Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2022 – 06:03 pm GMT

PDB ID	:	7P9Q
Title	:	Crystal structure of Indole 3-Carboxylic acid decarboxylase from Arthrobacter nicotianae FI1612 in complex with co-factor prFMN.
Authors	:	Gahloth, D.; Leys, D.
Deposited on	:	2021-07-27
Resolution	:	2.53 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 following versions of software and data (see references ⓘ) were used in the production of this report:

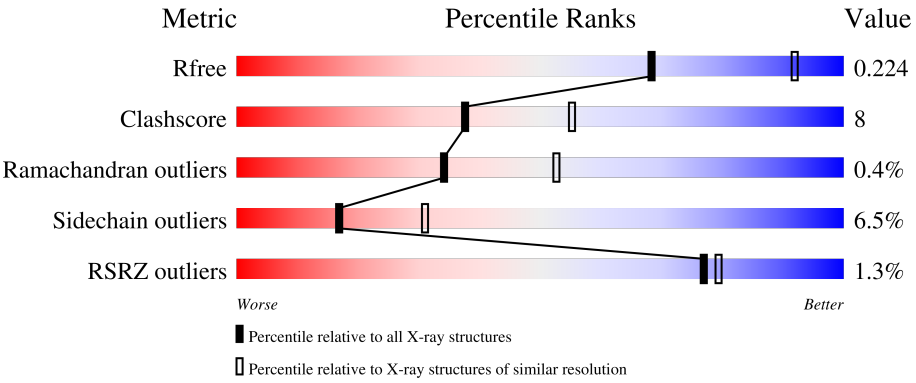
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.53 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	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (2.54-2.50)

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	461	83% 13%
1	B	461	83% 13%
1	C	461	% 84% 12%
1	D	461	% 83% 13%
1	E	461	2% 85% 12%

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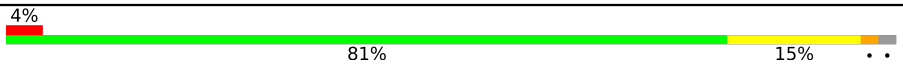
Mol	Chain	Length	Quality of chain
1	F	461	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21468 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called AnInD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3468	2199	600	657	12			
1	B	452	Total	C	N	O	S	0	0	0
			3459	2194	598	655	12			
1	C	452	Total	C	N	O	S	0	0	0
			3459	2194	598	655	12			
1	D	452	Total	C	N	O	S	0	0	0
			3459	2194	598	655	12			
1	E	452	Total	C	N	O	S	0	0	0
			3459	2194	598	655	12			
1	F	452	Total	C	N	O	S	0	0	0
			3459	2194	598	655	12			

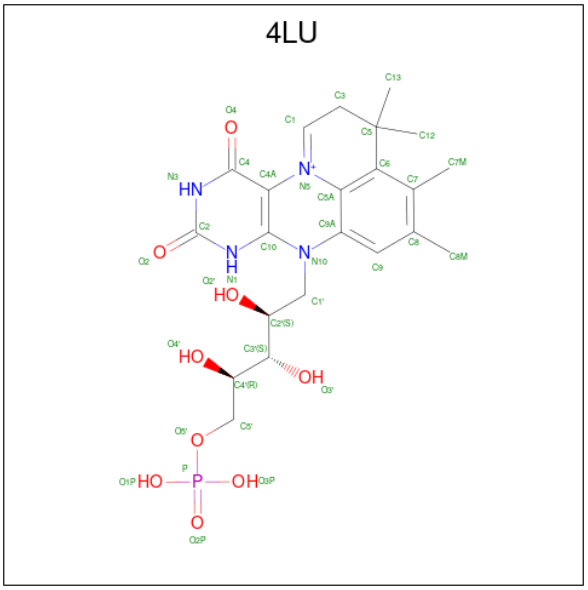
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is 1-deoxy-5-O-phosphono-1-(3,3,4,5-tetramethyl-9,11-dioxo-2,3,8,9,10,11-hexahydro-7H-quinolino[1,8-fg]pteridin-12-ium-7-y l)-D-ribitol (three-letter code: 4LU) (formula: $C_{22}H_{30}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 36 22 4 9 1	0	0
4	B	1	Total C N O P 36 22 4 9 1	0	0
4	C	1	Total C N O P 36 22 4 9 1	0	0
4	D	1	Total C N O P 36 22 4 9 1	0	0
4	E	1	Total C N O P 36 22 4 9 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	0	0
			36	22	4	9	1		

- Molecule 5 is water.

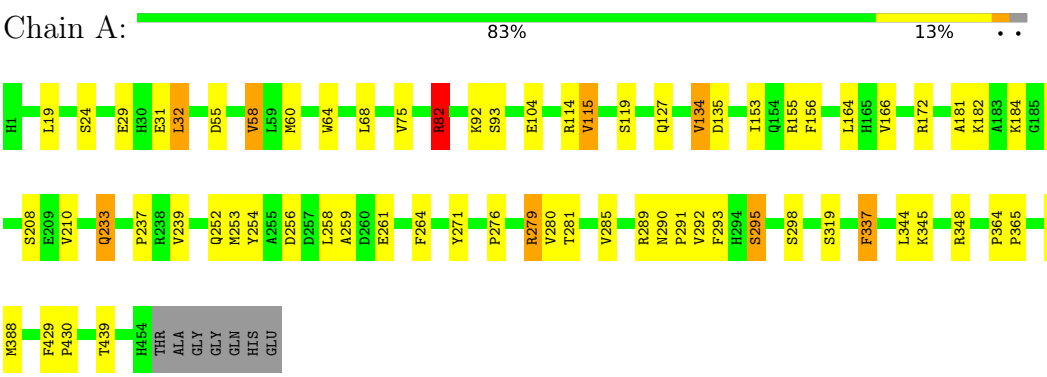
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	106	Total	O	0	0
			106	106		
5	B	100	Total	O	0	0
			100	100		
5	C	73	Total	O	0	0
			73	73		
5	D	75	Total	O	0	0
			75	75		
5	E	59	Total	O	0	0
			59	59		
5	F	64	Total	O	0	0
			64	64		

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.

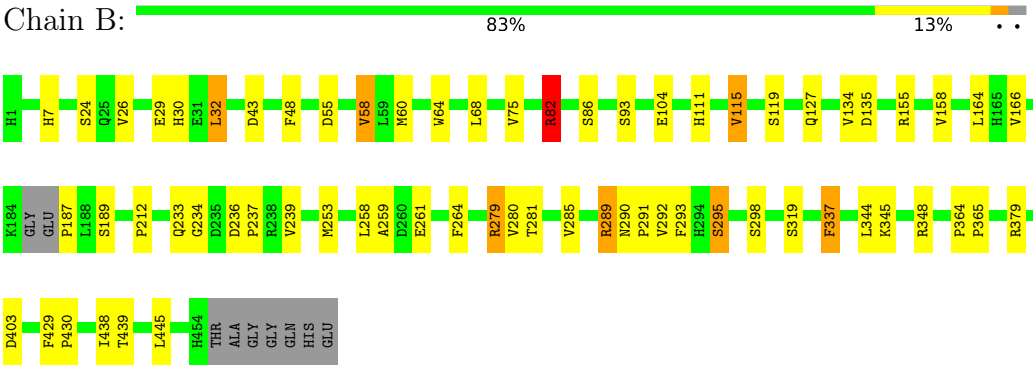
- Molecule 1: AnInD

Chain A:



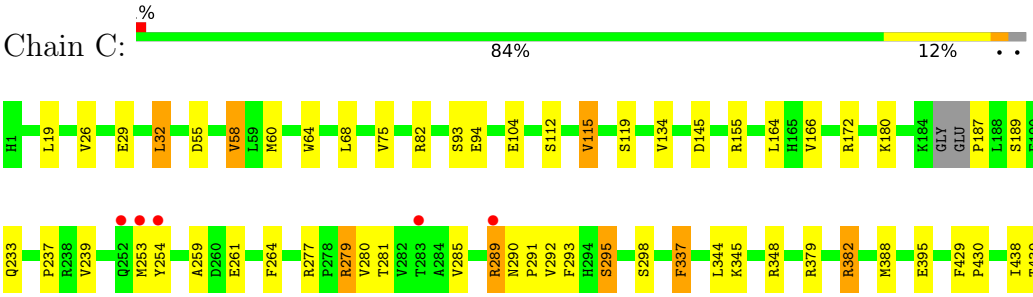
- Molecule 1: AnInD

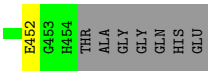
Chain B:



- Molecule 1: AnInD

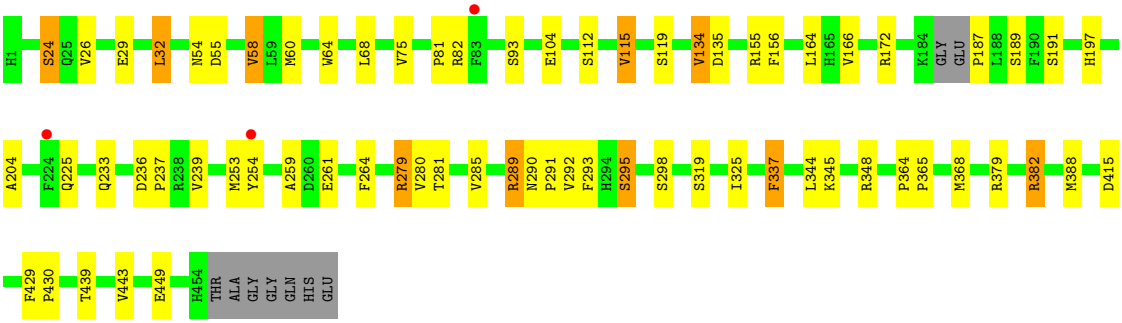
Chain C:





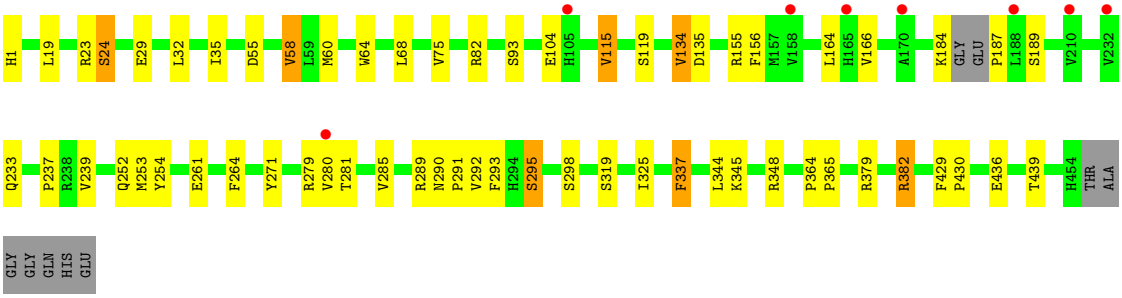
• Molecule 1: AnInD

Chain D:



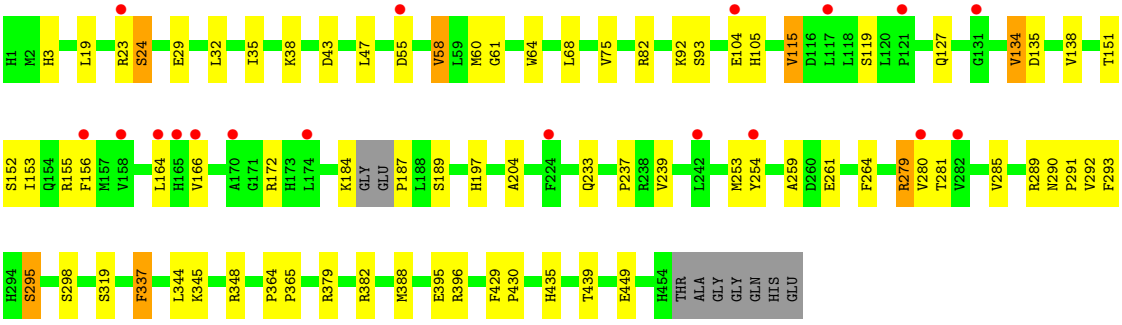
• Molecule 1: AnInD

Chain E:



• Molecule 1: AnInD

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	104.20Å 195.45Å 105.21Å 90.00° 116.35° 90.00°	Depositor
Resolution (Å)	43.42 – 2.53 43.38 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.42-2.53) 95.8 (43.38-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.184 , 0.221 0.189 , 0.224	Depositor DCC
R_{free} test set	6529 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å^2)	70.6	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.339 for l,-k,h	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21468	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: NA, MN, 4LU

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	0.81	2/3550 (0.1%)	0.94	4/4835 (0.1%)
1	B	0.83	1/3540 (0.0%)	0.94	5/4819 (0.1%)
1	C	0.77	2/3540 (0.1%)	0.91	1/4819 (0.0%)
1	D	0.75	1/3540 (0.0%)	0.90	1/4819 (0.0%)
1	E	0.77	0/3540	0.89	1/4819 (0.0%)
1	F	0.77	1/3540 (0.0%)	0.89	2/4819 (0.0%)
All	All	0.78	7/21250 (0.0%)	0.91	14/28930 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	24	SER	CB-OG	7.92	1.52	1.42
1	C	395	GLU	CD-OE1	5.64	1.31	1.25
1	A	382	ARG	NE-CZ	5.58	1.40	1.33
1	B	382	ARG	NE-CZ	5.42	1.40	1.33
1	C	382	ARG	NE-CZ	5.08	1.39	1.33
1	A	31	GLU	CD-OE2	5.04	1.31	1.25
1	F	395	GLU	CD-OE1	5.01	1.31	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	B	82	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	F	348	ARG	CG-CD-NE	-8.07	94.85	111.80
1	E	348	ARG	CG-CD-NE	-7.99	95.02	111.80
1	B	348	ARG	CG-CD-NE	-6.99	97.13	111.80
1	A	348	ARG	CG-CD-NE	-6.83	97.47	111.80
1	C	348	ARG	CG-CD-NE	-6.74	97.65	111.80
1	A	82	ARG	NE-CZ-NH1	6.57	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	348	ARG	CG-CD-NE	-6.19	98.81	111.80
1	B	82	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	319	SER	N-CA-CB	5.49	118.73	110.50
1	B	319	SER	N-CA-CB	5.16	118.24	110.50
1	B	388	MET	CG-SD-CE	-5.07	92.09	100.20
1	F	319	SER	N-CA-CB	5.03	118.05	110.50

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	3468	0	3368	53	0
1	B	3459	0	3363	59	0
1	C	3459	0	3363	42	0
1	D	3459	0	3363	54	0
1	E	3459	0	3363	42	0
1	F	3459	0	3363	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	36	0	28	10	0
4	B	36	0	28	8	0
4	C	36	0	28	7	0
4	D	36	0	28	10	0
4	E	36	0	28	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	36	0	28	8	0
5	A	106	0	0	20	0
5	B	100	0	0	31	0
5	C	73	0	0	16	0
5	D	75	0	0	17	0
5	E	59	0	0	14	0
5	F	64	0	0	24	0
All	All	21468	0	20351	320	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 8.

All (320) 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:B:187:PRO:HB2	5:B:682:HOH:O	1.18	1.34
1:B:237:PRO:HA	5:B:665:HOH:O	1.20	1.27
1:C:289:ARG:HD2	5:C:658:HOH:O	1.38	1.20
5:D:622:HOH:O	1:F:439:THR:HG22	1.46	1.13
4:C:503:4LU:H13	4:C:503:4LU:H14	1.35	1.08
4:D:503:4LU:H13	4:D:503:4LU:H14	1.35	1.08
5:C:668:HOH:O	1:E:382:ARG:HD2	1.54	1.05
1:D:382:ARG:HD2	5:F:655:HOH:O	1.54	1.05
1:E:23:ARG:NH1	5:E:601:HOH:O	1.88	1.05
4:E:503:4LU:H14	4:E:503:4LU:H13	1.39	1.04
4:F:503:4LU:H13	4:F:503:4LU:H14	1.41	1.02
1:F:43:ASP:HB2	5:F:652:HOH:O	1.59	1.00
4:B:503:4LU:H13	4:B:503:4LU:H14	1.46	0.97
1:C:388:MET:HE2	5:C:662:HOH:O	1.66	0.94
5:C:624:HOH:O	1:E:439:THR:HG22	1.68	0.92
1:A:237:PRO:HA	5:A:631:HOH:O	1.69	0.91
4:A:503:4LU:H13	4:A:503:4LU:H14	1.53	0.90
1:C:388:MET:CE	5:C:662:HOH:O	2.22	0.88
1:C:277:ARG:HD3	5:C:635:HOH:O	1.75	0.86
1:D:368:MET:SD	5:F:664:HOH:O	2.32	0.86
5:A:681:HOH:O	1:B:439:THR:HG22	1.75	0.86
5:C:664:HOH:O	1:E:436:GLU:HG2	1.77	0.85
1:D:439:THR:HG22	5:F:618:HOH:O	1.76	0.85
1:D:237:PRO:HA	5:D:604:HOH:O	1.76	0.85
1:A:114:ARG:CA	5:A:650:HOH:O	2.27	0.82
1:B:236:ASP:HB3	5:B:665:HOH:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:152:SER:N	5:F:601:HOH:O	2.13	0.81
1:A:439:THR:HG22	5:B:677:HOH:O	1.79	0.81
1:D:239:VAL:HG23	5:D:619:HOH:O	1.79	0.80
1:F:237:PRO:HA	5:F:640:HOH:O	1.81	0.80
1:B:182:LYS:CB	5:B:627:HOH:O	2.30	0.78
1:B:239:VAL:HG23	5:B:602:HOH:O	1.85	0.77
1:E:1:HIS:HD2	5:E:657:HOH:O	1.68	0.77
1:B:187:PRO:CB	5:B:682:HOH:O	1.92	0.76
1:A:210:VAL:O	5:A:601:HOH:O	2.03	0.76
1:D:187:PRO:HD2	5:D:612:HOH:O	1.84	0.76
1:D:187:PRO:CD	5:D:612:HOH:O	2.33	0.75
1:A:388:MET:CE	5:A:685:HOH:O	2.34	0.74
1:A:439:THR:HG23	1:B:127:GLN:HE21	1.52	0.74
1:A:184:LYS:HA	5:A:616:HOH:O	1.88	0.73
1:A:92:LYS:HD2	5:A:601:HOH:O	1.87	0.73
1:D:388:MET:CE	5:D:670:HOH:O	2.37	0.72
1:A:166:VAL:HG11	1:A:253:MET:HE1	1.72	0.71
1:F:152:SER:O	5:F:601:HOH:O	2.08	0.71
1:C:239:VAL:HG23	5:C:610:HOH:O	1.90	0.71
4:D:503:4LU:H14	4:D:503:4LU:C12	2.14	0.70
1:C:237:PRO:HA	5:C:625:HOH:O	1.92	0.69
4:C:503:4LU:H14	4:C:503:4LU:C12	2.14	0.69
4:E:503:4LU:H14	4:E:503:4LU:C12	2.17	0.68
4:B:503:4LU:H14	4:B:503:4LU:C12	2.23	0.68
1:D:239:VAL:CG2	5:D:619:HOH:O	2.40	0.68
1:A:135:ASP:HB2	4:A:503:4LU:H3	1.75	0.68
1:F:47:LEU:HB3	5:F:602:HOH:O	1.94	0.68
1:F:138:VAL:HG13	5:F:601:HOH:O	1.92	0.67
1:A:115:VAL:HB	5:A:604:HOH:O	1.94	0.67
1:B:279:ARG:HG2	5:B:604:HOH:O	1.93	0.67
1:F:197:HIS:ND1	5:F:603:HOH:O	2.26	0.67
1:A:172:ARG:HE	4:A:503:4LU:H7	1.43	0.67
1:B:172:ARG:HE	4:B:503:4LU:H7	1.41	0.66
1:E:237:PRO:HA	5:E:636:HOH:O	1.94	0.66
1:A:187:PRO:HG3	1:A:252:GLN:HE21	1.61	0.66
1:F:23:ARG:HD2	5:F:627:HOH:O	1.96	0.65
1:B:7:HIS:HB3	5:B:646:HOH:O	1.95	0.65
1:D:439:THR:HG23	1:F:127:GLN:HE21	1.61	0.65
1:F:92:LYS:HE2	5:F:663:HOH:O	1.95	0.65
1:A:276:PRO:HD2	5:A:607:HOH:O	1.97	0.64
1:B:158:VAL:HG23	5:B:661:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:503:4LU:H14	4:F:503:4LU:C12	2.20	0.64
1:B:237:PRO:C	5:B:665:HOH:O	2.31	0.62
1:C:115:VAL:HG12	1:C:285:VAL:HG23	1.82	0.62
1:B:111:HIS:NE2	5:B:601:HOH:O	2.22	0.62
1:B:187:PRO:CG	5:B:682:HOH:O	2.34	0.62
1:C:164:LEU:HB2	1:C:280:VAL:HG13	1.81	0.62
1:B:234:GLY:N	5:B:602:HOH:O	2.32	0.61
1:D:166:VAL:HG11	1:D:253:MET:HE1	1.81	0.61
1:A:388:MET:HE2	5:A:685:HOH:O	2.00	0.61
1:B:388:MET:CE	5:B:685:HOH:O	2.48	0.61
1:C:239:VAL:CG2	5:C:610:HOH:O	2.45	0.61
1:D:164:LEU:HB2	1:D:280:VAL:HG13	1.81	0.61
1:A:115:VAL:HG12	1:A:285:VAL:HG23	1.83	0.60
1:F:388:MET:CE	5:F:654:HOH:O	2.49	0.60
1:F:3:HIS:CE1	5:F:606:HOH:O	2.54	0.60
1:E:184:LYS:O	5:E:602:HOH:O	2.16	0.60
1:F:164:LEU:HB2	1:F:280:VAL:HG13	1.84	0.60
1:C:172:ARG:HE	4:C:503:4LU:H7	1.47	0.59
1:D:115:VAL:HG12	1:D:285:VAL:HG23	1.83	0.59
1:E:166:VAL:HG11	1:E:253:MET:HE1	1.83	0.59
1:F:115:VAL:HG12	1:F:285:VAL:HG23	1.84	0.59
4:A:503:4LU:H14	4:A:503:4LU:C12	2.31	0.59
1:B:115:VAL:HG12	1:B:285:VAL:HG23	1.85	0.59
1:E:164:LEU:HB2	1:E:280:VAL:HG13	1.83	0.59
1:D:189:SER:HB3	1:D:239:VAL:HG12	1.83	0.59
1:E:115:VAL:HG12	1:E:285:VAL:HG23	1.83	0.59
1:B:166:VAL:HG11	1:B:253:MET:HE1	1.85	0.59
1:C:189:SER:HB3	1:C:239:VAL:HG12	1.83	0.59
4:A:503:4LU:H6	4:A:503:4LU:O4	2.01	0.58
1:B:43:ASP:HB2	5:B:698:HOH:O	2.03	0.58
4:B:503:4LU:O4	4:B:503:4LU:H6	2.02	0.58
1:D:172:ARG:HE	4:D:503:4LU:H7	1.51	0.58
1:E:187:PRO:HB2	5:E:623:HOH:O	2.04	0.58
1:B:259:ALA:N	5:B:604:HOH:O	2.36	0.58
1:A:164:LEU:HB2	1:A:280:VAL:HG13	1.85	0.58
1:F:172:ARG:HE	4:F:503:4LU:H7	1.52	0.58
1:B:164:LEU:HB2	1:B:280:VAL:HG13	1.86	0.58
1:B:189:SER:HB3	1:B:239:VAL:HG12	1.85	0.58
1:F:19:LEU:HG	5:F:602:HOH:O	2.02	0.57
1:F:189:SER:HB3	1:F:239:VAL:HG12	1.87	0.57
1:A:189:SER:HB3	1:A:239:VAL:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:SER:HB3	1:E:239:VAL:HG12	1.87	0.57
1:D:388:MET:HE3	5:D:670:HOH:O	2.04	0.56
1:C:189:SER:HB3	1:C:239:VAL:CG1	2.36	0.56
1:B:388:MET:HE2	5:B:685:HOH:O	2.06	0.56
5:A:681:HOH:O	1:B:439:THR:CG2	2.43	0.56
4:D:503:4LU:H6	4:D:503:4LU:O4	2.04	0.56
4:F:503:4LU:H6	4:F:503:4LU:O4	2.06	0.56
1:D:189:SER:HB3	1:D:239:VAL:CG1	2.36	0.56
4:E:503:4LU:O4	4:E:503:4LU:H6	2.05	0.56
1:F:151:THR:HG22	5:F:601:HOH:O	2.05	0.55
1:D:54:ASN:HA	5:D:613:HOH:O	2.07	0.55
1:C:166:VAL:HG11	1:C:253:MET:HE1	1.89	0.55
1:B:86:SER:HB2	5:B:659:HOH:O	2.06	0.55
1:C:60:MET:CE	1:C:295:SER:HB3	2.37	0.55
1:A:189:SER:HB3	1:A:239:VAL:CG1	2.37	0.55
1:F:166:VAL:HG11	1:F:253:MET:HE1	1.88	0.55
1:E:189:SER:HB3	1:E:239:VAL:CG1	2.37	0.54
1:F:189:SER:HB3	1:F:239:VAL:CG1	2.37	0.54
1:A:208:SER:HB2	5:A:680:HOH:O	2.08	0.54
1:F:60:MET:CE	1:F:295:SER:HB3	2.38	0.54
1:A:233:GLN:HA	5:A:692:HOH:O	2.07	0.53
1:B:189:SER:HB3	1:B:239:VAL:CG1	2.38	0.53
1:D:60:MET:CE	1:D:295:SER:HB3	2.39	0.53
1:A:135:ASP:O	4:A:503:4LU:H4	2.09	0.53
1:B:82:ARG:NH1	5:B:607:HOH:O	2.42	0.53
1:E:187:PRO:C	5:E:623:HOH:O	2.47	0.53
1:A:187:PRO:HG3	1:A:252:GLN:NE2	2.23	0.53
4:C:503:4LU:O4	4:C:503:4LU:H6	2.07	0.53
1:C:191:SER:HB3	5:C:610:HOH:O	2.09	0.52
1:D:439:THR:CG2	5:F:618:HOH:O	2.44	0.52
1:A:181:ALA:O	1:A:186:GLU:O	2.27	0.52
1:B:60:MET:CE	1:B:295:SER:HB3	2.39	0.52
1:E:60:MET:CE	1:E:295:SER:HB3	2.39	0.52
1:D:439:THR:CG2	1:F:127:GLN:HE21	2.23	0.52
1:A:60:MET:CE	1:A:295:SER:HB3	2.41	0.51
1:F:184:LYS:C	5:F:637:HOH:O	2.49	0.51
1:B:187:PRO:HG2	5:B:682:HOH:O	2.03	0.50
1:E:239:VAL:HG22	5:E:636:HOH:O	2.11	0.50
5:D:622:HOH:O	1:F:439:THR:CG2	2.24	0.50
1:C:60:MET:HE2	1:C:295:SER:HB3	1.93	0.50
1:C:289:ARG:NH1	1:C:289:ARG:HB3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:HIS:HD2	5:B:675:HOH:O	1.92	0.50
1:D:388:MET:HE2	5:D:670:HOH:O	2.08	0.50
1:D:289:ARG:NH1	1:D:289:ARG:HB3	2.28	0.49
5:C:624:HOH:O	1:E:439:THR:CG2	2.40	0.49
1:F:105:HIS:C	5:F:611:HOH:O	2.50	0.49
1:E:252:GLN:HG3	5:E:623:HOH:O	2.12	0.49
1:B:279:ARG:CG	5:B:604:HOH:O	2.57	0.48
1:E:135:ASP:HB2	4:E:503:4LU:H3	1.95	0.48
4:F:503:4LU:O4	4:F:503:4LU:C1	2.61	0.48
1:D:290:ASN:N	1:D:291:PRO:CD	2.77	0.48
1:F:388:MET:HE2	5:F:654:HOH:O	2.11	0.48
1:A:187:PRO:HB3	1:A:254:TYR:CD2	2.48	0.48
1:A:439:THR:CG2	1:B:127:GLN:HE21	2.23	0.48
4:B:503:4LU:O4	4:B:503:4LU:C1	2.61	0.48
1:F:184:LYS:CA	5:F:637:HOH:O	2.61	0.48
4:A:503:4LU:O4	4:A:503:4LU:C1	2.61	0.48
1:A:258:LEU:HD11	5:A:698:HOH:O	2.14	0.48
1:B:60:MET:HE2	1:B:295:SER:HB3	1.96	0.47
1:D:135:ASP:HB2	4:D:503:4LU:H3	1.97	0.47
1:A:68:LEU:C	1:A:68:LEU:HD23	2.35	0.47
1:C:449:GLU:N	1:E:24:SER:OG	2.37	0.47
1:A:439:THR:HG23	1:B:127:GLN:NE2	2.27	0.47
1:C:439:THR:HG22	5:E:648:HOH:O	2.15	0.47
1:C:187:PRO:HB3	1:C:254:TYR:CD2	2.50	0.46
5:D:603:HOH:O	1:F:38:LYS:HE2	2.15	0.46
1:F:429:PHE:HA	1:F:430:PRO:C	2.36	0.46
1:A:82:ARG:HD2	5:A:684:HOH:O	2.15	0.46
1:D:134:VAL:HA	5:D:602:HOH:O	2.15	0.46
1:C:290:ASN:N	1:C:291:PRO:CD	2.78	0.46
1:A:182:LYS:CB	5:A:682:HOH:O	2.64	0.46
1:B:158:VAL:CG2	5:B:661:HOH:O	2.60	0.46
1:F:68:LEU:C	1:F:68:LEU:HD23	2.37	0.46
1:F:135:ASP:HB2	4:F:503:4LU:H3	1.98	0.46
1:B:68:LEU:C	1:B:68:LEU:HD23	2.36	0.46
1:C:429:PHE:HA	1:C:430:PRO:C	2.36	0.46
1:A:153:ILE:HG23	4:A:503:4LU:O2'	2.16	0.46
1:B:135:ASP:HB2	4:B:503:4LU:H3	1.98	0.45
4:D:503:4LU:O4	4:D:503:4LU:C1	2.63	0.45
1:E:187:PRO:CD	5:E:602:HOH:O	2.64	0.45
1:D:290:ASN:N	1:D:291:PRO:HD3	2.31	0.45
1:C:58:VAL:HA	1:C:293:PHE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:LEU:HD23	1:C:68:LEU:C	2.37	0.45
1:A:127:GLN:HE21	1:B:439:THR:HG23	1.80	0.45
1:C:208:SER:HB2	5:C:605:HOH:O	2.16	0.45
1:D:415:ASP:HB2	5:D:665:HOH:O	2.15	0.45
1:D:68:LEU:C	1:D:68:LEU:HD23	2.37	0.45
1:F:239:VAL:HG22	5:F:640:HOH:O	2.16	0.45
1:A:239:VAL:C	5:A:622:HOH:O	2.55	0.45
1:C:289:ARG:HB3	1:C:289:ARG:HH11	1.82	0.45
1:E:68:LEU:HD23	1:E:68:LEU:C	2.37	0.45
4:E:503:4LU:H1	4:E:503:4LU:H20	1.63	0.45
1:D:58:VAL:HA	1:D:293:PHE:O	2.16	0.45
1:D:259:ALA:HB2	1:D:279:ARG:HD2	1.99	0.45
1:B:445:LEU:HB3	5:B:687:HOH:O	2.17	0.44
1:E:429:PHE:HA	1:E:430:PRO:C	2.37	0.44
1:F:290:ASN:N	1:F:291:PRO:CD	2.81	0.44
1:B:429:PHE:HA	1:B:430:PRO:C	2.38	0.44
4:E:503:4LU:O4	4:E:503:4LU:C1	2.64	0.44
1:F:204:ALA:O	4:F:503:4LU:H26	2.16	0.44
1:B:58:VAL:HA	1:B:293:PHE:O	2.18	0.44
1:D:443:VAL:HG11	1:F:35:ILE:HG12	1.98	0.44
1:A:19:LEU:HD12	1:A:19:LEU:HA	1.87	0.44
1:A:429:PHE:HA	1:A:430:PRO:C	2.38	0.44
1:C:115:VAL:HG23	1:C:115:VAL:O	2.18	0.44
1:D:60:MET:HE2	1:D:295:SER:HB3	2.00	0.44
1:D:187:PRO:HB3	1:D:254:TYR:CD2	2.52	0.44
1:D:364:PRO:N	1:D:365:PRO:CD	2.80	0.44
1:A:60:MET:HE3	1:A:295:SER:HB3	1.99	0.44
1:D:344:LEU:C	1:D:344:LEU:HD12	2.38	0.44
1:C:443:VAL:HG11	1:E:35:ILE:HG12	1.99	0.44
1:E:115:VAL:HG23	1:E:115:VAL:O	2.18	0.44
1:E:135:ASP:O	4:E:503:4LU:H4	2.18	0.44
1:F:58:VAL:HA	1:F:293:PHE:O	2.18	0.44
1:B:111:HIS:CE1	5:B:601:HOH:O	2.67	0.44
1:E:290:ASN:N	1:E:291:PRO:CD	2.81	0.44
1:A:364:PRO:N	1:A:365:PRO:CD	2.81	0.43
1:C:290:ASN:N	1:C:291:PRO:HD3	2.33	0.43
1:A:259:ALA:HB2	1:A:279:ARG:HD2	1.99	0.43
1:C:19:LEU:HD12	1:C:19:LEU:HA	1.86	0.43
1:D:191:SER:HB3	5:D:619:HOH:O	2.18	0.43
1:F:61:GLY:N	5:F:613:HOH:O	2.50	0.43
1:F:187:PRO:HB3	1:F:254:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ASP:HA	5:A:698:HOH:O	2.18	0.43
1:C:26:VAL:HG21	1:C:32:LEU:HD12	1.99	0.43
1:C:94:GLU:O	5:C:601:HOH:O	2.20	0.43
4:C:503:4LU:O4	4:C:503:4LU:C1	2.66	0.43
1:E:58:VAL:HA	1:E:293:PHE:O	2.18	0.43
1:A:58:VAL:HA	1:A:293:PHE:O	2.18	0.43
1:B:115:VAL:O	1:B:115:VAL:HG23	2.18	0.43
1:F:115:VAL:HG23	1:F:115:VAL:O	2.18	0.43
1:B:364:PRO:N	1:B:365:PRO:CD	2.81	0.43
1:C:344:LEU:C	1:C:344:LEU:HD12	2.38	0.43
4:C:503:4LU:C12	4:C:503:4LU:C7M	2.92	0.43
1:E:187:PRO:N	5:E:602:HOH:O	2.51	0.43
1:A:115:VAL:HG23	1:A:115:VAL:O	2.19	0.43
1:B:237:PRO:HB2	5:B:695:HOH:O	2.17	0.43
1:D:24:SER:OG	1:F:449:GLU:N	2.36	0.43
1:D:449:GLU:H	1:F:24:SER:HG	1.64	0.43
1:E:19:LEU:HD12	1:E:19:LEU:HA	1.89	0.43
1:E:364:PRO:N	1:E:365:PRO:CD	2.82	0.43
1:B:290:ASN:N	1:B:291:PRO:CD	2.81	0.43
1:D:155:ARG:HD3	1:D:264:PHE:CD2	2.54	0.43
1:B:155:ARG:HD3	1:B:264:PHE:CD2	2.54	0.43
1:B:212:PRO:HG3	5:B:679:HOH:O	2.18	0.43
1:D:429:PHE:HA	1:D:430:PRO:C	2.38	0.43
4:D:503:4LU:C12	4:D:503:4LU:C7M	2.93	0.43
1:D:115:VAL:HG23	1:D:115:VAL:O	2.19	0.42
1:D:134:VAL:HG13	1:D:156:PHE:HB2	2.01	0.42
1:D:319:SER:HB3	1:D:325:ILE:HB	2.01	0.42
1:F:60:MET:HE3	1:F:295:SER:HB3	2.01	0.42
1:A:184:LYS:CB	5:A:679:HOH:O	2.67	0.42
1:E:60:MET:HE2	1:E:295:SER:HB3	2.00	0.42
1:A:32:LEU:HB3	5:A:632:HOH:O	2.19	0.42
1:A:290:ASN:N	1:A:291:PRO:CD	2.83	0.42
1:B:290:ASN:N	1:B:291:PRO:HD3	2.35	0.42
4:C:503:4LU:H1	4:C:503:4LU:H20	1.80	0.42
1:E:134:VAL:HG13	1:E:156:PHE:HB2	2.02	0.42
1:E:344:LEU:HD12	1:E:344:LEU:C	2.39	0.42
1:F:134:VAL:HG13	1:F:156:PHE:HB2	2.02	0.42
1:D:112:SER:HA	1:D:285:VAL:O	2.20	0.42
1:D:135:ASP:O	4:D:503:4LU:H4	2.20	0.42
1:A:271:TYR:CE2	1:B:438:ILE:HA	2.55	0.42
1:A:344:LEU:C	1:A:344:LEU:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LEU:HD12	1:B:344:LEU:C	2.39	0.42
1:C:259:ALA:HB2	1:C:279:ARG:HD2	2.01	0.42
1:B:259:ALA:HB2	1:B:279:ARG:HD2	2.02	0.42
1:C:449:GLU:H	1:E:24:SER:HG	1.60	0.42
1:A:134:VAL:HG13	1:A:156:PHE:HB2	2.02	0.42
1:B:135:ASP:O	4:B:503:4LU:H4	2.20	0.42
1:C:239:VAL:HB	5:C:610:HOH:O	2.20	0.42
1:E:155:ARG:HD3	1:E:264:PHE:CD2	2.55	0.42
1:A:155:ARG:HD3	1:A:264:PHE:CD2	2.55	0.41
1:C:452:GLU:CB	5:E:653:HOH:O	2.68	0.41
1:B:289:ARG:HD2	5:B:693:HOH:O	2.19	0.41
1:B:26:VAL:HG21	1:B:32:LEU:HD12	2.02	0.41
1:D:26:VAL:HG21	1:D:32:LEU:HD12	2.02	0.41
1:F:259:ALA:HB2	1:F:279:ARG:HD2	2.02	0.41
1:F:364:PRO:N	1:F:365:PRO:CD	2.82	0.41
1:A:439:THR:CG2	5:B:677:HOH:O	2.54	0.41
1:B:258:LEU:C	5:B:604:HOH:O	2.58	0.41
1:E:319:SER:HB3	1:E:325:ILE:HB	2.03	0.41
1:F:19:LEU:HD12	1:F:19:LEU:HA	1.87	0.41
1:C:155:ARG:HD3	1:C:264:PHE:CD2	2.56	0.41
1:D:197:HIS:NE2	1:D:225:GLN:NE2	2.67	0.41
1:D:289:ARG:HB3	1:D:289:ARG:HH11	1.85	0.41
1:E:252:GLN:CG	5:E:623:HOH:O	2.68	0.41
1:F:155:ARG:HD3	1:F:264:PHE:CD2	2.56	0.41
1:E:184:LYS:CB	5:E:602:HOH:O	2.68	0.41
1:E:290:ASN:N	1:E:291:PRO:HD3	2.35	0.41
1:F:290:ASN:N	1:F:291:PRO:HD3	2.35	0.41
1:A:155:ARG:HB3	4:A:503:4LU:H6	2.03	0.41
1:B:32:LEU:HD11	1:B:48:PHE:CD2	2.56	0.41
4:B:503:4LU:H1	4:B:503:4LU:H20	1.72	0.41
1:C:438:ILE:HA	1:E:271:TYR:CE2	2.56	0.41
1:D:236:ASP:N	5:D:604:HOH:O	2.41	0.41
1:D:449:GLU:OE1	1:F:23:ARG:HD3	2.20	0.41
1:E:187:PRO:HB3	1:E:254:TYR:CD2	2.56	0.41
1:F:344:LEU:C	1:F:344:LEU:HD12	2.40	0.41
1:F:435:HIS:HE1	5:F:604:HOH:O	2.03	0.41
4:A:503:4LU:H1	4:A:503:4LU:H20	1.78	0.41
1:C:112:SER:HA	1:C:285:VAL:O	2.21	0.41
1:F:153:ILE:HG23	4:F:503:4LU:O2'	2.21	0.41
1:A:290:ASN:N	1:A:291:PRO:HD3	2.36	0.40
1:C:145:ASP:OD2	1:C:180:LYS:HE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:VAL:HG22	5:C:625:HOH:O	2.21	0.40
4:D:503:4LU:H1	4:D:503:4LU:H20	1.72	0.40
1:B:403:ASP:CG	1:F:396:ARG:HH21	2.25	0.40
1:D:449:GLU:N	1:F:24:SER:OG	2.43	0.40
1:F:60:MET:HE2	1:F:295:SER:HB3	2.02	0.40
1:D:81:PRO:HD2	5:D:606:HOH:O	2.22	0.40
1:D:204:ALA:O	4:D:503:4LU:H26	2.21	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	452/461 (98%)	438 (97%)	12 (3%)	2 (0%)	34	53
1	B	448/461 (97%)	433 (97%)	13 (3%)	2 (0%)	34	53
1	C	448/461 (97%)	434 (97%)	12 (3%)	2 (0%)	34	53
1	D	448/461 (97%)	433 (97%)	13 (3%)	2 (0%)	34	53
1	E	448/461 (97%)	434 (97%)	12 (3%)	2 (0%)	34	53
1	F	448/461 (97%)	434 (97%)	12 (3%)	2 (0%)	34	53
All	All	2692/2766 (97%)	2606 (97%)	74 (3%)	12 (0%)	34	53

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	VAL
1	C	337	PHE
1	D	337	PHE
1	E	337	PHE
1	A	337	PHE

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Mol	Chain	Res	Type
1	B	337	PHE
1	F	337	PHE
1	B	115	VAL
1	E	115	VAL
1	F	115	VAL
1	C	115	VAL
1	D	115	VAL

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	364/376 (97%)	340 (93%)	24 (7%)	16	30
1	B	364/376 (97%)	340 (93%)	24 (7%)	16	30
1	C	364/376 (97%)	341 (94%)	23 (6%)	18	32
1	D	364/376 (97%)	341 (94%)	23 (6%)	18	32
1	E	364/376 (97%)	340 (93%)	24 (7%)	16	30
1	F	364/376 (97%)	340 (93%)	24 (7%)	16	30
All	All	2184/2256 (97%)	2042 (94%)	142 (6%)	17	31

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	29	GLU
1	A	32	LEU
1	A	55	ASP
1	A	58	VAL
1	A	64	TRP
1	A	75	VAL
1	A	82	ARG
1	A	93	SER
1	A	104	GLU
1	A	119	SER

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Mol	Chain	Res	Type
1	A	134	VAL
1	A	233	GLN
1	A	261	GLU
1	A	279	ARG
1	A	281	THR
1	A	289	ARG
1	A	292	VAL
1	A	295	SER
1	A	298	SER
1	A	337	PHE
1	A	345	LYS
1	A	379	ARG
1	A	382	ARG
1	B	24	SER
1	B	29	GLU
1	B	32	LEU
1	B	55	ASP
1	B	58	VAL
1	B	64	TRP
1	B	75	VAL
1	B	82	ARG
1	B	93	SER
1	B	104	GLU
1	B	119	SER
1	B	134	VAL
1	B	233	GLN
1	B	261	GLU
1	B	279	ARG
1	B	281	THR
1	B	289	ARG
1	B	292	VAL
1	B	295	SER
1	B	298	SER
1	B	337	PHE
1	B	345	LYS
1	B	379	ARG
1	B	382	ARG
1	C	29	GLU
1	C	32	LEU
1	C	55	ASP
1	C	58	VAL
1	C	64	TRP

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Mol	Chain	Res	Type
1	C	75	VAL
1	C	82	ARG
1	C	93	SER
1	C	104	GLU
1	C	119	SER
1	C	134	VAL
1	C	233	GLN
1	C	261	GLU
1	C	279	ARG
1	C	281	THR
1	C	289	ARG
1	C	292	VAL
1	C	295	SER
1	C	298	SER
1	C	337	PHE
1	C	345	LYS
1	C	379	ARG
1	C	382	ARG
1	D	29	GLU
1	D	32	LEU
1	D	55	ASP
1	D	58	VAL
1	D	64	TRP
1	D	75	VAL
1	D	82	ARG
1	D	93	SER
1	D	104	GLU
1	D	119	SER
1	D	134	VAL
1	D	233	GLN
1	D	261	GLU
1	D	279	ARG
1	D	281	THR
1	D	289	ARG
1	D	292	VAL
1	D	295	SER
1	D	298	SER
1	D	337	PHE
1	D	345	LYS
1	D	379	ARG
1	D	382	ARG
1	E	24	SER

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Mol	Chain	Res	Type
1	E	29	GLU
1	E	32	LEU
1	E	55	ASP
1	E	58	VAL
1	E	64	TRP
1	E	75	VAL
1	E	82	ARG
1	E	93	SER
1	E	104	GLU
1	E	119	SER
1	E	134	VAL
1	E	233	GLN
1	E	261	GLU
1	E	279	ARG
1	E	281	THR
1	E	289	ARG
1	E	292	VAL
1	E	295	SER
1	E	298	SER
1	E	337	PHE
1	E	345	LYS
1	E	379	ARG
1	E	382	ARG
1	F	24	SER
1	F	29	GLU
1	F	32	LEU
1	F	55	ASP
1	F	58	VAL
1	F	64	TRP
1	F	75	VAL
1	F	82	ARG
1	F	93	SER
1	F	104	GLU
1	F	119	SER
1	F	134	VAL
1	F	233	GLN
1	F	261	GLU
1	F	279	ARG
1	F	281	THR
1	F	289	ARG
1	F	292	VAL
1	F	295	SER

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Mol	Chain	Res	Type
1	F	298	SER
1	F	337	PHE
1	F	345	LYS
1	F	379	ARG
1	F	382	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	233	GLN
1	A	252	GLN
1	B	127	GLN
1	B	233	GLN
1	C	233	GLN
1	D	127	GLN
1	D	150	ASN
1	D	225	GLN
1	D	233	GLN
1	D	317	GLN
1	E	127	GLN
1	E	233	GLN
1	F	127	GLN
1	F	150	ASN
1	F	233	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	4LU	D	503	3,2	32,39,39	1.25	4 (12%)	41,62,62	2.41	6 (14%)
4	4LU	B	503	3,2	32,39,39	1.26	3 (9%)	41,62,62	2.51	8 (19%)
4	4LU	E	503	3,2	32,39,39	1.28	3 (9%)	41,62,62	2.45	7 (17%)
4	4LU	F	503	3,2	32,39,39	1.21	3 (9%)	41,62,62	2.43	6 (14%)
4	4LU	A	503	3,2	32,39,39	1.35	3 (9%)	41,62,62	2.51	7 (17%)
4	4LU	C	503	3	32,39,39	1.28	3 (9%)	41,62,62	2.35	5 (12%)

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
4	4LU	D	503	3,2	-	2/18/30/30	0/3/4/4
4	4LU	B	503	3,2	-	1/18/30/30	0/3/4/4
4	4LU	E	503	3,2	-	1/18/30/30	0/3/4/4
4	4LU	F	503	3,2	-	0/18/30/30	0/3/4/4
4	4LU	A	503	3,2	-	0/18/30/30	0/3/4/4
4	4LU	C	503	3	-	1/18/30/30	0/3/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	4LU	C4A-C4	4.53	1.49	1.41
4	A	503	4LU	C10-N1	4.48	1.39	1.33
4	E	503	4LU	C4A-C4	4.46	1.49	1.41
4	C	503	4LU	C10-N1	4.39	1.38	1.33
4	C	503	4LU	C4A-C4	4.32	1.48	1.41
4	D	503	4LU	C4A-C4	4.30	1.48	1.41
4	F	503	4LU	C10-N1	4.30	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	503	4LU	C10-N1	4.28	1.38	1.33
4	B	503	4LU	C10-N1	4.24	1.38	1.33
4	B	503	4LU	C4A-C4	4.00	1.48	1.41
4	D	503	4LU	C10-N1	3.96	1.38	1.33
4	F	503	4LU	C4A-C4	3.85	1.48	1.41
4	A	503	4LU	C4-N3	3.30	1.38	1.33
4	B	503	4LU	C4-N3	2.99	1.38	1.33
4	E	503	4LU	C4-N3	2.79	1.37	1.33
4	C	503	4LU	C4-N3	2.70	1.37	1.33
4	F	503	4LU	C4-N3	2.62	1.37	1.33
4	D	503	4LU	C4-N3	2.61	1.37	1.33
4	D	503	4LU	C9A-N10	2.14	1.41	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	503	4LU	C2-N3-C4	11.77	125.08	115.14
4	E	503	4LU	C2-N3-C4	11.66	124.99	115.14
4	F	503	4LU	C2-N3-C4	11.64	124.97	115.14
4	B	503	4LU	C2-N3-C4	11.64	124.97	115.14
4	A	503	4LU	C2-N3-C4	11.54	124.89	115.14
4	D	503	4LU	C2-N3-C4	11.53	124.88	115.14
4	B	503	4LU	C12-C5-C6	5.62	117.22	111.72
4	A	503	4LU	C4A-C4-N3	-5.29	116.19	123.43
4	E	503	4LU	C12-C5-C6	5.29	116.90	111.72
4	F	503	4LU	C12-C5-C6	5.27	116.88	111.72
4	E	503	4LU	C4A-C4-N3	-5.21	116.30	123.43
4	B	503	4LU	C4A-C4-N3	-5.13	116.41	123.43
4	F	503	4LU	C4A-C4-N3	-5.11	116.45	123.43
4	D	503	4LU	C4A-C4-N3	-5.05	116.52	123.43
4	C	503	4LU	C4A-C4-N3	-5.00	116.59	123.43
4	D	503	4LU	C12-C5-C6	4.97	116.58	111.72
4	A	503	4LU	C12-C5-C3	-4.83	101.23	109.60
4	A	503	4LU	C12-C5-C6	4.80	116.42	111.72
4	C	503	4LU	C12-C5-C6	4.21	115.84	111.72
4	F	503	4LU	C12-C5-C3	-3.84	102.94	109.60
4	E	503	4LU	C1'-N10-C10	3.56	121.59	118.41
4	D	503	4LU	C12-C5-C3	-3.33	103.84	109.60
4	B	503	4LU	C12-C5-C3	-3.19	104.08	109.60
4	E	503	4LU	C12-C5-C3	-3.14	104.16	109.60
4	C	503	4LU	C12-C5-C3	-3.09	104.24	109.60
4	B	503	4LU	C13-C5-C3	-2.98	104.44	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	503	4LU	C1'-N10-C10	2.86	120.97	118.41
4	A	503	4LU	O5'-P-O2P	-2.82	98.57	106.47
4	B	503	4LU	O2'-C2'-C1'	2.61	115.87	109.59
4	B	503	4LU	C1'-N10-C10	2.47	120.62	118.41
4	E	503	4LU	C1'-C2'-C3'	-2.38	103.12	109.79
4	F	503	4LU	C1'-C2'-C3'	-2.35	103.21	109.79
4	A	503	4LU	O2'-C2'-C1'	2.31	115.16	109.59
4	C	503	4LU	C10-C4A-C4	-2.16	118.52	119.95
4	E	503	4LU	C13-C5-C6	-2.15	109.62	111.72
4	A	503	4LU	C1'-N10-C10	2.09	120.28	118.41
4	B	503	4LU	C1'-C2'-C3'	-2.09	103.96	109.79
4	F	503	4LU	C1'-N10-C10	2.07	120.26	118.41
4	D	503	4LU	C4'-C3'-C2'	2.03	117.58	113.36

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	503	4LU	C2'-C1'-N10-C9A
4	E	503	4LU	C2'-C1'-N10-C9A
4	C	503	4LU	N10-C1'-C2'-O2'
4	D	503	4LU	C5'-O5'-P-O1P
4	B	503	4LU	C2'-C3'-C4'-C5'

There are no ring outliers.

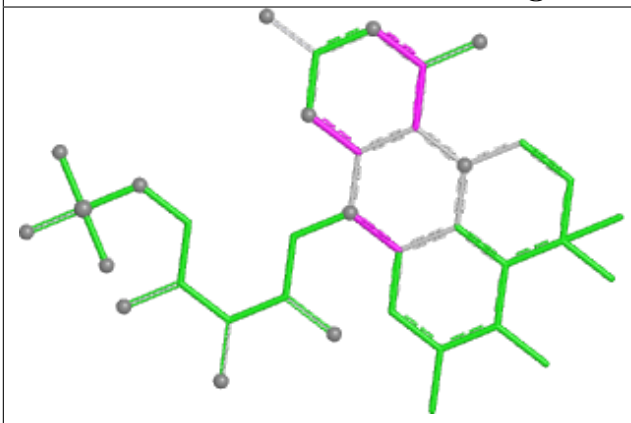
6 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	503	4LU	10	0
4	B	503	4LU	8	0
4	E	503	4LU	7	0
4	F	503	4LU	8	0
4	A	503	4LU	10	0
4	C	503	4LU	7	0

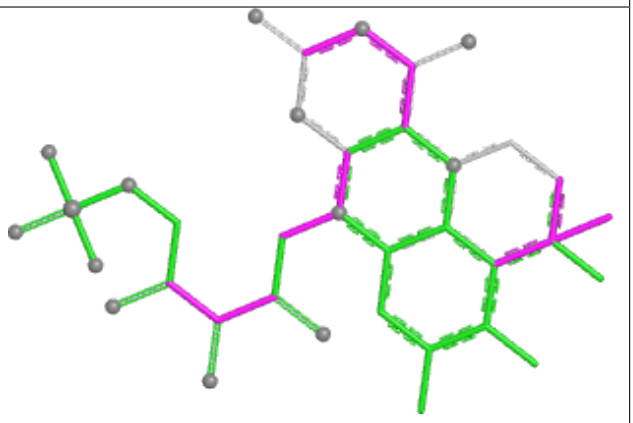
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

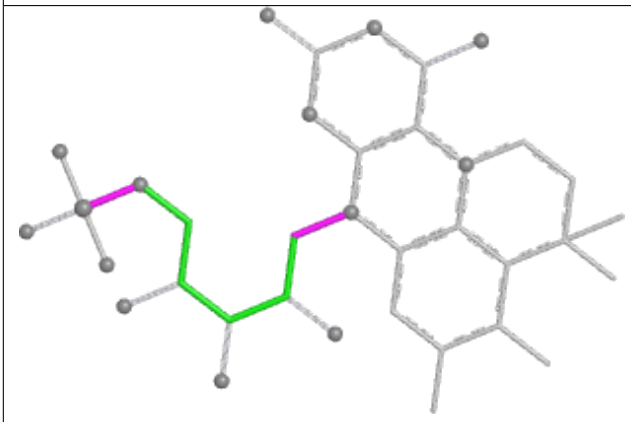
Ligand 4LU D 503



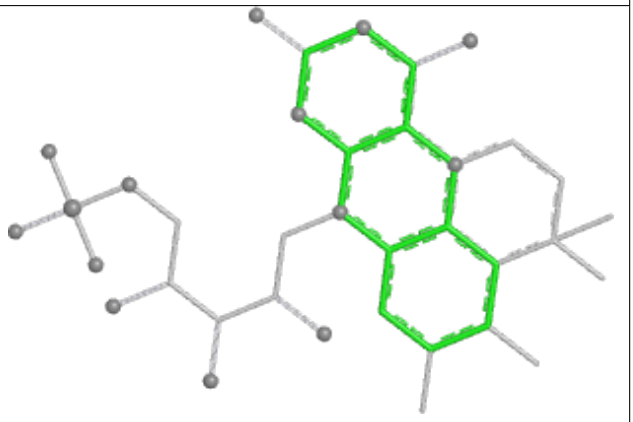
Bond lengths



Bond angles

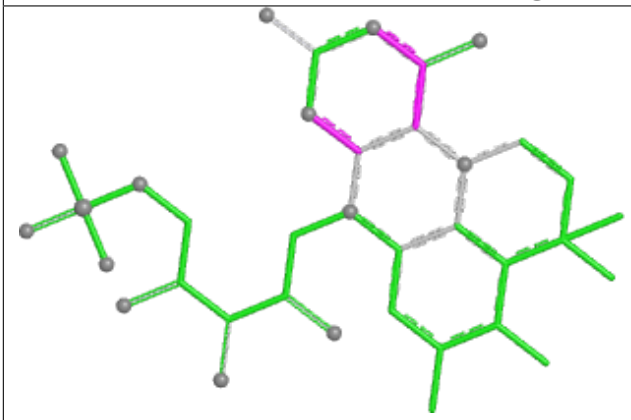


Torsions

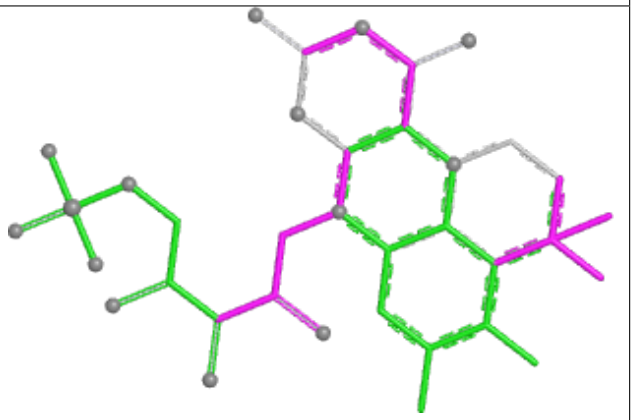


Rings

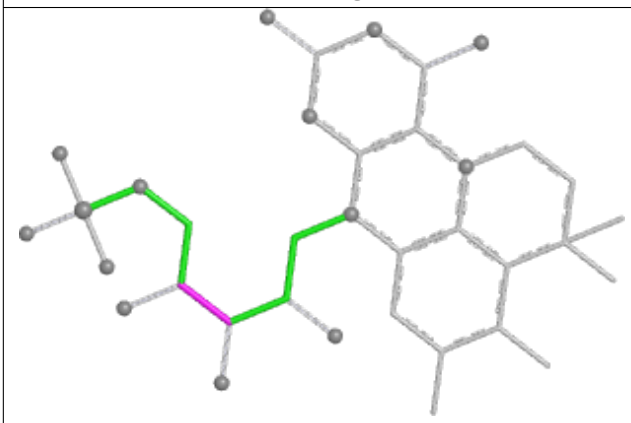
Ligand 4LU B 503



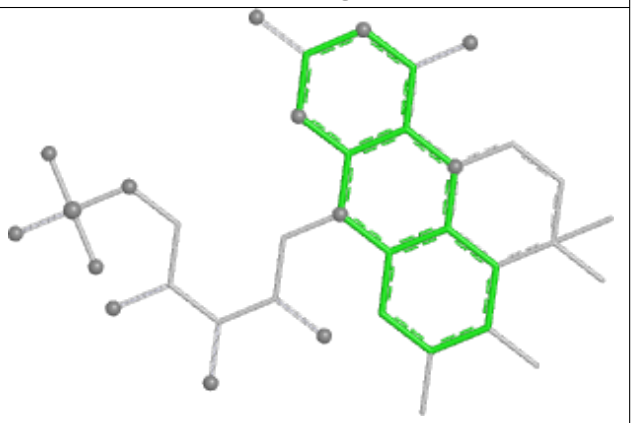
Bond lengths



Bond angles

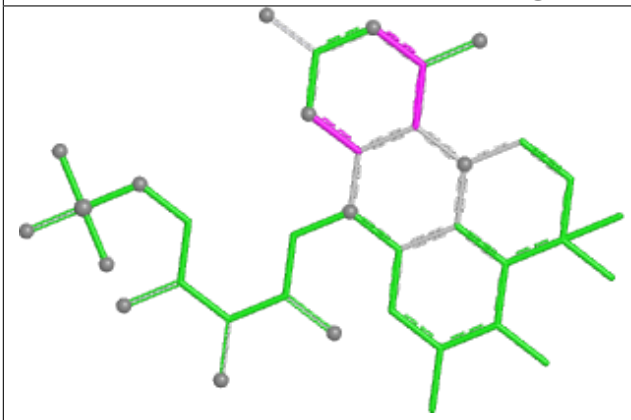


Torsions

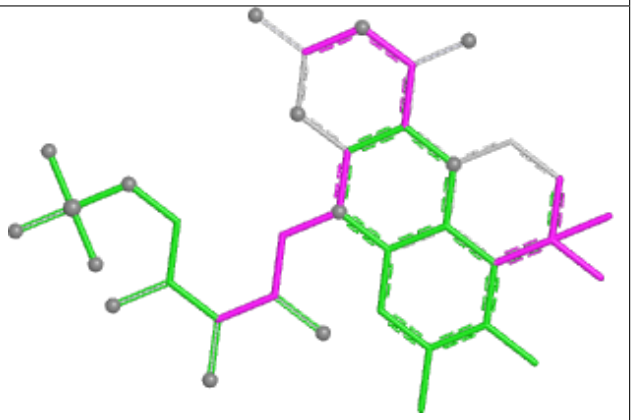


Rings

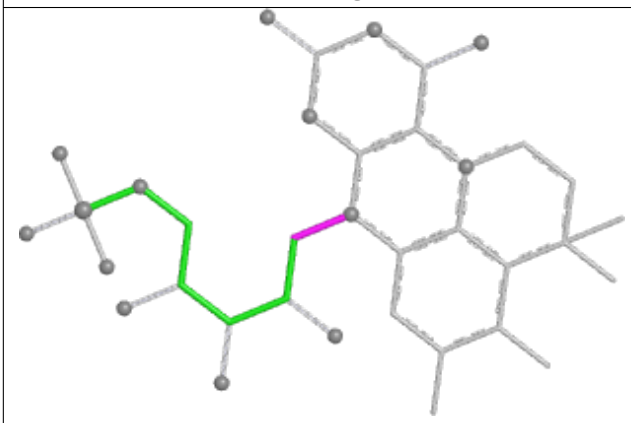
Ligand 4LU E 503



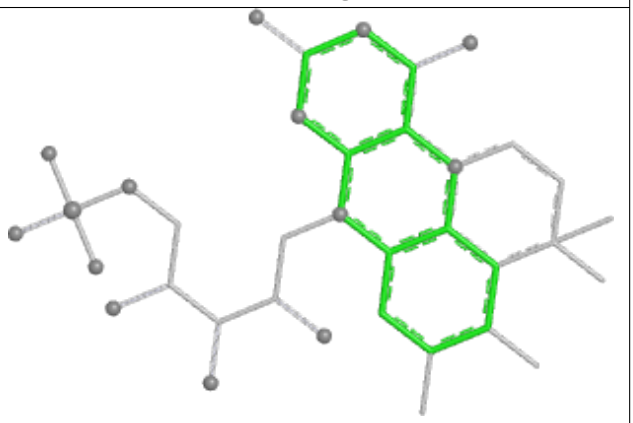
Bond lengths



Bond angles

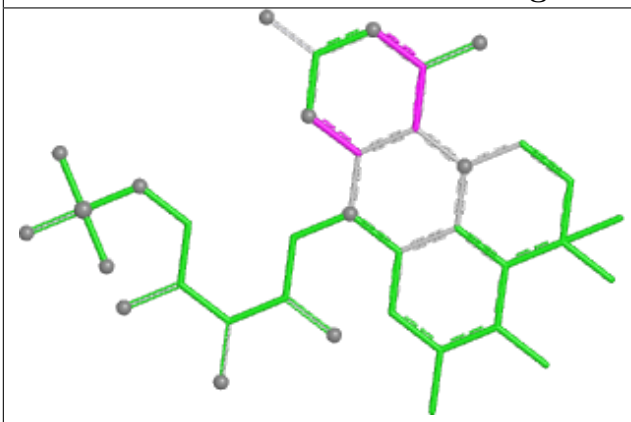


Torsions

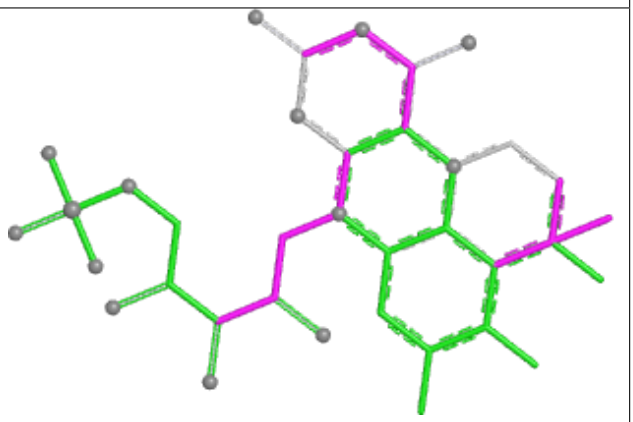


Rings

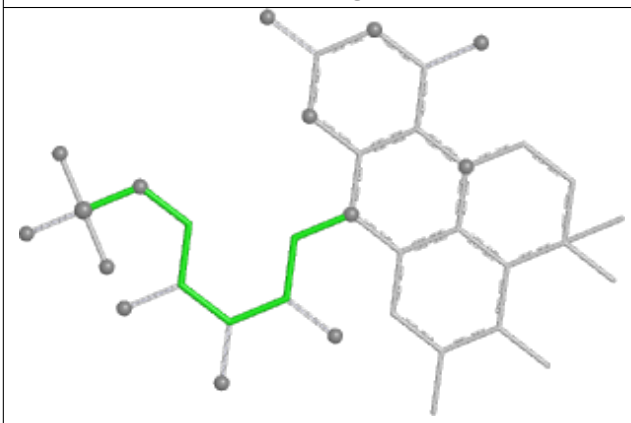
Ligand 4LU F 503



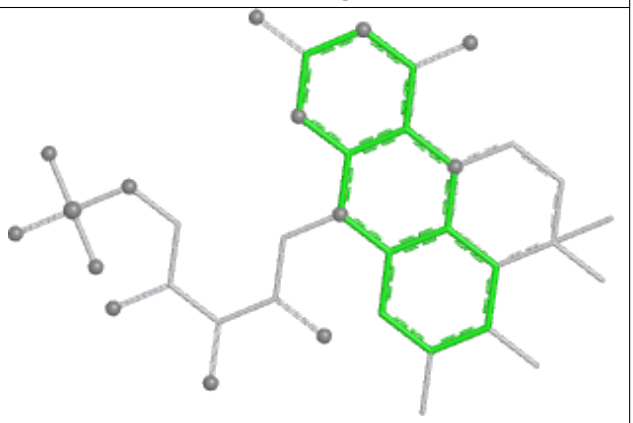
Bond lengths



Bond angles

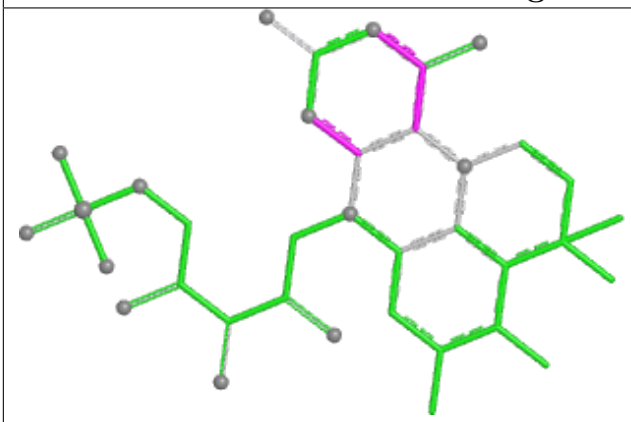


Torsions

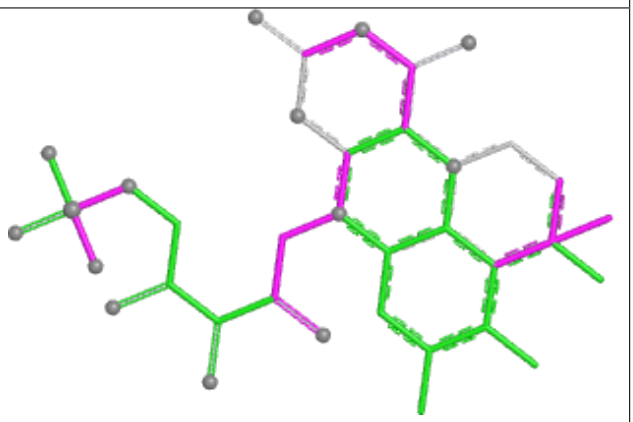


Rings

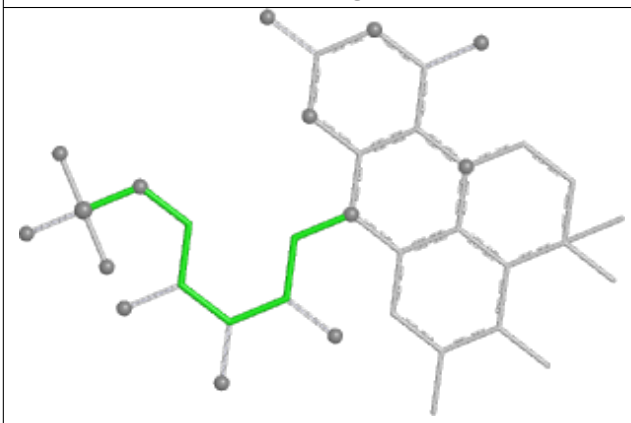
Ligand 4LU A 503



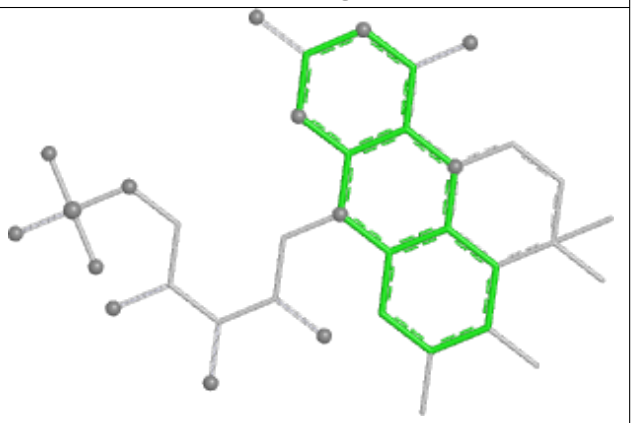
Bond lengths



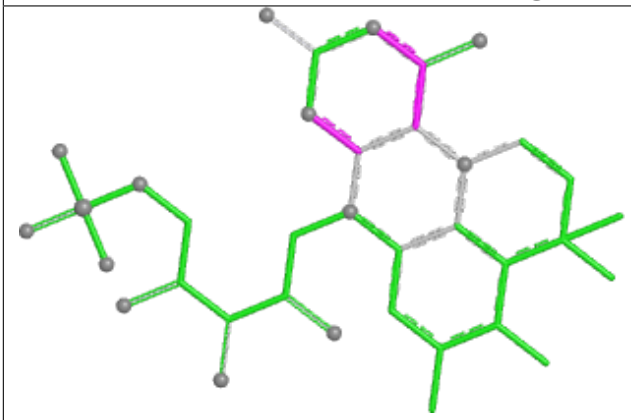
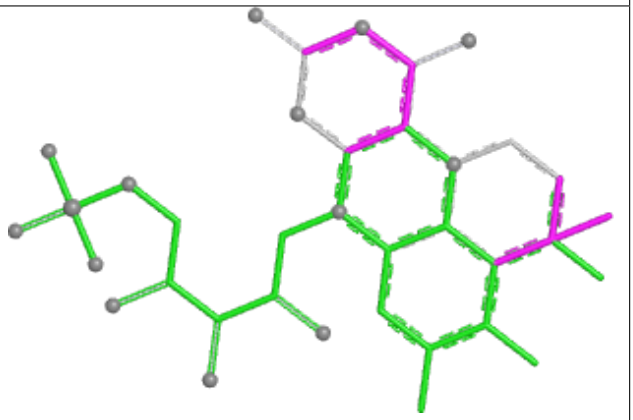
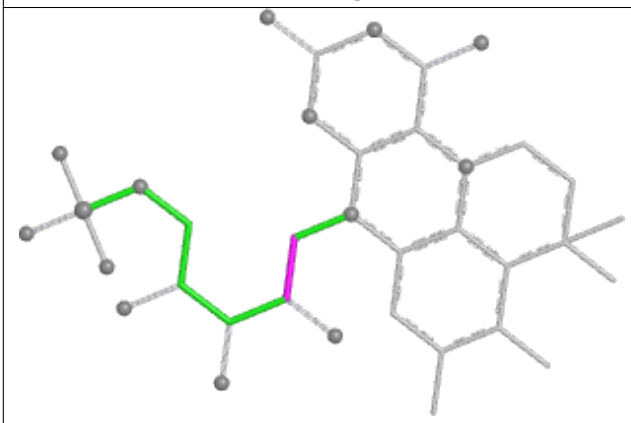
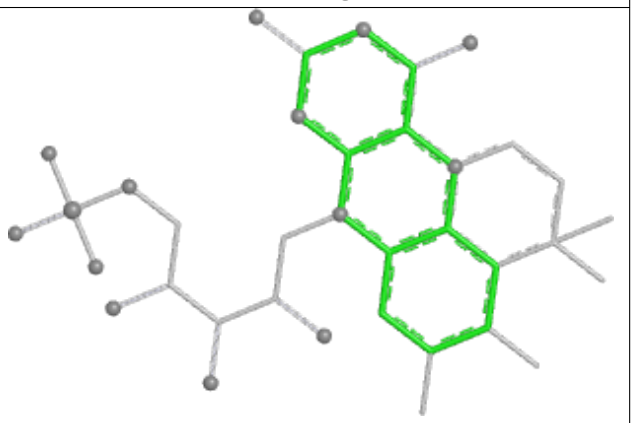
Bond angles



Torsions



Rings

Ligand 4LU C 503	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	454/461 (98%)	-0.19	0 100 100	47, 74, 107, 123	0
1	B	452/461 (98%)	-0.17	0 100 100	47, 76, 111, 131	0
1	C	452/461 (98%)	-0.12	5 (1%) 80 83	55, 93, 131, 149	0
1	D	452/461 (98%)	-0.10	3 (0%) 87 89	54, 92, 130, 142	0
1	E	452/461 (98%)	-0.05	8 (1%) 68 71	50, 100, 144, 164	0
1	F	452/461 (98%)	0.13	18 (3%) 38 42	52, 107, 158, 192	0
All	All	2714/2766 (98%)	-0.08	34 (1%) 77 79	47, 88, 140, 192	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	158	VAL	6.9
1	F	242	LEU	5.0
1	F	170	ALA	4.1
1	C	252	GLN	3.4
1	E	105	HIS	3.3
1	F	104	GLU	2.9
1	F	166	VAL	2.9
1	D	254	TYR	2.8
1	F	121	PRO	2.8
1	F	164	LEU	2.7
1	C	289	ARG	2.6
1	F	254	TYR	2.6
1	F	131	GLY	2.5
1	C	253	MET	2.5
1	F	280	VAL	2.5
1	F	165	HIS	2.5
1	D	83	PHE	2.4
1	E	280	VAL	2.4
1	F	23	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	224	PHE	2.3
1	E	188	LEU	2.3
1	C	283	THR	2.3
1	F	224	PHE	2.2
1	E	210	VAL	2.2
1	F	282	VAL	2.2
1	E	232	VAL	2.2
1	E	165	HIS	2.2
1	E	158	VAL	2.1
1	F	55	ASP	2.1
1	E	170	ALA	2.1
1	C	254	TYR	2.1
1	F	156	PHE	2.1
1	F	174	LEU	2.1
1	F	117	LEU	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
2	NA	D	501	1/1	0.87	0.05	78,78,78,78	0
2	NA	F	501	1/1	0.93	0.06	103,103,103,103	0
3	MN	D	502	1/1	0.93	0.12	137,137,137,137	0
3	MN	F	502	1/1	0.93	0.12	140,140,140,140	0
2	NA	C	501	1/1	0.95	0.09	81,81,81,81	0
4	4LU	B	503	36/36	0.95	0.12	69,91,103,105	0
4	4LU	D	503	36/36	0.95	0.15	92,116,134,140	0
4	4LU	F	503	36/36	0.95	0.17	101,122,140,148	0

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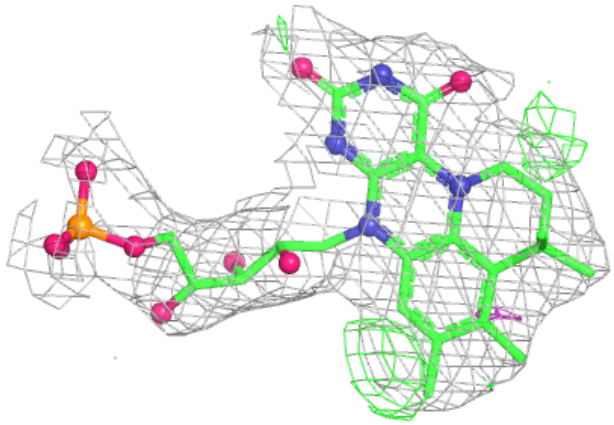
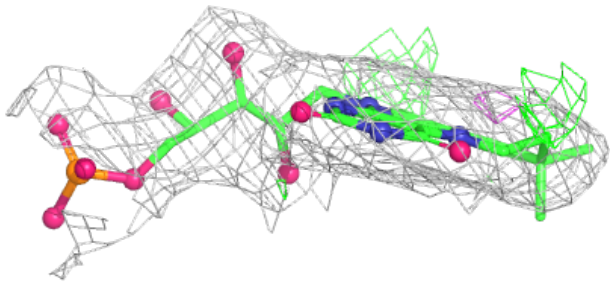
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	E	501	1/1	0.96	0.05	84,84,84,84	0
4	4LU	E	503	36/36	0.96	0.16	102,117,138,142	0
4	4LU	C	503	36/36	0.96	0.15	87,118,136,142	0
4	4LU	A	503	36/36	0.97	0.12	71,88,100,106	0
3	MN	C	502	1/1	0.97	0.10	136,136,136,136	0
2	NA	A	501	1/1	0.99	0.09	51,51,51,51	0
2	NA	B	501	1/1	0.99	0.07	52,52,52,52	0
3	MN	E	502	1/1	0.99	0.12	135,135,135,135	0
3	MN	A	502	1/1	0.99	0.11	93,93,93,93	0
3	MN	B	502	1/1	0.99	0.13	92,92,92,92	0

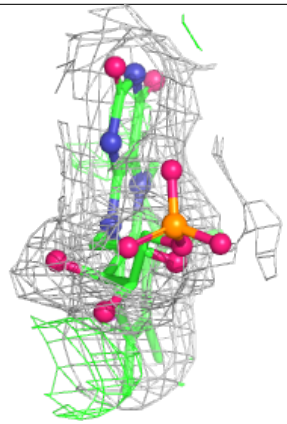
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4LU B 503:

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

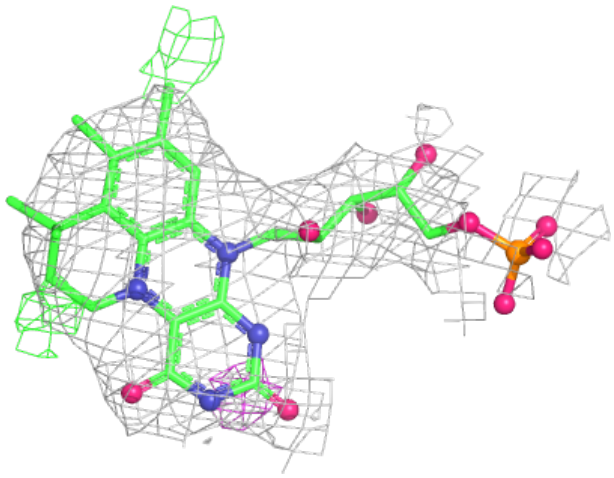


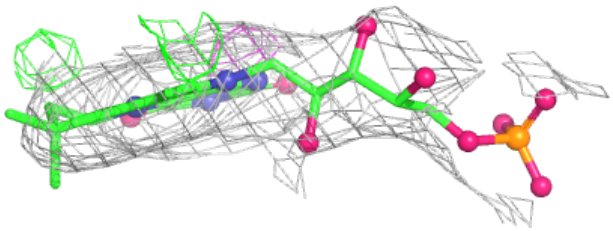


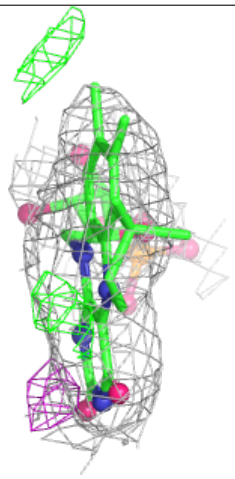


Electron density around 4LU D 503:

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

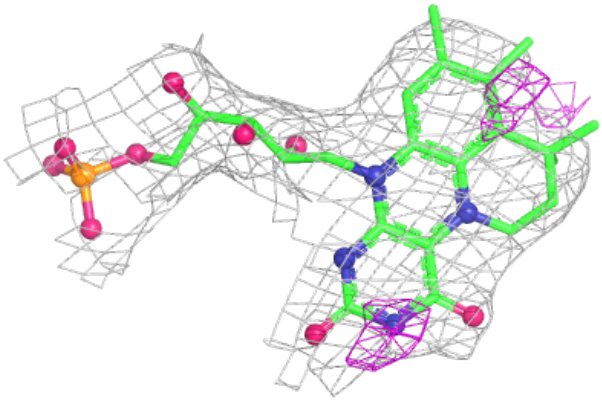


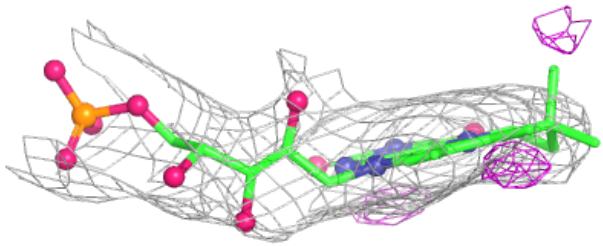


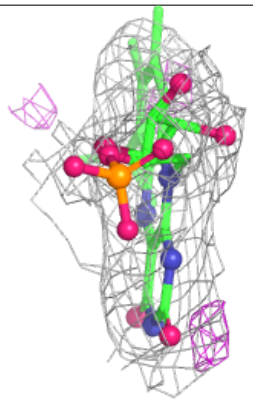


Electron density around 4LU F 503:

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

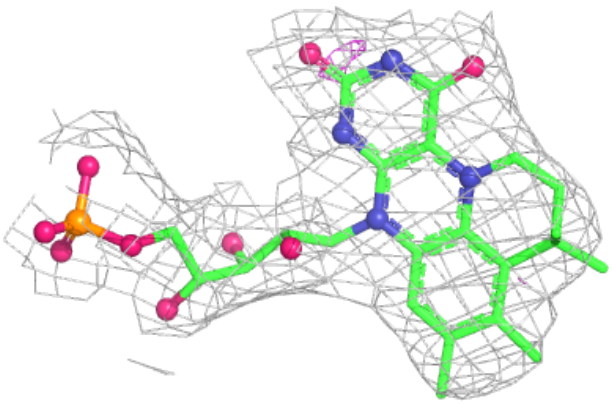


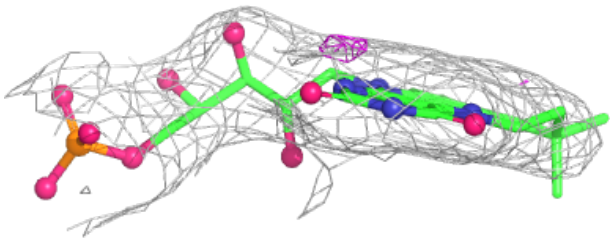


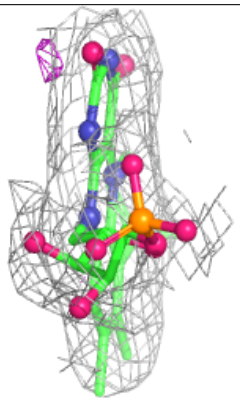


Electron density around 4LU E 503:

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

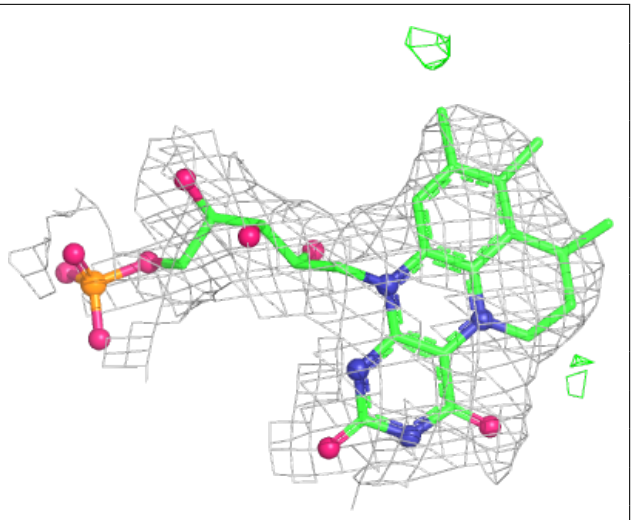


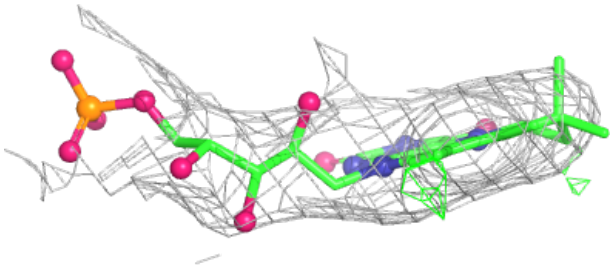


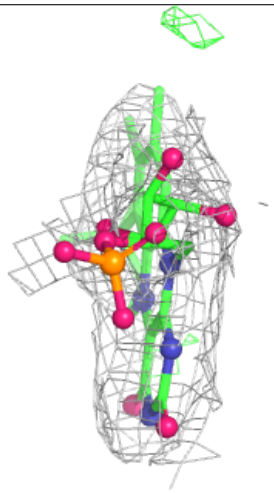


Electron density around 4LU C 503:

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

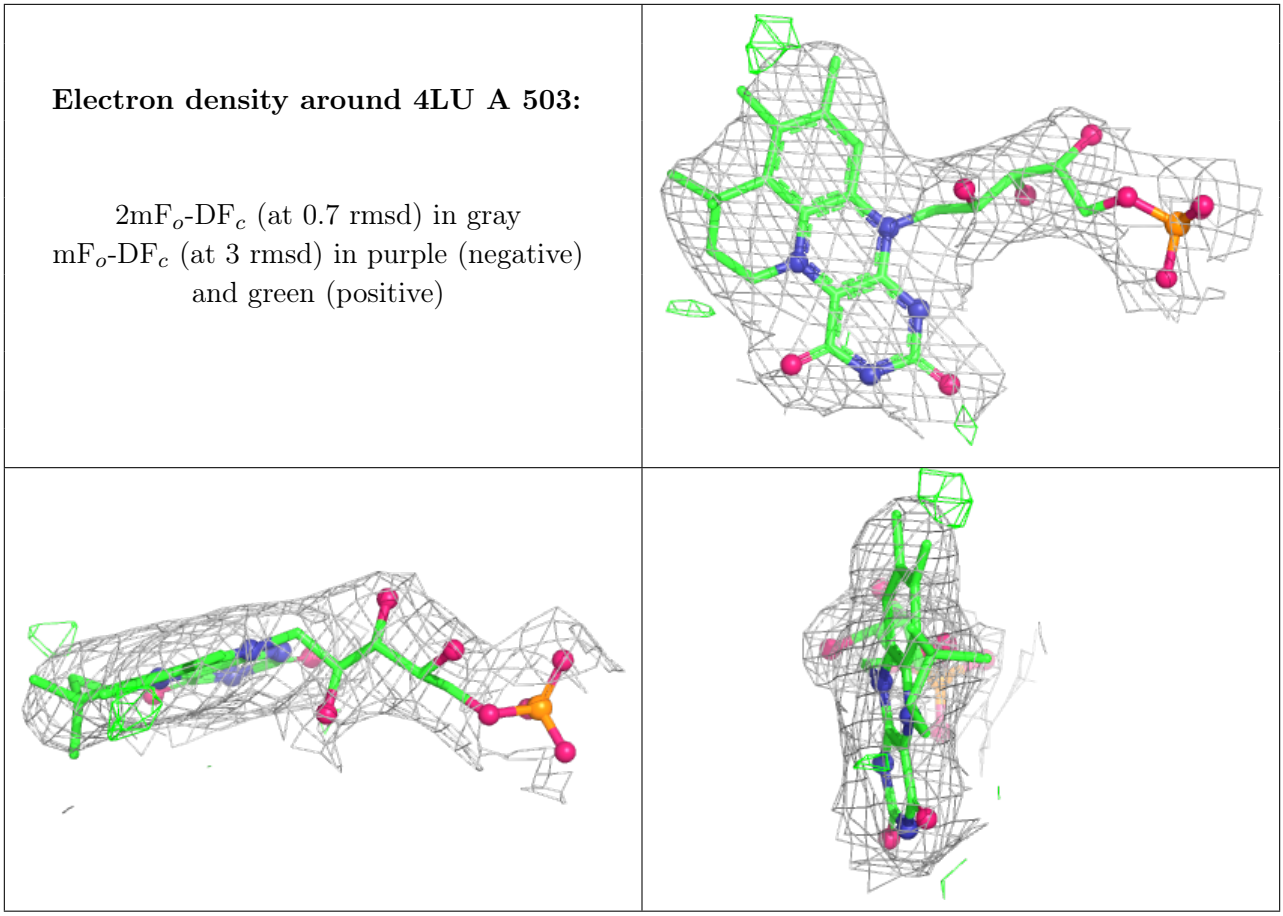






Electron density around 4LU A 503:

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



6.5 Other polymers

There are no such residues in this entry.