



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2024 – 02:16 pm BST

PDB ID : 9ENK
Title : L-amino acid oxidase 4 (HcLAAO4) from the fungus Hebeloma cylindrosporum
in complex with L-phenylalanine
Authors : Gilzer, D.; Koopmeiners, S.; Fischer von Mollard, G.; Niemann, H.H.
Deposited on : 2024-03-13
Resolution : 2.20 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

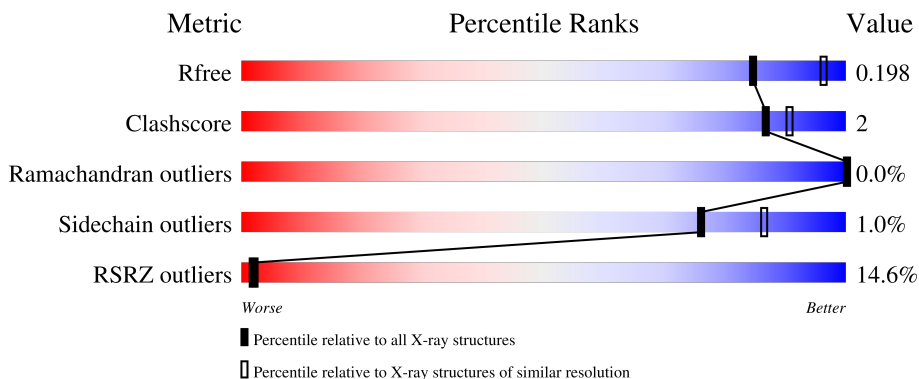
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	562	 12% 90% 5%
1	B	562	 12% 91% 6%
1	C	562	 15% 90% 6%
1	D	562	 17% 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	709	-	-	-	X
4	SO4	B	713	-	-	-	X
4	SO4	C	705	-	-	X	-
4	SO4	C	707	-	-	-	X
4	SO4	C	711	-	-	-	X
5	PGR	A	710	-	-	-	X
5	PGR	A	711	-	-	-	X
5	PGR	B	716	-	-	-	X
5	PGR	C	712	-	-	-	X
5	PGR	D	715	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35094 atoms, of which 16650 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.

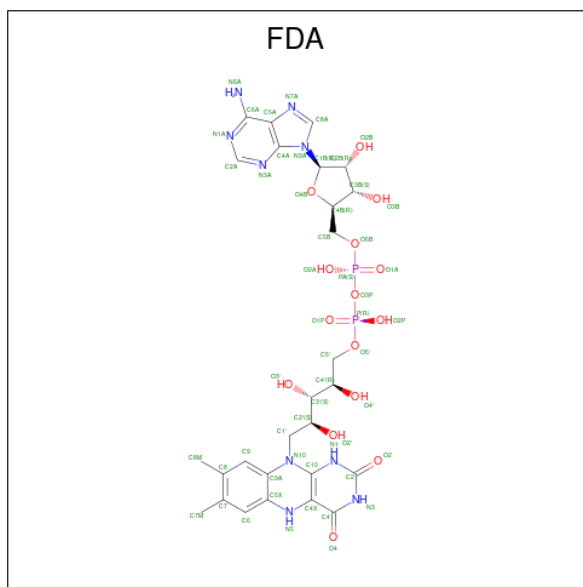
- Molecule 1 is a protein called L-amino acid oxidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	537	8401	2746	4132	716	796	11	0	9	0
1	B	528	8315	2724	4093	704	783	11	0	9	0
1	C	530	8291	2713	4078	705	784	11	0	6	0
1	D	533	8360	2732	4115	711	791	11	0	10	0

There are 8 discrepancies between the modelled and reference sequences:

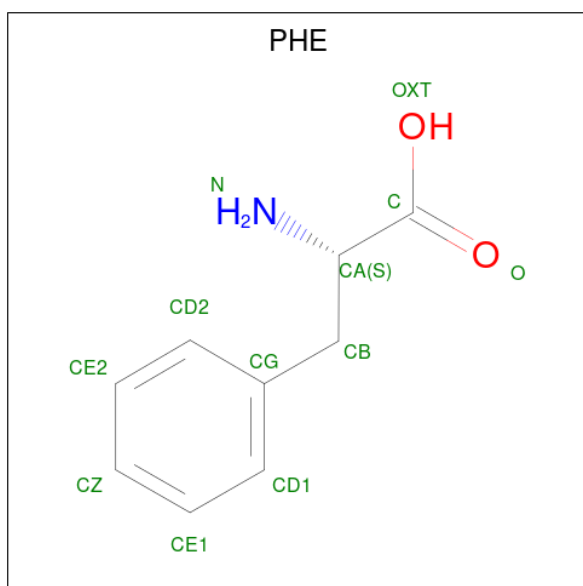
Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ALA	LYS	engineered mutation	UNP S4S6Z0
A	475	ALA	LYS	engineered mutation	UNP S4S6Z0
B	474	ALA	LYS	engineered mutation	UNP S4S6Z0
B	475	ALA	LYS	engineered mutation	UNP S4S6Z0
C	474	ALA	LYS	engineered mutation	UNP S4S6Z0
C	475	ALA	LYS	engineered mutation	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: C₂₇H₃₅N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



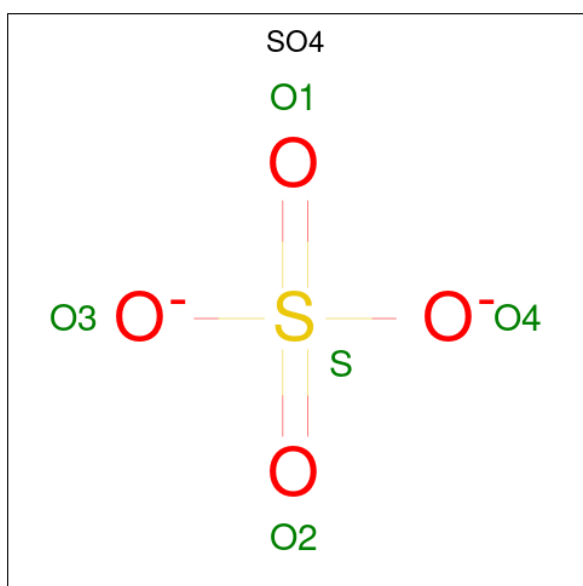
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
2	A	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		
2	D	1	Total	C	H	N	O	P	0	0
			85	27	32	9	15	2		

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	H	N	O	0	0
			20	9	8	1	2		
3	B	1	Total	C	H	N	O	0	0
			20	9	8	1	2		
3	C	1	Total	C	H	N	O	0	0
			20	9	8	1	2		
3	D	1	Total	C	H	N	O	0	0
			20	9	8	1	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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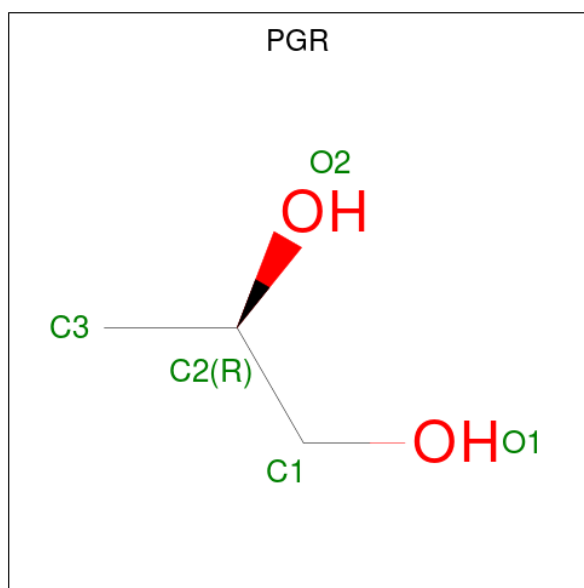
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	C	1	5	4	1	0	0
4	C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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
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: C₃H₈O₂).



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

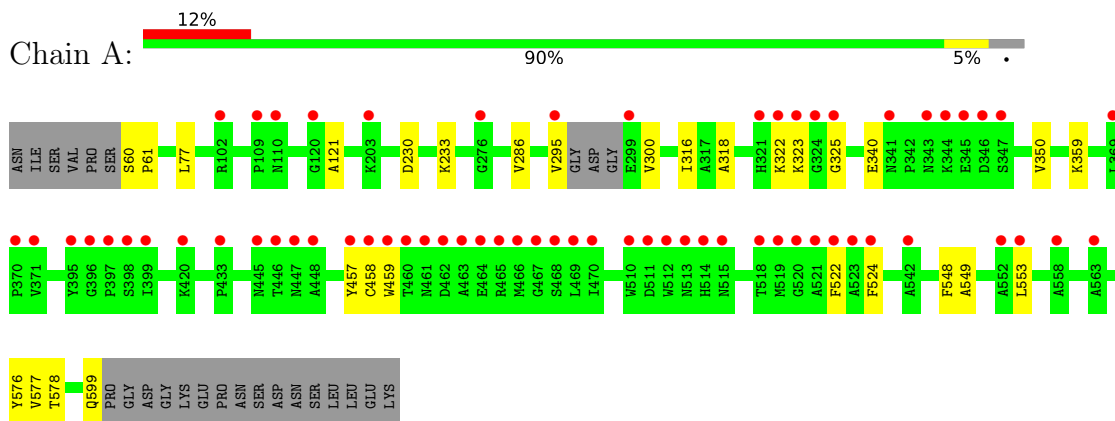
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	318	Total 319	O 319	0	1
6	B	278	Total 281	O 281	0	3
6	C	187	Total 188	O 188	0	1
6	D	197	Total 197	O 197	0	0

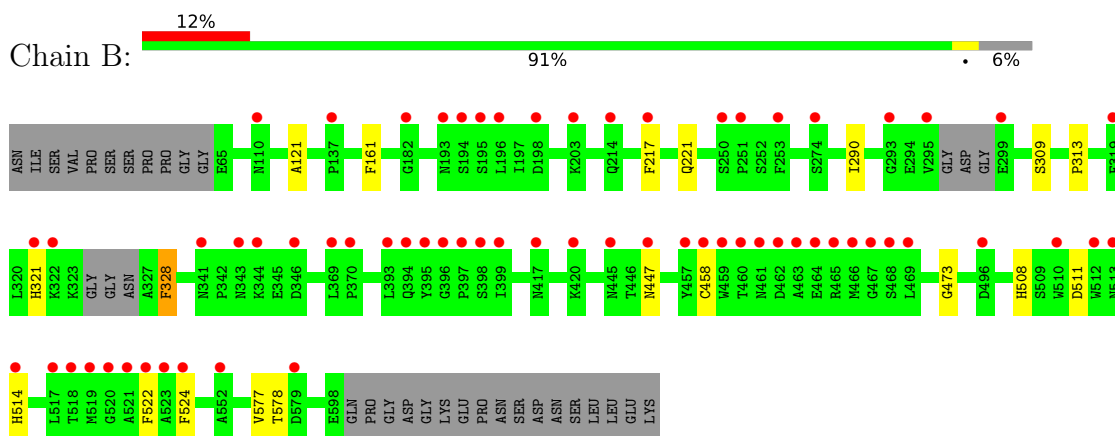
3 Residue-property plots

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

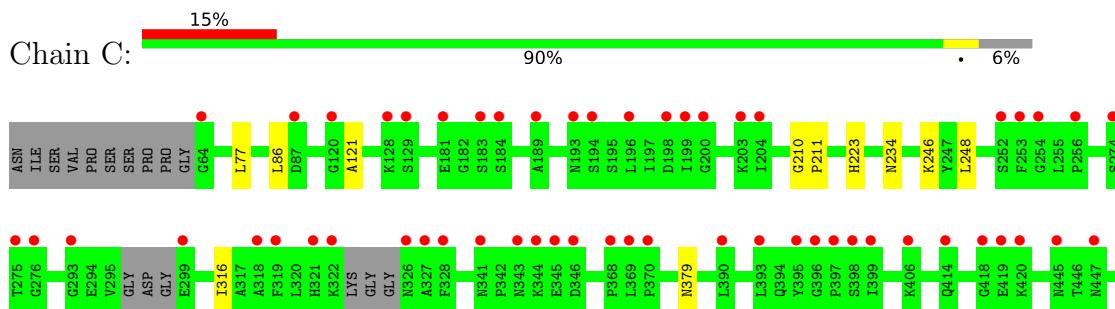
- Molecule 1: L-amino acid oxidase 4

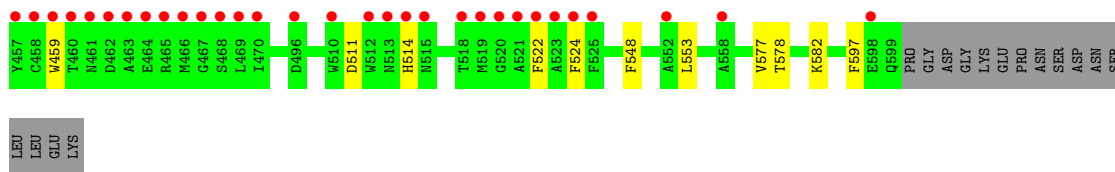


- Molecule 1: L-amino acid oxidase 4



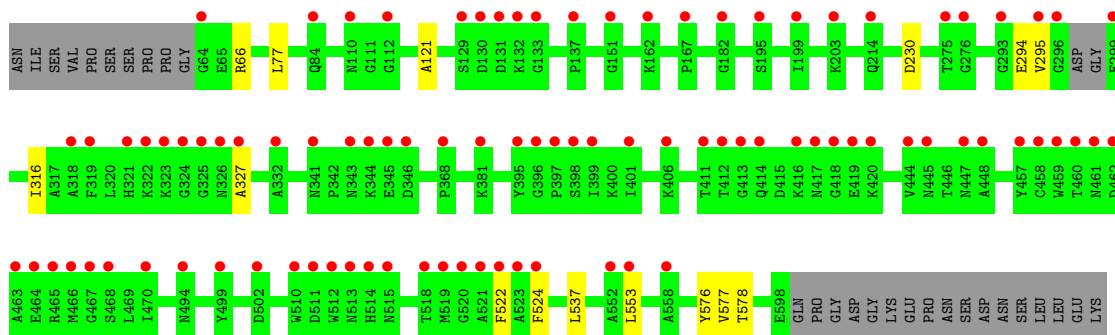
- Molecule 1: L-amino acid oxidase 4





LEU
LEU
GLU
LYS

● Molecule 1: L-amino acid oxidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.70Å 131.73Å 107.46Å 90.00° 96.04° 90.00°	Depositor
Resolution (Å)	40.67 – 2.20 45.53 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (40.67-2.20) 98.7 (45.53-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.170 , 0.202 0.167 , 0.198	Depositor DCC
R_{free} test set	5859 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtrriage
Anisotropy	0.189	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	35094	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGR, SO4, FDA

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	0.33	1/4420 (0.0%)	0.51	0/6011
1	B	0.34	1/4369 (0.0%)	0.51	0/5938
1	C	0.31	0/4350	0.49	0/5914
1	D	0.31	0/4395	0.49	0/5975
All	All	0.32	2/17534 (0.0%)	0.50	0/23838

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	458	CYS	CB-SG	-6.51	1.71	1.82
1	A	458	CYS	CB-SG	-5.14	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4269	4132	4132	22	1
1	B	4222	4093	4102	13	0
1	C	4213	4078	4084	14	0
1	D	4245	4115	4121	7	3
2	A	53	32	33	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	53	32	33	3	0
2	C	53	32	33	2	0
2	D	53	32	33	3	0
3	A	12	8	8	4	0
3	B	12	8	8	4	0
3	C	12	8	8	3	0
3	D	12	8	8	4	0
4	A	35	0	0	0	0
4	B	65	0	0	5	0
4	C	45	0	0	1	2
4	D	60	0	0	0	0
5	A	15	24	24	2	0
5	B	10	16	16	0	0
5	C	10	16	16	1	0
5	D	10	16	16	0	0
6	A	319	0	0	1	0
6	B	281	0	0	3	0
6	C	188	0	0	0	0
6	D	197	0	0	1	0
All	All	18444	16650	16675	72	3

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LYS:NZ	6:A:801:HOH:O	2.11	0.83
1:C:86:LEU:O	1:C:582:LYS:NZ	2.16	0.75
1:A:553:LEU:HD12	1:A:553:LEU:N	2.08	0.69
1:B:473:GLY:HA3	1:C:248:LEU:HD12	1.77	0.64
1:C:379:ASN:N	4:C:704:SO4:O4	2.27	0.64
2:C:701:FDA:N5	3:C:702:PHE:HA	2.13	0.63
2:A:701:FDA:N5	3:A:702:PHE:HA	2.14	0.62
2:B:701:FDA:N5	3:B:702:PHE:HA	2.15	0.62
1:A:340:GLU:OE2	1:A:359:LYS:NZ	2.31	0.61
1:A:457:TYR:O	5:A:710:PGR:H32	2.01	0.61
1:A:577:VAL:HG23	1:A:578:THR:HG23	1.84	0.60
1:D:294:GLU:O	1:D:295:VAL:HG23	2.02	0.59
1:A:548:PHE:O	1:A:553:LEU:CD2	2.50	0.59
1:B:511:ASP:OD2	1:B:514[B]:HIS:ND1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:712:SO4:O3	6:B:801:HOH:O	2.16	0.58
1:B:321:HIS:ND1	6:B:805:HOH:O	2.32	0.58
1:D:537:LEU:HB2	1:D:553:LEU:HD11	1.86	0.57
1:C:234:ASN:OD1	1:C:246:LYS:NZ	2.38	0.57
1:C:223:HIS:NE2	1:C:597:PHE:O	2.35	0.56
1:A:549:ALA:CA	1:A:553:LEU:HD22	2.35	0.56
1:C:121:ALA:HA	2:C:701:FDA:C4X	2.36	0.56
1:A:548:PHE:C	1:A:553:LEU:CD2	2.75	0.55
3:A:702:PHE:CD1	3:A:702:PHE:N	2.76	0.54
1:D:121:ALA:HA	2:D:701:FDA:C4X	2.37	0.54
2:A:701:FDA:C4X	3:A:702:PHE:HA	2.38	0.53
1:B:217[A]:PHE:CZ	1:B:221:GLN:NE2	2.76	0.53
4:B:710:SO4:O1	6:B:802:HOH:O	2.19	0.53
1:C:77:LEU:HB3	1:C:316:ILE:HG21	1.90	0.53
3:A:702:PHE:N	3:A:702:PHE:HD1	2.07	0.53
1:C:511:ASP:OD2	1:C:514[A]:HIS:ND1	2.42	0.52
3:B:702:PHE:CD1	3:B:702:PHE:N	2.77	0.52
1:A:121:ALA:HA	2:A:701:FDA:C4X	2.40	0.52
1:D:230:ASP:OD2	6:D:801:HOH:O	2.19	0.51
1:B:121:ALA:HA	2:B:701:FDA:C4X	2.40	0.51
1:A:548:PHE:HB3	1:A:553:LEU:HD21	1.93	0.51
1:A:549:ALA:HA	1:A:553:LEU:HD22	1.93	0.51
3:B:702:PHE:N	3:B:702:PHE:HD1	2.08	0.51
1:A:548:PHE:O	1:A:553:LEU:HD23	2.11	0.50
1:A:548:PHE:C	1:A:553:LEU:HD22	2.32	0.50
2:D:701:FDA:N5	3:D:702:PHE:HA	2.26	0.50
1:B:508:HIS:NE2	4:B:708:SO4:O2	2.40	0.49
1:A:553:LEU:N	1:A:553:LEU:CD1	2.75	0.49
1:B:217[B]:PHE:CE1	1:B:290:ILE:HG23	2.47	0.49
1:B:161:PHE:N	4:B:706:SO4:O3	2.44	0.48
1:C:577:VAL:HG23	1:C:578:THR:HG23	1.96	0.48
1:A:548:PHE:CB	1:A:553:LEU:HD21	2.43	0.48
1:C:459:TRP:CE2	5:C:712:PGR:H33	2.49	0.48
1:C:86:LEU:HB3	1:C:582:LYS:HD3	1.95	0.47
1:B:577:VAL:HG23	1:B:578:THR:HG23	1.97	0.47
2:B:701:FDA:C4X	3:B:702:PHE:HA	2.45	0.47
2:D:701:FDA:C4X	3:D:702:PHE:HA	2.44	0.47
1:A:323:LYS:O	1:A:325:GLY:N	2.47	0.46
1:D:577:VAL:HG23	1:D:578:THR:HG23	1.97	0.46
1:A:549:ALA:N	1:A:553:LEU:HD22	2.31	0.46
1:B:447:ASN:N	4:B:715:SO4:O4	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ALA:O	1:A:322:LYS:HG3	2.17	0.44
1:A:77:LEU:HB3	1:A:316:ILE:HG21	2.00	0.44
1:B:217[A]:PHE:CE2	1:B:221:GLN:NE2	2.85	0.44
1:D:77:LEU:HB3	1:D:316:ILE:HG21	2.00	0.44
1:C:548:PHE:O	1:C:553:LEU:HD22	2.18	0.43
3:D:702:PHE:CD1	3:D:702:PHE:N	2.86	0.43
3:C:702:PHE:N	3:C:702:PHE:CD1	2.87	0.43
3:D:702:PHE:N	3:D:702:PHE:HD1	2.17	0.43
1:C:86:LEU:O	1:C:582:LYS:CE	2.66	0.43
1:A:459:TRP:CZ3	5:A:710:PGR:H2	2.55	0.42
1:A:230:ASP:HA	1:A:233:LYS:HE2	2.01	0.42
3:C:702:PHE:N	3:C:702:PHE:HD1	2.17	0.42
1:C:210:GLY:N	1:C:211:PRO:HD2	2.35	0.42
1:A:60:SER:N	1:A:61:PRO:HD2	2.36	0.41
1:B:328:PHE:N	1:B:328:PHE:CD1	2.89	0.41
1:D:294:GLU:O	1:D:295:VAL:CG2	2.68	0.41
1:B:309:SER:O	1:B:313:PRO:HD2	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:TYR:O	1:D:576:TYR:OH[2_656]	2.05	0.15
1:D:66:ARG:NH1	4:C:705:SO4:O3[2_647]	2.08	0.12
1:D:66:ARG:HH12	4:C:705:SO4:O3[2_647]	1.54	0.06

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	542/562 (96%)	522 (96%)	20 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	531/562 (94%)	514 (97%)	17 (3%)	0	100	100
1	C	530/562 (94%)	514 (97%)	16 (3%)	0	100	100
1	D	539/562 (96%)	520 (96%)	18 (3%)	1 (0%)	47	55
All	All	2142/2248 (95%)	2070 (97%)	71 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	327	ALA

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	455/467 (97%)	448 (98%)	7 (2%)	65	78
1	B	450/467 (96%)	447 (99%)	3 (1%)	84	91
1	C	448/467 (96%)	446 (100%)	2 (0%)	91	96
1	D	452/467 (97%)	450 (100%)	2 (0%)	91	96
All	All	1805/1868 (97%)	1791 (99%)	14 (1%)	76	90

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	VAL
1	A	295	VAL
1	A	300	VAL
1	A	350	VAL
1	A	522	PHE
1	A	524	PHE
1	A	599	GLN
1	B	328	PHE
1	B	522	PHE
1	B	524	PHE

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Mol	Chain	Res	Type
1	C	522	PHE
1	C	524	PHE
1	D	522	PHE
1	D	524	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	326	ASN
1	B	221	GLN
1	D	106	HIS

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](#)

58 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	$\# Z > 2$
3	PHE	D	702	-	11,12,12	0.70	1 (9%)	14,15,15	0.88	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	A	709	-	4,4,4	0.63	0	6,6,6	0.05	0
4	SO4	D	714	-	4,4,4	0.65	0	6,6,6	0.09	0
2	FDA	B	701	-	52,58,58	0.63	0	60,89,89	0.78	2 (3%)
4	SO4	C	709	-	4,4,4	0.63	0	6,6,6	0.07	0
5	PGR	B	716	-	3,4,4	0.17	0	1,4,4	0.60	0
5	PGR	B	717	-	3,4,4	0.24	0	1,4,4	0.49	0
4	SO4	B	714	-	4,4,4	0.64	0	6,6,6	0.05	0
4	SO4	B	707	-	4,4,4	0.65	0	6,6,6	0.07	0
4	SO4	C	704	-	4,4,4	0.60	0	6,6,6	0.06	0
3	PHE	B	702	-	11,12,12	0.69	0	14,15,15	0.93	2 (14%)
5	PGR	D	715	-	3,4,4	0.20	0	1,4,4	0.68	0
4	SO4	B	711	-	4,4,4	0.63	0	6,6,6	0.08	0
4	SO4	A	705	-	4,4,4	0.59	0	6,6,6	0.11	0
4	SO4	A	706	-	4,4,4	0.63	0	6,6,6	0.19	0
4	SO4	A	708	-	4,4,4	0.62	0	6,6,6	0.07	0
4	SO4	C	707	-	4,4,4	0.65	0	6,6,6	0.06	0
4	SO4	D	706	-	4,4,4	0.63	0	6,6,6	0.11	0
4	SO4	D	707	-	4,4,4	0.58	0	6,6,6	0.07	0
2	FDA	C	701	-	52,58,58	0.65	0	60,89,89	0.78	2 (3%)
4	SO4	B	712	-	4,4,4	0.61	0	6,6,6	0.06	0
4	SO4	B	705	-	4,4,4	0.62	0	6,6,6	0.05	0
4	SO4	B	713	-	4,4,4	0.59	0	6,6,6	0.07	0
3	PHE	A	702	-	11,12,12	0.74	1 (9%)	14,15,15	0.91	2 (14%)
4	SO4	C	705	-	4,4,4	0.62	0	6,6,6	0.13	0
3	PHE	C	702	-	11,12,12	0.72	1 (9%)	14,15,15	0.89	2 (14%)
4	SO4	B	704	-	4,4,4	0.62	0	6,6,6	0.08	0
4	SO4	C	710	-	4,4,4	0.64	0	6,6,6	0.05	0
4	SO4	B	706	-	4,4,4	0.64	0	6,6,6	0.19	0
4	SO4	B	708	-	4,4,4	0.56	0	6,6,6	0.08	0
5	PGR	A	712	-	3,4,4	0.20	0	1,4,4	0.43	0
4	SO4	B	703	-	4,4,4	0.66	0	6,6,6	0.18	0
4	SO4	D	710	-	4,4,4	0.65	0	6,6,6	0.07	0
2	FDA	A	701	-	52,58,58	0.64	0	60,89,89	0.75	2 (3%)
5	PGR	A	710	-	3,4,4	0.17	0	1,4,4	0.62	0
4	SO4	D	709	-	4,4,4	0.64	0	6,6,6	0.06	0
5	PGR	A	711	-	3,4,4	0.23	0	1,4,4	0.53	0
4	SO4	C	706	-	4,4,4	0.64	0	6,6,6	0.10	0
4	SO4	C	708	-	4,4,4	0.64	0	6,6,6	0.08	0
4	SO4	C	711	-	4,4,4	0.64	0	6,6,6	0.08	0
4	SO4	D	705	-	4,4,4	0.59	0	6,6,6	0.12	0
4	SO4	D	704	-	4,4,4	0.59	0	6,6,6	0.07	0
4	SO4	D	703	-	4,4,4	0.67	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	708	-	4,4,4	0.61	0	6,6,6	0.07	0
4	SO4	D	713	-	4,4,4	0.61	0	6,6,6	0.06	0
4	SO4	A	707	-	4,4,4	0.62	0	6,6,6	0.11	0
4	SO4	B	715	-	4,4,4	0.63	0	6,6,6	0.07	0
4	SO4	B	709	-	4,4,4	0.64	0	6,6,6	0.09	0
4	SO4	C	703	-	4,4,4	0.62	0	6,6,6	0.05	0
5	PGR	C	712	-	3,4,4	0.23	0	1,4,4	0.53	0
4	SO4	A	704	-	4,4,4	0.59	0	6,6,6	0.14	0
5	PGR	C	713	-	3,4,4	0.25	0	1,4,4	0.59	0
2	FDA	D	701	-	52,58,58	0.61	0	60,89,89	0.77	2 (3%)
4	SO4	D	712	-	4,4,4	0.61	0	6,6,6	0.06	0
4	SO4	B	710	-	4,4,4	0.58	0	6,6,6	0.11	0
4	SO4	D	711	-	4,4,4	0.64	0	6,6,6	0.10	0
5	PGR	D	716	-	3,4,4	0.17	0	1,4,4	0.75	0
4	SO4	A	703	-	4,4,4	0.61	0	6,6,6	0.17	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	A	712	-	-	2/2/2/2	-
3	PHE	D	702	-	-	2/8/8/8	0/1/1/1
2	FDA	B	701	-	-	2/30/50/50	0/6/6/6
2	FDA	C	701	-	-	2/30/50/50	0/6/6/6
5	PGR	B	716	-	-	0/2/2/2	-
5	PGR	B	717	-	-	2/2/2/2	-
2	FDA	A	701	-	-	2/30/50/50	0/6/6/6
5	PGR	A	710	-	-	0/2/2/2	-
5	PGR	C	712	-	-	1/2/2/2	-
5	PGR	C	713	-	-	2/2/2/2	-
2	FDA	D	701	-	-	2/30/50/50	0/6/6/6
3	PHE	A	702	-	-	2/8/8/8	0/1/1/1
3	PHE	B	702	-	-	2/8/8/8	0/1/1/1
5	PGR	D	715	-	-	1/2/2/2	-
5	PGR	A	711	-	-	2/2/2/2	-
5	PGR	D	716	-	-	1/2/2/2	-
3	PHE	C	702	-	-	2/8/8/8	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	702	PHE	OXT-C	-2.18	1.23	1.30
3	A	702	PHE	OXT-C	-2.15	1.23	1.30
3	D	702	PHE	OXT-C	-2.12	1.23	1.30

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	FDA	C5A-C6A-N6A	2.38	123.97	120.35
2	B	701	FDA	C5A-C6A-N6A	2.37	123.96	120.35
2	B	701	FDA	O4B-C1B-C2B	-2.37	103.46	106.93
3	B	702	PHE	OXT-C-CA	2.33	121.32	113.38
2	A	701	FDA	O4B-C1B-C2B	-2.31	103.55	106.93
2	A	701	FDA	C5A-C6A-N6A	2.28	123.82	120.35
2	C	701	FDA	O4B-C1B-C2B	-2.23	103.66	106.93
2	D	701	FDA	O4B-C1B-C2B	-2.23	103.66	106.93
3	C	702	PHE	OXT-C-O	-2.20	119.10	124.09
3	D	702	PHE	OXT-C-O	-2.19	119.11	124.09
2	D	701	FDA	C5A-C6A-N6A	2.19	123.68	120.35
3	C	702	PHE	OXT-C-CA	2.18	120.83	113.38
3	A	702	PHE	OXT-C-CA	2.16	120.73	113.38
3	D	702	PHE	OXT-C-CA	2.14	120.66	113.38
3	B	702	PHE	OXT-C-O	-2.09	119.35	124.09
3	A	702	PHE	OXT-C-O	-2.05	119.42	124.09

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	711	PGR	O1-C1-C2-C3
5	A	711	PGR	O1-C1-C2-O2
5	A	712	PGR	O1-C1-C2-C3
5	A	712	PGR	O1-C1-C2-O2
5	B	717	PGR	O1-C1-C2-C3
5	B	717	PGR	O1-C1-C2-O2
5	C	713	PGR	O1-C1-C2-C3
5	C	713	PGR	O1-C1-C2-O2
5	D	716	PGR	O1-C1-C2-O2
3	C	702	PHE	CA-CB-CG-CD2
3	D	702	PHE	CA-CB-CG-CD2
3	A	702	PHE	CA-CB-CG-CD2
3	C	702	PHE	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
3	D	702	PHE	CA-CB-CG-CD1
3	A	702	PHE	CA-CB-CG-CD1
3	B	702	PHE	CA-CB-CG-CD2
3	B	702	PHE	CA-CB-CG-CD1
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'
5	D	715	PGR	O1-C1-C2-C3
2	A	701	FDA	O4B-C4B-C5B-O5B
2	D	701	FDA	O4B-C4B-C5B-O5B
5	C	712	PGR	O1-C1-C2-C3
2	B	701	FDA	O4B-C4B-C5B-O5B
2	C	701	FDA	O4B-C4B-C5B-O5B

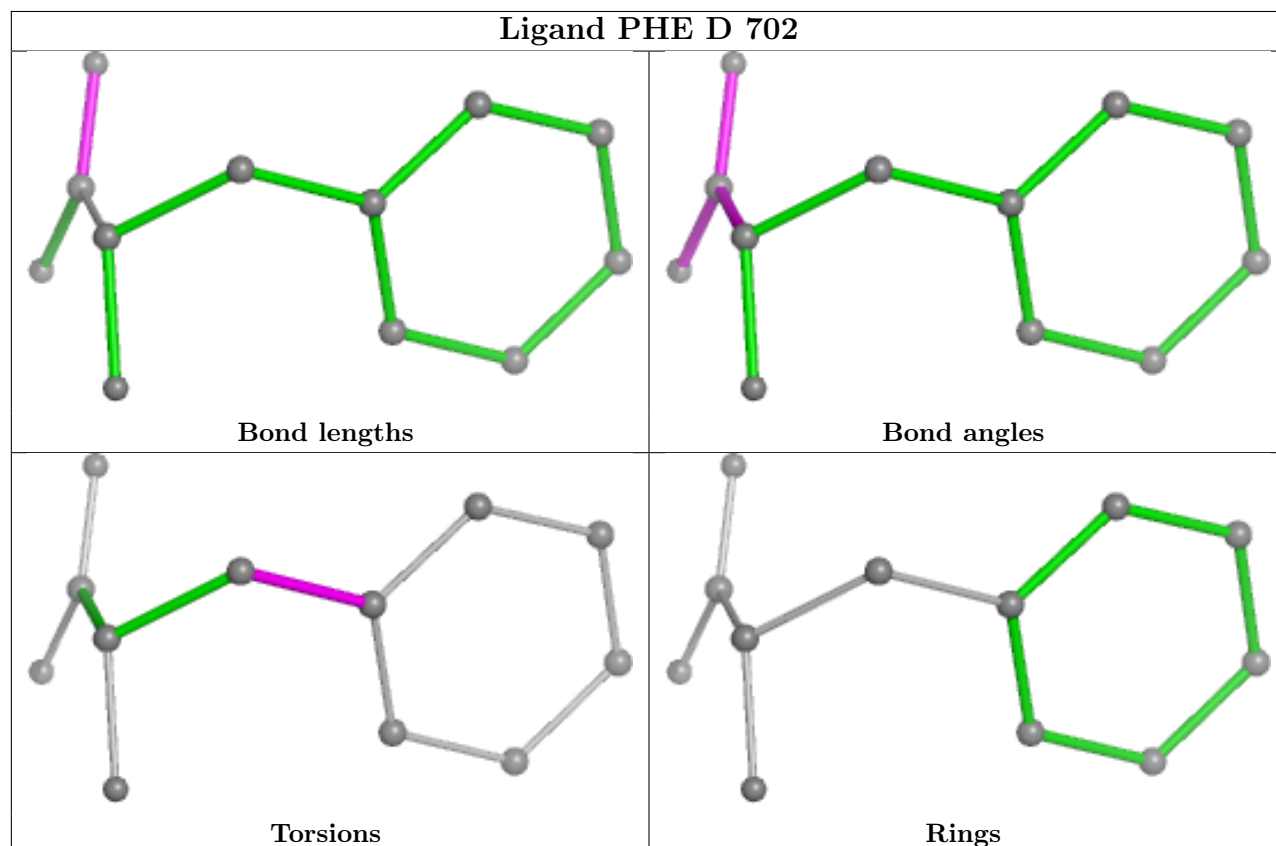
There are no ring outliers.

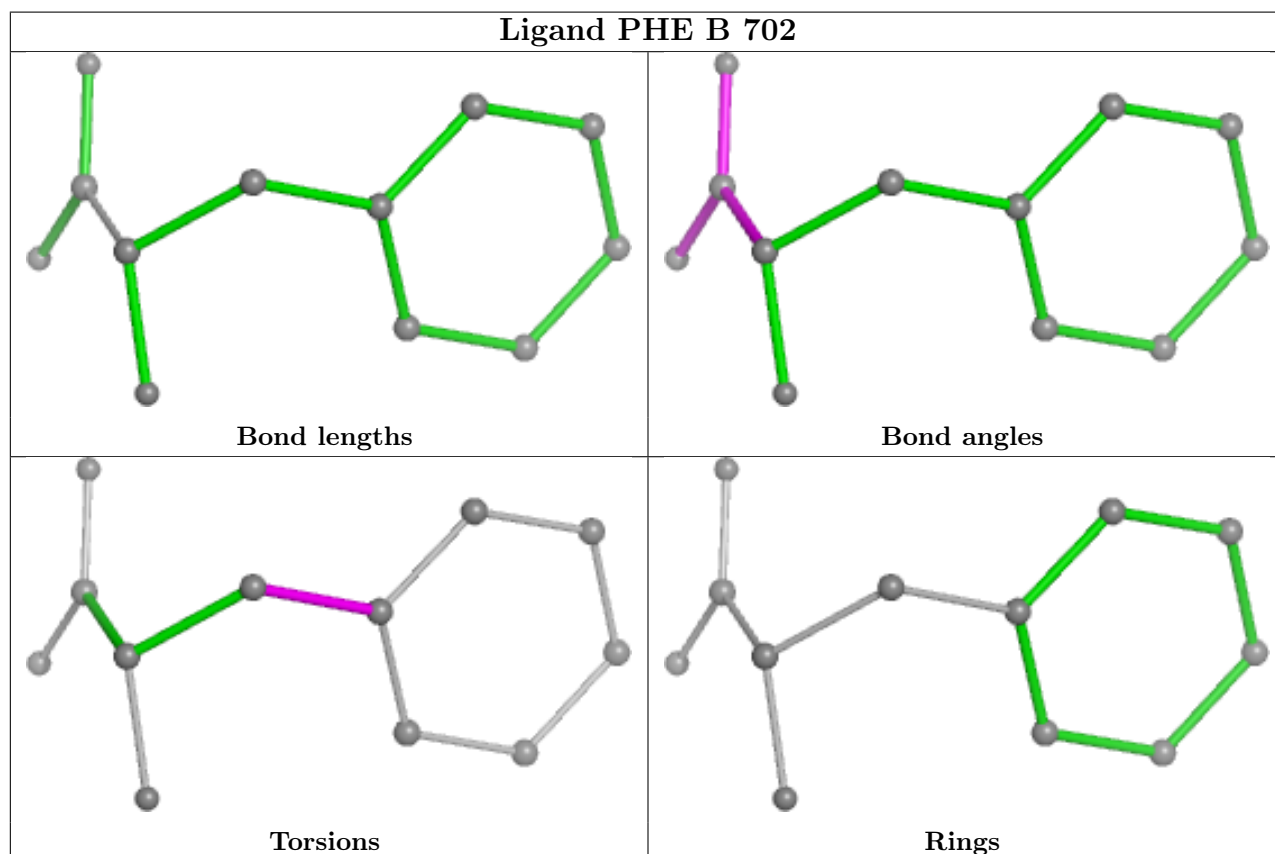
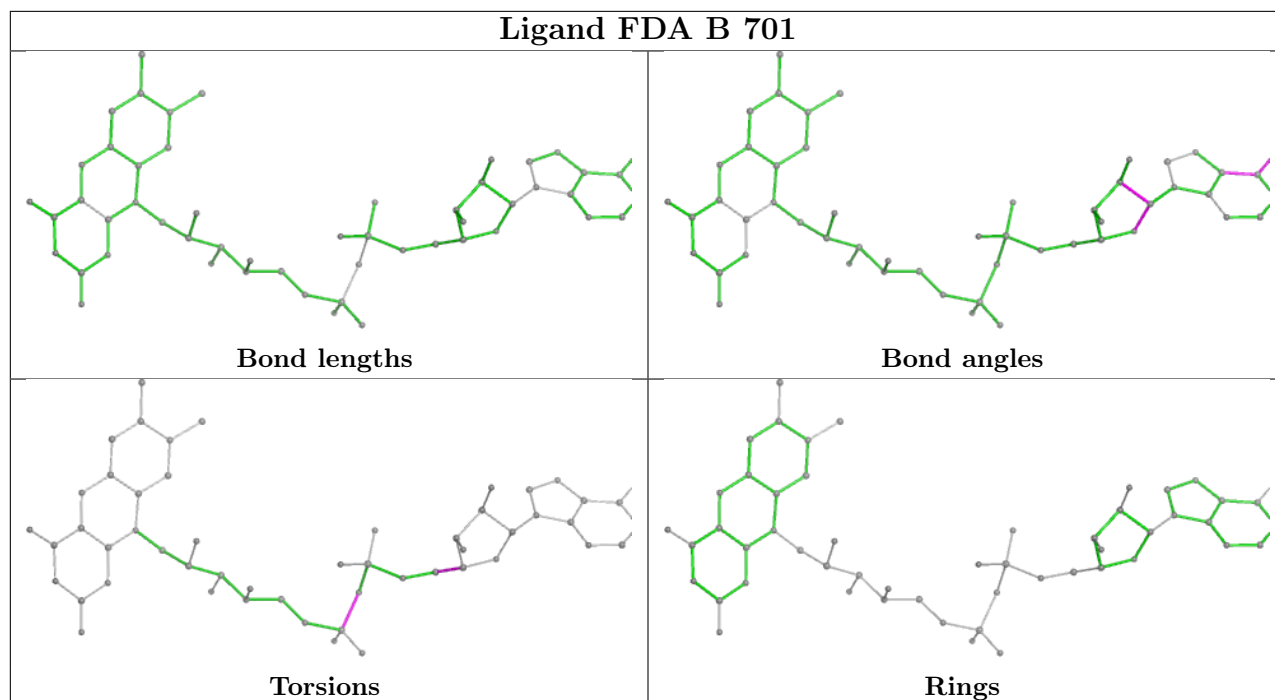
17 monomers are involved in 30 short contacts:

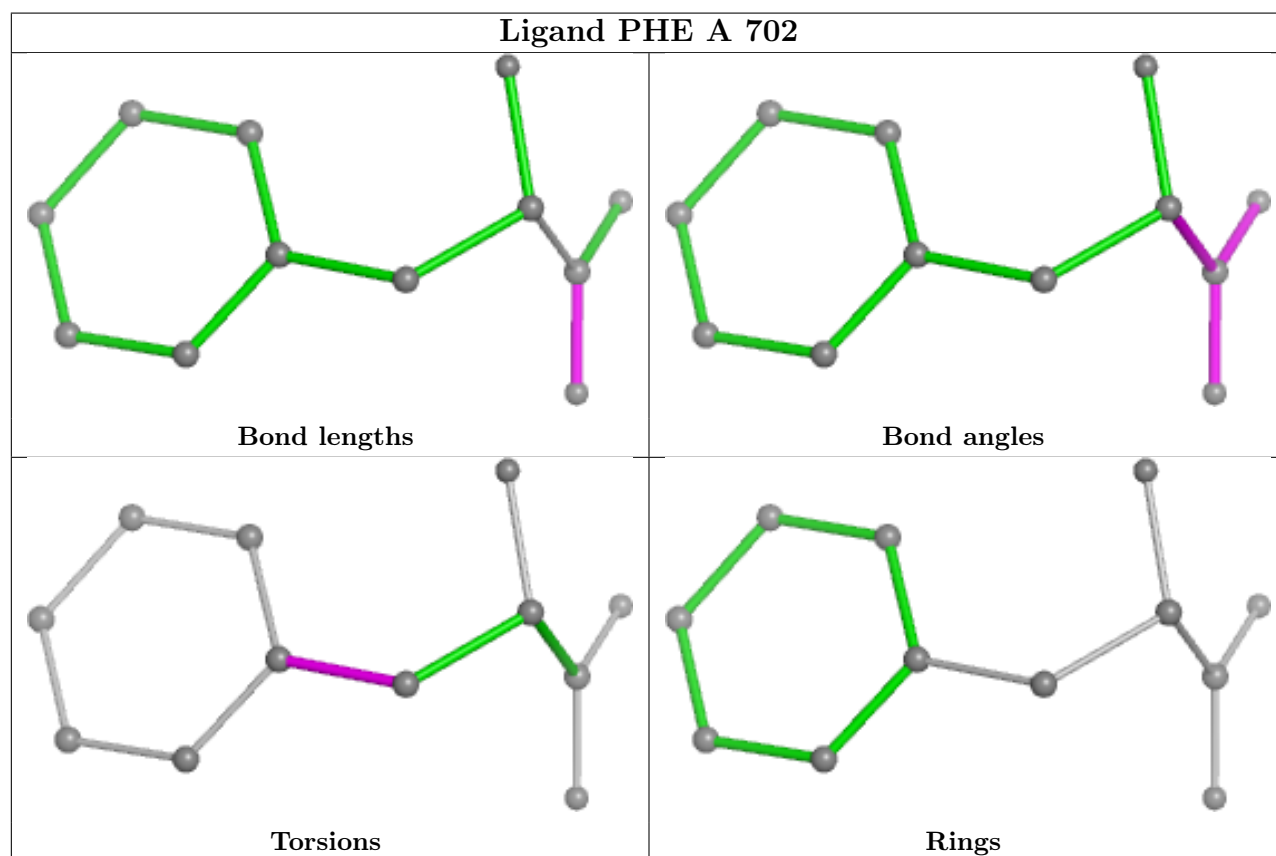
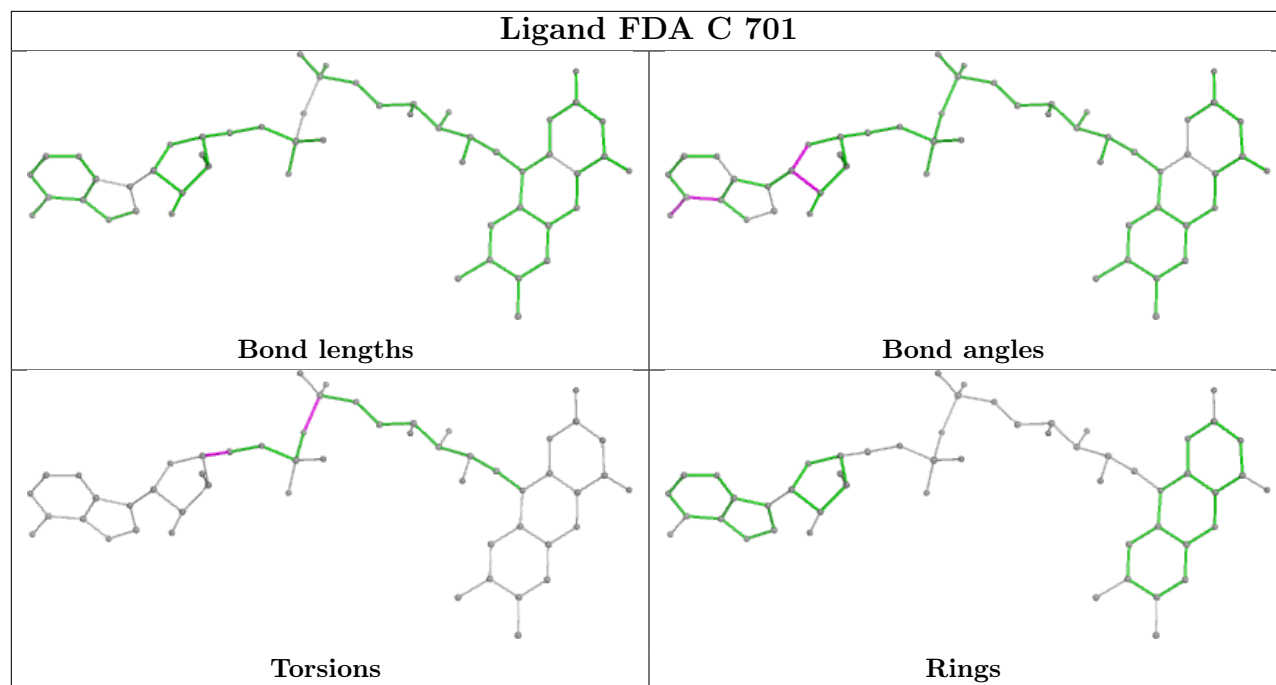
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	702	PHE	4	0
2	B	701	FDA	3	0
4	C	704	SO4	1	0
3	B	702	PHE	4	0
2	C	701	FDA	2	0
4	B	712	SO4	1	0
3	A	702	PHE	4	0
4	C	705	SO4	0	2
3	C	702	PHE	3	0
4	B	706	SO4	1	0
4	B	708	SO4	1	0
2	A	701	FDA	3	0
5	A	710	PGR	2	0
4	B	715	SO4	1	0
5	C	712	PGR	1	0
2	D	701	FDA	3	0
4	B	710	SO4	1	0

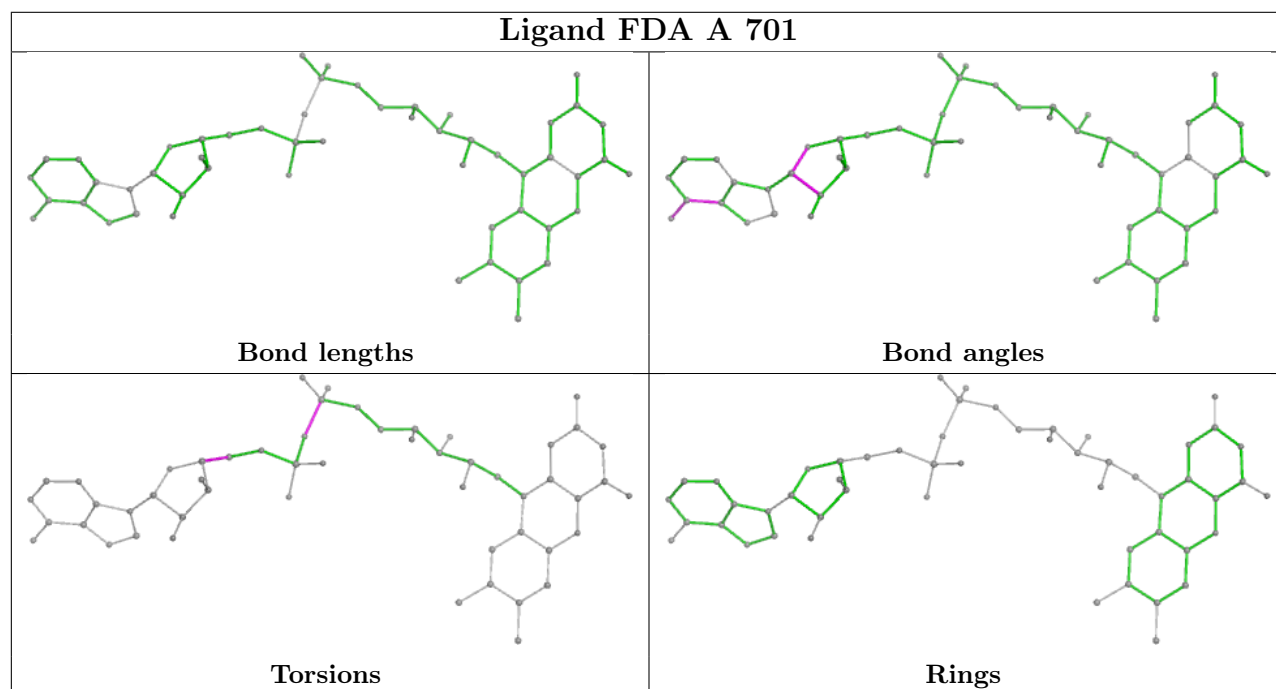
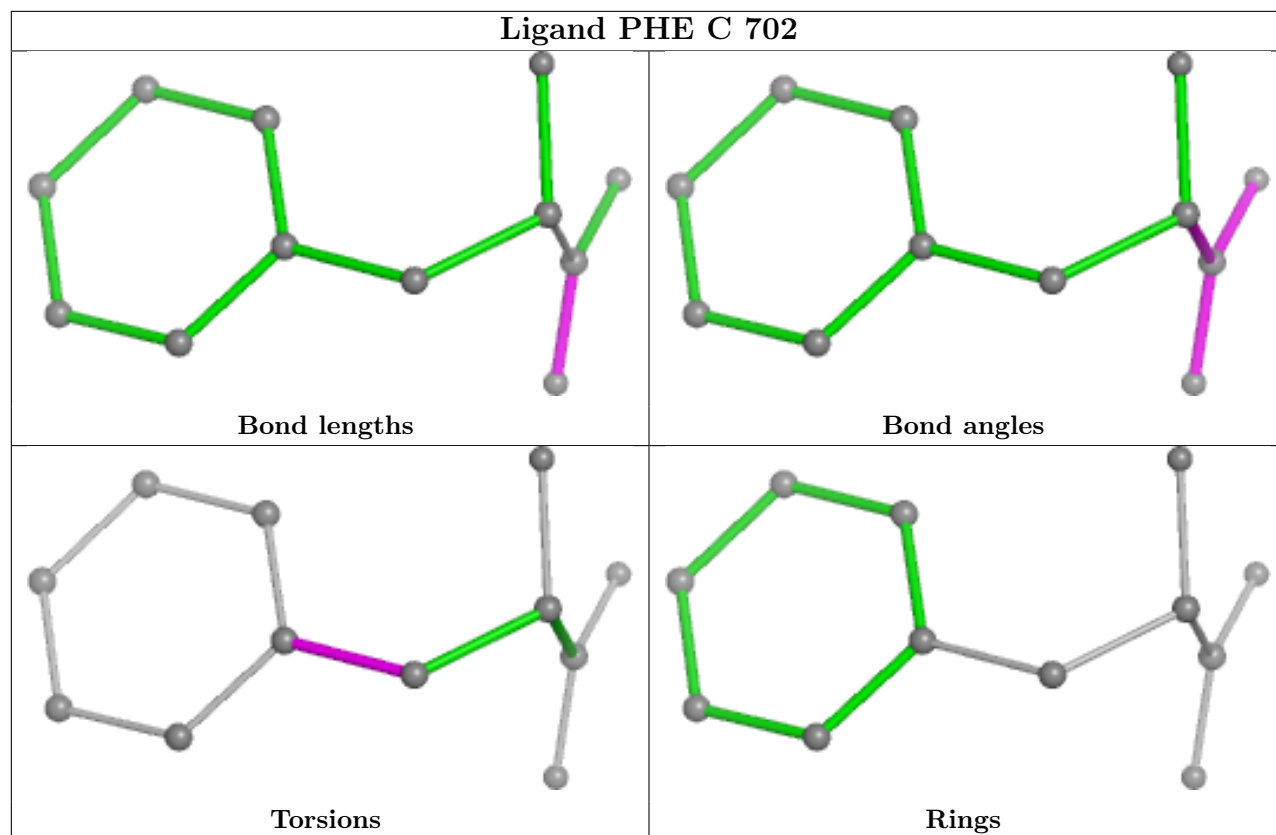
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

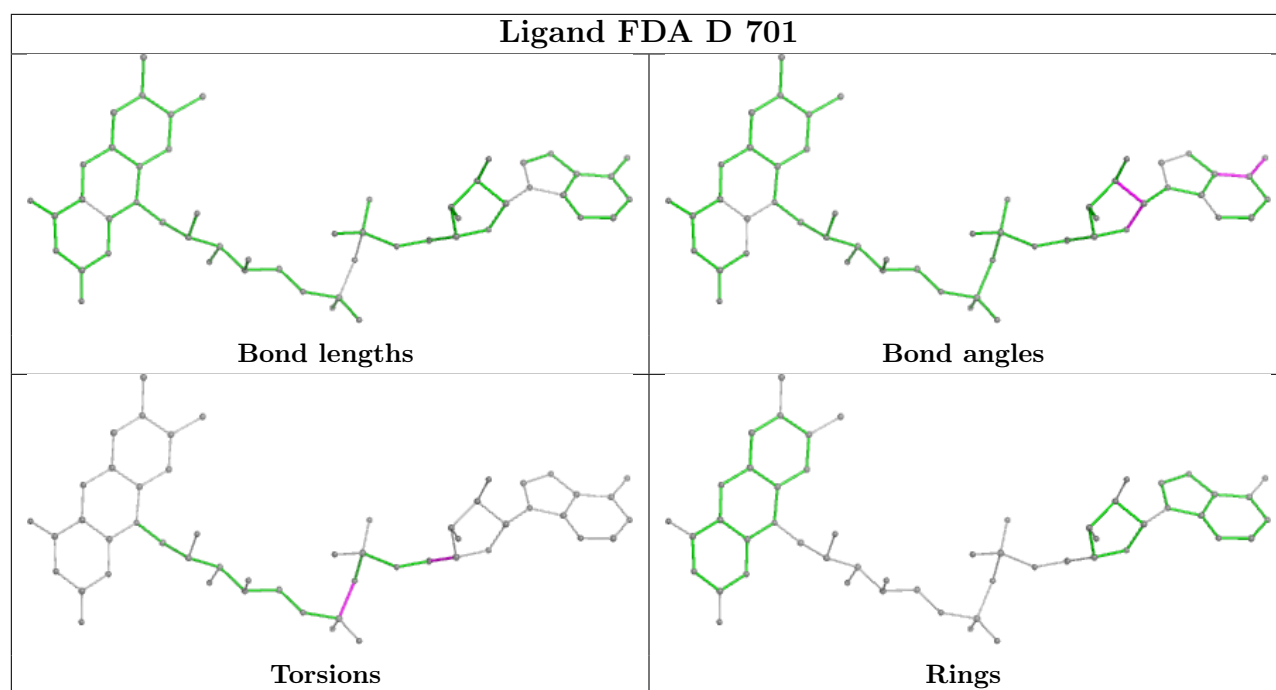
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD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











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	537/562 (95%)	0.65	65 (12%) 4 3	34, 42, 60, 131	0
1	B	528/562 (93%)	0.62	66 (12%) 3 3	34, 42, 60, 103	0
1	C	530/562 (94%)	0.81	86 (16%) 1 1	36, 48, 74, 122	0
1	D	533/562 (94%)	0.83	93 (17%) 1 1	37, 48, 76, 120	0
All	All	2128/2248 (94%)	0.73	310 (14%) 2 2	34, 45, 71, 131	0

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	LYS	8.0
1	B	321	HIS	7.8
1	D	323	LYS	7.3
1	C	299	GLU	7.1
1	D	325	GLY	5.7
1	A	448	ALA	5.6
1	A	514[A]	HIS	5.3
1	A	322	LYS	5.2
1	D	322	LYS	5.0
1	B	295	VAL	4.9
1	D	324	GLY	4.9
1	B	395	TYR	4.8
1	A	458	CYS	4.8
1	D	514[A]	HIS	4.7
1	B	514[A]	HIS	4.7
1	B	396	GLY	4.7
1	A	324	GLY	4.6
1	D	318	ALA	4.6
1	A	397	PRO	4.6
1	C	514[A]	HIS	4.5
1	B	522	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	319	PHE	4.4
1	D	397	PRO	4.4
1	D	418	GLY	4.4
1	C	397	PRO	4.4
1	A	343	ASN	4.3
1	B	343	ASN	4.3
1	C	395	TYR	4.3
1	A	522	PHE	4.3
1	D	395	TYR	4.3
1	D	321	HIS	4.3
1	D	463	ALA	4.3
1	B	458	CYS	4.2
1	B	397	PRO	4.2
1	B	463	ALA	4.2
1	D	182	GLY	4.2
1	B	398	SER	4.2
1	A	398	SER	4.1
1	A	399	ILE	4.1
1	C	512	TRP	4.1
1	C	522	PHE	4.0
1	C	521	ALA	4.0
1	D	458	CYS	3.9
1	D	459	TRP	3.9
1	C	343	ASN	3.9
1	C	420	LYS	3.9
1	C	399	ILE	3.9
1	B	459	TRP	3.9
1	C	396	GLY	3.9
1	C	256	PRO	3.9
1	D	512	TRP	3.8
1	C	345	GLU	3.8
1	D	412	THR	3.8
1	C	322	LYS	3.8
1	A	468	SER	3.8
1	B	399	ILE	3.8
1	C	458	CYS	3.8
1	D	468	SER	3.8
1	A	470	ILE	3.8
1	A	460	THR	3.8
1	A	523	ALA	3.8
1	D	399	ILE	3.7
1	D	417	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	445	ASN	3.7
1	A	512	TRP	3.7
1	A	295	VAL	3.7
1	B	519	MET	3.7
1	B	464	GLU	3.6
1	A	396	GLY	3.6
1	B	110	ASN	3.6
1	C	198	ASP	3.6
1	C	341	ASN	3.6
1	C	293	GLY	3.5
1	A	467	GLY	3.5
1	D	398	SER	3.5
1	A	521	ALA	3.5
1	A	345	GLU	3.5
1	A	463	ALA	3.5
1	B	198	ASP	3.5
1	C	523	ALA	3.4
1	D	465	ARG	3.4
1	D	420	LYS	3.4
1	B	467	GLY	3.4
1	D	396	GLY	3.4
1	C	327	ALA	3.4
1	D	129	SER	3.4
1	D	345	GLU	3.4
1	C	459	TRP	3.4
1	B	466	MET	3.4
1	A	513	ASN	3.4
1	D	460	THR	3.3
1	D	203	LYS	3.3
1	A	469	LEU	3.3
1	A	464	GLU	3.3
1	B	523	ALA	3.3
1	B	322	LYS	3.3
1	D	448	ALA	3.3
1	A	457	TYR	3.3
1	B	195	SER	3.3
1	B	420	LYS	3.3
1	C	193	ASN	3.2
1	D	167	PRO	3.2
1	D	110	ASN	3.2
1	B	447	ASN	3.1
1	B	513	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	518	THR	3.1
1	B	217[A]	PHE	3.1
1	C	328	PHE	3.1
1	A	552	ALA	3.1
1	B	460	THR	3.1
1	A	110	ASN	3.1
1	C	470	ILE	3.1
1	D	293	GLY	3.1
1	A	519	MET	3.1
1	B	512	TRP	3.1
1	B	299	GLU	3.1
1	D	511	ASP	3.0
1	D	132	LYS	3.0
1	A	447	ASN	3.0
1	D	520	GLY	3.0
1	D	522	PHE	3.0
1	C	398	SER	3.0
1	A	395	TYR	3.0
1	A	466	MET	3.0
1	C	519	MET	3.0
1	B	346	ASP	3.0
1	A	321	HIS	3.0
1	C	326	ASN	3.0
1	C	318	ALA	3.0
1	C	469	LEU	3.0
1	A	465	ARG	3.0
1	C	321	HIS	3.0
1	D	414	GLN	2.9
1	D	199	ILE	2.9
1	C	513	ASN	2.9
1	B	203	LYS	2.9
1	D	466	MET	2.9
1	C	463	ALA	2.9
1	D	524	PHE	2.9
1	B	468	SER	2.9
1	D	327	ALA	2.9
1	B	370	PRO	2.9
1	C	598	GLU	2.9
1	D	419[A]	GLU	2.9
1	D	461	ASN	2.9
1	D	296	GLY	2.9
1	B	520	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	344	LYS	2.8
1	D	344	LYS	2.8
1	D	131	ASP	2.8
1	B	469	LEU	2.8
1	D	464	GLU	2.8
1	C	393	LEU	2.8
1	B	461	ASN	2.8
1	B	462	ASP	2.8
1	D	411	THR	2.8
1	A	299	GLU	2.8
1	B	524	PHE	2.7
1	C	368	PRO	2.7
1	C	496	ASP	2.7
1	A	461	ASN	2.7
1	D	295	VAL	2.7
1	D	518	THR	2.7
1	A	462	ASP	2.7
1	C	276	GLY	2.7
1	D	64	GLY	2.7
1	B	521	ALA	2.7
1	D	467	GLY	2.7
1	A	433	PRO	2.7
1	C	319	PHE	2.7
1	D	553	LEU	2.7
1	C	183	SER	2.7
1	A	524	PHE	2.7
1	A	518	THR	2.7
1	C	406	LYS	2.6
1	D	519	MET	2.6
1	D	558	ALA	2.6
1	C	520	GLY	2.6
1	C	189	ALA	2.6
1	C	369	LEU	2.6
1	C	466	MET	2.6
1	D	513	ASN	2.6
1	D	523	ALA	2.6
1	D	447	ASN	2.6
1	C	203	LYS	2.6
1	C	465	ARG	2.6
1	C	87	ASP	2.6
1	B	293	GLY	2.6
1	A	341	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	347	SER	2.5
1	A	446	THR	2.5
1	B	579	ASP	2.5
1	D	133	GLY	2.5
1	C	419	GLU	2.5
1	A	553	LEU	2.5
1	A	558	ALA	2.5
1	D	84[A]	GLN	2.5
1	D	275	THR	2.5
1	C	467	GLY	2.5
1	C	184	SER	2.5
1	D	521	ALA	2.4
1	A	520	GLY	2.4
1	B	194	SER	2.4
1	C	196	LEU	2.4
1	C	344	LYS	2.4
1	D	162	LYS	2.4
1	B	214	GLN	2.4
1	B	496	ASP	2.4
1	A	510	TRP	2.4
1	C	370	PRO	2.4
1	C	129	SER	2.4
1	B	193	ASN	2.4
1	D	276	GLY	2.4
1	C	518	THR	2.4
1	C	445	ASN	2.4
1	A	102	ARG	2.3
1	B	552	ALA	2.3
1	B	465	ARG	2.3
1	D	462	ASP	2.3
1	C	457	TYR	2.3
1	D	368	PRO	2.3
1	D	499	TYR	2.3
1	A	203	LYS	2.3
1	C	64	GLY	2.3
1	D	151	GLY	2.3
1	D	470	ILE	2.3
1	B	137	PRO	2.3
1	A	542	ALA	2.3
1	A	459	TRP	2.3
1	D	214	GLN	2.3
1	D	552	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	393	LEU	2.3
1	D	444	VAL	2.3
1	D	326	ASN	2.3
1	D	401	ILE	2.3
1	A	563	ALA	2.3
1	C	460	THR	2.3
1	C	468	SER	2.3
1	A	276	GLY	2.3
1	D	112	GLY	2.3
1	C	510	TRP	2.3
1	A	344	LYS	2.3
1	B	251	PRO	2.3
1	A	325	GLY	2.2
1	D	299	GLU	2.2
1	B	457	TYR	2.2
1	D	416	LYS	2.2
1	C	204	ILE	2.2
1	A	369	LEU	2.2
1	C	461	ASN	2.2
1	D	457	TYR	2.2
1	C	524	PHE	2.2
1	C	252	SER	2.2
1	A	511	ASP	2.2
1	B	394	GLN	2.2
1	D	137	PRO	2.2
1	C	128	LYS	2.2
1	D	406	LYS	2.2
1	C	525	PHE	2.2
1	B	517	LEU	2.2
1	A	370	PRO	2.2
1	D	195	SER	2.2
1	D	346	ASP	2.2
1	B	341	ASN	2.2
1	C	199	ILE	2.2
1	D	381	LYS	2.2
1	C	390	LEU	2.2
1	C	253	PHE	2.2
1	B	510	TRP	2.2
1	B	274	SER	2.2
1	B	417	ASN	2.1
1	D	515	ASN	2.1
1	C	275	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	552	ALA	2.1
1	C	274	SER	2.1
1	D	510	TRP	2.1
1	C	447	ASN	2.1
1	B	319	PHE	2.1
1	C	346	ASP	2.1
1	D	130	ASP	2.1
1	A	445	ASN	2.1
1	C	194	SER	2.1
1	C	515	ASN	2.1
1	D	343	ASN	2.1
1	C	181	GLU	2.1
1	A	515[A]	ASN	2.1
1	A	109	PRO	2.1
1	C	418	GLY	2.1
1	A	420	LYS	2.1
1	B	253	PHE	2.1
1	C	200	GLY	2.1
1	A	371	VAL	2.1
1	C	254	GLY	2.1
1	C	462	ASP	2.0
1	B	196	LEU	2.0
1	B	369	LEU	2.0
1	D	341	ASN	2.0
1	D	413	GLY	2.0
1	C	464	GLU	2.0
1	C	414	GLN	2.0
1	A	346	ASP	2.0
1	D	502	ASP	2.0
1	B	445	ASN	2.0
1	D	494	ASN	2.0
1	A	120	GLY	2.0
1	B	182	GLY	2.0
1	C	120	GLY	2.0
1	B	250	SER	2.0
1	C	558	ALA	2.0
1	D	332	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

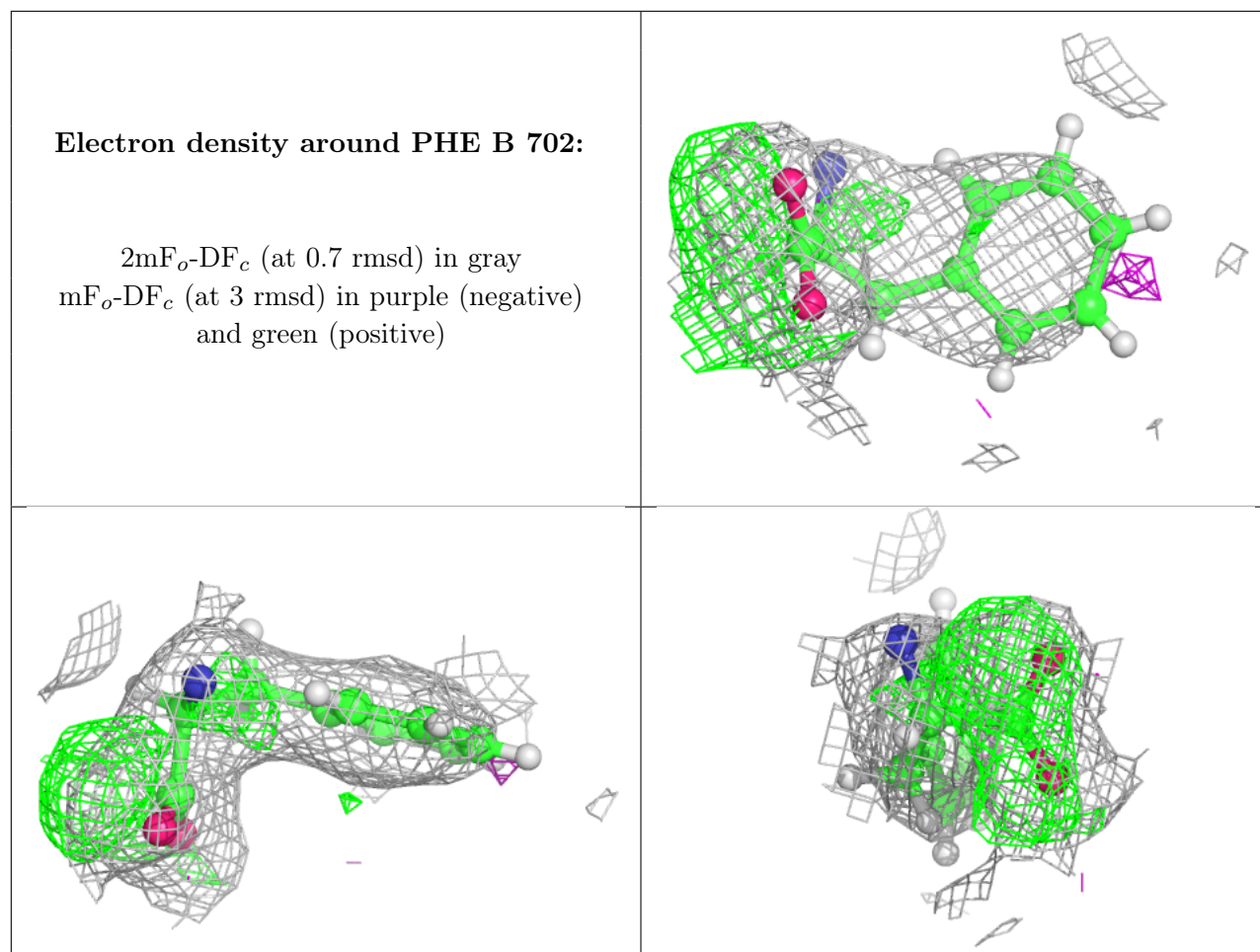
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PGR	B	716	5/5	0.41	0.75	39,47,49,50	13
4	SO4	A	709	5/5	0.44	0.49	94,95,101,102	5
5	PGR	A	710	5/5	0.52	0.77	39,47,49,49	13
5	PGR	D	715	5/5	0.55	0.79	45,54,55,56	13
4	SO4	D	714	5/5	0.63	0.39	53,53,57,59	5
4	SO4	D	711	5/5	0.64	0.39	84,84,94,105	5
4	SO4	D	712	5/5	0.65	0.39	89,91,96,110	5
4	SO4	C	705	5/5	0.67	0.24	70,71,77,77	5
5	PGR	C	712	5/5	0.67	0.70	45,55,56,58	13
4	SO4	C	707	5/5	0.67	0.43	82,84,94,98	5
4	SO4	C	711	5/5	0.72	0.40	57,61,62,67	5
4	SO4	B	715	5/5	0.72	0.38	64,65,70,73	5
4	SO4	B	711	5/5	0.73	0.33	51,52,60,62	5
4	SO4	B	703	5/5	0.73	0.30	43,46,51,53	5
4	SO4	D	713	5/5	0.75	0.34	70,76,80,85	5
4	SO4	B	713	5/5	0.76	0.48	69,71,74,75	5
4	SO4	C	708	5/5	0.76	0.23	56,58,62,64	5
4	SO4	B	714	5/5	0.76	0.20	69,70,74,77	5
4	SO4	D	710	5/5	0.76	0.31	45,47,51,55	5
5	PGR	A	711	5/5	0.77	0.49	34,44,47,53	13
4	SO4	D	709	5/5	0.77	0.33	72,74,83,85	5
4	SO4	B	709	5/5	0.78	0.16	57,62,65,66	5
4	SO4	B	712	5/5	0.79	0.34	51,51,52,55	5
4	SO4	D	705	5/5	0.81	0.26	49,50,52,54	5
4	SO4	C	710	5/5	0.82	0.28	94,100,105,116	5
4	SO4	C	709	5/5	0.82	0.18	74,75,85,88	5
5	PGR	A	712	5/5	0.84	0.14	49,59,65,71	0
4	SO4	A	703	5/5	0.84	0.28	44,47,51,54	5
4	SO4	B	708	5/5	0.85	0.48	42,43,45,48	5
4	SO4	B	706	5/5	0.85	0.28	42,44,48,51	5
3	PHE	B	702	12/12	0.86	0.57	37,43,52,54	20
3	PHE	C	702	12/12	0.86	0.53	41,48,58,61	20

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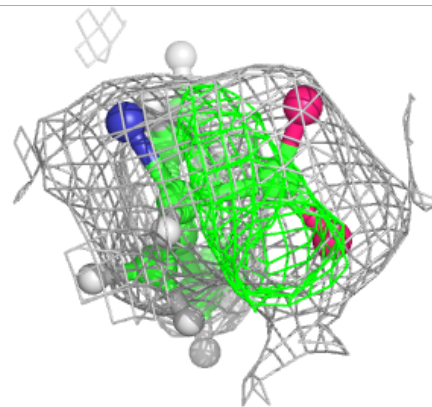
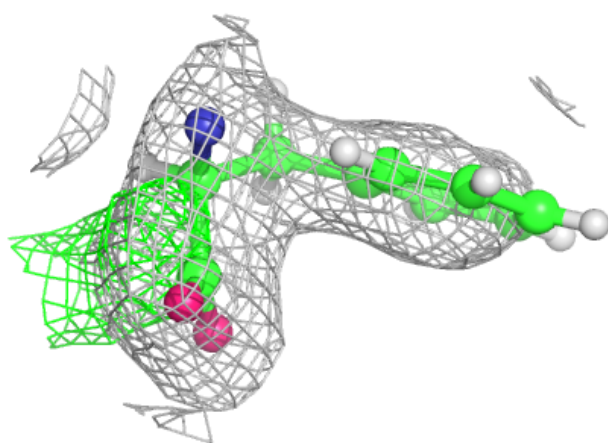
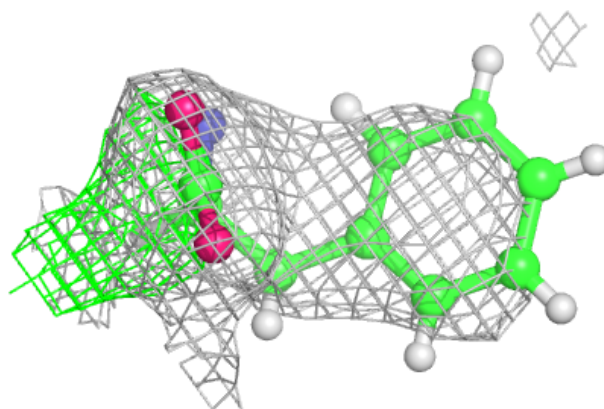
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	710	5/5	0.86	0.30	49,51,53,55	5
4	SO4	D	707	5/5	0.86	0.28	53,55,57,57	5
4	SO4	B	704	5/5	0.87	0.23	45,50,51,53	5
3	PHE	D	702	12/12	0.88	0.47	43,49,59,60	20
4	SO4	C	703	5/5	0.88	0.19	58,59,65,66	5
3	PHE	A	702	12/12	0.89	0.45	35,43,52,55	20
5	PGR	C	713	5/5	0.89	0.17	47,58,70,70	0
4	SO4	D	703	5/5	0.89	0.19	58,59,61,61	5
4	SO4	C	706	5/5	0.90	0.20	54,56,64,66	5
4	SO4	D	706	5/5	0.90	0.14	56,57,62,63	5
4	SO4	A	705	5/5	0.91	0.40	41,47,48,50	5
4	SO4	A	707	5/5	0.91	0.21	41,42,45,46	5
4	SO4	D	708	5/5	0.91	0.23	50,54,57,59	5
4	SO4	B	707	5/5	0.91	0.17	56,57,62,66	5
5	PGR	D	716	5/5	0.91	0.23	51,62,64,64	0
5	PGR	B	717	5/5	0.92	0.19	46,56,61,61	0
2	FDA	D	701	53/53	0.92	0.19	35,41,50,51	0
4	SO4	D	704	5/5	0.92	0.28	50,52,55,57	5
4	SO4	A	706	5/5	0.92	0.24	47,52,56,58	5
2	FDA	C	701	53/53	0.92	0.20	35,41,50,50	0
2	FDA	A	701	53/53	0.93	0.21	33,36,44,45	0
2	FDA	B	701	53/53	0.93	0.21	29,36,44,46	0
4	SO4	A	708	5/5	0.94	0.15	50,50,56,58	5
4	SO4	C	704	5/5	0.95	0.13	56,59,62,66	5
4	SO4	B	705	5/5	0.96	0.19	51,52,52,59	5
4	SO4	A	704	5/5	0.97	0.17	47,53,54,55	5

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.



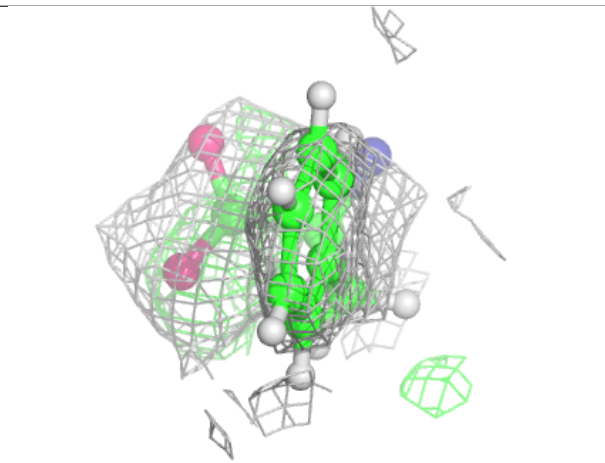
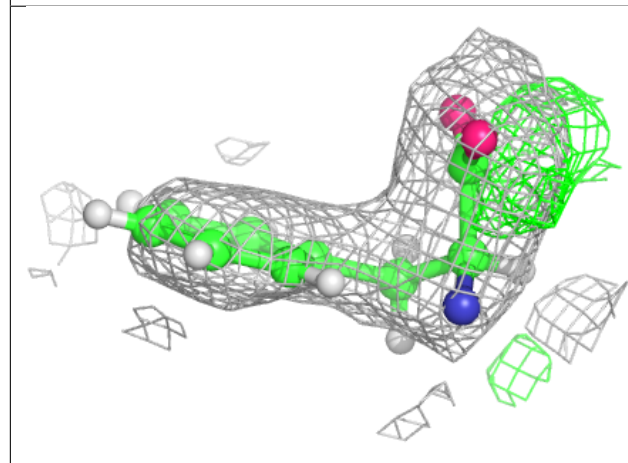
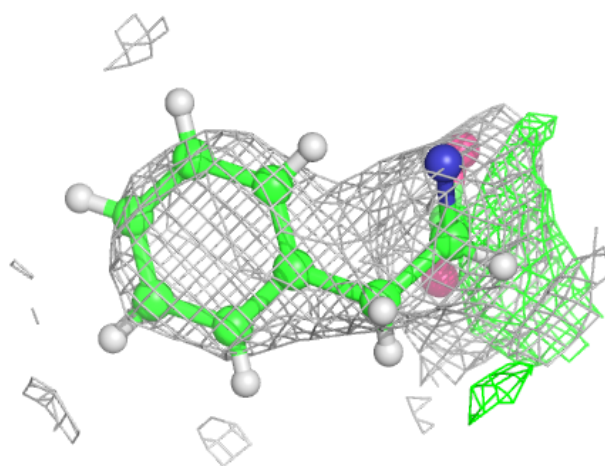
Electron density around PHE C 702:

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



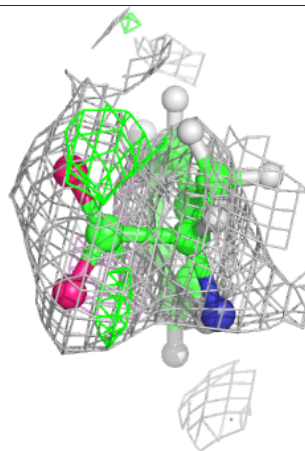
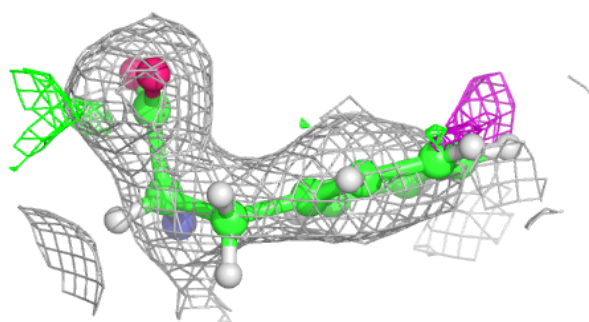
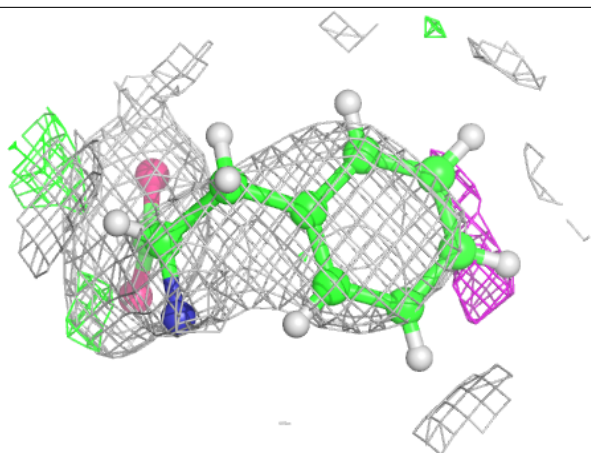
Electron density around PHE D 702:

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

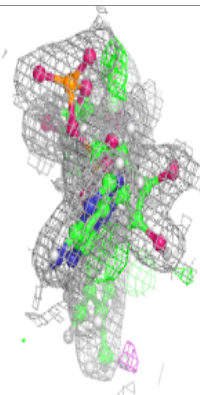
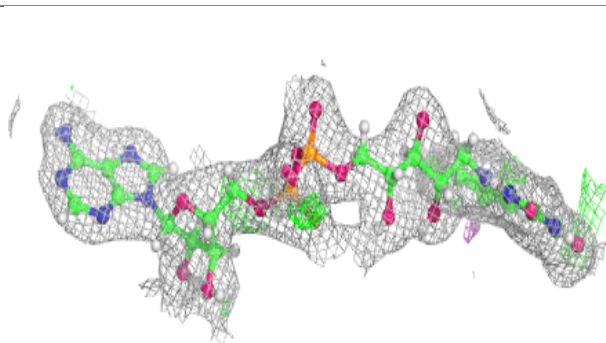
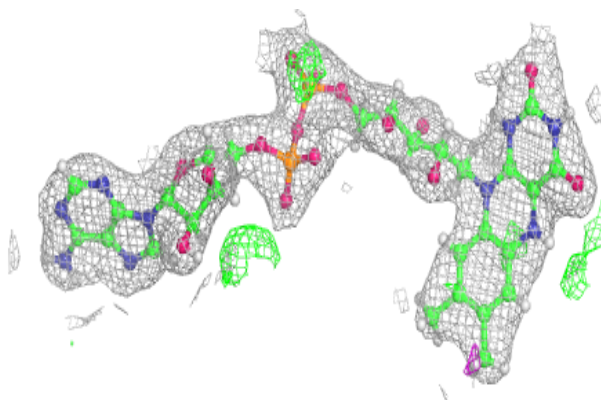


Electron density around PHE A 702:

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

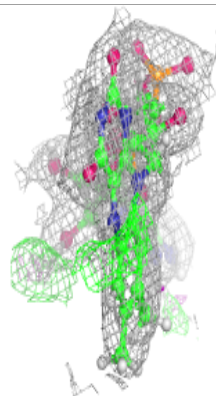
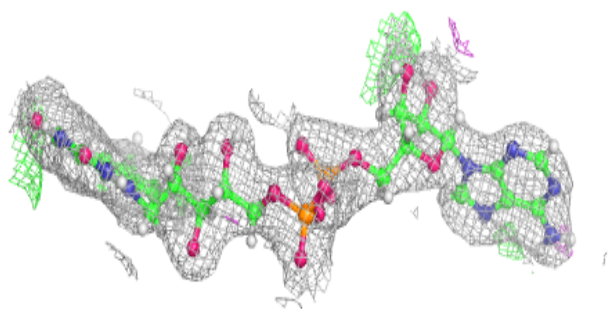
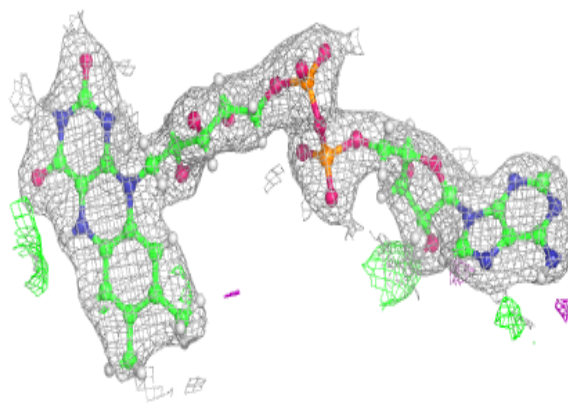
**Electron density around FDA D 701:**

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

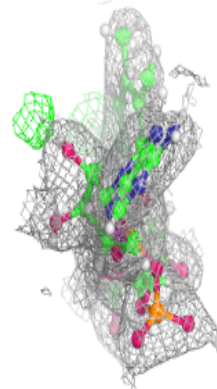
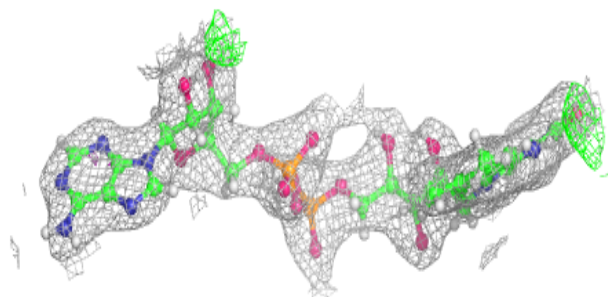
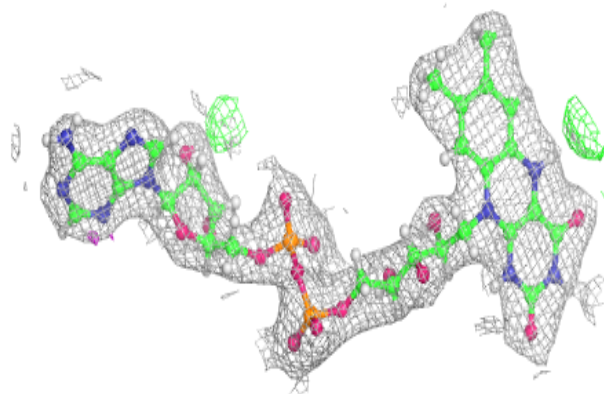


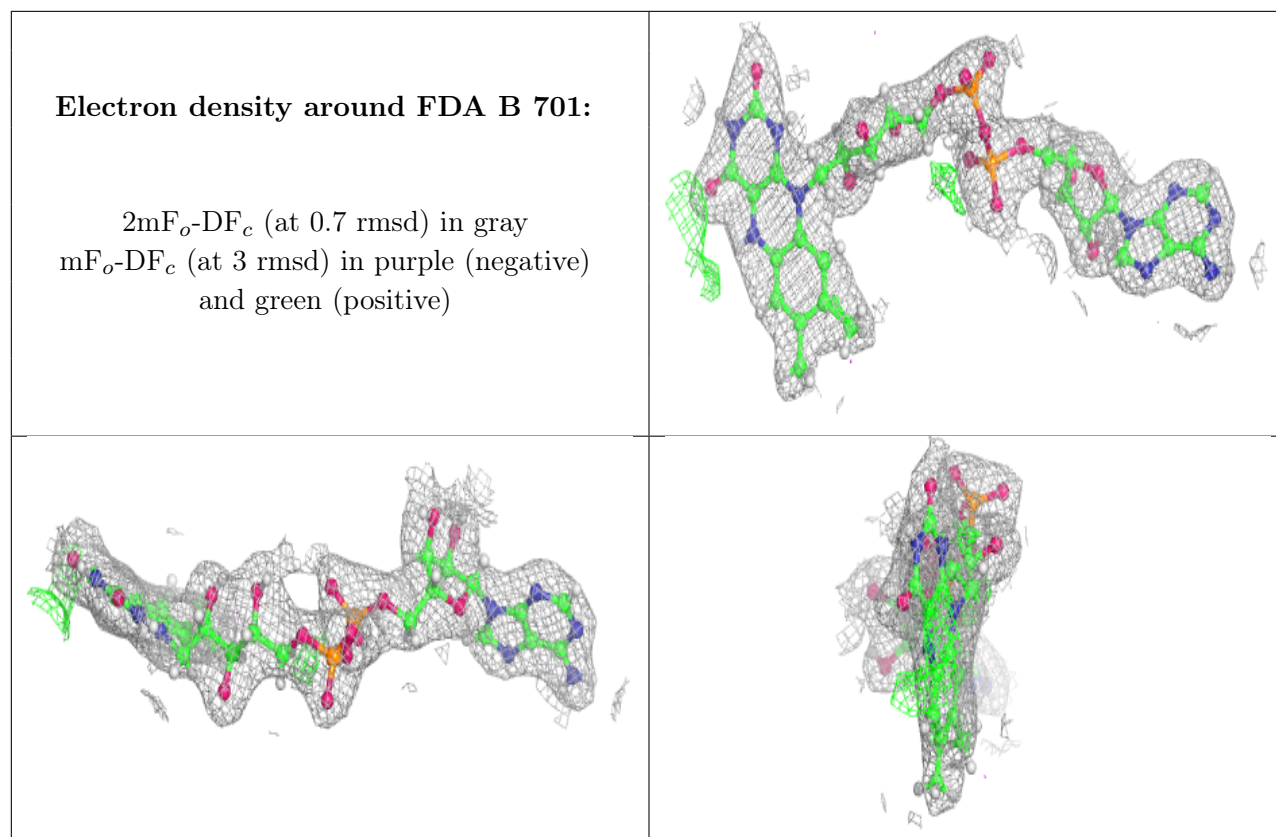
Electron density around FDA C 701:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.