Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2024 – 03:10 pm BST

PDB ID	:	9ENN
Title	:	L-amino acid oxidase 4 (HcLAAO4) from the fungus Hebeloma cylindrosporum in complex with N-epsilon-acetyl-L-lysine
Authors	:	Gilzer, D.; Koopmeiners, S.; Fischer von Mollard, G.; Niemann, H.H.
Deposited on	:	2024-03-13
Resolution	:	1.80 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:

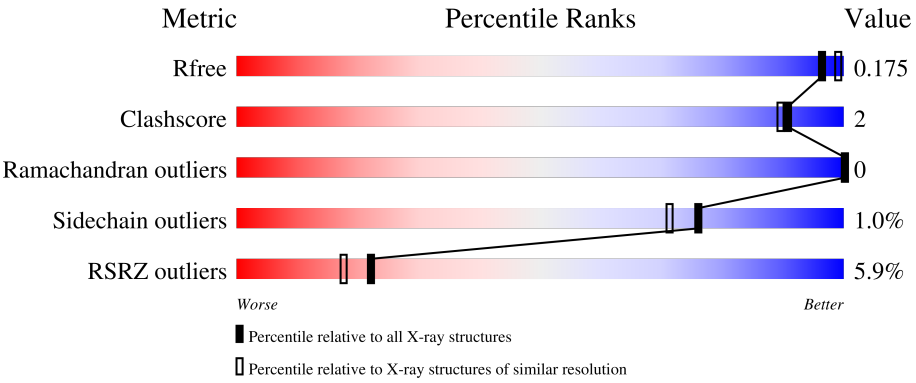
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	562	6% 93% · 5%
1	B	562	5% 90% · 6%
1	C	562	5% 91% · 5%
1	D	562	7% 92% · 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	711	-	-	-	X
4	SO4	C	712	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 35880 atoms, of which 16797 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.

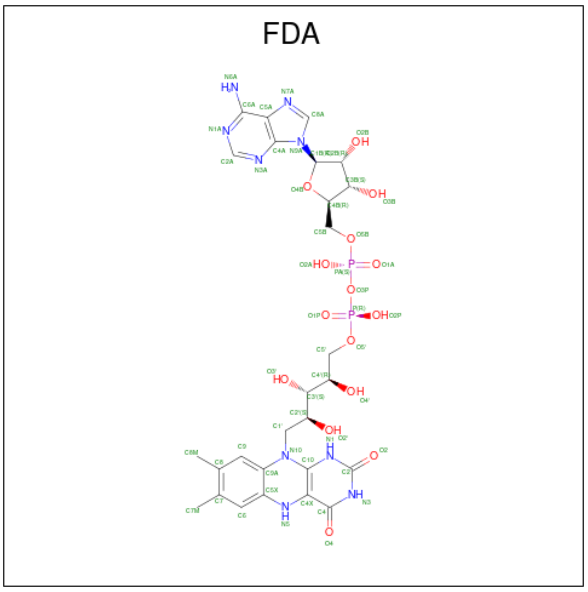
- Molecule 1 is a protein called L-amino acid oxidase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	536	Total	C	H	N	O	S	0	12	0
			8442	2755	4163	716	797	11			
1	B	531	Total	C	H	N	O	S	0	8	0
			8325	2719	4101	709	785	11			
1	C	532	Total	C	H	N	O	S	0	8	0
			8326	2721	4097	709	788	11			
1	D	535	Total	C	H	N	O	S	0	9	0
			8382	2736	4128	715	792	11			

There are 8 discrepancies between the modelled and reference sequences:

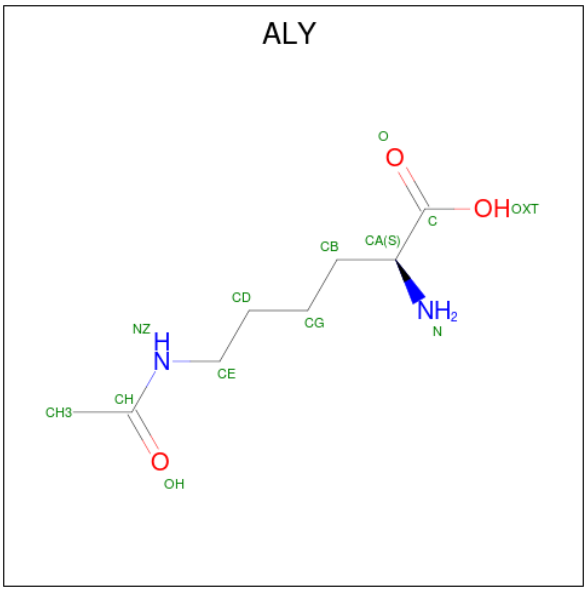
Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ALA	LYS	engineered mutation	UNP S4S6Z0
A	475	ALA	LYS	engineered mutation	UNP S4S6Z0
B	474	ALA	LYS	engineered mutation	UNP S4S6Z0
B	475	ALA	LYS	engineered mutation	UNP S4S6Z0
C	474	ALA	LYS	engineered mutation	UNP S4S6Z0
C	475	ALA	LYS	engineered mutation	UNP S4S6Z0
D	474	ALA	LYS	engineered mutation	UNP S4S6Z0
D	475	ALA	LYS	engineered mutation	UNP S4S6Z0

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



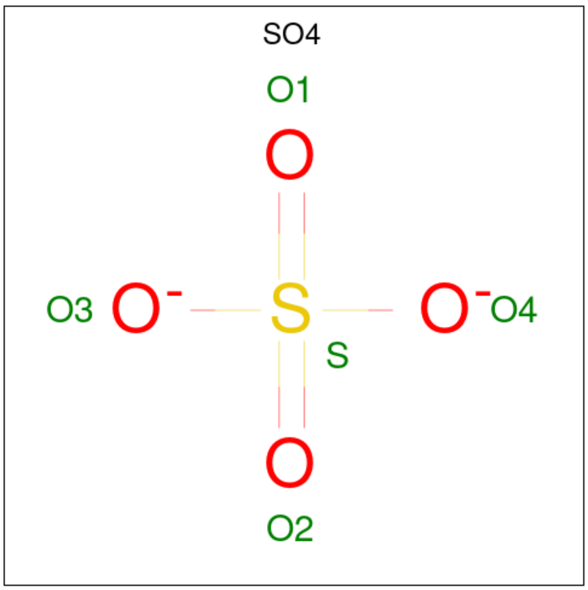
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		
2	D	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		

- Molecule 3 is N(6)-ACETYLLYSINE (three-letter code: ALY) (formula: $C_8H_{16}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 28	C 8	H 15	N 2	O 3	0	0
3	B	1	Total 28	C 8	H 15	N 2	O 3	0	0
3	C	1	Total 28	C 8	H 15	N 2	O 3	0	0
3	D	1	Total 28	C 8	H 15	N 2	O 3	0	0

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



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

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

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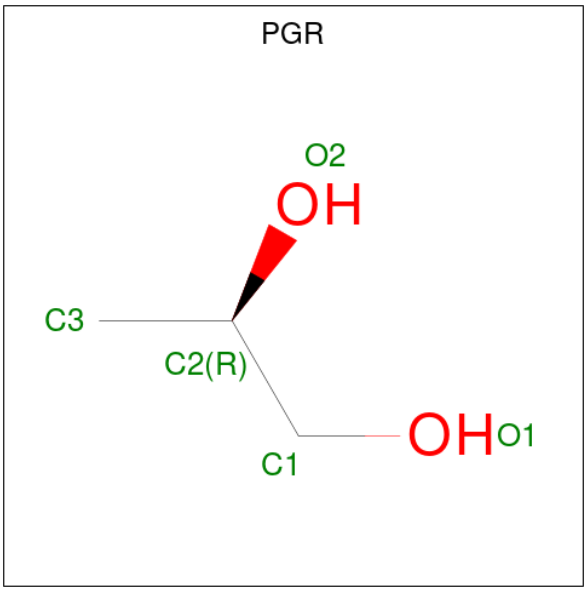
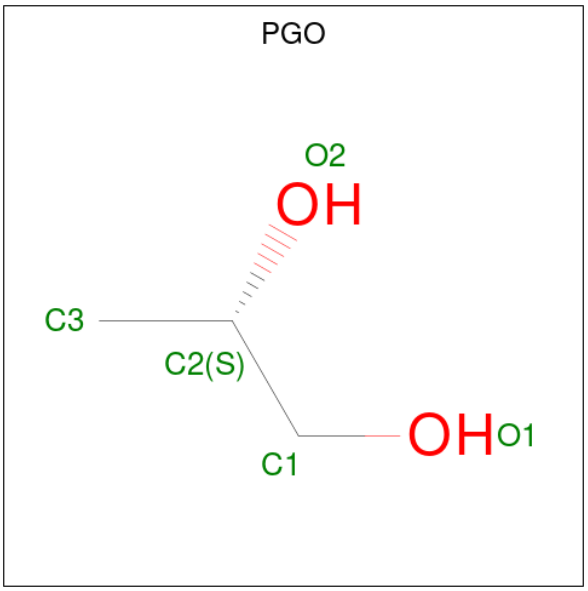
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0

- Molecule 5 is R-1,2-PROPANEDIOL (three-letter code: PGR) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 13 3 8 2	0	0
5	A	1	Total C H O 13 3 8 2	0	0
5	A	1	Total C H O 13 3 8 2	0	0
5	B	1	Total C H O 13 3 8 2	0	0
5	B	1	Total C H O 13 3 8 2	0	0
5	C	1	Total C H O 13 3 8 2	0	0
5	C	1	Total C H O 13 3 8 2	0	0
5	C	1	Total C H O 13 3 8 2	0	0
5	D	1	Total C H O 13 3 8 2	0	0
5	D	1	Total C H O 13 3 8 2	0	0

- Molecule 6 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C H O 13 3 8 2	0	0
6	A	1	Total C H O 13 3 8 2	0	0
6	B	1	Total C H O 13 3 8 2	0	0
6	C	1	Total C H O 13 3 8 2	0	0
6	D	1	Total C H O 13 3 8 2	0	0

- Molecule 7 is water.

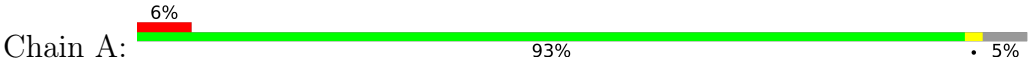
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	437	Total O 442 442	0	5
7	B	420	Total O 424 424	0	6
7	C	329	Total O 332 332	0	3
7	D	316	Total O 320 320	0	4

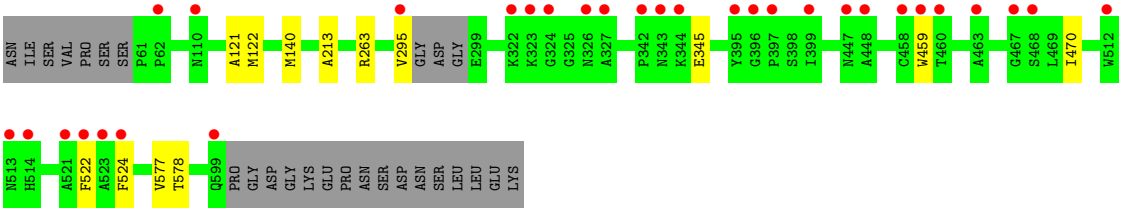
3 Residue-property plots (i)

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: L-amino acid oxidase 4

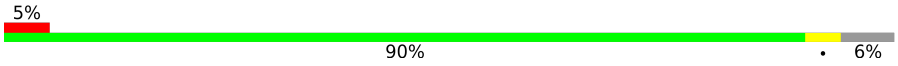
Chain A:

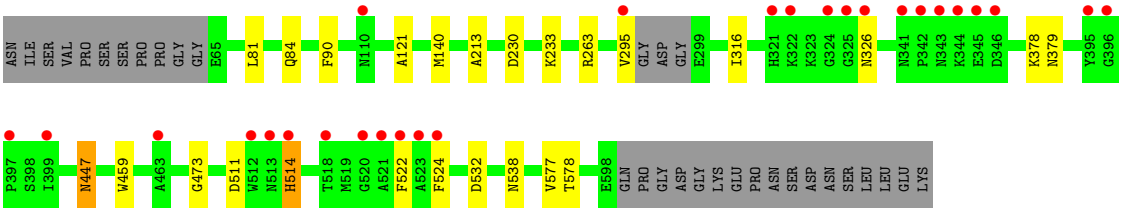




• Molecule 1: L-amino acid oxidase 4

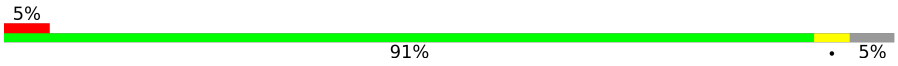
Chain B:

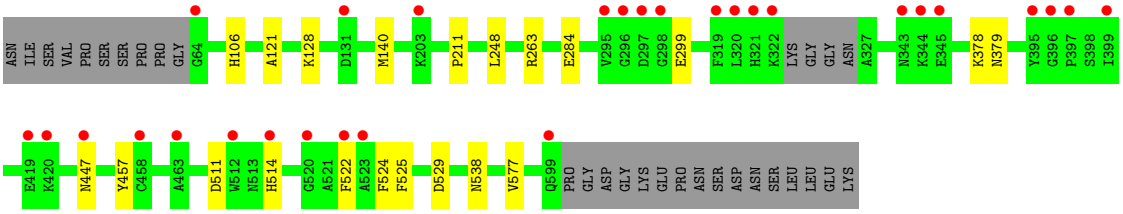




• Molecule 1: L-amino acid oxidase 4

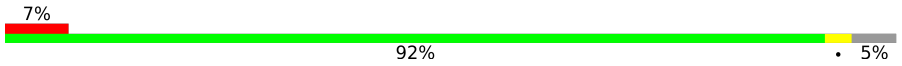
Chain C:

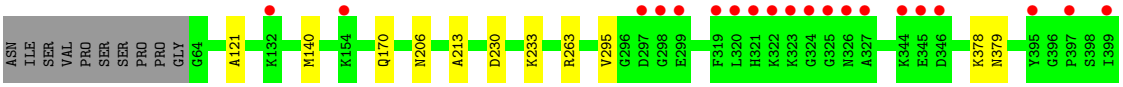


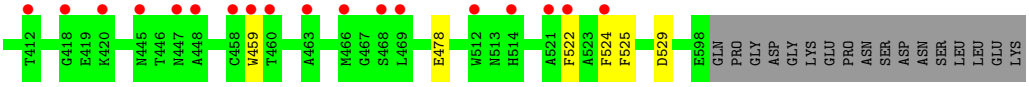


• Molecule 1: L-amino acid oxidase 4

Chain D:






T412
G418
E419
K420
N445
T446
N447
A448
C458
W459
T460
A463
M466
G467
S468
L469
E478
W512
N513
H514
A521
F522
A523
F524
F525
D529
E598
GLN
PRO
GLY
ASP
GLY
LYS
GLU
PRO
ASN
SER
ASP
ASN
SER
LEU
LEU
GLU
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.88Å 132.12Å 107.32Å 90.00° 95.93° 90.00°	Depositor
Resolution (Å)	47.38 – 1.80 47.38 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.38-1.80) 98.8 (47.38-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.154 , 0.177 0.152 , 0.175	Depositor DCC
R_{free} test set	10729 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 48.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	35880	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: PGR, ALY, FDA, SO4, PGO

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	0.34	0/4437	0.60	0/6031
1	B	0.34	0/4370	0.60	0/5941
1	C	0.32	0/4375	0.58	0/5949
1	D	0.32	0/4402	0.57	0/5985
All	All	0.33	0/17584	0.59	0/23906

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	4279	4163	4161	8	0
1	B	4224	4101	4093	19	0
1	C	4229	4097	4093	14	0
1	D	4254	4128	4130	12	0
2	A	53	32	33	1	0
2	B	53	32	33	1	0
2	C	53	32	33	1	0
2	D	53	32	33	1	0
3	A	13	15	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	15	15	0	0
3	C	13	15	15	0	0
3	D	13	15	15	0	0
4	A	45	0	0	2	0
4	B	60	0	0	2	0
4	C	70	0	0	2	0
4	D	65	0	0	2	0
5	A	15	24	24	3	0
5	B	10	16	16	3	0
5	C	15	24	24	3	0
5	D	10	16	16	2	0
6	A	10	16	16	1	0
6	B	5	8	8	0	0
6	C	5	8	8	0	0
6	D	5	8	8	0	0
7	A	442	0	0	4	0
7	B	424	0	0	5	0
7	C	332	0	0	4	0
7	D	320	0	0	4	0
All	All	19083	16797	16789	58	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 2.

All (58) 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)
4:A:703:SO4:O4	7:A:801:HOH:O	1.88	0.91
4:B:711:SO4:O3	7:B:801:HOH:O	1.89	0.88
1:B:230:ASP:HA	1:B:233:LYS:HE2	1.56	0.88
4:B:713:SO4:O1	7:B:802:HOH:O	1.93	0.87
1:D:206[A]:ASN:OD1	7:D:801:HOH:O	2.03	0.76
6:A:713:PGO:H32	7:A:946:HOH:O	1.89	0.73
1:C:379:ASN:N	4:C:704:SO4:O4	2.22	0.71
4:D:710:SO4:O2	7:D:802:HOH:O	2.10	0.69
1:B:230:ASP:HA	1:B:233:LYS:CE	2.27	0.65
1:B:473:GLY:HA3	1:C:248:LEU:HD12	1.83	0.60
1:C:447:ASN:N	4:C:705:SO4:O4	2.33	0.59
1:D:121:ALA:HA	2:D:701:FDA:C4X	2.35	0.56
1:A:121:ALA:HA	2:A:701:FDA:C4X	2.37	0.54
1:C:121:ALA:HA	2:C:701:FDA:C4X	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:ASP:OD1	7:B:803:HOH:O	2.18	0.53
1:B:213:ALA:HB1	1:B:295:VAL:HG21	1.92	0.52
1:A:577:VAL:HG23	1:A:578:THR:HG23	1.91	0.52
1:A:345:GLU:N	4:A:711:SO4:O3	2.37	0.51
1:D:378:LYS:O	7:D:803:HOH:O	2.19	0.50
1:B:121:ALA:HA	2:B:701:FDA:C4X	2.42	0.50
1:C:447:ASN:ND2	7:C:806:HOH:O	2.39	0.50
1:C:457:TYR:O	5:C:718:PGR:H32	2.12	0.49
1:B:447:ASN:OD1	1:B:447:ASN:N	2.35	0.48
1:C:511:ASP:OD2	1:C:514[A]:HIS:ND1	2.46	0.47
1:B:81:LEU:HD13	1:B:316:ILE:HG23	1.96	0.47
1:D:378:LYS:O	1:D:379:ASN:HB2	2.15	0.46
1:C:106:HIS:HD2	7:C:1102:HOH:O	1.98	0.46
1:B:577:VAL:HG23	1:B:578:THR:HG23	1.98	0.45
5:C:719:PGR:H31	1:D:263:ARG:HH12	1.81	0.45
1:B:90:PHE:O	1:B:326:ASN:HA	2.17	0.45
1:B:90:PHE:CZ	1:B:326:ASN:CB	3.00	0.45
1:B:378:LYS:O	1:B:379:ASN:HB2	2.17	0.45
5:B:716:PGR:H11	7:B:1008:HOH:O	2.17	0.45
1:A:263:ARG:HH22	5:B:717:PGR:H2	1.82	0.44
1:A:459:TRP:CZ3	5:A:714:PGR:H2	2.53	0.44
1:D:213:ALA:HB1	1:D:295:VAL:HG21	1.99	0.44
1:B:90:PHE:CE1	1:B:326:ASN:HB2	2.52	0.44
5:A:714:PGR:H11	7:A:921:HOH:O	2.18	0.43
1:A:213:ALA:HB1	1:A:295:VAL:HG21	2.00	0.43
1:B:459:TRP:CZ3	5:B:716:PGR:H2	2.53	0.43
5:C:719:PGR:H2	1:D:263:ARG:HH22	1.84	0.43
1:B:538:ASN:HB2	7:B:924:HOH:O	2.19	0.42
1:C:538:ASN:HB2	7:C:989:HOH:O	2.19	0.42
1:B:511:ASP:OD2	1:B:514[B]:HIS:ND1	2.53	0.42
1:A:470:ILE:O	1:B:514[A]:HIS:HE1	2.02	0.42
1:C:378:LYS:O	1:C:379:ASN:HB2	2.19	0.42
1:B:230:ASP:OD1	1:B:233:LYS:HE3	2.18	0.42
1:D:478:GLU:HG2	7:D:1090[A]:HOH:O	2.18	0.42
1:C:525:PHE:HB3	1:C:529:ASP:HB2	2.02	0.42
1:D:230:ASP:HA	1:D:233:LYS:CE	2.50	0.42
1:C:284:GLU:HG2	7:C:1067:HOH:O	2.20	0.41
1:D:459:TRP:CZ3	5:D:717:PGR:H2	2.55	0.41
1:A:122:MET:HG2	7:A:1118:HOH:O	2.20	0.41
1:D:525:PHE:HB3	1:D:529:ASP:HB2	2.02	0.41
1:D:170:GLN:NE2	4:D:703:SO4:O4	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LYS:HE3	1:C:299:GLU:HB2	2.04	0.40
1:C:263:ARG:HH22	5:D:718:PGR:C2	2.34	0.40
5:A:716:PGR:H31	1:B:263:ARG:HH12	1.87	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	544/562 (97%)	527 (97%)	17 (3%)	0	100	100
1	B	535/562 (95%)	518 (97%)	17 (3%)	0	100	100
1	C	536/562 (95%)	520 (97%)	16 (3%)	0	100	100
1	D	542/562 (96%)	526 (97%)	16 (3%)	0	100	100
All	All	2157/2248 (96%)	2091 (97%)	66 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	457/467 (98%)	454 (99%)	3 (1%)	84	81
1	B	450/467 (96%)	442 (98%)	8 (2%)	59	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	450/467 (96%)	445 (99%)	5 (1%)	73 68
1	D	452/467 (97%)	449 (99%)	3 (1%)	84 81
All	All	1809/1868 (97%)	1790 (99%)	19 (1%)	76 68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	MET
1	A	522	PHE
1	A	524	PHE
1	B	84[A]	GLN
1	B	84[B]	GLN
1	B	140	MET
1	B	447	ASN
1	B	514[A]	HIS
1	B	514[B]	HIS
1	B	522	PHE
1	B	524	PHE
1	C	140	MET
1	C	211	PRO
1	C	522	PHE
1	C	524	PHE
1	C	577	VAL
1	D	140	MET
1	D	522	PHE
1	D	524	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	543	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)

71 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	D	715	-	4,4,4	0.60	0	6,6,6	0.24	0
4	SO4	A	704	-	4,4,4	0.58	0	6,6,6	0.33	0
4	SO4	B	708	-	4,4,4	0.63	0	6,6,6	0.08	0
4	SO4	C	712	-	4,4,4	0.61	0	6,6,6	0.11	0
5	PGR	C	718	-	3,4,4	0.33	0	1,4,4	0.78	0
2	FDA	C	701	-	52,58,58	0.64	0	60,89,89	0.84	2 (3%)
4	SO4	C	714	-	4,4,4	0.63	0	6,6,6	0.14	0
5	PGR	D	717	-	3,4,4	0.29	0	1,4,4	0.86	0
2	FDA	A	701	-	52,58,58	0.65	0	60,89,89	0.80	2 (3%)
4	SO4	D	705	-	4,4,4	0.57	0	6,6,6	0.15	0
4	SO4	C	710	-	4,4,4	0.60	0	6,6,6	0.06	0
4	SO4	D	714	-	4,4,4	0.60	0	6,6,6	0.13	0
4	SO4	B	713	-	4,4,4	0.62	0	6,6,6	0.14	0
5	PGR	C	717	-	3,4,4	0.26	0	1,4,4	0.35	0
3	ALY	A	702	-	11,12,12	0.95	1 (9%)	13,14,14	0.86	0
4	SO4	C	715	-	4,4,4	0.61	0	6,6,6	0.06	0
4	SO4	D	710	-	4,4,4	0.61	0	6,6,6	0.11	0
4	SO4	D	708	-	4,4,4	0.61	0	6,6,6	0.10	0
5	PGR	D	718	-	3,4,4	0.20	0	1,4,4	0.96	0
4	SO4	D	703	-	4,4,4	0.59	0	6,6,6	0.12	0
4	SO4	D	709	-	4,4,4	0.60	0	6,6,6	0.07	0
4	SO4	C	708	-	4,4,4	0.61	0	6,6,6	0.06	0
6	PGO	A	713	-	3,4,4	0.35	0	1,4,4	0.50	0
4	SO4	B	707	-	4,4,4	0.61	0	6,6,6	0.08	0
4	SO4	C	707	-	4,4,4	0.62	0	6,6,6	0.26	0
2	FDA	B	701	-	52,58,58	0.63	0	60,89,89	0.78	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	B	706	-	4,4,4	0.57	0	6,6,6	0.32	0
4	SO4	D	713	-	4,4,4	0.60	0	6,6,6	0.09	0
4	SO4	A	706	-	4,4,4	0.57	0	6,6,6	0.32	0
4	SO4	D	706	-	4,4,4	0.61	0	6,6,6	0.12	0
4	SO4	C	711	-	4,4,4	0.61	0	6,6,6	0.16	0
4	SO4	A	707	-	4,4,4	0.58	0	6,6,6	0.08	0
5	PGR	A	714	-	3,4,4	0.40	0	1,4,4	0.76	0
4	SO4	B	711	-	4,4,4	0.59	0	6,6,6	0.10	0
4	SO4	B	704	-	4,4,4	0.63	0	6,6,6	0.13	0
4	SO4	D	707	-	4,4,4	0.59	0	6,6,6	0.08	0
4	SO4	D	711	-	4,4,4	0.61	0	6,6,6	0.13	0
4	SO4	B	714	-	4,4,4	0.60	0	6,6,6	0.34	0
3	ALY	C	702	-	11,12,12	1.01	1 (9%)	13,14,14	0.71	0
4	SO4	C	705	-	4,4,4	0.61	0	6,6,6	0.08	0
4	SO4	D	712	-	4,4,4	0.61	0	6,6,6	0.08	0
3	ALY	B	702	-	11,12,12	0.98	1 (9%)	13,14,14	0.80	0
5	PGR	C	719	-	3,4,4	0.18	0	1,4,4	0.66	0
6	PGO	D	716	-	3,4,4	0.29	0	1,4,4	0.64	0
3	ALY	D	702	-	11,12,12	1.15	2 (18%)	13,14,14	0.99	1 (7%)
4	SO4	A	708	-	4,4,4	0.61	0	6,6,6	0.10	0
2	FDA	D	701	-	52,58,58	0.63	0	60,89,89	0.80	1 (1%)
4	SO4	C	706	-	4,4,4	0.62	0	6,6,6	0.12	0
4	SO4	C	703	-	4,4,4	0.59	0	6,6,6	0.09	0
4	SO4	B	703	-	4,4,4	0.61	0	6,6,6	0.31	0
4	SO4	A	711	-	4,4,4	0.60	0	6,6,6	0.10	0
6	PGO	B	715	-	3,4,4	0.27	0	1,4,4	0.60	0
4	SO4	C	709	-	4,4,4	0.60	0	6,6,6	0.10	0
6	PGO	C	720	-	3,4,4	0.28	0	1,4,4	0.29	0
4	SO4	A	710	-	4,4,4	0.61	0	6,6,6	0.07	0
4	SO4	C	704	-	4,4,4	0.58	0	6,6,6	0.10	0
4	SO4	B	709	-	4,4,4	0.62	0	6,6,6	0.19	0
4	SO4	A	703	-	4,4,4	0.61	0	6,6,6	0.43	0
4	SO4	A	709	-	4,4,4	0.62	0	6,6,6	0.13	0
4	SO4	D	704	-	4,4,4	0.59	0	6,6,6	0.14	0
5	PGR	A	716	-	3,4,4	0.17	0	1,4,4	0.75	0
4	SO4	A	705	-	4,4,4	0.61	0	6,6,6	0.22	0
4	SO4	C	716	-	4,4,4	0.60	0	6,6,6	0.10	0
4	SO4	B	712	-	4,4,4	0.63	0	6,6,6	0.14	0
6	PGO	A	715	-	3,4,4	0.36	0	1,4,4	0.40	0
4	SO4	B	710	-	4,4,4	0.61	0	6,6,6	0.09	0
5	PGR	B	717	-	3,4,4	0.22	0	1,4,4	0.58	0
4	SO4	C	713	-	4,4,4	0.62	0	6,6,6	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PGR	B	716	-	3,4,4	0.30	0	1,4,4	0.91	0
4	SO4	B	705	-	4,4,4	0.60	0	6,6,6	0.15	0
5	PGR	A	712	-	3,4,4	0.24	0	1,4,4	0.36	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
5	PGR	C	718	-	-	0/2/2/2	-
2	FDA	C	701	-	-	2/30/50/50	0/6/6/6
5	PGR	D	717	-	-	0/2/2/2	-
2	FDA	A	701	-	-	2/30/50/50	0/6/6/6
5	PGR	C	717	-	-	0/2/2/2	-
3	ALY	A	702	-	-	3/12/12/12	-
5	PGR	D	718	-	-	0/2/2/2	-
6	PGO	A	713	-	-	2/2/2/2	-
2	FDA	B	701	-	-	2/30/50/50	0/6/6/6
5	PGR	A	714	-	-	0/2/2/2	-
3	ALY	C	702	-	-	3/12/12/12	-
3	ALY	B	702	-	-	3/12/12/12	-
5	PGR	C	719	-	-	2/2/2/2	-
6	PGO	D	716	-	-	2/2/2/2	-
3	ALY	D	702	-	-	3/12/12/12	-
2	FDA	D	701	-	-	2/30/50/50	0/6/6/6
6	PGO	B	715	-	-	2/2/2/2	-
6	PGO	C	720	-	-	0/2/2/2	-
5	PGR	A	716	-	-	0/2/2/2	-
6	PGO	A	715	-	-	0/2/2/2	-
5	PGR	B	717	-	-	2/2/2/2	-
5	PGR	B	716	-	-	0/2/2/2	-
5	PGR	A	712	-	-	0/2/2/2	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	ALY	CH3-CH	2.78	1.56	1.50
3	C	702	ALY	CH3-CH	2.70	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	ALY	CH3-CH	2.68	1.56	1.50
3	A	702	ALY	CH3-CH	2.48	1.55	1.50
3	D	702	ALY	OXT-C	-2.25	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	FDA	C5A-C6A-N6A	2.39	123.98	120.35
2	C	701	FDA	C5A-C6A-N6A	2.38	123.97	120.35
2	C	701	FDA	O4B-C1B-C2B	-2.34	103.51	106.93
2	A	701	FDA	C5A-C6A-N6A	2.30	123.84	120.35
2	A	701	FDA	O4B-C1B-C2B	-2.29	103.58	106.93
2	B	701	FDA	C5A-C6A-N6A	2.16	123.63	120.35
3	D	702	ALY	OXT-C-CA	2.04	120.32	113.38

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	717	PGR	O1-C1-C2-C3
5	B	717	PGR	O1-C1-C2-O2
5	C	719	PGR	O1-C1-C2-C3
5	C	719	PGR	O1-C1-C2-O2
6	A	713	PGO	O1-C1-C2-O2
6	D	716	PGO	O1-C1-C2-C3
6	D	716	PGO	O1-C1-C2-O2
3	A	702	ALY	CG-CD-CE-NZ
3	B	702	ALY	CG-CD-CE-NZ
3	C	702	ALY	CG-CD-CE-NZ
3	D	702	ALY	CG-CD-CE-NZ
3	C	702	ALY	CE-CD-CG-CB
3	B	702	ALY	CE-CD-CG-CB
3	A	702	ALY	CE-CD-CG-CB
3	D	702	ALY	CE-CD-CG-CB
2	A	701	FDA	PA-O3P-P-O5'
2	B	701	FDA	PA-O3P-P-O5'
2	C	701	FDA	PA-O3P-P-O5'
2	D	701	FDA	PA-O3P-P-O5'
6	A	713	PGO	O1-C1-C2-C3
2	A	701	FDA	O4B-C4B-C5B-O5B
2	B	701	FDA	O4B-C4B-C5B-O5B
3	C	702	ALY	CA-CB-CG-CD

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Mol	Chain	Res	Type	Atoms
3	B	702	ALY	CA-CB-CG-CD
2	C	701	FDA	O4B-C4B-C5B-O5B
2	D	701	FDA	O4B-C4B-C5B-O5B
6	B	715	PGO	O1-C1-C2-C3
3	A	702	ALY	CA-CB-CG-CD
3	D	702	ALY	CA-CB-CG-CD
6	B	715	PGO	O1-C1-C2-O2

There are no ring outliers.

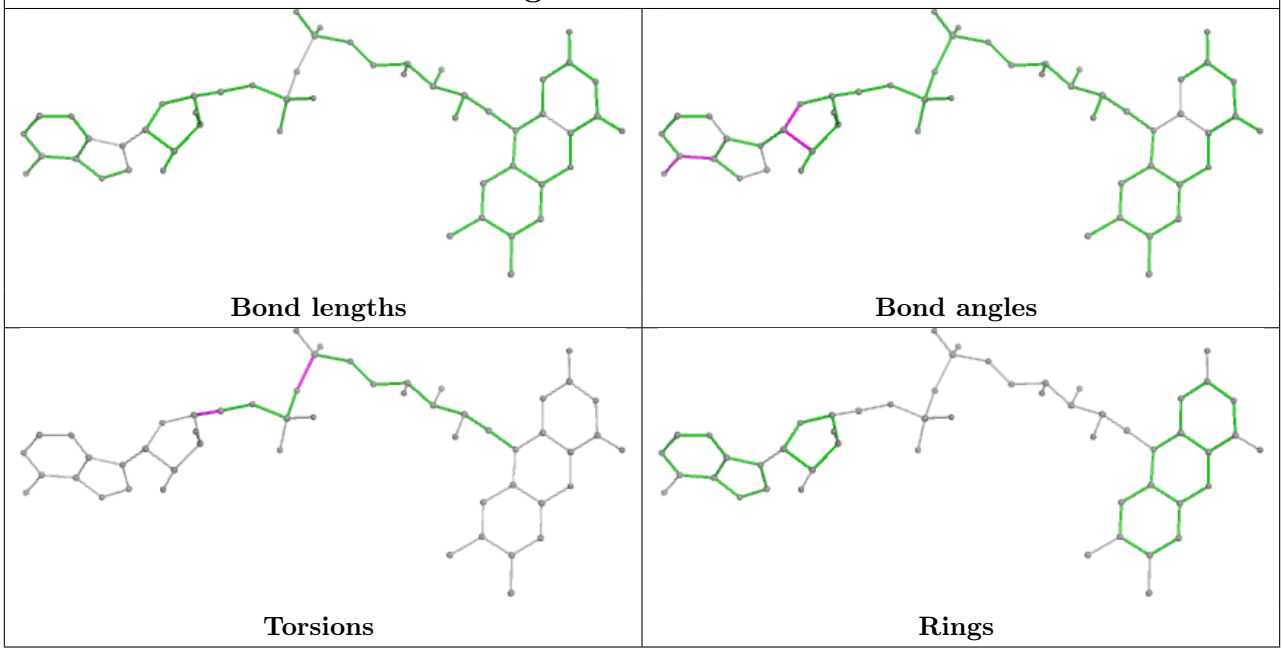
21 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	718	PGR	1	0
2	C	701	FDA	1	0
5	D	717	PGR	1	0
2	A	701	FDA	1	0
4	B	713	SO4	1	0
4	D	710	SO4	1	0
5	D	718	PGR	1	0
4	D	703	SO4	1	0
6	A	713	PGO	1	0
2	B	701	FDA	1	0
5	A	714	PGR	2	0
4	B	711	SO4	1	0
4	C	705	SO4	1	0
5	C	719	PGR	2	0
2	D	701	FDA	1	0
4	A	711	SO4	1	0
4	C	704	SO4	1	0
4	A	703	SO4	1	0
5	A	716	PGR	1	0
5	B	717	PGR	1	0
5	B	716	PGR	2	0

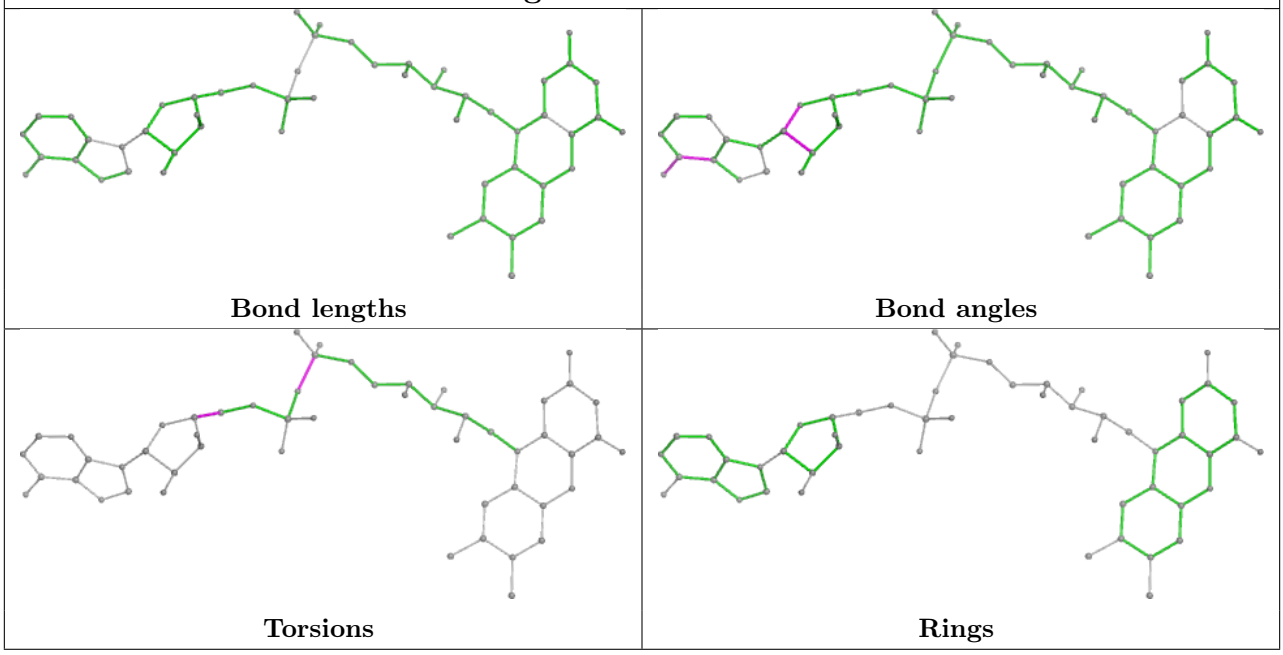
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

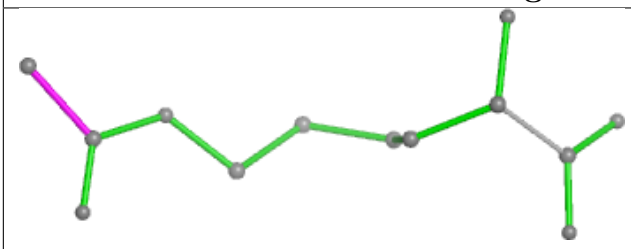
Ligand FDA C 701



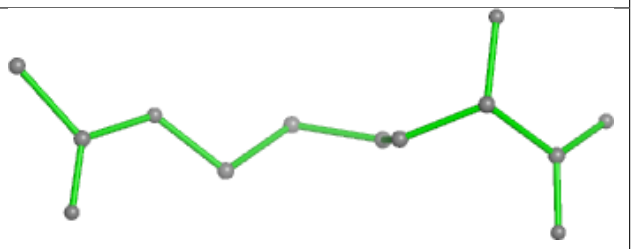
Ligand FDA A 701



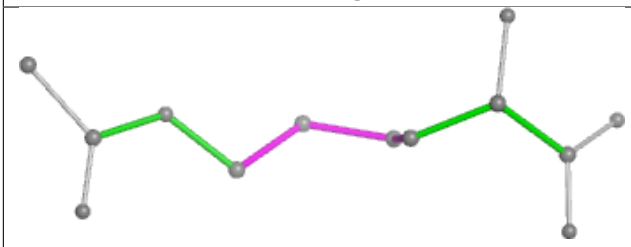
Ligand ALY A 702



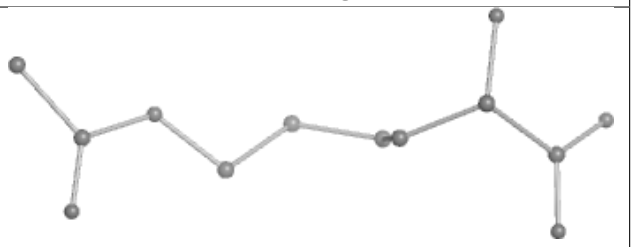
Bond lengths



Bond angles

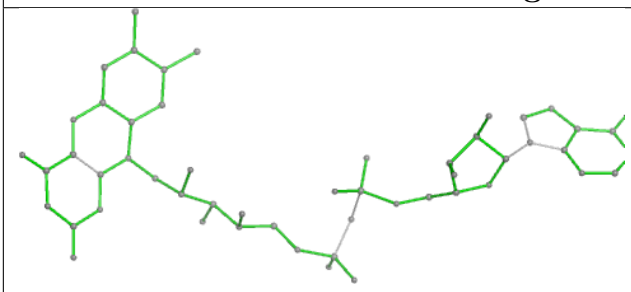


Torsions

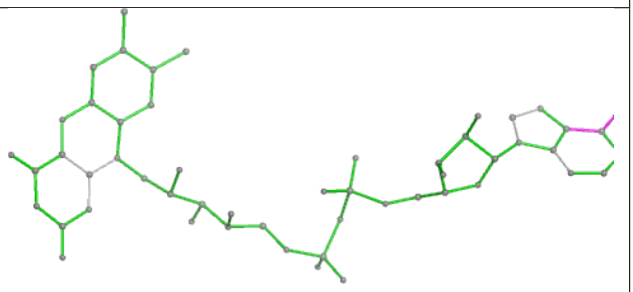


Rings

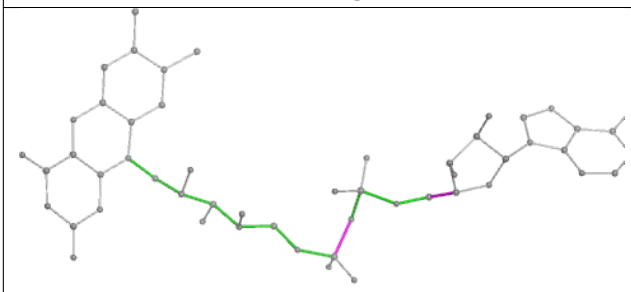
Ligand FDA B 701



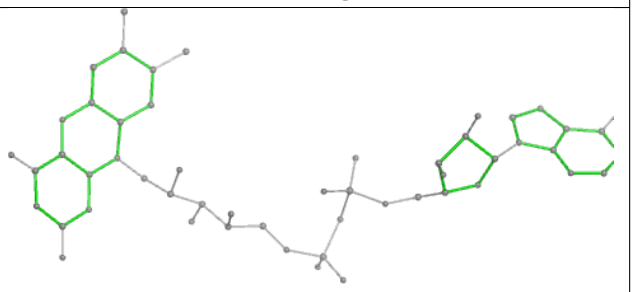
Bond lengths



Bond angles

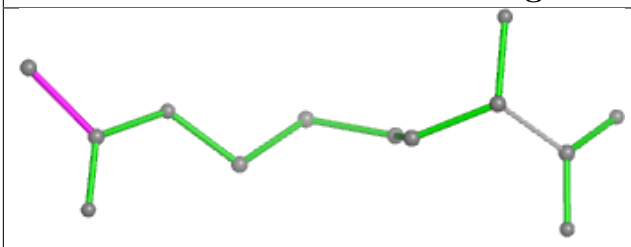


Torsions

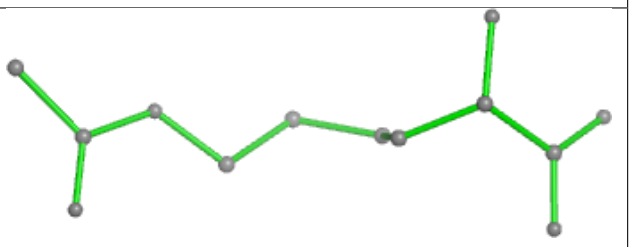


Rings

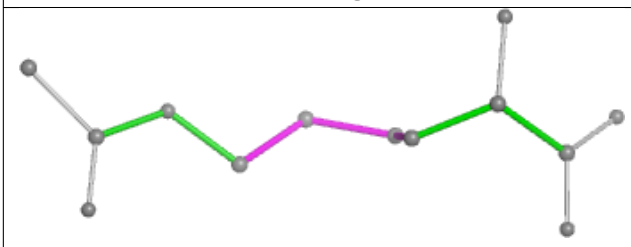
Ligand ALY C 702



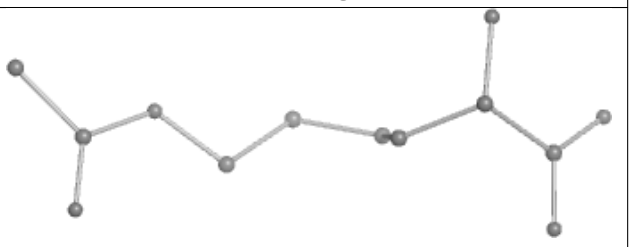
Bond lengths



Bond angles

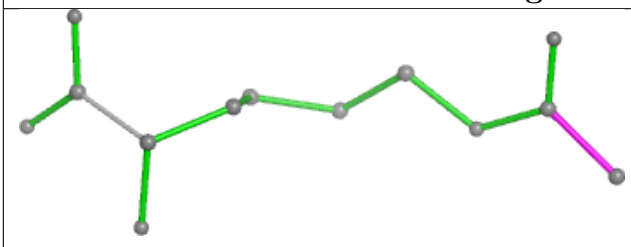


Torsions

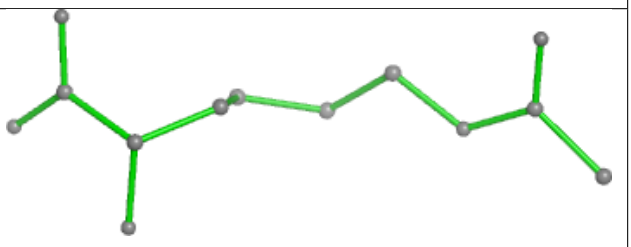


Rings

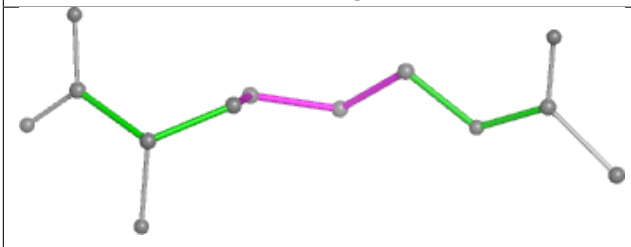
Ligand ALY B 702



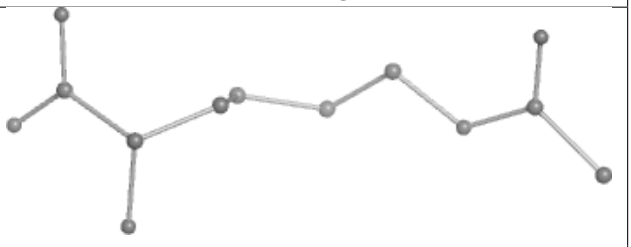
Bond lengths



Bond angles

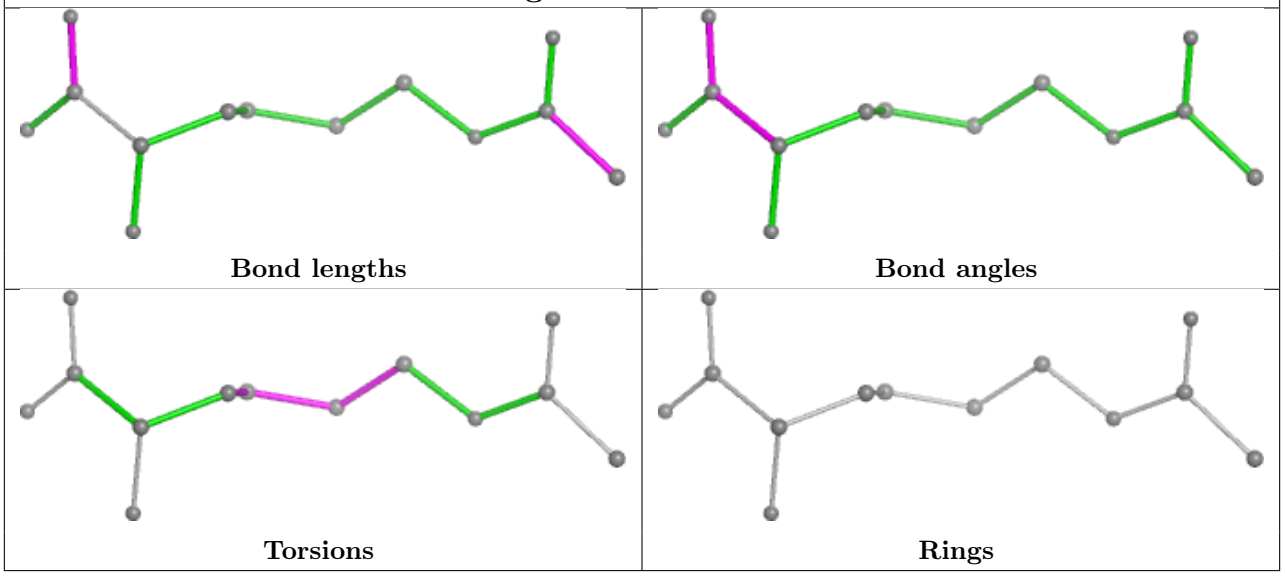


Torsions

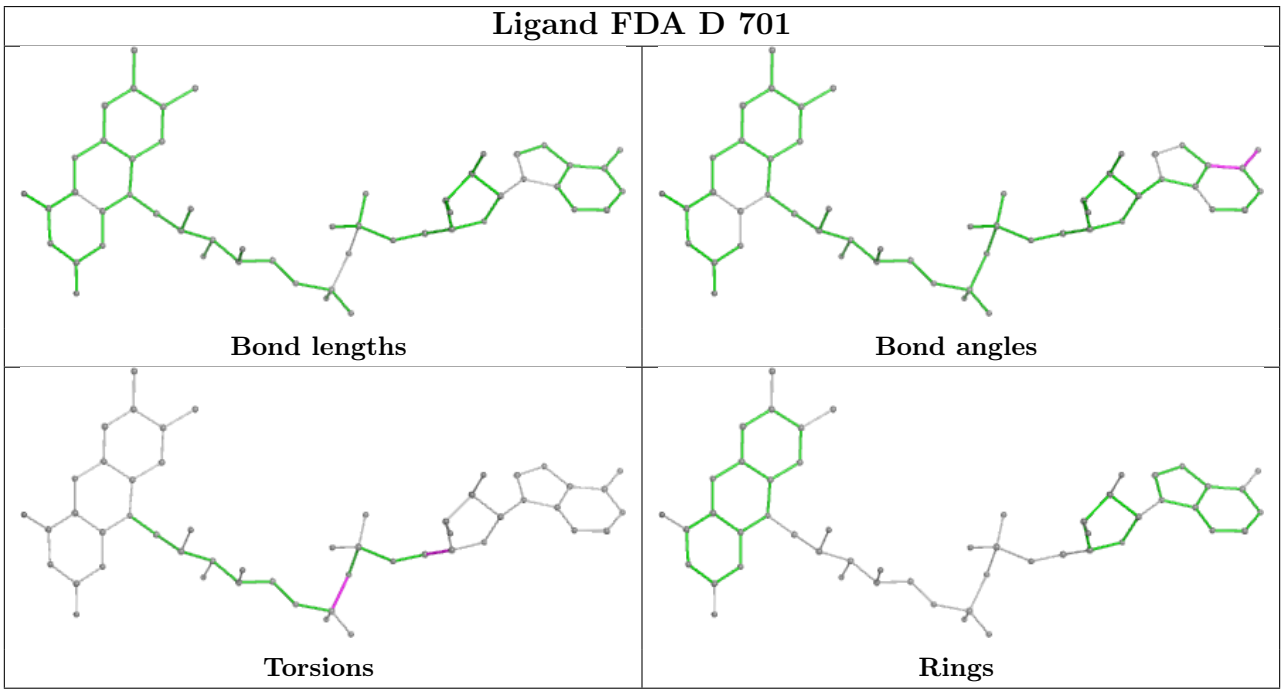


Rings

Ligand ALY D 702



Ligand FDA D 701



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	536/562 (95%)	0.00	31 (5%)	23	18	23, 32, 51, 98	0
1	B	531/562 (94%)	-0.08	27 (5%)	28	22	22, 31, 52, 93	0
1	C	532/562 (94%)	0.06	29 (5%)	25	20	25, 38, 61, 111	0
1	D	535/562 (95%)	0.13	38 (7%)	16	12	26, 38, 65, 117	0
All	All	2134/2248 (94%)	0.03	125 (5%)	22	17	22, 35, 60, 117	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	324	GLY	7.3
1	D	323	LYS	6.8
1	A	323	LYS	5.6
1	B	326	ASN	5.5
1	D	325	GLY	5.3
1	A	295	VAL	5.0
1	A	324	GLY	5.0
1	C	297	ASP	5.0
1	D	322	LYS	5.0
1	B	295	VAL	4.8
1	D	297	ASP	4.6
1	C	322	LYS	4.6
1	B	325	GLY	4.6
1	D	298	GLY	4.5
1	D	299	GLU	4.3
1	A	322	LYS	4.1
1	D	321	HIS	4.0
1	C	321	HIS	3.8
1	A	343	ASN	3.8
1	D	399	ILE	3.6
1	A	514[A]	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	343	ASN	3.5
1	D	447	ASN	3.5
1	C	319	PHE	3.5
1	A	512	TRP	3.4
1	C	345	GLU	3.3
1	D	345	GLU	3.3
1	B	514[A]	HIS	3.3
1	B	344	LYS	3.2
1	D	463	ALA	3.2
1	A	397	PRO	3.1
1	D	324	GLY	3.1
1	A	327	ALA	3.1
1	B	395	TYR	3.0
1	B	463	ALA	3.0
1	D	418	GLY	2.9
1	D	154	LYS	2.9
1	D	514[A]	HIS	2.9
1	B	345	GLU	2.8
1	C	395	TYR	2.8
1	D	458	CYS	2.8
1	A	62	PRO	2.8
1	A	448	ALA	2.8
1	C	447	ASN	2.8
1	B	399	ILE	2.8
1	A	459	TRP	2.8
1	D	132	LYS	2.8
1	A	344	LYS	2.7
1	B	523	ALA	2.7
1	D	344	LYS	2.7
1	A	523	ALA	2.7
1	B	512	TRP	2.7
1	D	468	SER	2.7
1	A	326	ASN	2.7
1	A	110	ASN	2.6
1	C	344	LYS	2.6
1	B	346	ASP	2.6
1	C	420	LYS	2.6
1	D	459	TRP	2.6
1	C	463	ALA	2.6
1	B	341	ASN	2.6
1	C	343	ASN	2.6
1	C	298	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	447	ASN	2.5
1	D	319	PHE	2.5
1	C	599	GLN	2.5
1	C	397	PRO	2.5
1	C	522	PHE	2.5
1	D	395	TYR	2.5
1	D	346	ASP	2.5
1	B	522	PHE	2.5
1	D	412	THR	2.4
1	A	458	CYS	2.4
1	D	326	ASN	2.4
1	C	458	CYS	2.4
1	C	520	GLY	2.4
1	D	466	MET	2.4
1	C	396	GLY	2.4
1	D	320	LEU	2.4
1	C	514[A]	HIS	2.4
1	A	399	ILE	2.4
1	D	420	LYS	2.3
1	A	467	GLY	2.3
1	B	342	PRO	2.3
1	A	513	ASN	2.3
1	A	599	GLN	2.3
1	A	524	PHE	2.3
1	B	397	PRO	2.3
1	B	518	THR	2.3
1	B	524	PHE	2.3
1	D	524	PHE	2.3
1	D	512	TRP	2.3
1	B	396	GLY	2.3
1	D	445	ASN	2.3
1	D	522	PHE	2.3
1	A	460	THR	2.2
1	A	395	TYR	2.2
1	C	320	LEU	2.2
1	A	342	PRO	2.2
1	A	522	PHE	2.2
1	B	110	ASN	2.2
1	D	397	PRO	2.1
1	D	460	THR	2.1
1	A	463	ALA	2.1
1	C	512	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	448	ALA	2.1
1	A	396	GLY	2.1
1	D	327	ALA	2.1
1	D	521	ALA	2.1
1	B	520	GLY	2.1
1	C	523	ALA	2.1
1	D	469	LEU	2.1
1	C	64	GLY	2.1
1	C	131	ASP	2.1
1	A	521	ALA	2.1
1	B	521	ALA	2.1
1	B	513	ASN	2.0
1	C	203	LYS	2.0
1	C	399	ILE	2.0
1	B	321	HIS	2.0
1	B	322	LYS	2.0
1	C	295	VAL	2.0
1	C	296	GLY	2.0
1	C	419	GLU	2.0
1	A	468	SER	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
4	SO4	C	711	5/5	0.56	0.30	59,63,72,81	5
4	SO4	B	709	5/5	0.68	0.31	39,46,60,66	5
4	SO4	C	709	5/5	0.70	0.37	66,70,78,83	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	714	5/5	0.72	0.32	36,50,71,72	5
4	SO4	D	712	5/5	0.72	0.36	62,64,85,86	5
4	SO4	C	716	5/5	0.73	0.36	62,63,84,93	5
4	SO4	C	712	5/5	0.75	0.42	47,61,68,71	5
4	SO4	D	708	5/5	0.76	0.21	68,68,79,91	5
4	SO4	C	705	5/5	0.77	0.14	63,64,75,80	5
4	SO4	D	715	5/5	0.78	0.34	37,40,45,57	5
4	SO4	D	711	5/5	0.79	0.20	61,70,82,85	5
4	SO4	B	711	5/5	0.79	0.37	46,50,55,57	5
4	SO4	A	711	5/5	0.79	0.42	71,76,84,84	5
4	SO4	C	715	5/5	0.80	0.24	49,59,60,64	5
4	SO4	A	709	5/5	0.81	0.29	36,45,57,63	5
4	SO4	B	712	5/5	0.81	0.18	52,62,68,73	5
4	SO4	D	710	5/5	0.81	0.28	44,57,62,65	5
4	SO4	C	713	5/5	0.82	0.49	61,71,94,112	0
5	PGR	C	718	5/5	0.82	0.49	35,42,51,57	13
4	SO4	C	703	5/5	0.83	0.25	48,57,72,72	5
4	SO4	C	708	5/5	0.83	0.29	71,72,85,93	5
4	SO4	C	714	5/5	0.84	0.36	77,78,100,106	0
4	SO4	C	710	5/5	0.84	0.41	48,55,60,65	5
5	PGR	A	714	5/5	0.84	0.37	27,34,41,44	13
4	SO4	B	707	5/5	0.84	0.18	43,51,63,66	5
4	SO4	D	714	5/5	0.85	0.33	60,68,73,81	5
5	PGR	B	716	5/5	0.85	0.42	28,34,40,47	13
4	SO4	D	709	5/5	0.85	0.27	59,69,73,78	5
4	SO4	B	713	5/5	0.86	0.25	30,51,55,64	5
4	SO4	B	703	5/5	0.87	0.20	34,39,58,67	5
5	PGR	B	717	5/5	0.87	0.12	40,52,63,75	0
4	SO4	A	710	5/5	0.87	0.25	48,59,67,73	5
6	PGO	B	715	5/5	0.87	0.25	45,54,64,65	13
4	SO4	C	707	5/5	0.89	0.24	45,48,63,67	5
4	SO4	B	710	5/5	0.89	0.35	50,64,71,75	5
4	SO4	B	708	5/5	0.90	0.12	38,54,60,66	5
6	PGO	A	713	5/5	0.90	0.20	47,57,69,69	13
4	SO4	D	703	5/5	0.90	0.23	46,47,51,60	5
6	PGO	D	716	5/5	0.90	0.20	51,61,73,73	0
4	SO4	D	705	5/5	0.91	0.19	46,48,52,55	5
4	SO4	B	706	5/5	0.91	0.15	41,44,48,52	5
4	SO4	A	703	5/5	0.91	0.15	33,40,54,62	5
5	PGR	C	717	5/5	0.92	0.21	31,42,49,59	13
4	SO4	D	706	5/5	0.92	0.13	44,45,47,54	5
5	PGR	C	719	5/5	0.92	0.12	41,51,73,88	0

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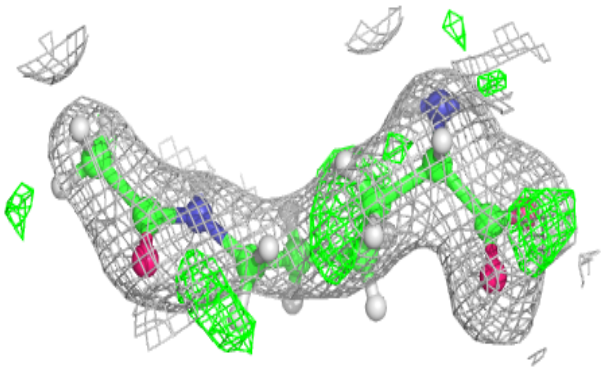
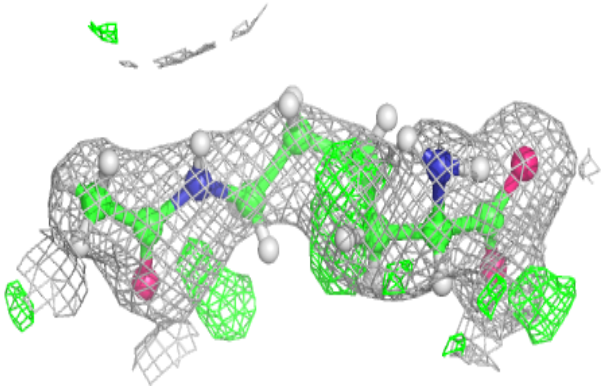
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGR	D	717	5/5	0.92	0.39	38,45,52,54	13
5	PGR	A	716	5/5	0.92	0.12	41,49,77,80	0
4	SO4	A	708	5/5	0.92	0.17	51,56,69,71	5
5	PGR	A	712	5/5	0.92	0.18	25,34,43,51	13
4	SO4	B	704	5/5	0.93	0.20	41,47,59,60	5
5	PGR	D	718	5/5	0.93	0.11	43,56,68,81	0
3	ALY	B	702	13/13	0.93	0.34	27,35,49,55	28
4	SO4	C	704	5/5	0.93	0.14	49,52,66,71	5
6	PGO	C	720	5/5	0.93	0.26	25,38,46,46	13
3	ALY	D	702	13/13	0.93	0.29	34,46,56,64	28
4	SO4	A	705	5/5	0.94	0.18	34,47,53,57	5
4	SO4	D	713	5/5	0.94	0.17	61,62,73,75	5
4	SO4	B	705	5/5	0.94	0.14	43,43,47,49	5
4	SO4	C	706	5/5	0.94	0.12	42,52,60,60	5
3	ALY	A	702	13/13	0.94	0.31	27,38,53,54	28
3	ALY	C	702	13/13	0.94	0.26	31,42,62,65	28
6	PGO	A	715	5/5	0.95	0.24	25,42,51,54	13
4	SO4	D	704	5/5	0.95	0.14	52,53,58,61	5
4	SO4	D	707	5/5	0.95	0.14	50,54,60,62	5
4	SO4	A	707	5/5	0.95	0.15	34,36,45,48	5
4	SO4	A	706	5/5	0.96	0.16	41,42,47,49	5
4	SO4	A	704	5/5	0.97	0.13	40,45,50,55	5
2	FDA	D	701	53/53	0.98	0.12	25,30,37,40	0
2	FDA	A	701	53/53	0.98	0.14	21,26,32,33	0
2	FDA	B	701	53/53	0.98	0.15	21,25,31,33	0
2	FDA	C	701	53/53	0.98	0.13	25,30,36,38	0

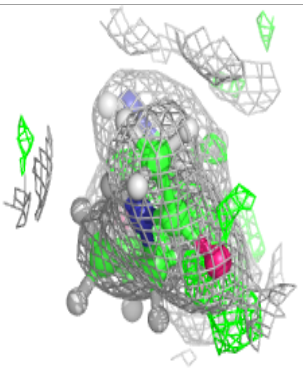
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ALY B 702:

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

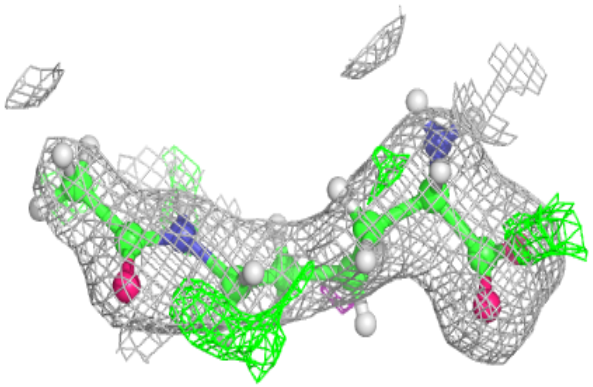


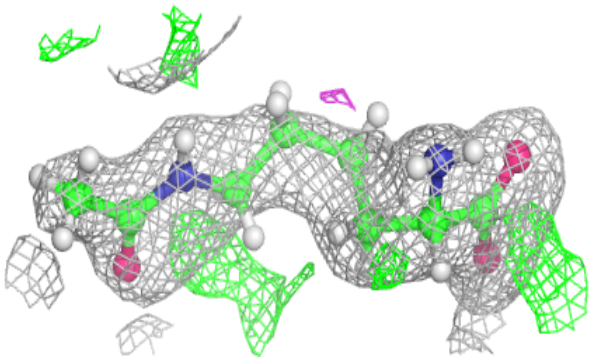


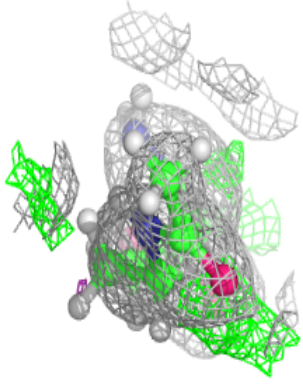


Electron density around ALY D 702:

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

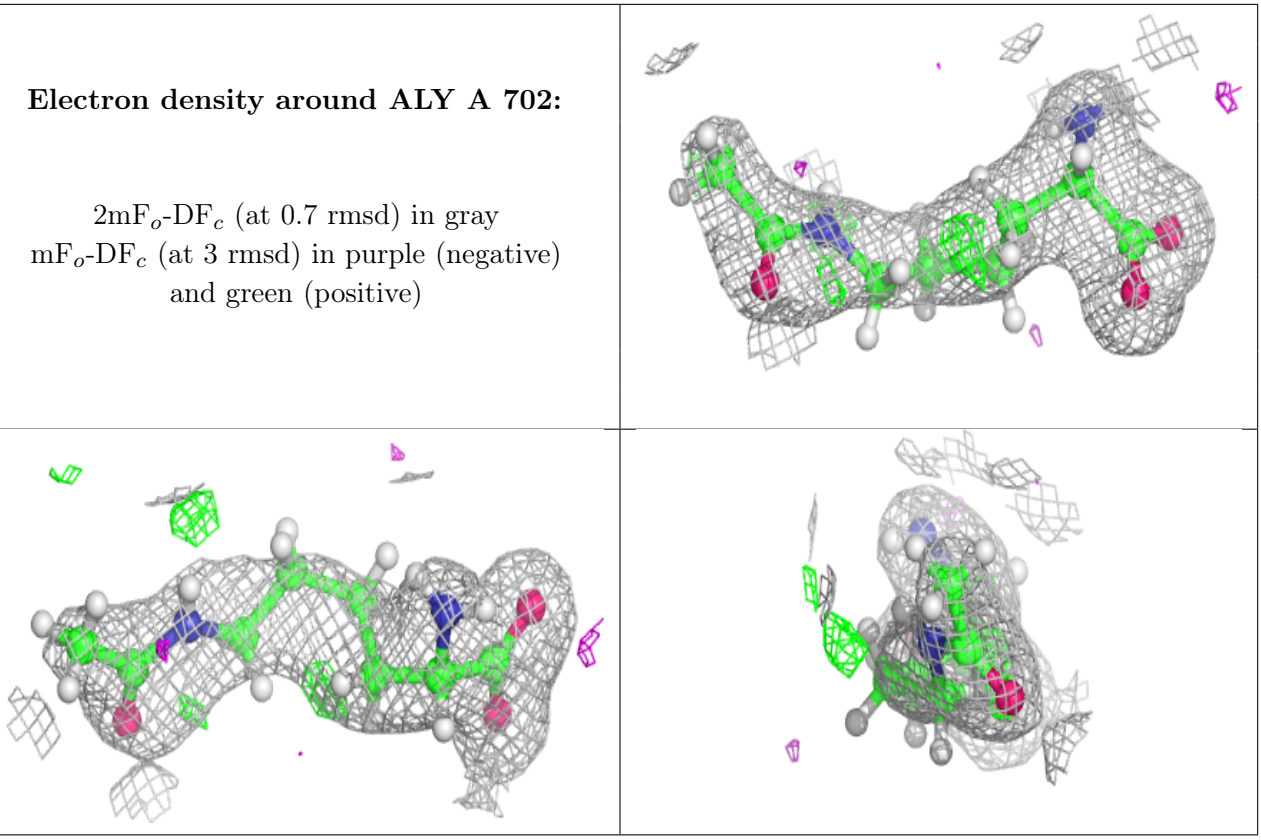






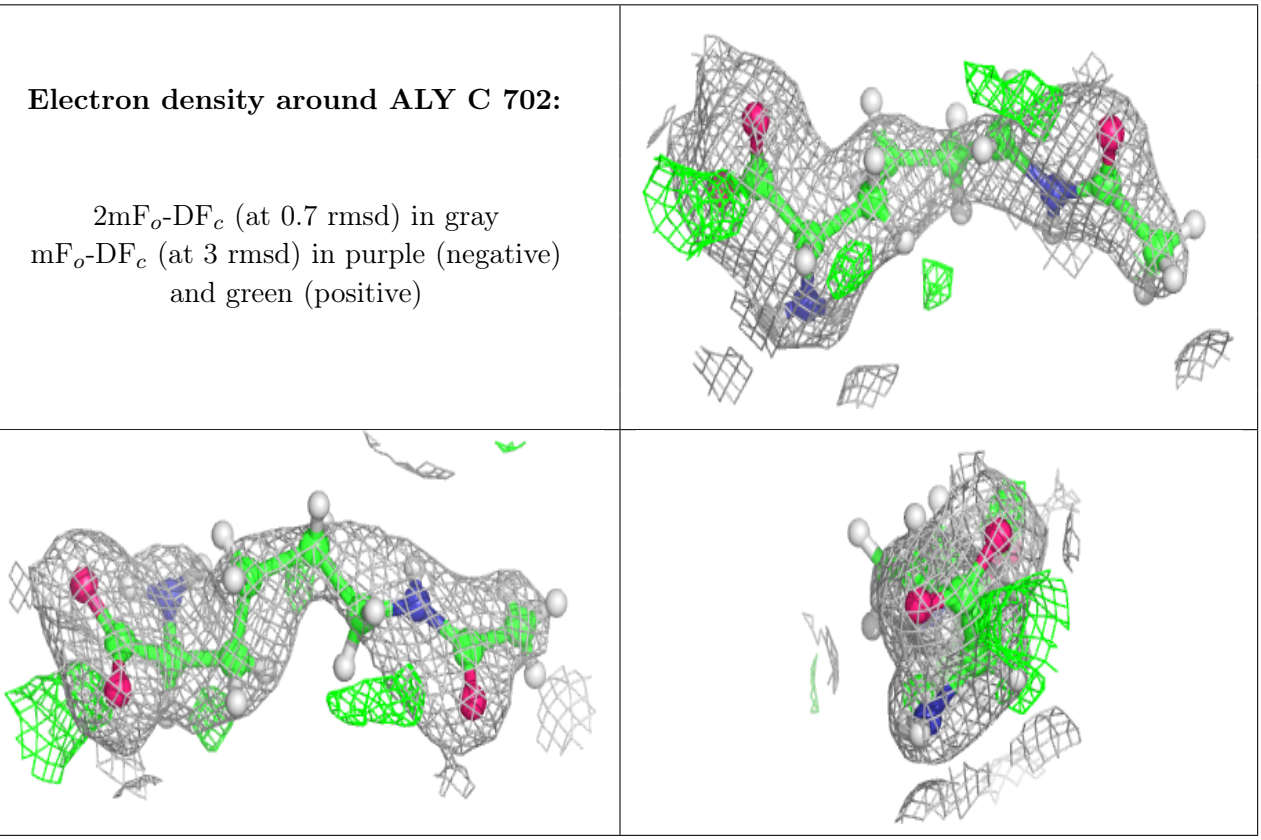
Electron density around ALY A 702:

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



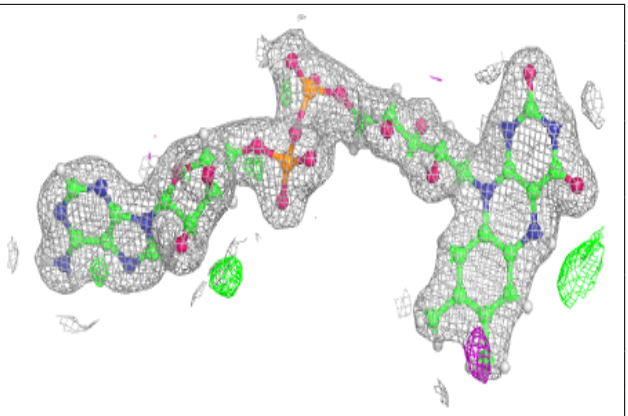
Electron density around ALY C 702:

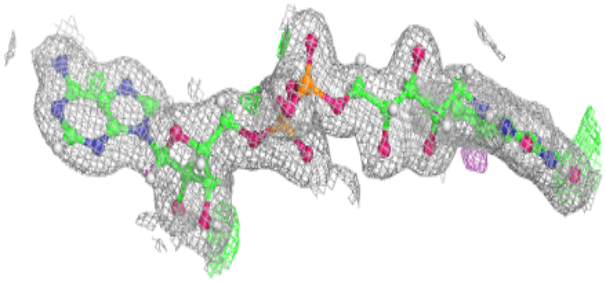
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

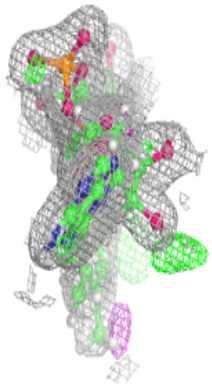


Electron density around FDA D 701:

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

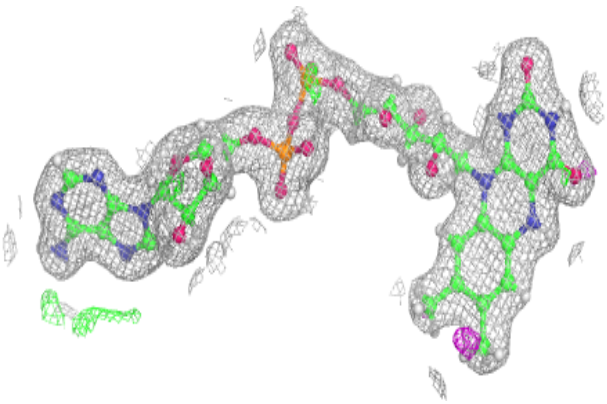


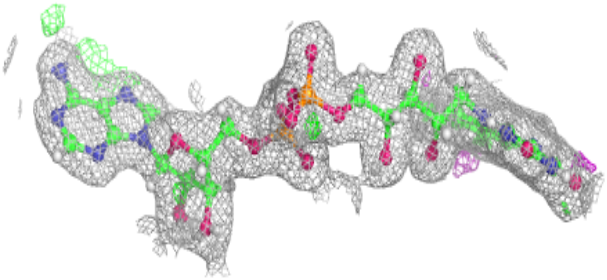


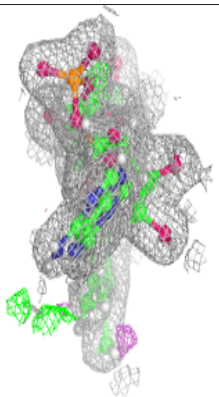


Electron density around FDA A 701:

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

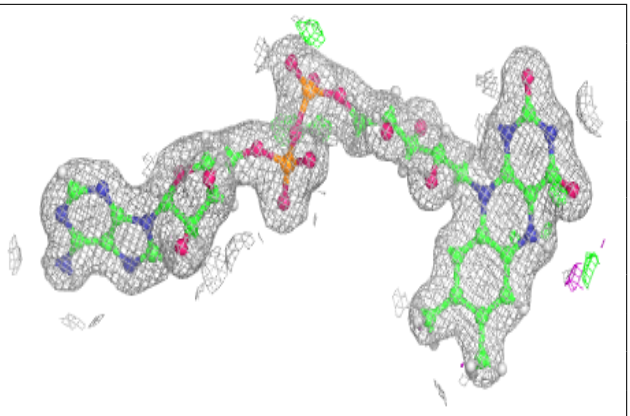


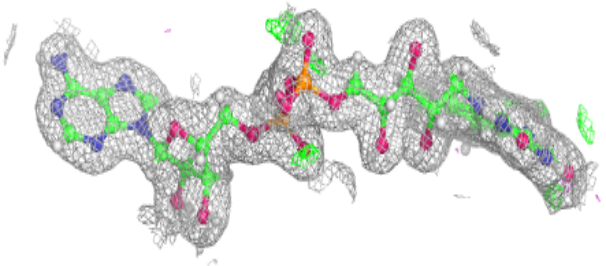


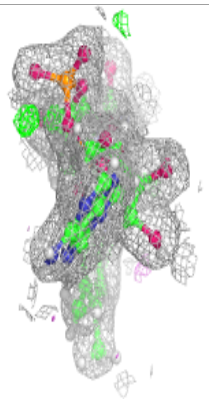


Electron density around FDA B 701:

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

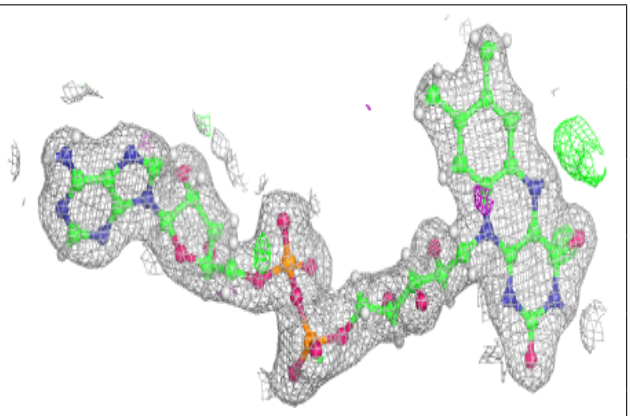


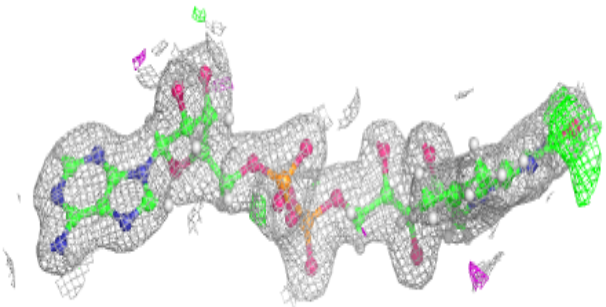


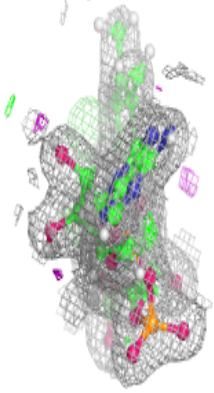


Electron density around FDA C 701:

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







6.5 Other polymers (i)

There are no such residues in this entry.