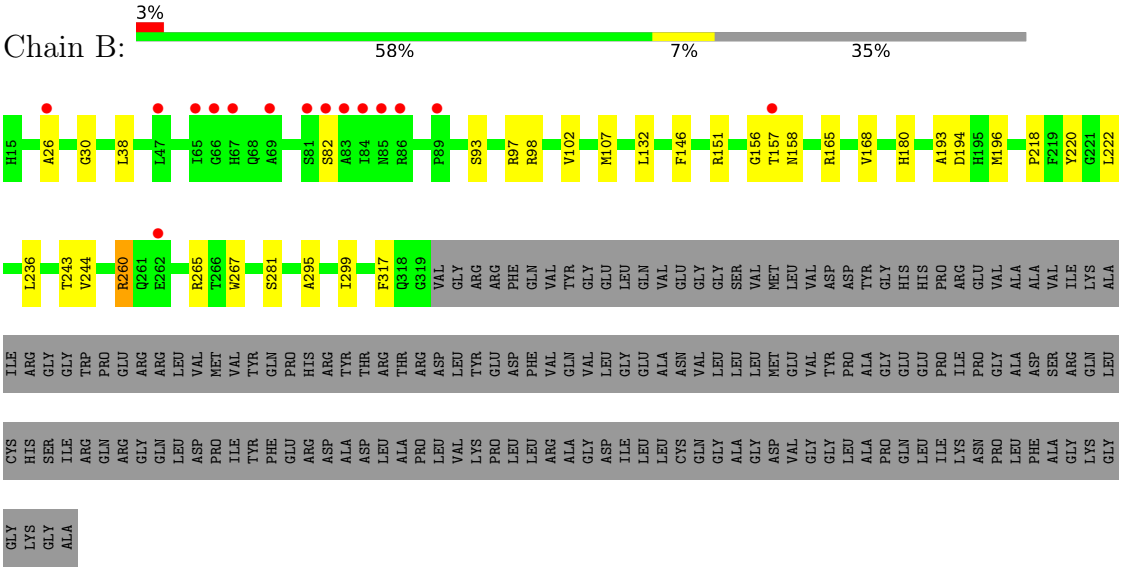
• Molecule 1: UDP-N-acetylmuramate--L-alanine ligase

Chain A:



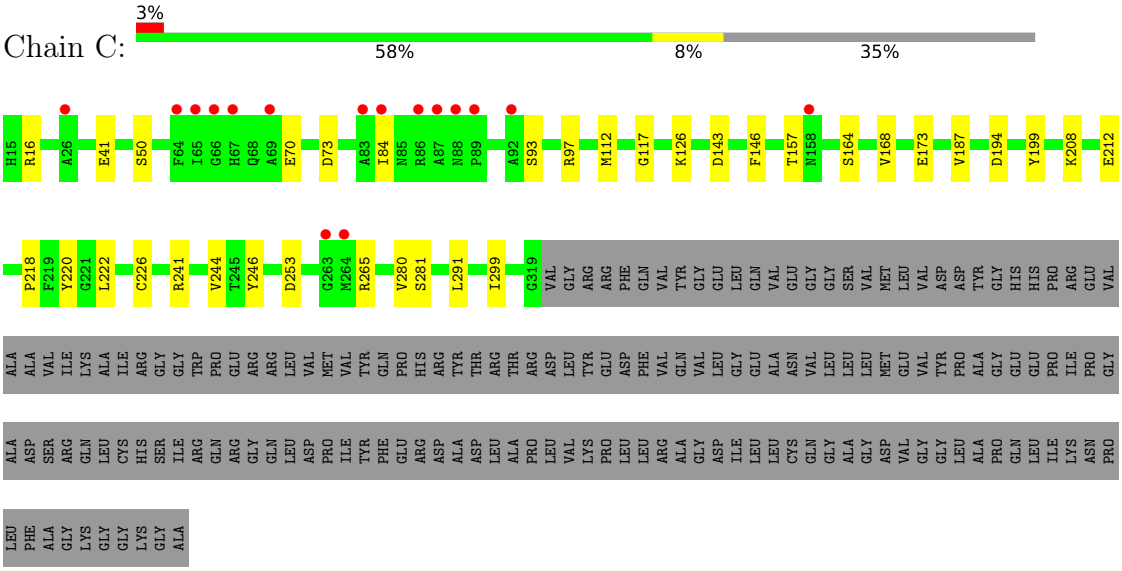
• Molecule 1: UDP-N-acetylmuramate--L-alanine ligase

Chain B:



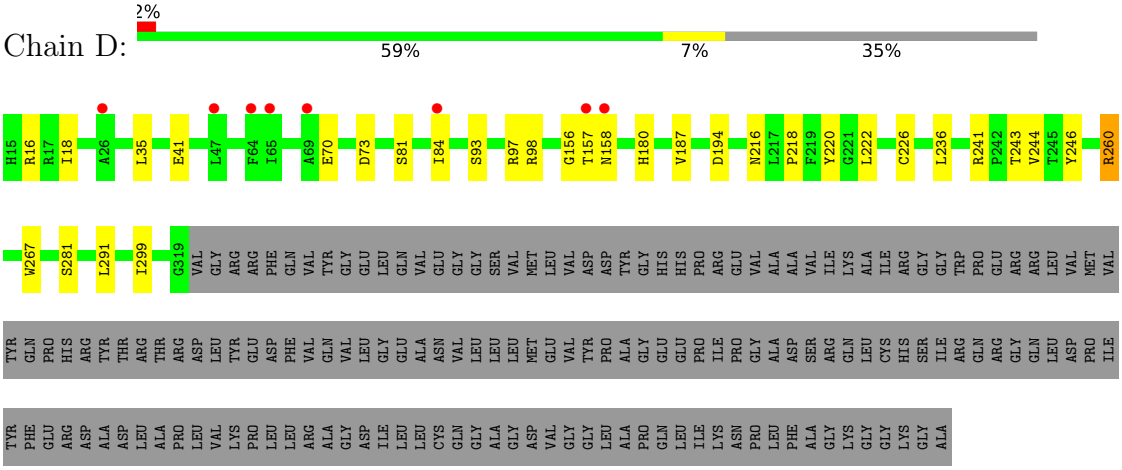
• Molecule 1: UDP-N-acetylmuramate--L-alanine ligase

Chain C:



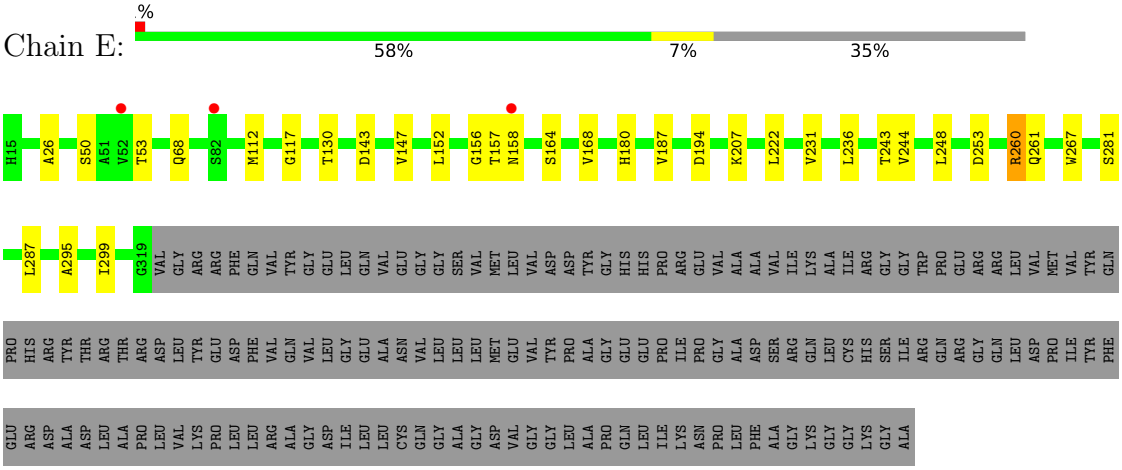
• Molecule 1: UDP-N-acetylmuramate--L-alanine ligase

Chain D:



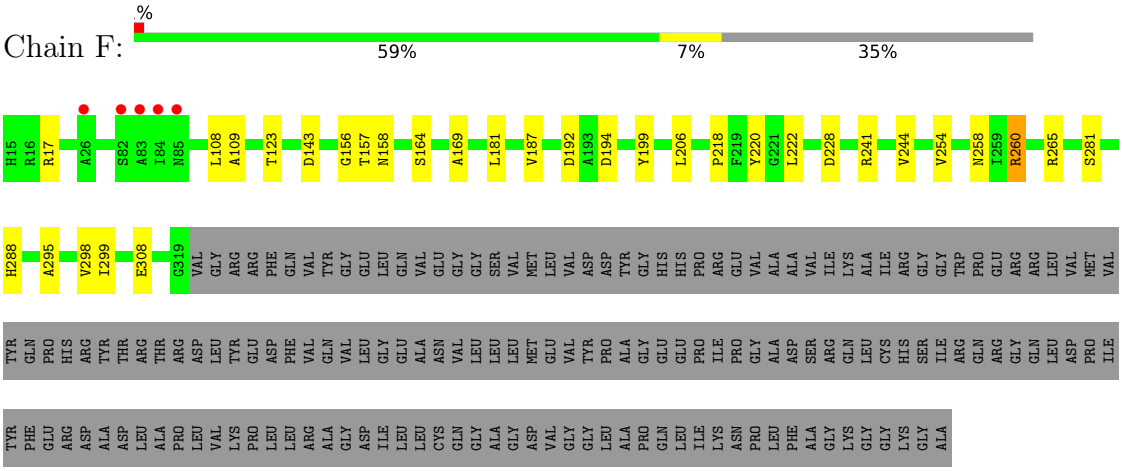
• Molecule 1: UDP-N-acetylmuramate--L-alanine ligase

Chain E:



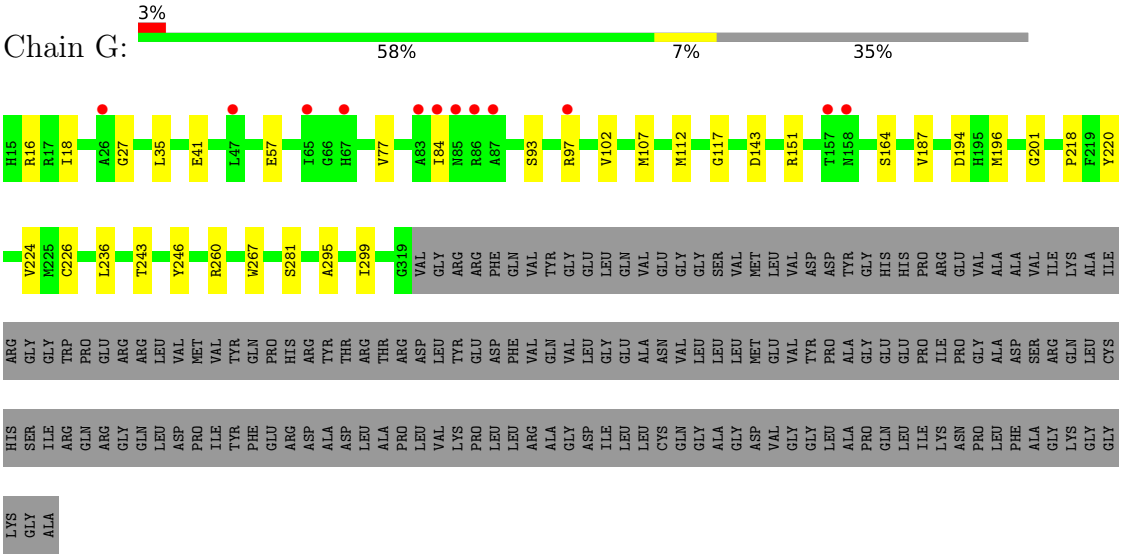
• Molecule 1: UDP-N-acetylmuramate--L-alanine ligase

Chain F:



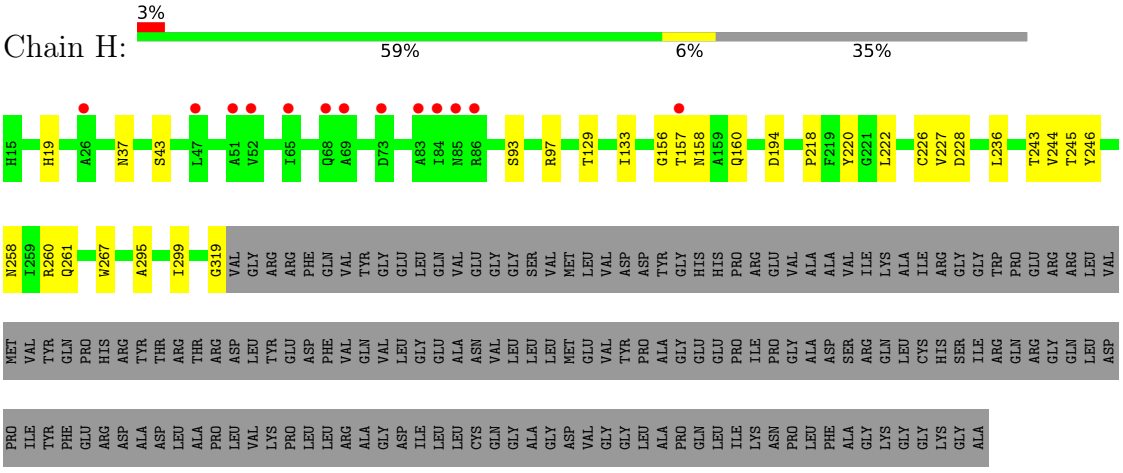
• Molecule 1: UDP-N-acetylmuramate--L-alanine ligase

Chain G:



• Molecule 1: UDP-N-acetylmuramate--L-alanine ligase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	285.65Å 109.10Å 108.43Å 90.00° 112.28° 90.00°	Depositor
Resolution (Å)	47.75 – 2.25 47.92 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.75-2.25) 92.4 (47.92-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.51 (at 2.24Å)	Xtriage
Refinement program	PHENIX (dev_2744: ???)	Depositor
R, R_{free}	0.181 , 0.222 0.182 , 0.224	Depositor DCC
R_{free} test set	2005 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å^2)	34.8	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	0.025 for -h-k-l,l,k 0.022 for -h+k-l,-l,-k 0.036 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19389	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8676e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: CL, UYD, DMS, EDO

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	0.39	0/2288	0.55	0/3117
1	B	0.40	0/2324	0.58	0/3162
1	C	0.38	0/2280	0.56	0/3106
1	D	0.39	0/2291	0.56	0/3121
1	E	0.41	0/2338	0.59	0/3180
1	F	0.40	0/2305	0.56	0/3137
1	G	0.39	0/2308	0.55	0/3143
1	H	0.42	0/2306	0.59	0/3140
All	All	0.40	0/18440	0.57	0/25106

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2240	0	2194	24	0
1	B	2273	0	2243	21	0
1	C	2235	0	2182	19	0
1	D	2246	0	2204	18	0
1	E	2287	0	2268	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2260	0	2220	21	0
1	G	2260	0	2235	20	0
1	H	2261	0	2227	20	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0
2	E	30	0	0	0	0
2	F	30	0	0	0	0
2	G	30	0	0	0	0
2	H	30	0	0	1	0
3	A	16	0	24	1	0
3	B	28	0	42	5	0
3	C	16	0	24	2	0
3	D	16	0	24	4	0
3	E	16	0	24	0	0
3	F	20	0	30	5	0
3	G	12	0	18	0	0
3	H	12	0	18	3	0
4	A	4	0	6	0	0
4	B	16	0	24	2	0
4	C	4	0	6	0	0
4	D	8	0	12	0	0
4	E	8	0	12	0	0
4	F	8	0	12	0	0
4	G	4	0	6	0	0
4	H	4	0	6	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	H	7	0	8	2	0
7	A	108	0	0	1	0
7	B	113	0	0	2	0
7	C	100	0	0	0	0
7	D	109	0	0	2	0
7	E	110	0	0	4	0
7	F	111	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	102	0	0	0	0
7	H	127	0	0	2	0
All	All	19389	0	18069	163	0

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

All (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:LEU:HG	3:F:502:EDO:H11	1.68	0.75
1:G:27:GLY:HA2	1:G:151:ARG:HH11	1.52	0.74
1:C:291:LEU:HD11	3:C:503:EDO:H12	1.69	0.73
1:D:291:LEU:HD11	3:D:504:EDO:H12	1.71	0.72
1:F:288:HIS:ND1	7:F:601:HOH:O	2.22	0.71
1:F:181:LEU:HD21	3:F:502:EDO:H21	1.72	0.71
1:F:241:ARG:HH12	3:H:503:EDO:H21	1.56	0.69
1:C:265:ARG:NH1	1:C:281:SER:OG	2.26	0.68
3:C:502:EDO:H21	1:D:241:ARG:HH22	1.58	0.68
1:C:241:ARG:HH22	3:D:503:EDO:H21	1.59	0.67
1:G:93:SER:OG	1:G:97:ARG:NH1	2.29	0.66
1:H:93:SER:HG	1:H:97:ARG:HH12	1.43	0.66
1:E:156:GLY:O	1:E:158:ASN:N	2.28	0.66
1:E:50:SER:H	1:E:53:THR:HG22	1.60	0.66
1:F:258:ASN:O	1:F:260[B]:ARG:HD3	1.99	0.63
1:E:261:GLN:NE2	7:E:601:HOH:O	2.30	0.63
1:A:16:ARG:HH21	1:A:41:GLU:HG3	1.64	0.62
1:G:16:ARG:NH2	1:G:41:GLU:HG3	2.15	0.62
1:A:93:SER:O	1:A:97:ARG:HG3	2.01	0.60
1:G:16:ARG:HH21	1:G:41:GLU:HG3	1.67	0.59
1:H:37:ASN:HD22	1:H:160:GLN:HE21	1.51	0.59
1:E:260[B]:ARG:HG3	1:E:267:TRP:HB2	1.84	0.59
1:B:93:SER:O	1:B:97:ARG:HG3	2.02	0.59
1:E:50:SER:O	1:E:53:THR:HG22	2.03	0.59
1:G:187:VAL:CG2	1:G:299[B]:ILE:HD11	2.33	0.59
1:A:187:VAL:CG2	1:A:299[B]:ILE:HD11	2.34	0.58
1:C:253:ASP:OD2	1:D:98:ARG:NH1	2.38	0.56
3:B:504:EDO:H12	7:B:706:HOH:O	2.06	0.56
1:C:208:LYS:O	1:C:212:GLU:HG2	2.06	0.56
1:F:156:GLY:O	1:F:158:ASN:N	2.38	0.56
1:G:18:ILE:HD13	1:G:35:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:MET:HG2	1:E:117:GLY:HA3	1.89	0.55
1:D:156:GLY:O	1:D:158:ASN:N	2.40	0.55
1:E:222:LEU:HD11	1:E:244:VAL:HG23	1.88	0.55
1:C:212:GLU:HB3	3:D:502:EDO:H22	1.88	0.55
1:E:50:SER:H	1:E:53:THR:CG2	2.20	0.54
1:H:37:ASN:HD22	1:H:160:GLN:NE2	2.06	0.54
1:E:187:VAL:HG22	1:E:299:ILE:HD11	1.89	0.54
1:D:260[B]:ARG:HG3	1:D:267:TRP:HB2	1.89	0.53
1:F:218:PRO:HB2	1:F:220:TYR:CE1	2.43	0.53
1:H:93:SER:OG	1:H:97:ARG:NH1	2.29	0.53
1:C:112:MET:HG2	1:C:117:GLY:HA3	1.89	0.53
1:D:70:GLU:HA	1:D:73:ASP:OD2	2.09	0.53
1:G:218:PRO:HB2	1:G:220:TYR:CE1	2.44	0.53
1:B:218:PRO:HB2	1:B:220:TYR:CE1	2.43	0.52
1:H:222:LEU:HD11	1:H:244:VAL:HG23	1.90	0.52
1:D:226:CYS:HB2	1:D:246:TYR:CZ	2.45	0.52
1:E:236:LEU:HD11	1:E:243:THR:HG21	1.91	0.52
1:G:295:ALA:O	1:G:299[A]:ILE:HG12	2.10	0.52
1:C:218:PRO:HB2	1:C:220:TYR:CE1	2.45	0.52
1:B:260[B]:ARG:HG3	1:B:267:TRP:HB2	1.91	0.51
1:A:226:CYS:HB2	1:A:246:TYR:CZ	2.45	0.51
1:D:236:LEU:HD11	1:D:243:THR:HG21	1.93	0.51
1:A:187:VAL:HG22	1:A:299[B]:ILE:HD11	1.92	0.51
1:D:187:VAL:CG2	1:D:299:ILE:HD11	2.41	0.50
1:A:295:ALA:O	1:A:299[A]:ILE:HG12	2.11	0.50
1:C:222:LEU:HD11	1:C:244:VAL:HG23	1.94	0.50
1:D:18:ILE:HD13	1:D:35:LEU:HD13	1.92	0.50
1:A:254:VAL:HG21	1:A:298:VAL:HG22	1.94	0.50
1:A:218:PRO:HB2	1:A:220:TYR:CE1	2.47	0.50
1:A:156:GLY:O	1:A:158:ASN:N	2.45	0.49
1:G:260[B]:ARG:HG3	1:G:267:TRP:HB2	1.93	0.49
1:H:260[B]:ARG:HG3	1:H:267:TRP:HB2	1.93	0.49
1:B:30:GLY:H	3:B:508:EDO:H12	1.77	0.49
1:H:236:LEU:HD11	1:H:243:THR:HG21	1.94	0.49
1:A:228:ASP:OD1	1:A:249:SER:OG	2.23	0.49
1:D:93:SER:O	1:D:97:ARG:HG3	2.13	0.49
1:H:156:GLY:O	1:H:158:ASN:N	2.45	0.49
1:B:156:GLY:O	1:B:158:ASN:N	2.47	0.48
1:G:112:MET:HG2	1:G:117:GLY:HA3	1.94	0.48
1:A:16:ARG:NH2	1:A:41:GLU:HG3	2.28	0.48
1:D:187:VAL:HG22	1:D:299:ILE:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ALA:HA	3:F:502:EDO:H22	1.95	0.48
1:E:295:ALA:O	1:E:299:ILE:HG12	2.13	0.48
1:G:224:VAL:HG21	1:G:299[A]:ILE:HD13	1.95	0.47
1:B:236:LEU:HD11	1:B:243:THR:HG21	1.97	0.47
1:B:222:LEU:HD11	1:B:244:VAL:HG23	1.95	0.47
1:B:295:ALA:O	1:B:299:ILE:HG12	2.15	0.47
1:C:173:GLU:O	1:C:199:TYR:OH	2.30	0.47
1:D:267:TRP:CE3	1:D:281:SER:HB3	2.50	0.47
1:H:226:CYS:HB2	1:H:246:TYR:CZ	2.49	0.47
1:H:228:ASP:HB3	3:H:504:EDO:H11	1.96	0.47
2:H:502:UYD:C18	3:H:504:EDO:H22	2.45	0.47
1:G:27:GLY:HA2	1:G:151:ARG:HD2	1.97	0.47
1:C:187:VAL:HG22	1:C:299:ILE:HD11	1.97	0.46
1:A:224:VAL:HG21	1:A:299[A]:ILE:HD13	1.97	0.46
4:B:510:DMS:H11	7:D:665:HOH:O	2.16	0.46
1:F:199:TYR:CE2	1:F:206:LEU:HD23	2.50	0.46
1:F:199:TYR:CD2	1:F:206:LEU:HD23	2.50	0.46
1:B:165:ARG:HG3	3:B:502:EDO:H21	1.98	0.46
1:E:207:LYS:HD3	1:E:231:VAL:HG13	1.98	0.46
1:F:265:ARG:NH1	1:F:281:SER:OG	2.47	0.46
3:B:503:EDO:H21	1:E:180:HIS:NE2	2.31	0.46
1:A:288:HIS:HD2	7:A:686:HOH:O	1.98	0.45
1:A:236:LEU:HD11	1:A:243:THR:HG21	1.98	0.45
1:F:222:LEU:HD11	1:F:244:VAL:HG23	1.98	0.45
1:H:245:THR:HG21	7:H:654:HOH:O	2.17	0.45
1:A:222:LEU:HD11	1:A:244:VAL:HG23	1.98	0.45
1:B:317:PHE:O	7:B:601:HOH:O	2.21	0.45
1:B:98:ARG:NH2	1:E:253:ASP:OD2	2.39	0.45
1:D:180:HIS:NE2	3:D:502:EDO:H21	2.31	0.45
1:H:319:GLY:C	6:H:501:VAL:HG23	2.37	0.45
1:F:169:ALA:HB1	3:F:502:EDO:H12	1.99	0.44
1:H:227:VAL:HG22	1:H:245:THR:HG23	1.98	0.44
1:C:112:MET:CG	1:C:117:GLY:HA3	2.47	0.44
1:E:267:TRP:CE3	1:E:281:SER:HB3	2.52	0.44
1:H:129:THR:O	1:H:133:ILE:HG13	2.18	0.43
1:D:218:PRO:HB2	1:D:220:TYR:CE1	2.53	0.43
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.88	0.43
1:D:222:LEU:HD11	1:D:244:VAL:HG23	2.00	0.43
1:A:31:ILE:HG23	1:A:111:LEU:HD11	2.01	0.43
1:C:93:SER:O	1:C:97:ARG:HG3	2.19	0.43
1:F:295:ALA:O	1:F:299:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:THR:HG21	1:A:192:ASP:HB3	2.00	0.43
1:B:26:ALA:O	3:B:508:EDO:H11	2.18	0.43
1:B:180:HIS:HE1	7:E:602:HOH:O	2.00	0.43
1:C:70:GLU:HA	1:C:73:ASP:OD2	2.19	0.43
1:D:216:ASN:ND2	7:D:601:HOH:O	2.30	0.43
1:G:196:MET:HB3	1:G:201:GLY:HA2	2.00	0.43
1:C:16:ARG:HH21	1:C:41:GLU:HG3	1.82	0.43
1:G:102:VAL:HG21	1:G:107:MET:CE	2.49	0.43
1:G:236:LEU:HD11	1:G:243:THR:HG21	2.01	0.42
1:B:265:ARG:NH1	1:B:281:SER:OG	2.49	0.42
1:F:123:THR:HG21	1:F:192:ASP:HB3	2.01	0.42
1:F:228:ASP:HB3	3:F:505:EDO:H11	2.01	0.42
1:E:147:VAL:HG22	1:E:152:LEU:HD23	2.02	0.42
1:C:146:PHE:HA	1:C:168:VAL:O	2.18	0.42
1:F:254:VAL:HG21	1:F:298:VAL:HG22	2.02	0.42
1:B:38:LEU:O	4:B:512:DMS:H13	2.19	0.42
1:E:53:THR:HG23	7:E:693:HOH:O	2.20	0.42
1:G:267:TRP:CE3	1:G:281:SER:HB3	2.55	0.42
1:B:102:VAL:HG21	1:B:107:MET:CE	2.50	0.42
1:F:187:VAL:HG22	1:F:299:ILE:HD11	2.00	0.42
1:H:218:PRO:HB2	1:H:220:TYR:CE1	2.54	0.42
1:E:143:ASP:O	1:E:164:SER:HB2	2.20	0.42
1:A:143:ASP:O	1:A:164:SER:HB2	2.20	0.41
1:B:132:LEU:HD23	1:B:132:LEU:HA	1.90	0.41
1:F:308[A]:GLU:OE2	1:G:57:GLU:HG2	2.20	0.41
1:A:112:MET:HG2	1:A:117:GLY:HA3	2.02	0.41
1:H:261:GLN:NE2	7:H:612:HOH:O	2.51	0.41
1:E:248:LEU:HD21	1:E:287:LEU:HD22	2.02	0.41
1:G:143:ASP:O	1:G:164:SER:HB2	2.20	0.41
1:H:319:GLY:C	6:H:501:VAL:HA	2.40	0.41
1:B:151:ARG:CZ	1:B:151:ARG:HB3	2.50	0.41
1:C:226:CYS:HB2	1:C:246:TYR:CZ	2.55	0.41
1:D:16:ARG:NH1	1:D:41:GLU:HG3	2.36	0.41
1:B:180:HIS:CE1	7:E:602:HOH:O	2.73	0.41
1:G:226:CYS:HB2	1:G:246:TYR:CZ	2.55	0.41
1:H:19:HIS:HA	1:H:43:SER:O	2.20	0.41
1:G:18:ILE:HG23	1:G:77:VAL:HG13	2.02	0.41
1:C:143:ASP:O	1:C:164:SER:HB2	2.21	0.41
1:B:193:ALA:HB1	1:B:196:MET:CE	2.50	0.41
1:C:126:LYS:HB2	1:C:126:LYS:HE2	1.90	0.41
1:H:258:ASN:O	1:H:260[B]:ARG:NH1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:ARG:NH2	7:F:602:HOH:O	2.54	0.41
1:H:295:ALA:O	1:H:299:ILE:HG12	2.20	0.41
1:A:130:THR:HG23	1:A:168:VAL:HG12	2.03	0.40
1:E:130:THR:HG23	1:E:168:VAL:HG12	2.02	0.40
1:B:146:PHE:HA	1:B:168:VAL:O	2.21	0.40
1:A:207:LYS:HD3	1:A:231:VAL:HG13	2.04	0.40
1:A:291:LEU:HD11	3:A:504:EDO:H11	2.04	0.40
1:F:143:ASP:O	1:F:164:SER:HB2	2.22	0.40
1:A:267:TRP:CE3	1:A:281:SER:HB3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/466 (66%)	297 (97%)	7 (2%)	1 (0%)	41	46
1	B	307/466 (66%)	301 (98%)	4 (1%)	2 (1%)	22	21
1	C	305/466 (66%)	295 (97%)	8 (3%)	2 (1%)	22	21
1	D	305/466 (66%)	299 (98%)	4 (1%)	2 (1%)	22	21
1	E	307/466 (66%)	295 (96%)	10 (3%)	2 (1%)	22	21
1	F	305/466 (66%)	299 (98%)	5 (2%)	1 (0%)	41	46
1	G	306/466 (66%)	296 (97%)	9 (3%)	1 (0%)	41	46
1	H	305/466 (66%)	294 (96%)	10 (3%)	1 (0%)	41	46
All	All	2445/3728 (66%)	2376 (97%)	57 (2%)	12 (0%)	29	29

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	THR

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Mol	Chain	Res	Type
1	B	157	THR
1	C	84	ILE
1	D	157	THR
1	E	157	THR
1	F	157	THR
1	H	157	THR
1	G	84	ILE
1	B	82	SER
1	E	26	ALA
1	C	157	THR
1	D	84	ILE

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	225/368 (61%)	221 (98%)	4 (2%)	59	68
1	B	233/368 (63%)	230 (99%)	3 (1%)	69	79
1	C	223/368 (61%)	220 (99%)	3 (1%)	69	79
1	D	227/368 (62%)	223 (98%)	4 (2%)	59	68
1	E	235/368 (64%)	231 (98%)	4 (2%)	60	71
1	F	229/368 (62%)	226 (99%)	3 (1%)	69	79
1	G	230/368 (62%)	229 (100%)	1 (0%)	91	94
1	H	231/368 (63%)	230 (100%)	1 (0%)	91	94
All	All	1833/2944 (62%)	1810 (99%)	23 (1%)	76	79

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	SER
1	A	148	ILE
1	A	194	ASP
1	A	280	VAL

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Mol	Chain	Res	Type
1	B	194	ASP
1	B	260[A]	ARG
1	B	260[B]	ARG
1	C	50	SER
1	C	194	ASP
1	C	280	VAL
1	D	81	SER
1	D	194	ASP
1	D	260[A]	ARG
1	D	260[B]	ARG
1	E	68	GLN
1	E	194	ASP
1	E	260[A]	ARG
1	E	260[B]	ARG
1	F	194	ASP
1	F	260[A]	ARG
1	F	260[B]	ARG
1	G	194	ASP
1	H	194	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	B	292	ASN
1	C	37	ASN
1	C	288	HIS
1	C	292	ASN
1	D	288	HIS
1	D	292	ASN
1	E	292	ASN
1	H	160	GLN
1	H	216	ASN

5.3.3 RNA

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 65 ligands modelled in this entry, 8 are monoatomic - leaving 57 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	UYD	B	501	-	31,33,33	1.66	4 (12%)	34,48,48	1.58	5 (14%)
3	EDO	B	503	-	3,3,3	0.53	0	2,2,2	0.23	0
6	VAL	H	501	-	4,6,7	0.54	0	6,7,9	0.98	0
4	DMS	H	506	-	3,3,3	0.60	0	3,3,3	0.65	0
3	EDO	B	506	-	3,3,3	0.58	0	2,2,2	0.12	0
3	EDO	E	504	-	3,3,3	0.63	0	2,2,2	0.26	0
3	EDO	A	503	-	3,3,3	0.49	0	2,2,2	0.27	0
3	EDO	F	502	-	3,3,3	0.52	0	2,2,2	0.04	0
3	EDO	D	503	-	3,3,3	0.45	0	2,2,2	0.37	0
3	EDO	C	504	-	3,3,3	0.38	0	2,2,2	0.63	0
3	EDO	G	503	-	3,3,3	0.50	0	2,2,2	0.18	0
2	UYD	F	501	-	31,33,33	1.70	5 (16%)	34,48,48	1.55	4 (11%)
4	DMS	D	507	-	3,3,3	0.59	0	3,3,3	0.47	0
4	DMS	E	506	-	3,3,3	0.66	0	3,3,3	0.87	0
3	EDO	H	503	-	3,3,3	0.45	0	2,2,2	0.39	0
3	EDO	C	505	-	3,3,3	0.44	0	2,2,2	0.58	0
4	DMS	B	512	-	3,3,3	0.62	0	3,3,3	0.52	0
4	DMS	G	505	-	3,3,3	0.65	0	3,3,3	0.76	0
2	UYD	C	501	-	31,33,33	1.78	3 (9%)	34,48,48	1.42	4 (11%)
3	EDO	C	502	-	3,3,3	0.42	0	2,2,2	0.44	0
3	EDO	D	504	-	3,3,3	0.40	0	2,2,2	0.51	0
4	DMS	B	511	-	3,3,3	0.64	0	3,3,3	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	G	504	-	3,3,3	0.50	0	2,2,2	0.31	0
3	EDO	B	505	-	3,3,3	0.45	0	2,2,2	0.32	0
2	UYD	E	501	-	31,33,33	1.71	4 (12%)	34,48,48	1.40	3 (8%)
3	EDO	E	503	-	3,3,3	0.49	0	2,2,2	0.19	0
3	EDO	B	502	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.28	0
3	EDO	H	504	-	3,3,3	0.50	0	2,2,2	0.19	0
3	EDO	D	505	-	3,3,3	0.51	0	2,2,2	0.20	0
2	UYD	G	501	-	31,33,33	1.74	4 (12%)	34,48,48	1.45	5 (14%)
3	EDO	A	502	-	3,3,3	0.50	0	2,2,2	0.15	0
3	EDO	B	507	-	3,3,3	0.46	0	2,2,2	0.33	0
2	UYD	A	501	-	31,33,33	1.67	4 (12%)	34,48,48	1.55	5 (14%)
3	EDO	F	503	-	3,3,3	0.33	0	2,2,2	0.66	0
3	EDO	F	506	-	3,3,3	0.43	0	2,2,2	0.39	0
2	UYD	H	502	-	31,33,33	1.69	4 (12%)	34,48,48	1.60	7 (20%)
4	DMS	E	507	-	3,3,3	0.64	0	3,3,3	0.61	0
4	DMS	C	506	-	3,3,3	0.57	0	3,3,3	0.69	0
4	DMS	F	507	-	3,3,3	0.66	0	3,3,3	0.59	0
3	EDO	A	504	-	3,3,3	0.56	0	2,2,2	0.10	0
3	EDO	F	504	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	E	502	-	3,3,3	0.47	0	2,2,2	0.40	0
3	EDO	B	504	-	3,3,3	0.41	0	2,2,2	0.39	0
3	EDO	H	505	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	C	503	-	3,3,3	0.54	0	2,2,2	0.35	0
4	DMS	A	506	-	3,3,3	0.59	0	3,3,3	0.47	0
4	DMS	B	510	-	3,3,3	0.59	0	3,3,3	0.50	0
3	EDO	D	502	-	3,3,3	0.52	0	2,2,2	0.14	0
3	EDO	F	505	-	3,3,3	0.55	0	2,2,2	0.11	0
3	EDO	G	502	-	3,3,3	0.45	0	2,2,2	0.35	0
3	EDO	E	505	-	3,3,3	0.56	0	2,2,2	0.12	0
4	DMS	B	509	-	3,3,3	0.63	0	3,3,3	0.79	0
4	DMS	F	508	-	3,3,3	0.52	0	3,3,3	0.17	0
3	EDO	B	508	-	3,3,3	0.45	0	2,2,2	0.25	0
4	DMS	D	506	-	3,3,3	0.67	0	3,3,3	0.72	0
2	UYD	D	501	-	31,33,33	1.74	4 (12%)	34,48,48	1.58	5 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UYD	B	501	-	-	4/18/20/20	0/4/4/4
3	EDO	B	503	-	-	1/1/1/1	-
6	VAL	H	501	-	-	0/5/6/8	-
3	EDO	B	506	-	-	0/1/1/1	-
3	EDO	E	504	-	-	1/1/1/1	-
3	EDO	A	503	-	-	0/1/1/1	-
3	EDO	F	502	-	-	0/1/1/1	-
3	EDO	D	503	-	-	1/1/1/1	-
3	EDO	C	504	-	-	0/1/1/1	-
3	EDO	G	503	-	-	1/1/1/1	-
2	UYD	F	501	-	-	2/18/20/20	0/4/4/4
3	EDO	H	503	-	-	0/1/1/1	-
3	EDO	C	505	-	-	1/1/1/1	-
2	UYD	C	501	-	-	3/18/20/20	0/4/4/4
3	EDO	C	502	-	-	0/1/1/1	-
3	EDO	D	504	-	-	0/1/1/1	-
3	EDO	G	504	-	-	0/1/1/1	-
3	EDO	B	505	-	-	0/1/1/1	-
2	UYD	E	501	-	-	4/18/20/20	0/4/4/4
3	EDO	E	503	-	-	0/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	H	504	-	-	1/1/1/1	-
3	EDO	D	505	-	-	1/1/1/1	-
2	UYD	G	501	-	-	0/18/20/20	0/4/4/4
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	B	507	-	-	0/1/1/1	-
2	UYD	A	501	-	-	3/18/20/20	0/4/4/4
3	EDO	F	503	-	-	1/1/1/1	-
3	EDO	F	506	-	-	1/1/1/1	-
2	UYD	H	502	-	-	0/18/20/20	0/4/4/4
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	F	504	-	-	1/1/1/1	-
3	EDO	E	502	-	-	1/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
3	EDO	H	505	-	-	1/1/1/1	-
3	EDO	C	503	-	-	1/1/1/1	-
3	EDO	D	502	-	-	1/1/1/1	-
3	EDO	F	505	-	-	0/1/1/1	-
3	EDO	G	502	-	-	0/1/1/1	-
3	EDO	E	505	-	-	1/1/1/1	-
3	EDO	B	508	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UYD	D	501	-	-	1/18/20/20	0/4/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	UYD	C20-N21	6.85	1.45	1.34
2	G	501	UYD	C20-N21	6.83	1.45	1.34
2	E	501	UYD	C20-N21	6.72	1.45	1.34
2	A	501	UYD	C20-N21	6.59	1.45	1.34
2	F	501	UYD	C20-N21	6.55	1.45	1.34
2	B	501	UYD	C20-N21	6.45	1.45	1.34
2	D	501	UYD	C20-N21	6.40	1.45	1.34
2	H	502	UYD	C20-N21	6.15	1.44	1.34
2	C	501	UYD	C06-C24	-4.47	1.39	1.44
2	D	501	UYD	C06-C24	-4.02	1.39	1.44
2	G	501	UYD	C06-C24	-4.00	1.39	1.44
2	H	502	UYD	C06-C24	-3.99	1.39	1.44
2	E	501	UYD	C06-C24	-3.96	1.39	1.44
2	C	501	UYD	C20-N19	-3.85	1.29	1.36
2	A	501	UYD	C06-C24	-3.84	1.40	1.44
2	D	501	UYD	C20-N19	-3.72	1.29	1.36
2	F	501	UYD	C06-C24	-3.71	1.40	1.44
2	H	502	UYD	C20-N19	-3.55	1.29	1.36
2	G	501	UYD	C20-N19	-3.50	1.29	1.36
2	E	501	UYD	C20-N19	-3.42	1.30	1.36
2	B	501	UYD	C06-C24	-3.35	1.40	1.44
2	B	501	UYD	C20-N19	-3.30	1.30	1.36
2	A	501	UYD	C20-N19	-3.27	1.30	1.36
2	F	501	UYD	C20-N19	-3.07	1.30	1.36
2	F	501	UYD	C23-C24	2.40	1.46	1.40
2	D	501	UYD	C23-C24	2.21	1.45	1.40
2	H	502	UYD	C06-N07	2.20	1.35	1.32
2	B	501	UYD	C23-C24	2.10	1.45	1.40
2	E	501	UYD	C23-C24	2.10	1.45	1.40
2	G	501	UYD	C23-C24	2.06	1.45	1.40
2	A	501	UYD	C23-C24	2.03	1.45	1.40
2	F	501	UYD	C06-N07	2.02	1.35	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	UYD	C24-C06-N05	5.56	125.85	119.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	UYD	C24-C06-N05	5.43	125.70	119.73
2	F	501	UYD	C24-C06-N05	5.39	125.67	119.73
2	H	502	UYD	C24-C06-N05	4.97	125.20	119.73
2	E	501	UYD	C24-C06-N05	4.84	125.06	119.73
2	C	501	UYD	C24-C06-N05	4.68	124.88	119.73
2	A	501	UYD	C24-C06-N05	4.54	124.73	119.73
2	G	501	UYD	C24-C06-N05	4.26	124.41	119.73
2	A	501	UYD	C01-N02-C26	4.07	135.20	129.18
2	F	501	UYD	C01-N02-C26	3.94	135.02	129.18
2	H	502	UYD	C01-N02-C26	3.94	135.01	129.18
2	D	501	UYD	C01-N02-C26	3.93	134.99	129.18
2	G	501	UYD	C01-N02-C26	3.83	134.85	129.18
2	E	501	UYD	C01-N02-C26	3.72	134.69	129.18
2	C	501	UYD	C01-N02-C26	3.68	134.62	129.18
2	B	501	UYD	C01-N02-C26	3.60	134.51	129.18
2	D	501	UYD	C13-C10-N09	-2.88	109.12	113.44
2	A	501	UYD	C26-N02-N03	-2.86	109.76	111.96
2	B	501	UYD	C24-C06-N07	-2.80	117.39	121.98
2	H	502	UYD	C26-N02-N03	-2.73	109.86	111.96
2	F	501	UYD	C24-C06-N07	-2.70	117.55	121.98
2	A	501	UYD	C13-C10-N09	-2.64	109.47	113.44
2	G	501	UYD	C24-C06-N07	-2.59	117.74	121.98
2	D	501	UYD	N05-C06-N07	-2.52	116.29	118.66
2	C	501	UYD	C24-C06-N07	-2.47	117.94	121.98
2	E	501	UYD	C24-C06-N07	-2.43	118.00	121.98
2	D	501	UYD	C24-C06-N07	-2.42	118.00	121.98
2	B	501	UYD	C26-N02-N03	-2.36	110.15	111.96
2	F	501	UYD	C08-N07-C06	2.32	121.71	116.39
2	H	502	UYD	N05-C06-N07	-2.27	116.53	118.66
2	A	501	UYD	C24-C06-N07	-2.27	118.26	121.98
2	H	502	UYD	C24-C06-N07	-2.26	118.27	121.98
2	H	502	UYD	C11-C10-N09	-2.13	106.44	109.12
2	C	501	UYD	C26-N02-N03	-2.04	110.39	111.96
2	G	501	UYD	C08-N07-C06	2.03	121.04	116.39
2	G	501	UYD	C11-C10-N09	-2.03	106.56	109.12
2	B	501	UYD	N05-C06-N07	-2.02	116.76	118.66
2	H	502	UYD	N09-C08-N07	2.01	120.20	117.18

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	UYD	C13-C10-C11-O12
2	A	501	UYD	N09-C10-C11-O12
2	B	501	UYD	C13-C10-C11-O12
2	B	501	UYD	N09-C10-C11-O12
2	C	501	UYD	N09-C10-C11-O12
2	E	501	UYD	C13-C10-C11-O12
2	E	501	UYD	N09-C10-C11-O12
2	F	501	UYD	C13-C10-C11-O12
2	F	501	UYD	N09-C10-C11-O12
3	B	503	EDO	O1-C1-C2-O2
3	B	508	EDO	O1-C1-C2-O2
3	D	502	EDO	O1-C1-C2-O2
3	D	505	EDO	O1-C1-C2-O2
3	F	504	EDO	O1-C1-C2-O2
2	C	501	UYD	C13-C10-C11-O12
2	D	501	UYD	N09-C10-C11-O12
3	E	505	EDO	O1-C1-C2-O2
3	F	506	EDO	O1-C1-C2-O2
2	B	501	UYD	N09-C10-C13-C14
2	B	501	UYD	N09-C10-C13-C18
3	C	503	EDO	O1-C1-C2-O2
3	D	503	EDO	O1-C1-C2-O2
2	E	501	UYD	N09-C10-C13-C18
3	E	504	EDO	O1-C1-C2-O2
2	A	501	UYD	N09-C10-C13-C18
3	F	503	EDO	O1-C1-C2-O2
3	H	505	EDO	O1-C1-C2-O2
2	C	501	UYD	N09-C10-C13-C18
2	E	501	UYD	N09-C10-C13-C14
3	C	505	EDO	O1-C1-C2-O2
3	E	502	EDO	O1-C1-C2-O2
3	G	503	EDO	O1-C1-C2-O2
3	H	504	EDO	O1-C1-C2-O2

There are no ring outliers.

18 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	EDO	1	0
6	H	501	VAL	2	0
3	F	502	EDO	4	0
3	D	503	EDO	1	0
3	H	503	EDO	1	0

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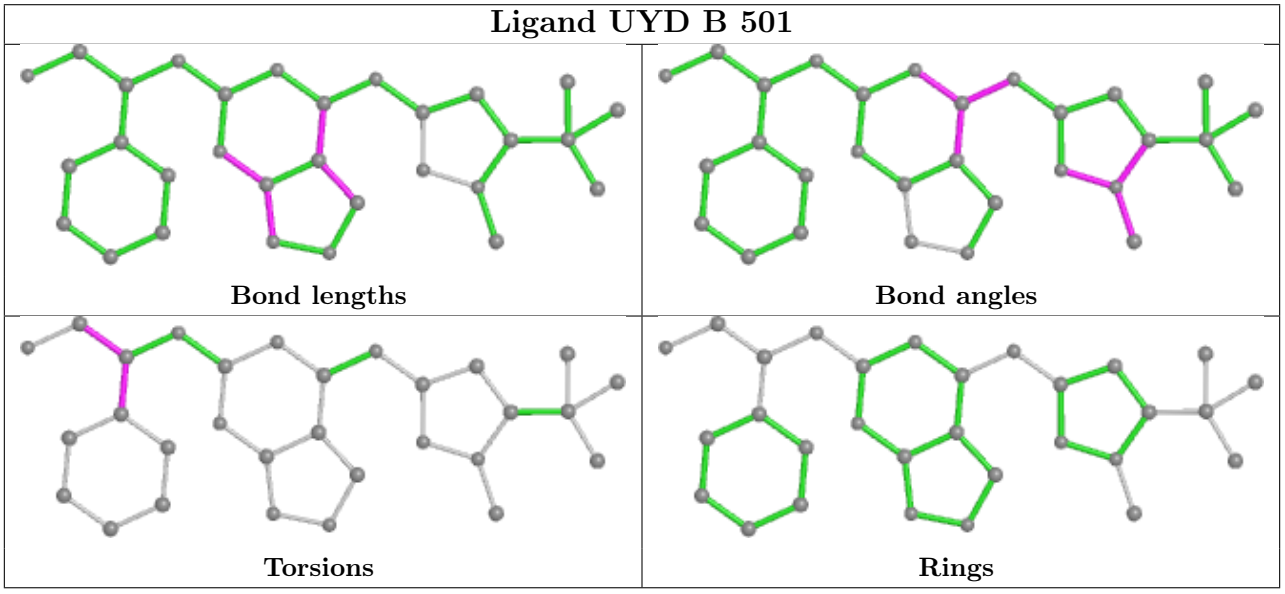
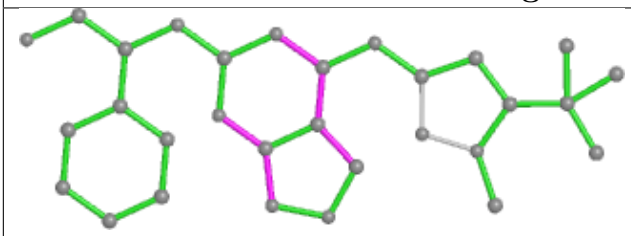
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	512	DMS	1	0
3	C	502	EDO	1	0
3	D	504	EDO	1	0
3	B	502	EDO	1	0
3	H	504	EDO	2	0
2	H	502	UYD	1	0
3	A	504	EDO	1	0
3	B	504	EDO	1	0
3	C	503	EDO	1	0
4	B	510	DMS	1	0
3	D	502	EDO	2	0
3	F	505	EDO	1	0
3	B	508	EDO	2	0

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 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.

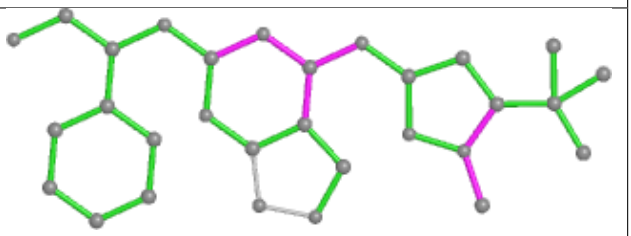
Ligand UYD B 501



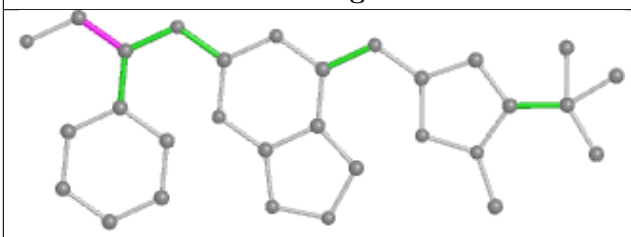
Ligand UYD F 501



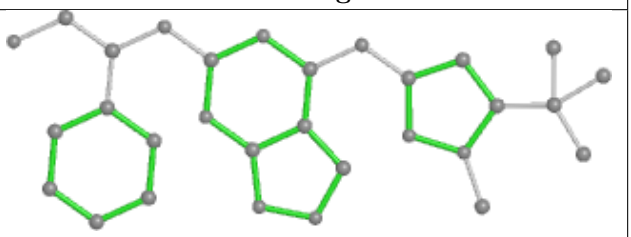
Bond lengths



Bond angles

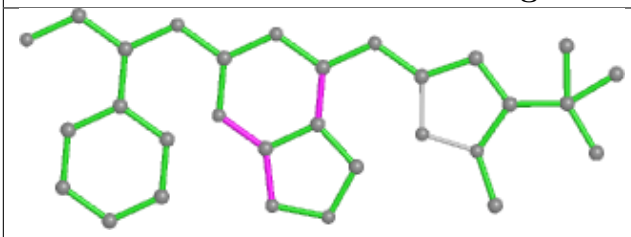


Torsions

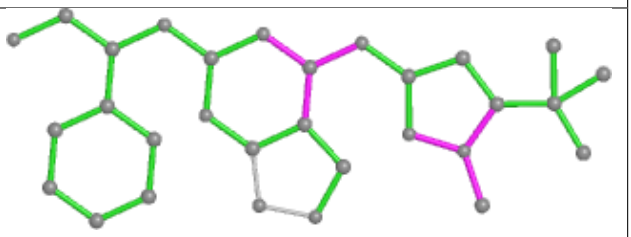


Rings

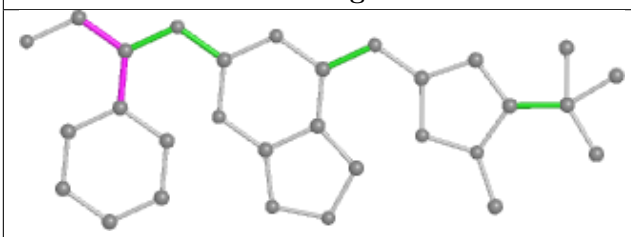
Ligand UYD C 501



Bond lengths



Bond angles



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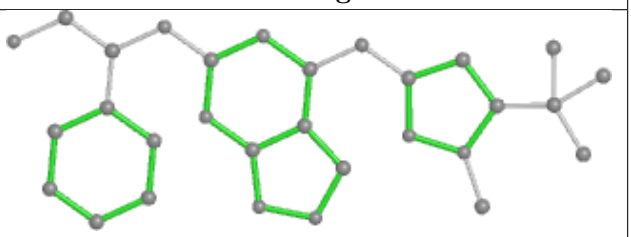
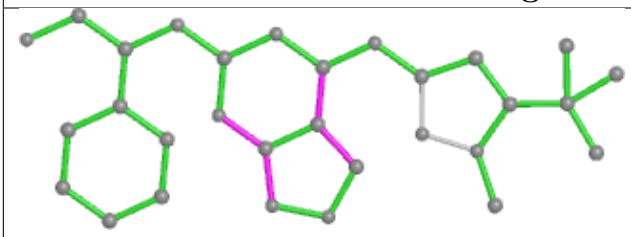
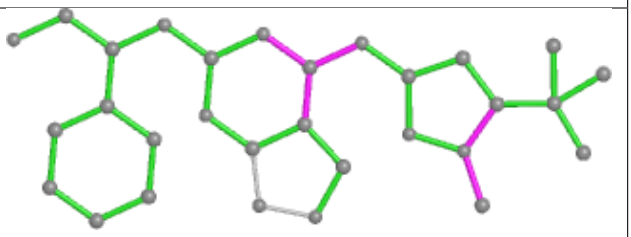


Rings

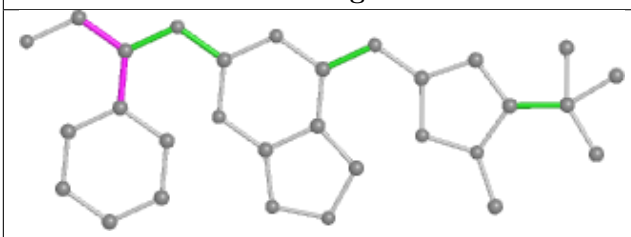
Ligand UYD E 501



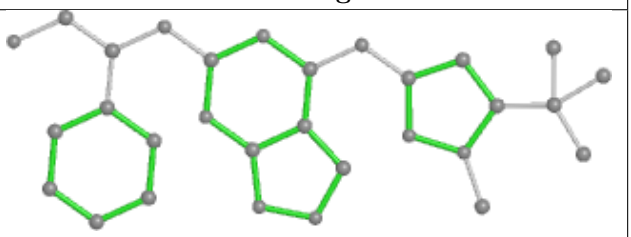
Bond lengths



Bond angles

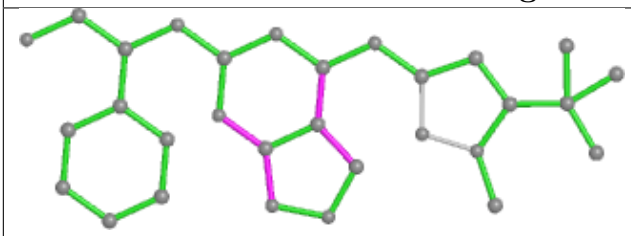


Torsions

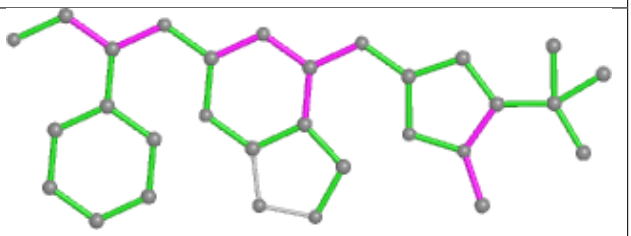


Rings

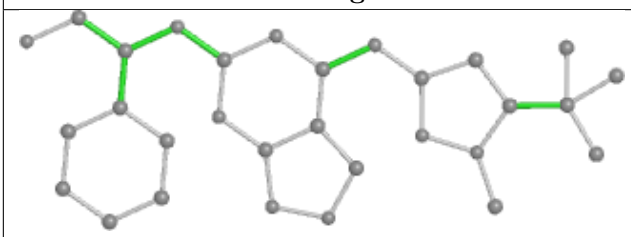
Ligand UYD G 501



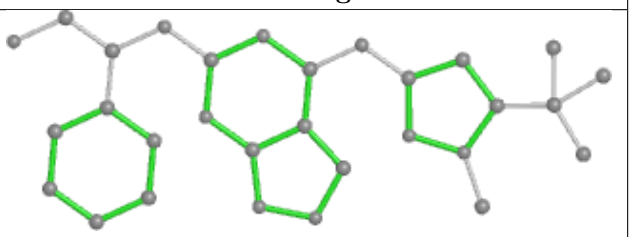
Bond lengths



Bond angles

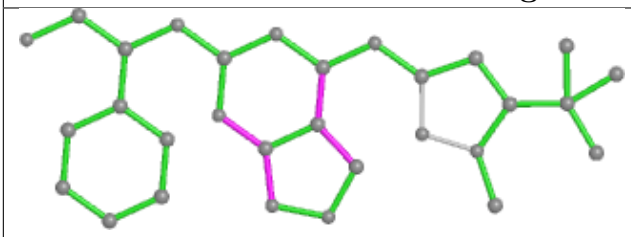


Torsions

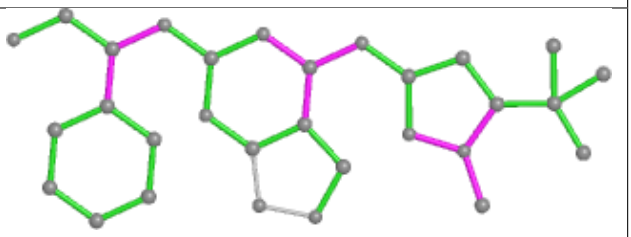


Rings

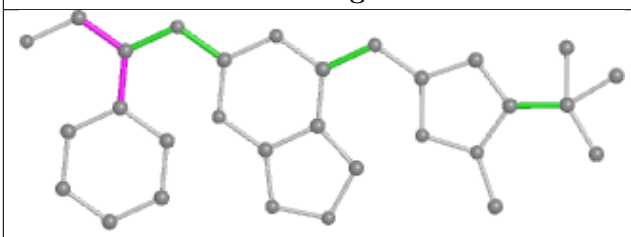
Ligand UYD A 501



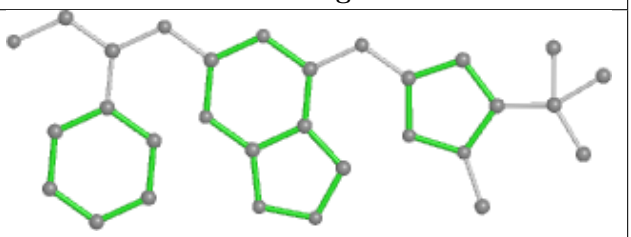
Bond lengths



Bond angles

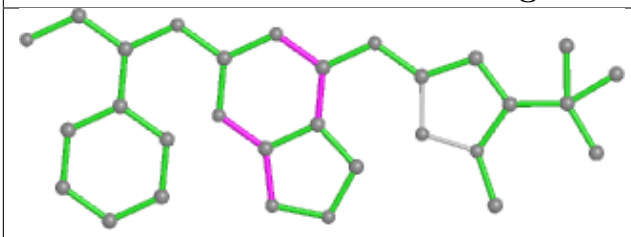


Torsions

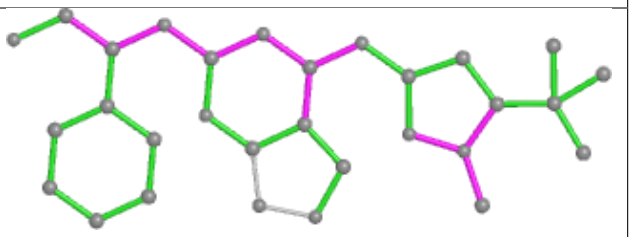


Rings

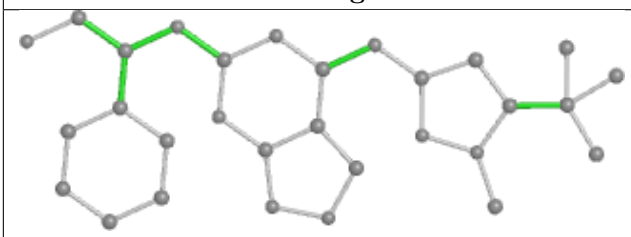
Ligand UYD H 502



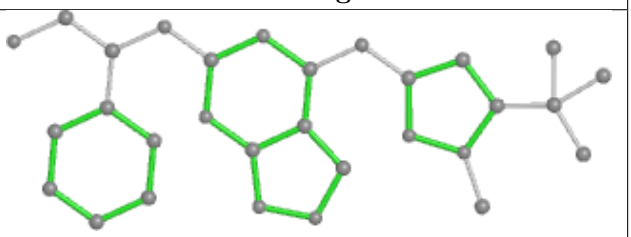
Bond lengths



Bond angles

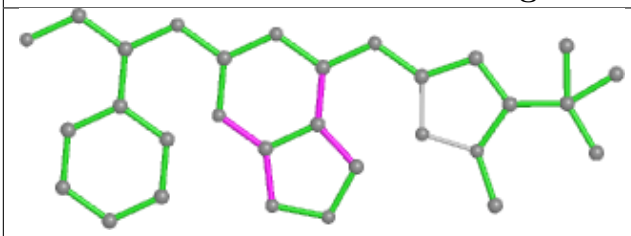


Torsions

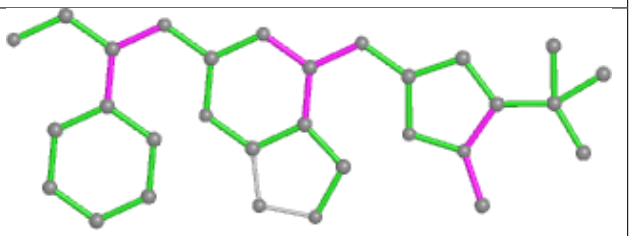


Rings

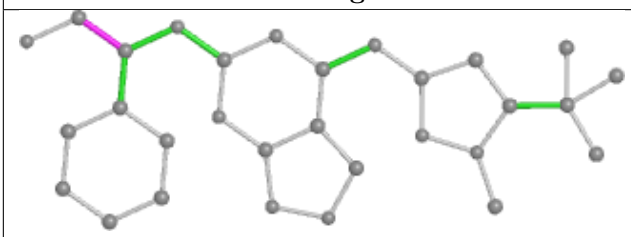
Ligand UYD D 501



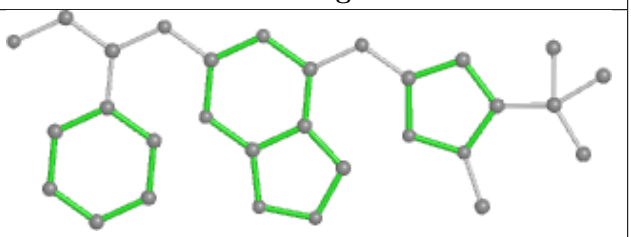
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	304/466 (65%)	0.07	12 (3%)	39	42	28, 41, 75, 106	0
1	B	305/466 (65%)	0.06	15 (4%)	29	32	25, 37, 75, 112	0
1	C	305/466 (65%)	0.12	16 (5%)	27	30	29, 40, 78, 109	0
1	D	305/466 (65%)	0.00	8 (2%)	56	59	30, 41, 75, 105	0
1	E	305/466 (65%)	-0.13	3 (0%)	82	84	27, 37, 68, 101	0
1	F	305/466 (65%)	-0.05	5 (1%)	72	74	29, 40, 79, 111	0
1	G	305/466 (65%)	0.05	12 (3%)	39	42	29, 42, 77, 104	0
1	H	305/466 (65%)	0.09	13 (4%)	35	37	25, 37, 74, 108	0
All	All	2439/3728 (65%)	0.03	84 (3%)	45	47	25, 40, 77, 112	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	26	ALA	6.0
1	C	84	ILE	5.5
1	C	87	ALA	5.2
1	F	83	ALA	5.2
1	A	67	HIS	4.9
1	C	65	ILE	4.8
1	G	84	ILE	4.4
1	F	84	ILE	4.3
1	D	84	ILE	4.2
1	G	67	HIS	4.0
1	B	157	THR	3.9
1	G	26	ALA	3.9
1	H	157	THR	3.9
1	G	87	ALA	3.8
1	H	84	ILE	3.8
1	B	86	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	89	PRO	3.8
1	B	84	ILE	3.7
1	B	262	GLU	3.6
1	H	47	LEU	3.6
1	B	83	ALA	3.6
1	H	83	ALA	3.6
1	H	65	ILE	3.5
1	F	26	ALA	3.4
1	C	83	ALA	3.4
1	A	69	ALA	3.4
1	D	26	ALA	3.4
1	B	47	LEU	3.4
1	G	86	ARG	3.3
1	F	85	ASN	3.3
1	D	65	ILE	3.3
1	G	47	LEU	3.3
1	D	157	THR	3.3
1	A	65	ILE	3.2
1	G	157	THR	3.2
1	C	69	ALA	3.2
1	C	67	HIS	3.2
1	D	158	ASN	3.1
1	C	88	ASN	3.0
1	A	49	ALA	3.0
1	A	26	ALA	2.9
1	A	47	LEU	2.9
1	E	52	VAL	2.8
1	C	264	MET	2.8
1	A	84	ILE	2.8
1	F	82	SER	2.8
1	H	26	ALA	2.8
1	B	89	PRO	2.7
1	C	158	ASN	2.7
1	A	83	ALA	2.7
1	H	85	ASN	2.7
1	C	86	ARG	2.6
1	A	158	ASN	2.6
1	G	65	ILE	2.6
1	B	85	ASN	2.6
1	B	69	ALA	2.5
1	D	47	LEU	2.5
1	E	158	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	82	SER	2.5
1	C	263	GLY	2.5
1	B	26	ALA	2.5
1	G	85	ASN	2.5
1	B	65	ILE	2.4
1	B	81	SER	2.4
1	H	52	VAL	2.4
1	H	69	ALA	2.3
1	A	89	PRO	2.3
1	G	83	ALA	2.3
1	H	86	ARG	2.2
1	H	73	ASP	2.2
1	G	158	ASN	2.2
1	E	82	SER	2.2
1	D	64	PHE	2.1
1	B	67	HIS	2.1
1	C	66	GLY	2.1
1	D	69	ALA	2.1
1	C	92	ALA	2.1
1	C	64	PHE	2.1
1	A	66	GLY	2.1
1	B	66	GLY	2.1
1	G	97	ARG	2.0
1	A	46	ASP	2.0
1	H	68	GLN	2.0
1	H	51	ALA	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 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	VAL	H	501	7/8	0.50	0.32	98,101,108,110	0
3	EDO	E	505	4/4	0.68	0.23	49,60,67,72	0
3	EDO	G	503	4/4	0.74	0.28	65,66,71,76	0
3	EDO	F	506	4/4	0.77	0.39	55,56,60,66	0
3	EDO	A	504	4/4	0.78	0.28	61,62,66,66	0
3	EDO	C	502	4/4	0.79	0.21	75,78,82,86	0
3	EDO	C	505	4/4	0.79	0.26	56,64,72,82	0
3	EDO	B	503	4/4	0.79	0.21	59,64,66,68	0
3	EDO	A	503	4/4	0.80	0.19	73,75,77,78	0
3	EDO	C	503	4/4	0.81	0.29	52,55,66,69	0
3	EDO	D	502	4/4	0.82	0.27	70,70,71,72	0
3	EDO	F	504	4/4	0.83	0.15	63,67,67,68	0
3	EDO	H	504	4/4	0.84	0.26	59,61,68,74	0
3	EDO	B	507	4/4	0.85	0.26	56,68,75,75	0
3	EDO	D	505	4/4	0.85	0.27	54,60,68,72	0
3	EDO	E	504	4/4	0.86	0.26	48,56,56,60	0
3	EDO	F	505	4/4	0.86	0.24	50,52,54,62	0
4	DMS	B	512	4/4	0.86	0.31	103,106,107,110	0
3	EDO	D	504	4/4	0.86	0.25	66,72,73,74	0
3	EDO	C	504	4/4	0.87	0.33	71,71,72,77	0
3	EDO	H	505	4/4	0.87	0.31	49,60,69,74	0
4	DMS	F	508	4/4	0.88	0.25	70,81,84,91	0
3	EDO	E	502	4/4	0.88	0.15	60,63,64,66	0
3	EDO	H	503	4/4	0.89	0.22	59,61,67,77	0
5	CL	A	507	1/1	0.89	0.11	64,64,64,64	0
5	CL	G	506	1/1	0.89	0.21	78,78,78,78	0
3	EDO	B	505	4/4	0.89	0.28	70,70,75,79	0
3	EDO	E	503	4/4	0.90	0.16	51,54,55,57	0
3	EDO	D	503	4/4	0.90	0.21	68,69,71,74	0
5	CL	E	508	1/1	0.90	0.14	60,60,60,60	0
3	EDO	A	502	4/4	0.90	0.25	51,56,59,66	0
3	EDO	F	502	4/4	0.90	0.24	68,71,74,78	0
3	EDO	G	502	4/4	0.91	0.17	68,69,70,72	0
5	CL	C	507	1/1	0.91	0.16	78,78,78,78	0
5	CL	D	508	1/1	0.91	0.21	75,75,75,75	0
3	EDO	B	502	4/4	0.91	0.26	50,55,57,58	0
3	EDO	G	504	4/4	0.91	0.21	54,62,70,78	0
3	EDO	B	508	4/4	0.91	0.21	65,66,71,79	0
4	DMS	E	507	4/4	0.92	0.24	94,97,98,98	0
4	DMS	A	506	4/4	0.92	0.21	71,74,77,82	0
4	DMS	C	506	4/4	0.93	0.15	59,69,71,78	0
4	DMS	D	507	4/4	0.93	0.24	74,79,83,89	0
3	EDO	B	504	4/4	0.93	0.15	65,67,68,69	0

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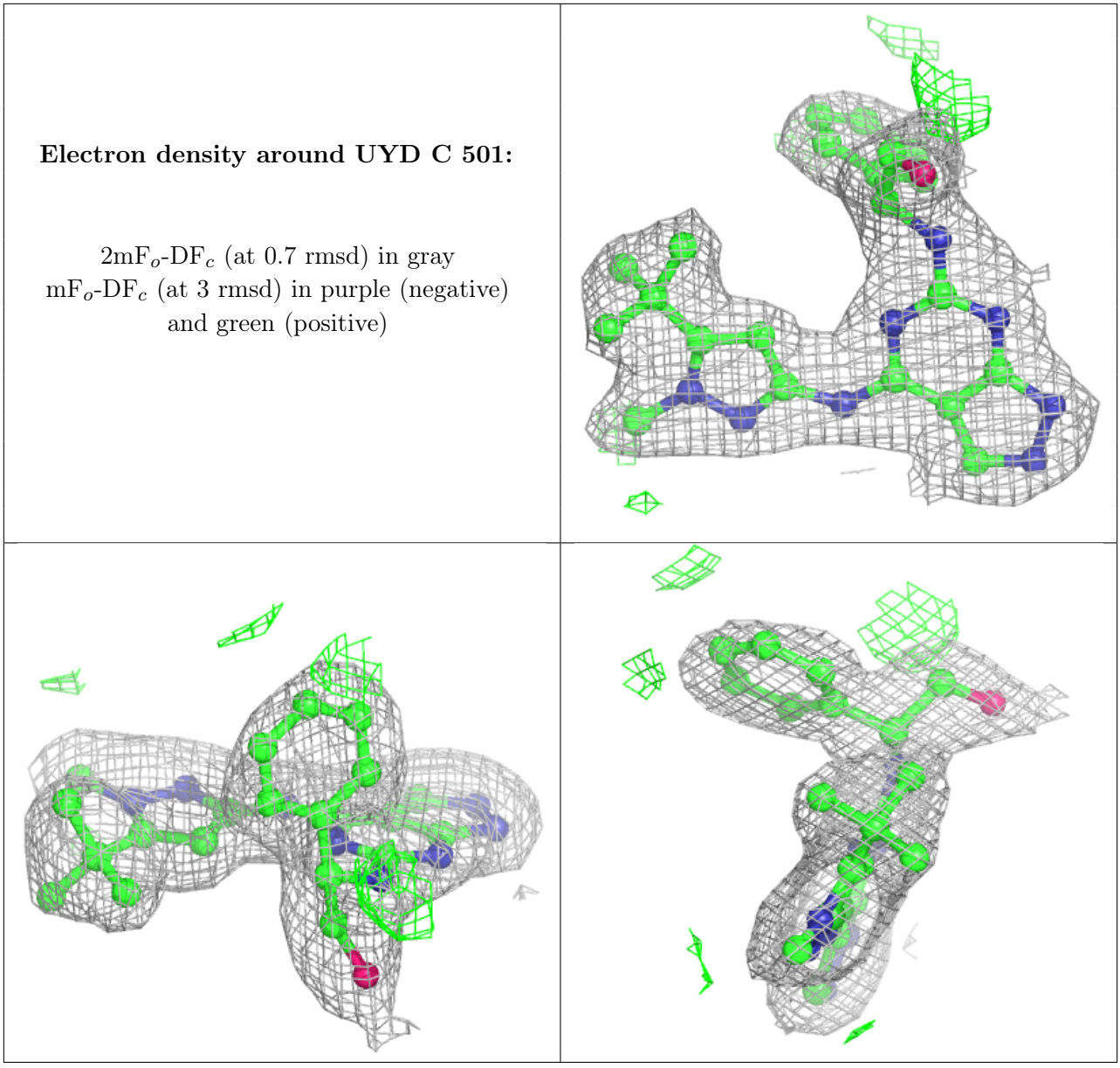
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	CL	F	509	1/1	0.93	0.12	68,68,68,68	0
4	DMS	B	509	4/4	0.93	0.19	57,76,78,79	0
3	EDO	B	506	4/4	0.93	0.26	44,47,52,54	0
3	EDO	F	503	4/4	0.94	0.19	46,46,53,63	0
4	DMS	B	510	4/4	0.94	0.18	62,68,70,75	0
4	DMS	B	511	4/4	0.94	0.21	74,76,78,80	0
4	DMS	H	506	4/4	0.95	0.16	50,69,74,79	0
5	CL	H	507	1/1	0.95	0.08	69,69,69,69	0
3	EDO	A	505	4/4	0.95	0.31	56,64,66,70	0
4	DMS	D	506	4/4	0.96	0.20	71,71,76,78	0
2	UYD	C	501	30/30	0.97	0.12	29,38,48,59	0
2	UYD	D	501	30/30	0.97	0.12	33,41,52,57	0
5	CL	B	513	1/1	0.97	0.15	64,64,64,64	0
2	UYD	F	501	30/30	0.97	0.13	29,37,42,57	0
2	UYD	G	501	30/30	0.97	0.14	28,39,47,54	0
2	UYD	H	502	30/30	0.97	0.12	24,33,44,62	0
4	DMS	E	506	4/4	0.97	0.11	61,62,64,65	0
2	UYD	A	501	30/30	0.97	0.12	32,37,51,59	0
2	UYD	B	501	30/30	0.97	0.11	24,33,41,56	0
4	DMS	G	505	4/4	0.97	0.17	65,68,70,72	0
2	UYD	E	501	30/30	0.98	0.10	28,36,47,62	0
4	DMS	F	507	4/4	0.98	0.16	69,70,70,71	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.

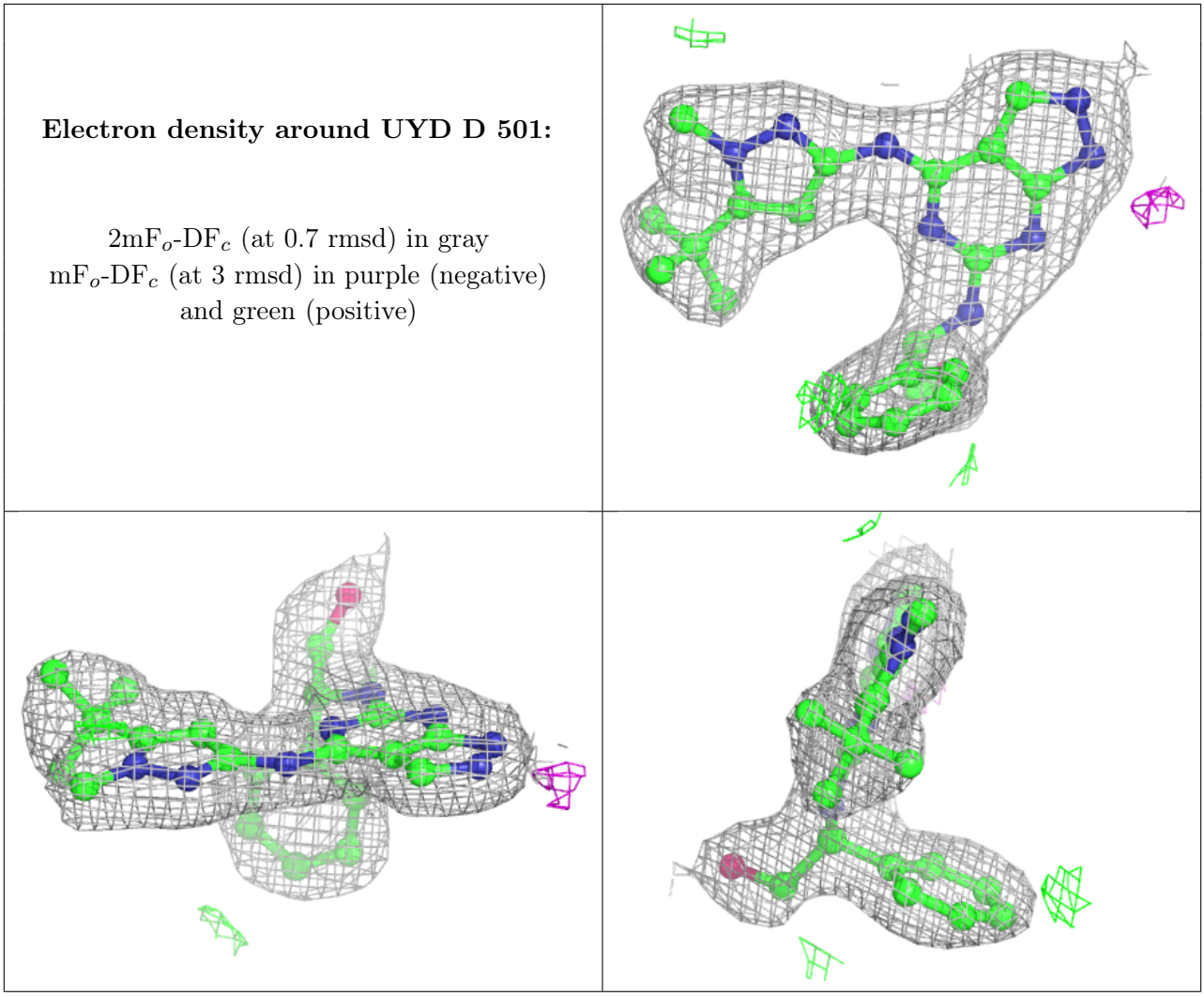
Electron density around UYD C 501:

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



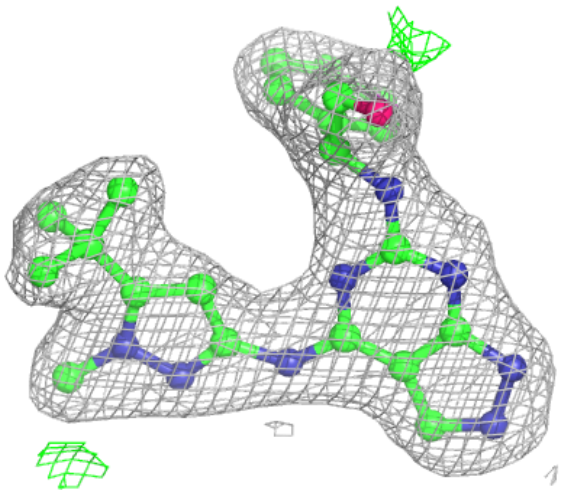
Electron density around UYD D 501:

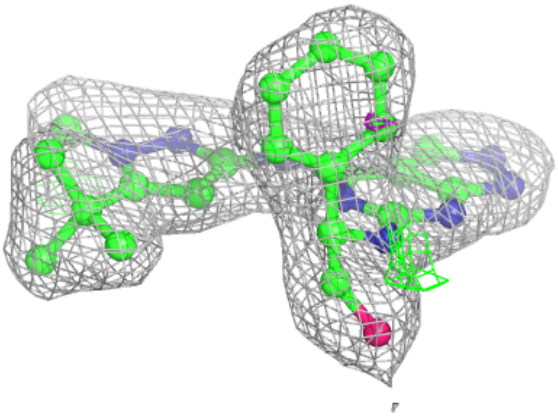
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

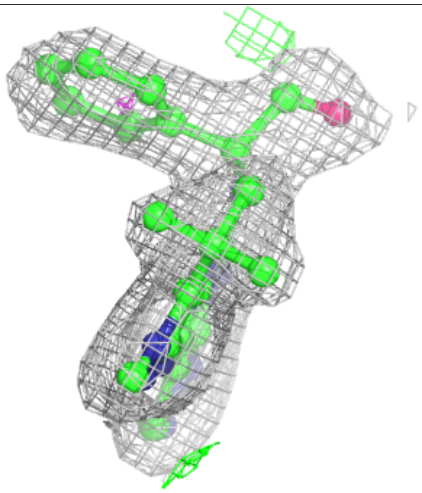


Electron density around UYD F 501:

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

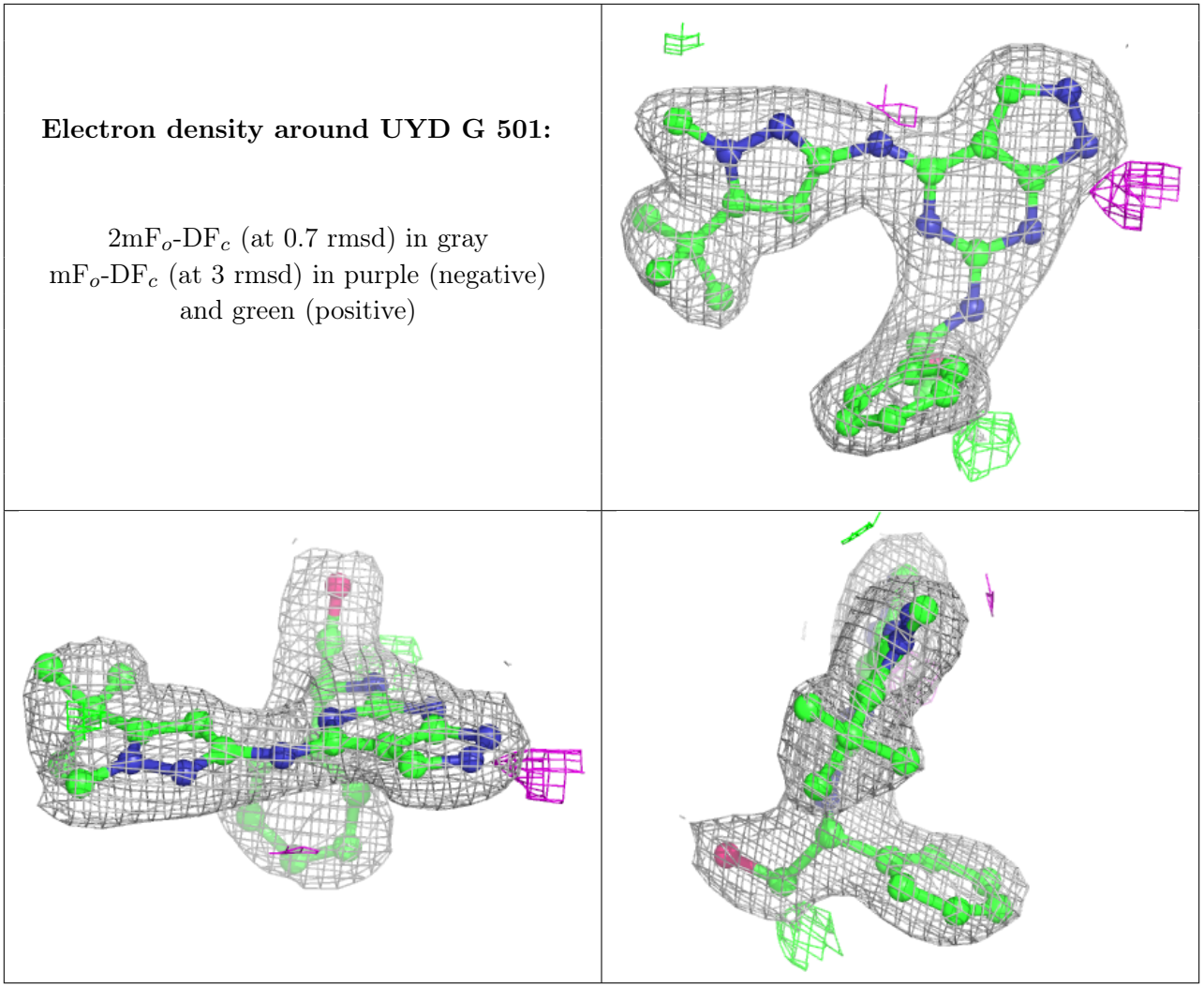






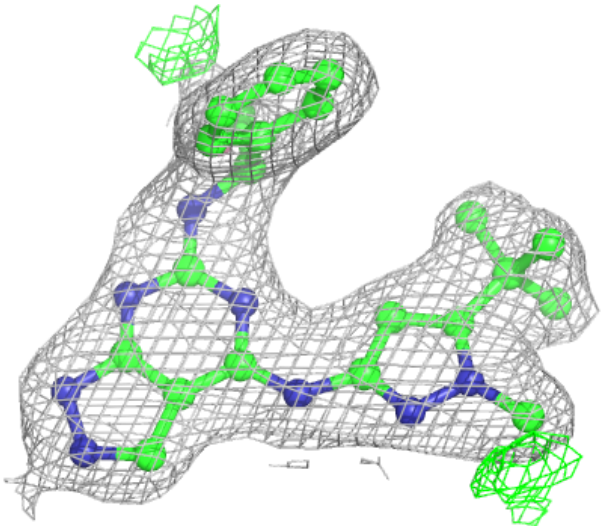
Electron density around UYD G 501:

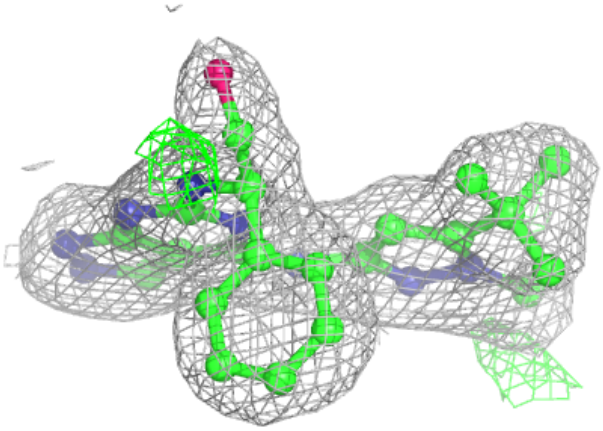
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

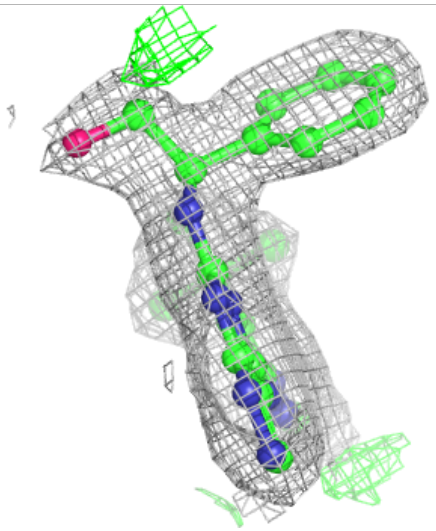


Electron density around UYD H 502:

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

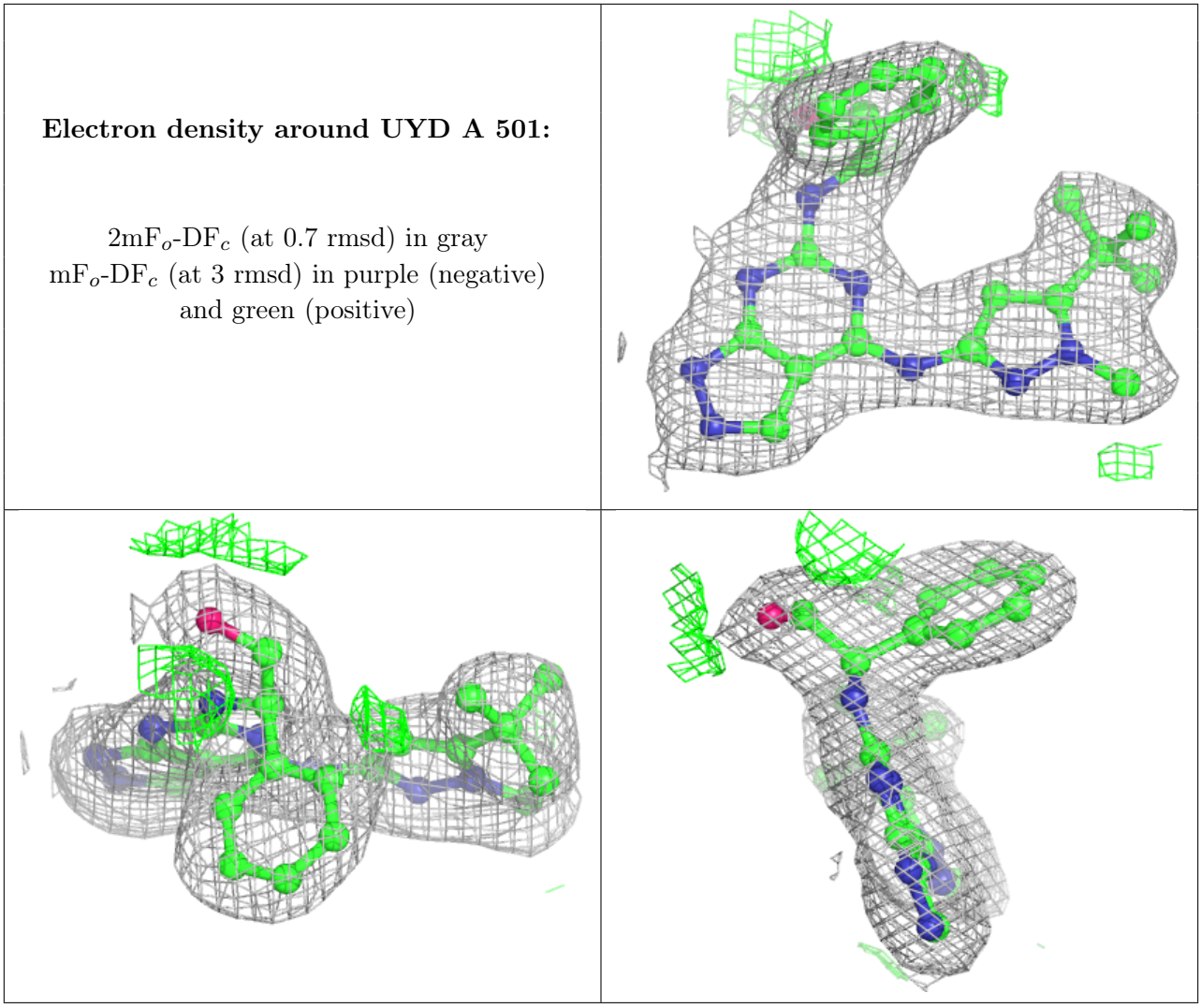






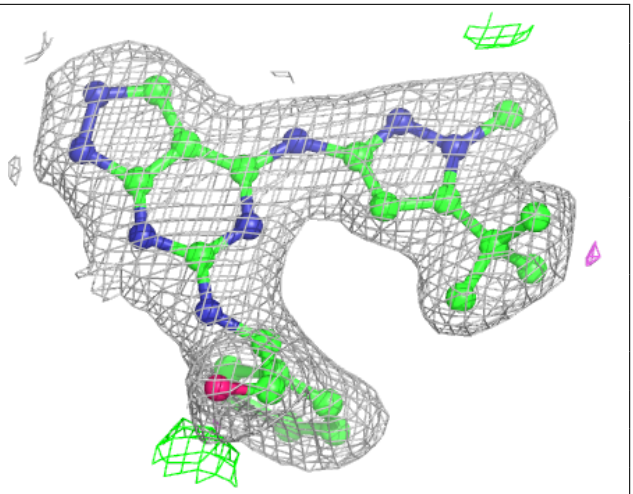
Electron density around UYD A 501:

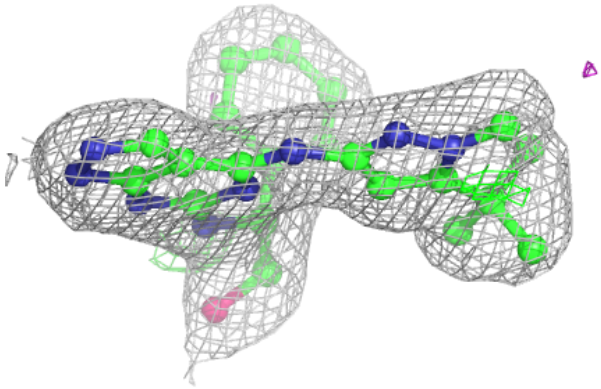
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

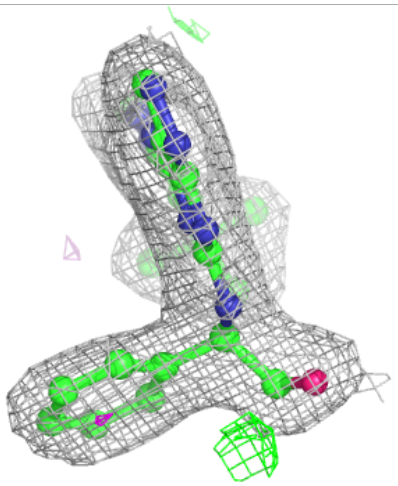


Electron density around UYD B 501:

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

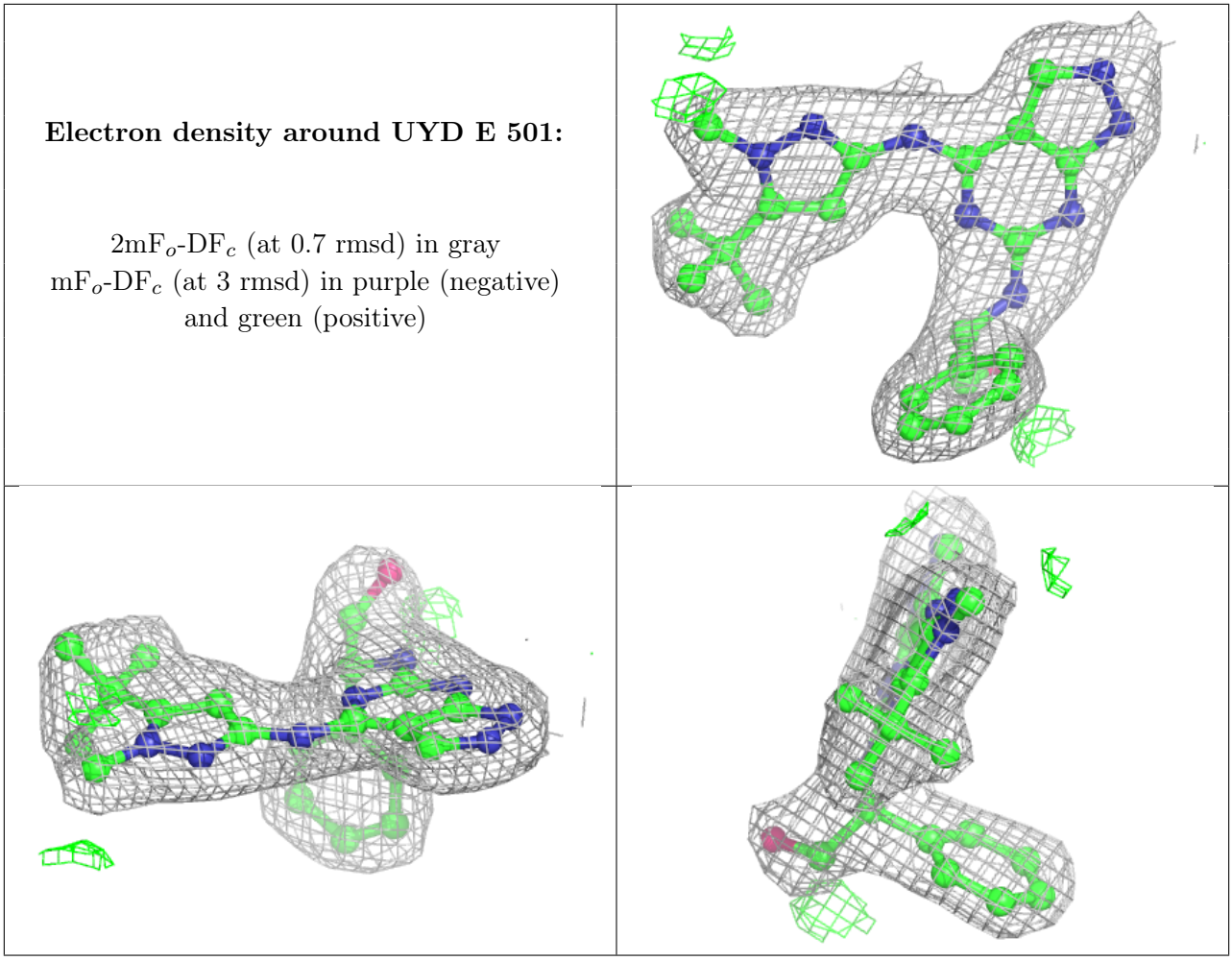






Electron density around UYD E 501:

$2mF_o$-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

There are no such residues in this entry.