Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2024 – 08:13 PM EDT

PDB ID	:	8VYX
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with k-410
Authors	:	Min, C.K.; Nwachukwu, J.C.; Hou, Y.; Russo, R.J.; Papa, A.; Min, J.; Peng, R.; Kim, S.H.; Ziegler, Y.; Rangarajan, E.S.; Izard, T.; Katzenellenbogen, B.S.; Katzenellenbogen, J.A.; Nettles, K.W.
Deposited on	:	2024-02-09
Resolution	:	1.69 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 (1)) were used in the production of this report:

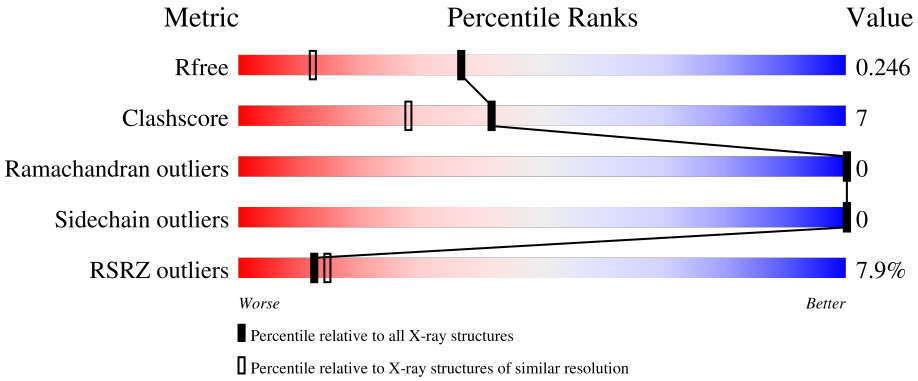
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.69 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	242	6% 81% 14% ·
1	B	242	7% 76% 14% · 9%
1	C	242	8% 82% 13% · ·
1	D	242	9% 83% 8% · 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15146 atoms, of which 7300 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.

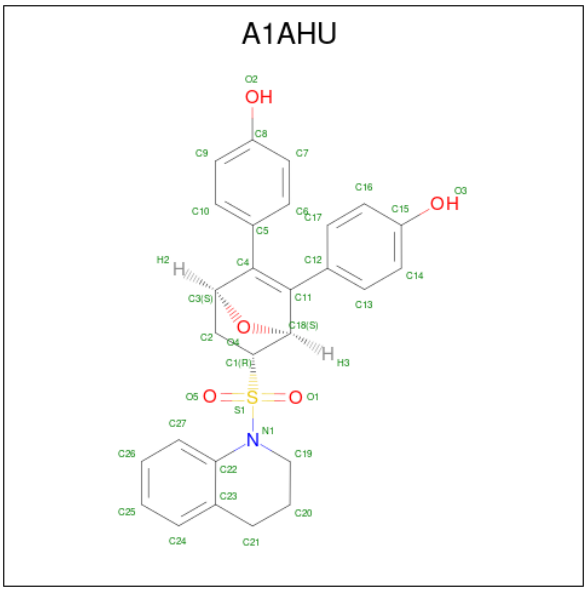
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	233	Total	C	H	N	O	S	0	1	0
			3661	1170	1834	311	330	16			
1	B	221	Total	C	H	N	O	S	0	0	0
			3451	1108	1724	295	307	17			
1	C	234	Total	C	H	N	O	S	1	1	0
			3601	1157	1792	309	327	16			
1	D	228	Total	C	H	N	O	S	0	0	0
			3656	1160	1850	304	324	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	372	SER	LEU	engineered mutation	UNP P03372
A	536	SER	LEU	engineered mutation	UNP P03372
B	372	SER	LEU	engineered mutation	UNP P03372
B	536	SER	LEU	engineered mutation	UNP P03372
C	372	SER	LEU	engineered mutation	UNP P03372
C	536	SER	LEU	engineered mutation	UNP P03372
D	372	SER	LEU	engineered mutation	UNP P03372
D	536	SER	LEU	engineered mutation	UNP P03372

- Molecule 2 is 4,4'-[(1S,4S,5R)-5-(3,4-dihydroquinoline-1(2H)-sulfonyl)-7-oxabicyclo[2.2.1]hept-2-ene-2,3-diyl]diphenol (three-letter code: A1AHU) (formula: $C_{27}H_{25}NO_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			59	27	25	1	5	1		
2	B	1	Total	C	H	N	O	S	0	0
			59	27	25	1	5	1		
2	C	1	Total	C	H	N	O	S	0	0
			59	27	25	1	5	1		
2	D	1	Total	C	H	N	O	S	0	0
			59	27	25	1	5	1		

- Molecule 3 is water.

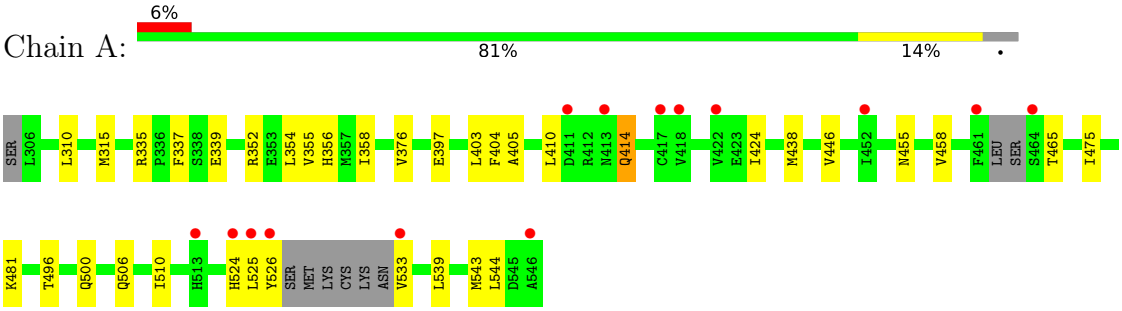
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	153	Total	O	0	0
			153	153		
3	B	117	Total	O	0	0
			117	117		
3	C	144	Total	O	0	0
			144	144		
3	D	127	Total	O	0	0
			127	127		

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.

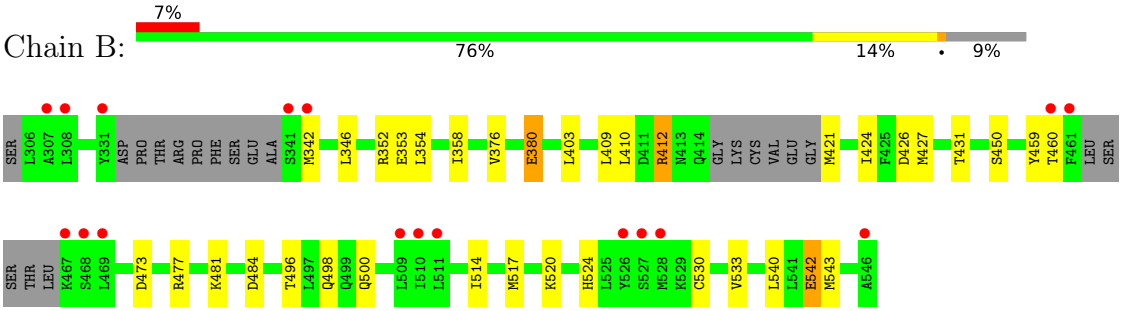
• Molecule 1: Estrogen receptor

Chain A:



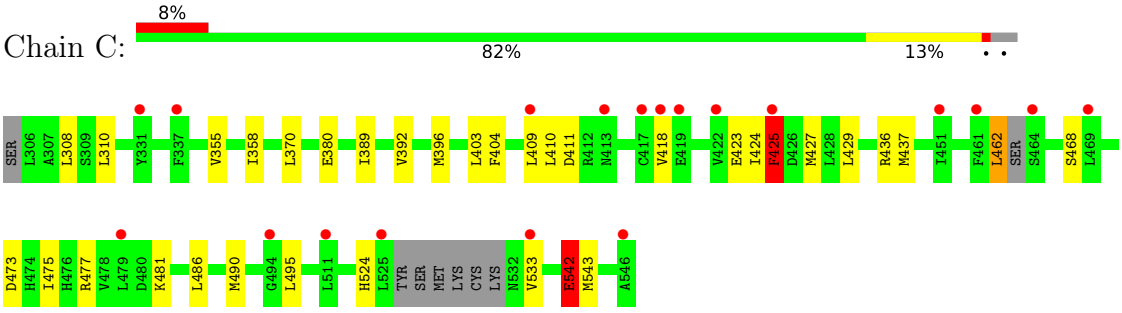
• Molecule 1: Estrogen receptor

Chain B:



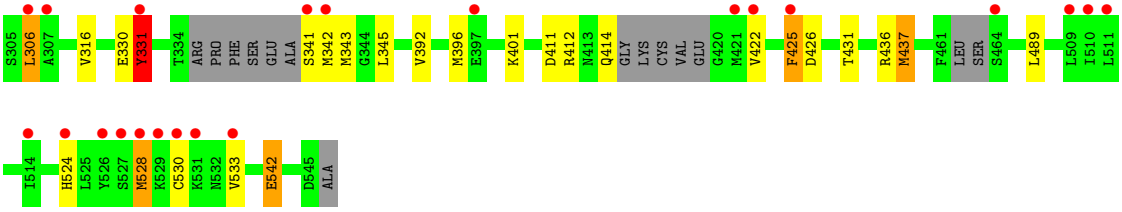
• Molecule 1: Estrogen receptor

Chain C:



• Molecule 1: Estrogen receptor

Chain D:


S305
L306
A307
V316
E330
V331
T334
ARG
PRO
PHE
SER
GLU
ALA
S341
M342
M343
G344
L345
V392
M396
E397
K401
D411
R412
N413
Q414
GLY
LYS
CYS
VAL
GLU
G420
M421
V422
F425
D426
T431
R436
M437
F461
LEU
SER
S464
L489
L509
I510
L511
I514
H524
L525
Y526
S527
M528
K529
C530
K531
N532
V533
E542
D545
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.81Å 58.87Å 94.13Å 86.75° 74.98° 62.91°	Depositor
Resolution (Å)	33.10 – 1.69 38.56 – 1.69	Depositor EDS
% Data completeness (in resolution range)	68.3 (33.10-1.69) 68.3 (38.56-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.209 , 0.246 0.208 , 0.246	Depositor DCC
R_{free} test set	3719 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	17.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.107 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15146	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.40% 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: A1AHU

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	0.74	2/1872 (0.1%)	0.74	1/2536 (0.0%)
1	B	0.79	4/1756 (0.2%)	1.37	9/2376 (0.4%)
1	C	0.97	6/1853 (0.3%)	1.38	9/2515 (0.4%)
1	D	1.02	6/1836 (0.3%)	2.38	22/2478 (0.9%)
All	All	0.89	18/7317 (0.2%)	1.58	41/9905 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	3
1	D	0	3
All	All	0	7

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	542	GLU	CB-CG	15.07	1.80	1.52
1	D	331	TYR	CG-CD2	15.06	1.58	1.39
1	D	331	TYR	CE1-CZ	-14.63	1.19	1.38
1	C	542	GLU	CD-OE1	13.11	1.40	1.25
1	C	542	GLU	CD-OE2	-10.50	1.14	1.25
1	D	330	GLU	CD-OE1	-8.70	1.16	1.25
1	D	331	TYR	CD1-CE1	-8.36	1.26	1.39
1	D	425	PHE	CB-CG	-8.27	1.37	1.51
1	C	425	PHE	CE1-CZ	-7.73	1.22	1.37
1	B	352	ARG	CZ-NH2	-7.58	1.23	1.33
1	B	542	GLU	CD-OE2	-6.34	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	380	GLU	CD-OE2	6.21	1.32	1.25
1	B	450	SER	CB-OG	5.94	1.50	1.42
1	C	425	PHE	CB-CG	-5.74	1.41	1.51
1	A	414	GLN	CB-CG	-5.64	1.37	1.52
1	C	380	GLU	CB-CG	-5.61	1.41	1.52
1	A	446	VAL	CB-CG1	5.24	1.63	1.52
1	D	425	PHE	CE2-CZ	-5.13	1.27	1.37

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	331	TYR	CB-CG-CD2	-68.50	79.90	121.00
1	D	331	TYR	CB-CG-CD1	54.77	153.86	121.00
1	B	380	GLU	OE1-CD-OE2	-47.83	65.91	123.30
1	D	425	PHE	CB-CG-CD2	-45.05	89.27	120.80
1	C	425	PHE	CB-CG-CD2	-42.18	91.27	120.80
1	C	425	PHE	CB-CG-CD1	32.82	143.77	120.80
1	D	331	TYR	CD1-CG-CD2	-31.30	83.47	117.90
1	D	425	PHE	CB-CG-CD1	25.02	138.31	120.80
1	B	380	GLU	CG-CD-OE1	16.29	150.88	118.30
1	B	380	GLU	CG-CD-OE2	-16.01	86.28	118.30
1	C	425	PHE	CD1-CG-CD2	-13.41	100.87	118.30
1	D	342	MET	CB-CG-SD	-12.41	75.16	112.40
1	D	437	MET	CB-CA-C	-10.71	88.99	110.40
1	D	528	MET	CG-SD-CE	10.46	116.94	100.20
1	D	425	PHE	CD1-CG-CD2	-10.26	104.96	118.30
1	D	306	LEU	CB-CG-CD2	-10.11	93.81	111.00
1	C	462	LEU	CB-CG-CD2	-9.70	94.52	111.00
1	C	542	GLU	CA-CB-CG	-8.83	93.97	113.40
1	D	331	TYR	N-CA-C	-8.39	88.34	111.00
1	D	331	TYR	CG-CD2-CE2	8.32	127.96	121.30
1	D	331	TYR	CE1-CZ-CE2	-7.21	108.26	119.80
1	B	542	GLU	CG-CD-OE1	7.13	132.56	118.30
1	C	542	GLU	CG-CD-OE2	-7.07	104.16	118.30
1	B	412	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	D	401	LYS	CD-CE-NZ	6.37	126.35	111.70
1	D	542	GLU	CA-CB-CG	6.27	127.20	113.40
1	D	425	PHE	CG-CD2-CE2	6.21	127.63	120.80
1	D	330	GLU	CA-CB-CG	6.10	126.83	113.40
1	D	437	MET	CA-CB-CG	-6.09	102.95	113.30
1	D	437	MET	CB-CG-SD	-6.02	94.35	112.40
1	C	542	GLU	N-CA-CB	-5.95	99.90	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	306	LEU	CB-CG-CD1	5.82	120.90	111.00
1	C	542	GLU	CB-CG-CD	5.79	129.83	114.20
1	B	542	GLU	OE1-CD-OE2	-5.77	116.37	123.30
1	A	465	THR	OG1-CB-CG2	5.58	122.84	110.00
1	B	484	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	B	410	LEU	CB-CG-CD2	-5.54	101.59	111.00
1	B	380	GLU	N-CA-C	-5.50	96.15	111.00
1	D	425	PHE	CB-CA-C	5.47	121.34	110.40
1	C	437	MET	CG-SD-CE	5.20	108.52	100.20
1	D	331	TYR	CG-CD1-CE1	5.14	125.41	121.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414	GLN	Sidechain
1	C	418	VAL	Peptide
1	C	425	PHE	Sidechain
1	C	542	GLU	Sidechain
1	D	331	TYR	Sidechain
1	D	425	PHE	Sidechain
1	D	542	GLU	Sidechain

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	1827	1834	1824	31	0
1	B	1727	1724	1734	33	2
1	C	1809	1792	1783	28	0
1	D	1806	1850	1851	13	0
2	A	34	25	0	3	0
2	B	34	25	0	1	0
2	C	34	25	0	2	0
2	D	34	25	0	1	0
3	A	153	0	0	3	2
3	B	117	0	0	2	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	144	0	0	0	0
3	D	127	0	0	1	0
All	All	7846	7300	7192	102	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (102) 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:C:542:GLU:CG	1:C:542:GLU:CB	1.80	1.59
1:C:370:LEU:HD11	1:C:475:ILE:HD11	1.36	1.05
1:C:542:GLU:CG	1:C:542:GLU:CA	2.51	0.88
1:B:424:ILE:HD11	1:B:520:LYS:HG2	1.55	0.87
1:B:542:GLU:OE1	3:B:701:HOH:O	1.95	0.84
1:A:339:GLU:OE2	3:A:701:HOH:O	1.95	0.83
1:C:462:LEU:O	1:C:468:SER:HB2	1.80	0.81
1:A:352:ARG:O	1:A:355:VAL:HG12	1.85	0.76
1:D:411:ASP:OD1	1:D:414:GLN:NE2	2.22	0.73
1:A:354:LEU:O	1:A:358:ILE:HD12	1.91	0.69
1:B:358:ILE:HD13	1:B:543:MET:HE1	1.75	0.68
1:D:524:HIS:CE1	1:D:528:MET:SD	2.87	0.67
1:B:424:ILE:CD1	1:B:520:LYS:HG2	2.25	0.67
1:A:355:VAL:HG11	3:A:782:HOH:O	1.95	0.66
1:D:306:LEU:H	1:D:306:LEU:HD23	1.60	0.66
1:D:412:ARG:NH2	1:D:426:ASP:OD2	2.31	0.63
1:B:354:LEU:O	1:B:358:ILE:HD12	2.01	0.61
1:B:358:ILE:HD13	1:B:543:MET:CE	2.31	0.61
1:C:462:LEU:C	1:C:468:SER:HB2	2.21	0.60
1:B:431:THR:HG21	1:B:514:ILE:HD11	1.84	0.59
1:C:490:MET:HB3	1:C:495:LEU:HD12	1.86	0.57
1:B:354:LEU:HG	1:B:543:MET:HE1	1.86	0.57
1:B:412:ARG:HD2	1:B:426:ASP:OD1	2.06	0.56
1:A:404:PHE:CE1	1:A:410:LEU:HD12	2.40	0.56
1:C:389:ILE:HA	1:C:392:VAL:HG22	1.88	0.55
1:C:424:ILE:HB	2:C:600:A1AHU:C19	2.37	0.55
1:B:530:CYS:O	1:B:533:VAL:HG22	2.08	0.54
1:C:404:PHE:CE1	1:C:410:LEU:HD12	2.44	0.53
1:A:510:ILE:HD13	1:B:459:TYR:OH	2.09	0.53
1:C:486:LEU:O	1:C:490:MET:HG3	2.09	0.53
1:A:533:VAL:HG13	2:A:600:A1AHU:O3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:ARG:NH1	1:D:422:VAL:HG21	2.24	0.52
1:D:530:CYS:O	1:D:533:VAL:HG22	2.10	0.52
1:A:510:ILE:HD13	1:B:459:TYR:CZ	2.45	0.52
1:B:514:ILE:HD13	1:B:517:MET:CE	2.40	0.52
1:B:424:ILE:CG1	1:B:520:LYS:HG2	2.40	0.51
1:C:425:PHE:HE1	1:C:429:LEU:HD11	1.75	0.51
1:C:355:VAL:HG22	1:C:543:MET:CE	2.41	0.51
1:C:358:ILE:HD13	1:C:543:MET:CB	2.40	0.51
1:D:316:VAL:HG21	1:D:489:LEU:HD21	1.93	0.49
1:C:308:LEU:HD22	1:C:308:LEU:N	2.26	0.49
1:C:473:ASP:O	1:C:477:ARG:HG3	2.13	0.49
1:A:355:VAL:HA	1:A:543:MET:CE	2.43	0.48
1:D:331:TYR:O	1:D:331:TYR:CG	2.58	0.48
1:C:524:HIS:N	1:C:524:HIS:ND1	2.59	0.47
1:B:342:MET:O	1:B:346:LEU:HG	2.14	0.47
1:A:404:PHE:CD1	1:A:410:LEU:HD12	2.50	0.47
1:A:403:LEU:HD12	1:A:405:ALA:O	2.14	0.47
1:A:376:VAL:HG22	1:A:544:LEU:HD12	1.96	0.47
1:A:397:GLU:HG2	3:A:778:HOH:O	2.15	0.47
1:B:403:LEU:HA	1:B:409:LEU:HD12	1.97	0.47
1:B:353:GLU:OE1	2:B:600:A1AHU:O2	2.33	0.46
1:B:477:ARG:HH11	1:B:477:ARG:HG2	1.79	0.46
1:B:496:THR:O	1:B:500:GLN:HG3	2.15	0.46
1:A:524:HIS:O	1:A:526:TYR:CE2	2.69	0.46
1:C:358:ILE:HD13	1:C:543:MET:HB2	1.96	0.46
1:B:403:LEU:HA	1:B:409:LEU:CD1	2.46	0.46
1:A:525:LEU:O	1:A:526:TYR:HB2	2.16	0.46
1:B:514:ILE:HD13	1:B:517:MET:HE2	1.97	0.46
1:D:396:MET:O	1:D:436:ARG:NE	2.43	0.45
1:A:438:MET:HE1	1:A:506:GLN:HB2	1.98	0.45
1:C:358:ILE:HD12	1:C:543:MET:SD	2.56	0.45
1:C:423:GLU:O	1:C:427:MET:HG3	2.16	0.45
1:A:510:ILE:CD1	1:B:459:TYR:CE1	3.00	0.45
1:B:460:THR:HG23	3:B:713:HOH:O	2.16	0.45
1:A:424:ILE:HG21	2:A:600:A1AHU:O5	2.17	0.44
1:C:310:LEU:O	1:C:481:LYS:HE3	2.17	0.44
1:A:355:VAL:HG13	1:A:356:HIS:N	2.32	0.44
1:C:396:MET:O	1:C:436:ARG:HD3	2.17	0.44
1:C:403:LEU:HD13	1:C:409:LEU:HD13	1.99	0.44
1:A:496:THR:O	1:A:500:GLN:HG3	2.17	0.44
1:A:539:LEU:O	1:A:543:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:VAL:HA	1:A:543:MET:HE2	1.99	0.43
1:A:525:LEU:HD22	1:A:533:VAL:HG11	2.01	0.43
1:D:343:MET:HE2	2:D:600:A1AHU:C26	2.48	0.43
1:D:341:SER:O	1:D:345:LEU:HG	2.19	0.43
1:B:473:ASP:O	1:B:477:ARG:HG2	2.19	0.42
1:D:392:VAL:HG11	1:D:431:THR:HG22	2.01	0.42
1:C:411:ASP:OD1	1:C:411:ASP:C	2.58	0.42
1:B:421:MET:HE3	1:B:524:HIS:NE2	2.34	0.42
1:A:315:MET:HE2	1:A:481:LYS:HG3	2.01	0.42
2:A:600:A1AHU:O1	2:A:600:A1AHU:C27	2.67	0.42
1:A:455:ASN:O	1:A:458:VAL:HG12	2.19	0.42
1:B:376:VAL:O	1:B:380:GLU:HB2	2.20	0.42
1:B:477:ARG:HG2	1:B:477:ARG:NH1	2.35	0.42
1:A:510:ILE:CD1	1:B:459:TYR:CZ	3.03	0.42
1:B:380:GLU:HA	1:B:540:LEU:CD1	2.50	0.42
1:C:355:VAL:HG22	1:C:543:MET:HE2	2.01	0.42
1:B:403:LEU:O	1:B:403:LEU:HD23	2.21	0.41
1:A:335:ARG:CD	1:A:337:PHE:CZ	3.04	0.41
1:B:427:MET:CE	1:B:520:LYS:HD2	2.51	0.41
1:A:358:ILE:HG23	1:A:544:LEU:HD23	2.02	0.41
1:B:427:MET:HE2	1:B:520:LYS:HD2	2.02	0.41
1:B:481:LYS:HA	1:B:481:LYS:HD2	1.93	0.40
1:C:533:VAL:CG1	2:C:600:A1AHU:O3	2.70	0.40
1:C:542:GLU:CG	1:C:542:GLU:HA	2.44	0.40
1:D:437:MET:CE	3:D:818:HOH:O	2.69	0.40
1:A:525:LEU:O	1:A:526:TYR:CB	2.69	0.40
1:A:310:LEU:O	1:A:481:LYS:HE3	2.22	0.40
1:C:358:ILE:HD13	1:C:543:MET:HB3	2.04	0.40
1:C:462:LEU:HA	1:C:462:LEU:HD23	1.66	0.40
1:A:458:VAL:CG2	1:A:475:ILE:HG21	2.51	0.40

All (5) 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)
3:A:843:HOH:O	3:B:809:HOH:O[1_655]	2.14	0.06
3:B:701:HOH:O	3:B:751:HOH:O[1_455]	2.14	0.06
3:A:820:HOH:O	3:B:815:HOH:O[1_565]	2.16	0.04
1:B:498:GLN:CD	1:B:542:GLU:OE2[1_655]	2.17	0.03
1:B:498:GLN:OE1	1:B:542:GLU:OE2[1_655]	2.18	0.02

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	228/242 (94%)	226 (99%)	2 (1%)	0	100	100
1	B	213/242 (88%)	211 (99%)	2 (1%)	0	100	100
1	C	229/242 (95%)	227 (99%)	2 (1%)	0	100	100
1	D	220/242 (91%)	218 (99%)	2 (1%)	0	100	100
All	All	890/968 (92%)	882 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	201/218 (92%)	201 (100%)	0	100	100
1	B	188/218 (86%)	188 (100%)	0	100	100
1	C	196/218 (90%)	196 (100%)	0	100	100
1	D	203/218 (93%)	203 (100%)	0	100	100
All	All	788/872 (90%)	788 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 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	$\#\|Z\| > 2$
2	A1AHU	C	600	-	37,39,39	2.34	8 (21%)	46,59,59	1.35	5 (10%)
2	A1AHU	D	600	-	37,39,39	1.89	4 (10%)	46,59,59	1.76	10 (21%)
2	A1AHU	B	600	-	37,39,39	2.14	10 (27%)	46,59,59	1.20	5 (10%)
2	A1AHU	A	600	-	37,39,39	2.22	7 (18%)	46,59,59	1.95	7 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1AHU	C	600	-	-	2/18/54/54	0/7/6/6
2	A1AHU	D	600	-	-	4/18/54/54	0/7/6/6
2	A1AHU	B	600	-	-	8/18/54/54	0/7/6/6
2	A1AHU	A	600	-	-	5/18/54/54	0/7/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	A1AHU	O1-S1	9.65	1.51	1.43
2	C	600	A1AHU	O1-S1	7.79	1.50	1.43
2	B	600	A1AHU	O1-S1	6.73	1.49	1.43
2	D	600	A1AHU	O1-S1	6.71	1.49	1.43
2	C	600	A1AHU	C19-N1	-5.88	1.43	1.48
2	D	600	A1AHU	S1-N1	5.72	1.78	1.67
2	C	600	A1AHU	O5-S1	5.69	1.48	1.43
2	D	600	A1AHU	C19-N1	-4.85	1.44	1.48
2	B	600	A1AHU	S1-N1	4.65	1.76	1.67
2	B	600	A1AHU	C19-N1	-4.64	1.44	1.48
2	C	600	A1AHU	S1-N1	4.25	1.76	1.67
2	A	600	A1AHU	S1-N1	4.15	1.75	1.67
2	B	600	A1AHU	O5-S1	4.10	1.47	1.43
2	B	600	A1AHU	C18-C11	4.04	1.55	1.50
2	A	600	A1AHU	O5-S1	3.89	1.46	1.43
2	A	600	A1AHU	C18-C11	3.34	1.54	1.50
2	A	600	A1AHU	C19-N1	-3.20	1.46	1.48
2	C	600	A1AHU	C6-C5	2.97	1.44	1.39
2	C	600	A1AHU	C18-C11	2.75	1.53	1.50
2	C	600	A1AHU	C7-C6	2.56	1.43	1.38
2	B	600	A1AHU	C10-C5	2.55	1.43	1.39
2	D	600	A1AHU	O2-C8	-2.52	1.31	1.37
2	B	600	A1AHU	C3-C4	2.52	1.55	1.51
2	A	600	A1AHU	C7-C6	2.21	1.42	1.38
2	A	600	A1AHU	C6-C5	2.16	1.43	1.39
2	B	600	A1AHU	C22-N1	-2.11	1.41	1.43
2	B	600	A1AHU	O4-C18	-2.09	1.40	1.43
2	C	600	A1AHU	O4-C18	-2.06	1.41	1.43
2	B	600	A1AHU	C24-C23	2.02	1.43	1.39

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	A1AHU	O5-S1-N1	7.51	116.75	107.56
2	A	600	A1AHU	C19-N1-S1	5.18	125.42	117.46
2	D	600	A1AHU	C23-C22-N1	4.44	121.81	118.31
2	D	600	A1AHU	O5-S1-O1	4.36	122.02	119.22
2	C	600	A1AHU	O5-S1-N1	4.10	112.58	107.56
2	A	600	A1AHU	C23-C22-N1	4.06	121.51	118.31
2	D	600	A1AHU	C3-C2-C1	3.89	104.05	100.61
2	A	600	A1AHU	O4-C3-C2	-3.44	97.88	104.64
2	D	600	A1AHU	C24-C23-C22	3.43	122.78	118.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	A1AHU	O4-C3-C2	-3.31	98.13	104.64
2	B	600	A1AHU	O4-C3-C2	-3.08	98.58	104.64
2	A	600	A1AHU	O1-S1-N1	3.01	111.24	107.56
2	A	600	A1AHU	C10-C5-C4	-2.92	117.13	120.91
2	C	600	A1AHU	C17-C12-C11	-2.92	117.13	120.91
2	A	600	A1AHU	C17-C12-C11	-2.87	117.19	120.91
2	C	600	A1AHU	C19-N1-S1	2.87	121.88	117.46
2	B	600	A1AHU	O1-S1-N1	2.82	111.01	107.56
2	D	600	A1AHU	C17-C12-C11	-2.73	117.38	120.91
2	D	600	A1AHU	C27-C22-C23	-2.72	115.83	119.87
2	C	600	A1AHU	C10-C5-C4	-2.66	117.47	120.91
2	C	600	A1AHU	O4-C3-C2	-2.61	99.50	104.64
2	D	600	A1AHU	C21-C23-C24	-2.57	115.59	120.98
2	B	600	A1AHU	C12-C11-C18	2.52	125.42	121.27
2	B	600	A1AHU	C9-C10-C5	-2.49	117.88	120.78
2	D	600	A1AHU	C10-C5-C4	-2.37	117.84	120.91
2	D	600	A1AHU	O4-C3-C4	-2.35	98.72	101.99
2	B	600	A1AHU	C3-C2-C1	2.26	102.61	100.61

There are no chirality outliers.

All (19) torsion outliers are listed below:

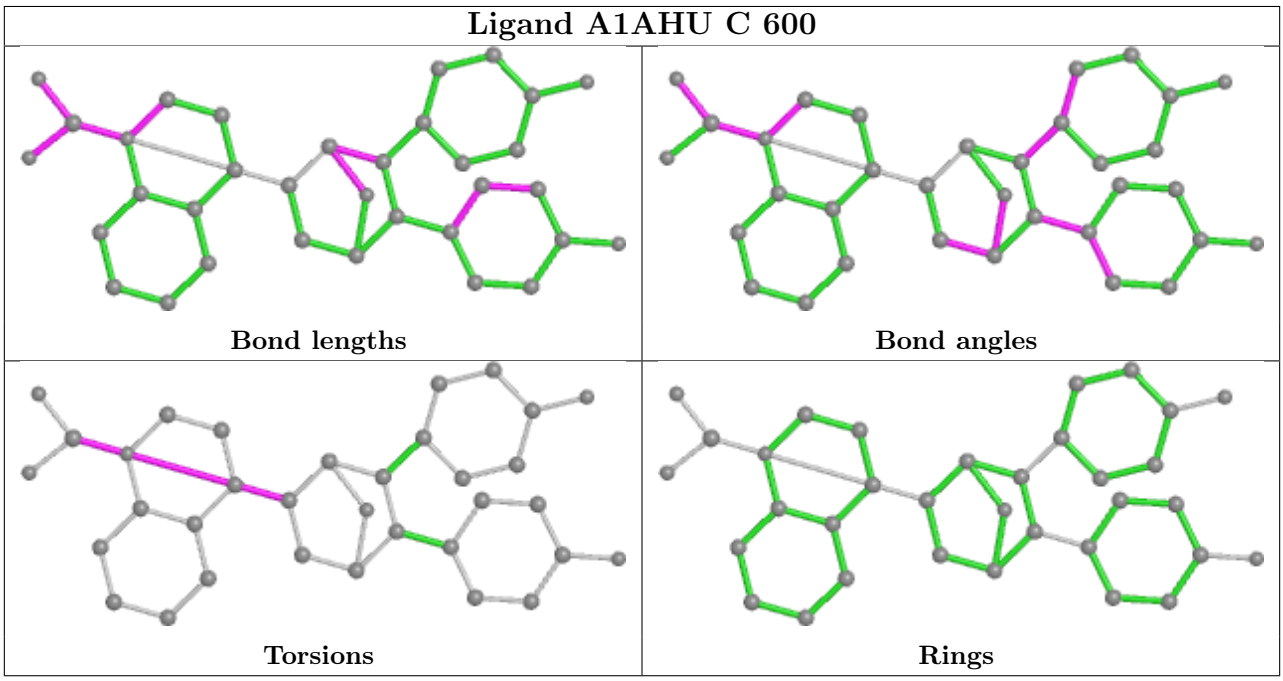
Mol	Chain	Res	Type	Atoms
2	A	600	A1AHU	C22-N1-S1-C1
2	A	600	A1AHU	C18-C1-S1-O1
2	A	600	A1AHU	C18-C1-S1-O5
2	B	600	A1AHU	C18-C1-S1-O5
2	C	600	A1AHU	C18-C1-S1-O5
2	B	600	A1AHU	C11-C4-C5-C6
2	B	600	A1AHU	C19-N1-S1-O1
2	B	600	A1AHU	C11-C4-C5-C10
2	A	600	A1AHU	C2-C1-S1-O1
2	B	600	A1AHU	C18-C1-S1-O1
2	A	600	A1AHU	C2-C1-S1-O5
2	B	600	A1AHU	C2-C1-S1-O1
2	B	600	A1AHU	C2-C1-S1-O5
2	B	600	A1AHU	C19-N1-S1-C1
2	D	600	A1AHU	C4-C11-C12-C17
2	C	600	A1AHU	C19-N1-S1-O5
2	D	600	A1AHU	C19-N1-S1-O5
2	D	600	A1AHU	C4-C11-C12-C13
2	D	600	A1AHU	C19-N1-S1-O1

There are no ring outliers.

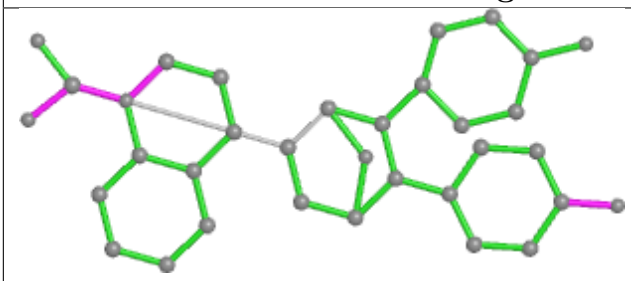
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	A1AHU	2	0
2	D	600	A1AHU	1	0
2	B	600	A1AHU	1	0
2	A	600	A1AHU	3	0

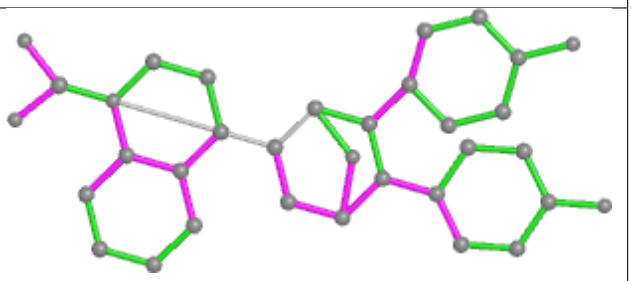
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



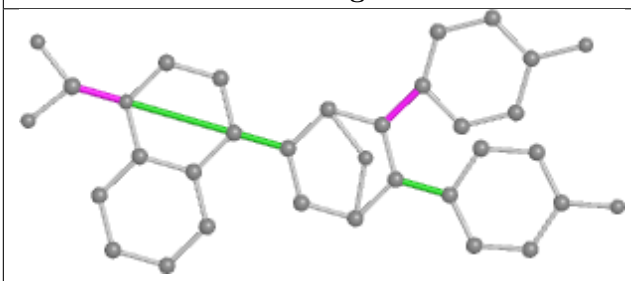
Ligand A1AHU D 600



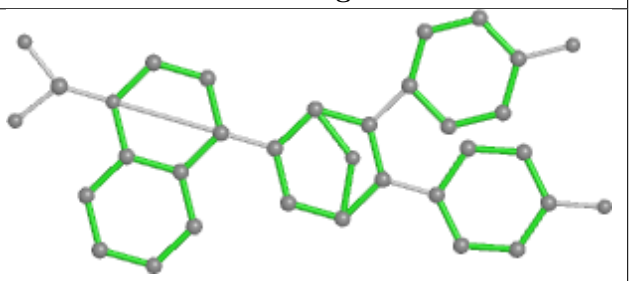
Bond lengths



Bond angles

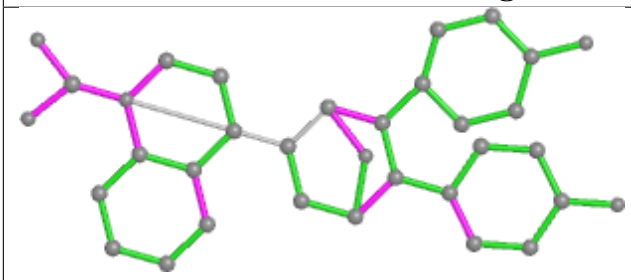


Torsions

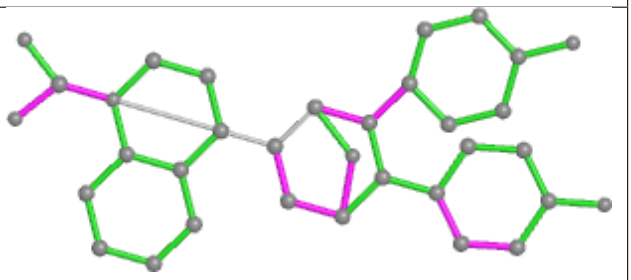


Rings

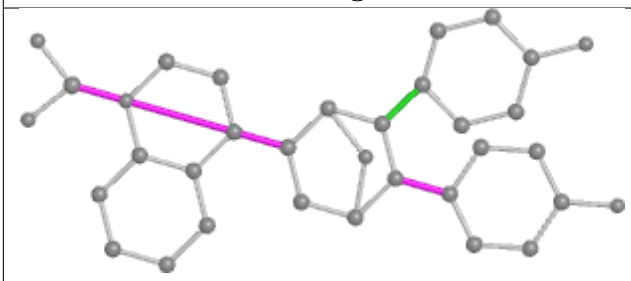
Ligand A1AHU B 600



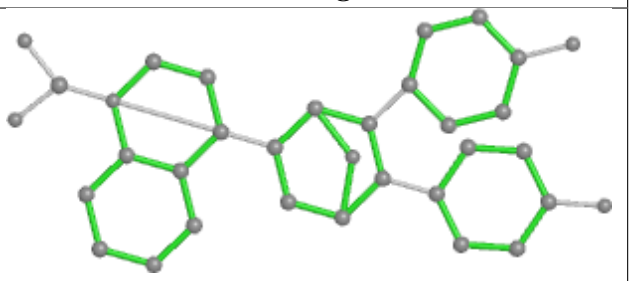
Bond lengths



Bond angles

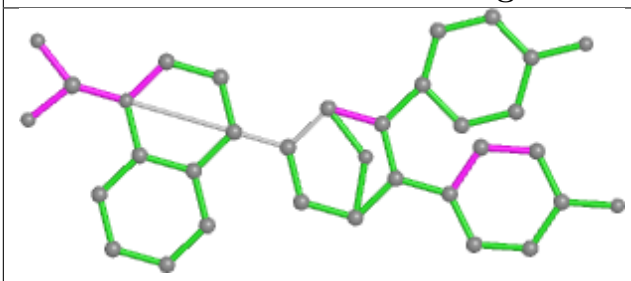


Torsions

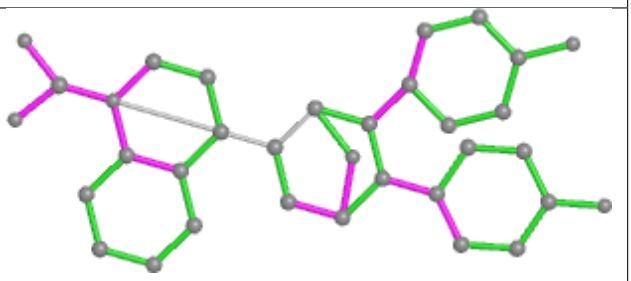


Rings

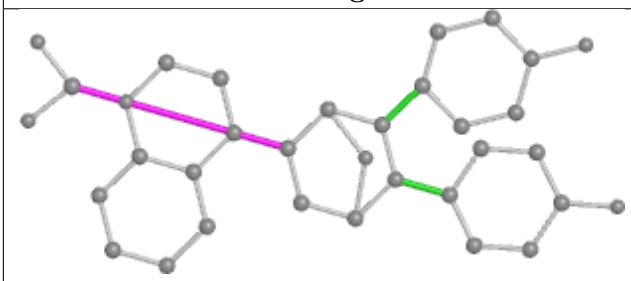
Ligand A1AHU A 600



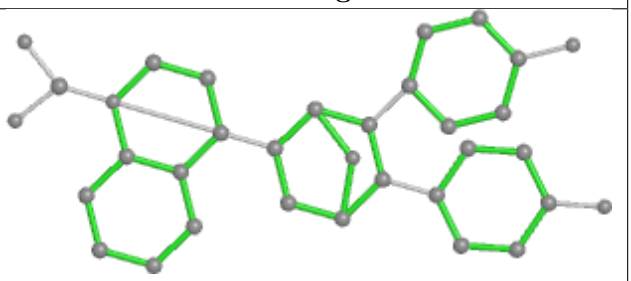
Bond lengths



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	233/242 (96%)	0.43	14 (6%)	21	24	9, 20, 45, 56	0
1	B	221/242 (91%)	0.58	17 (7%)	13	15	10, 21, 46, 63	0
1	C	234/242 (96%)	0.49	19 (8%)	12	14	10, 24, 51, 61	0
1	D	228/242 (94%)	0.66	22 (9%)	8	9	10, 22, 49, 60	0
All	All	916/968 (94%)	0.54	72 (7%)	12	14	9, 22, 48, 63	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	528	MET	6.1
1	A	526	TYR	6.0
1	A	417	CYS	5.9
1	D	527	SER	5.7
1	D	331	TYR	5.6
1	A	418	VAL	5.4
1	C	417	CYS	5.1
1	D	306	LEU	4.8
1	B	469	LEU	4.7
1	C	425	PHE	4.5
1	B	528	MET	4.4
1	C	418	VAL	4.3
1	B	527	SER	4.1
1	A	422	VAL	3.9
1	B	342	MET	3.9
1	D	526	TYR	3.8
1	A	533	VAL	3.7
1	D	342	MET	3.6
1	C	422	VAL	3.5
1	A	546	ALA	3.5
1	B	511	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	341	SER	3.3
1	D	530	CYS	3.3
1	D	533	VAL	3.3
1	C	494	GLY	3.3
1	C	546	ALA	3.1
1	C	464	SER	3.1
1	B	307	ALA	3.1
1	D	511	LEU	3.1
1	C	469	LEU	3.0
1	D	425	PHE	2.9
1	B	341	SER	2.9
1	B	468	SER	2.9
1	C	533	VAL	2.9
1	B	467	LYS	2.9
1	B	461	PHE	2.9
1	D	514	ILE	2.7
1	A	525	LEU	2.7
1	C	409	LEU	2.7
1	D	421	MET	2.6
1	B	526	TYR	2.6
1	C	461	PHE	2.6
1	A	513	HIS	2.6
1	A	524	HIS	2.6
1	D	529	LYS	2.6
1	A	411	ASP	2.6
1	C	413	ASN	2.6
1	D	464	SER	2.6
1	C	419	GLU	2.5
1	D	509	LEU	2.5
1	C	331	TYR	2.4
1	B	331	TYR	2.4
1	C	337	PHE	2.4
1	B	510	ILE	2.3
1	C	511	LEU	2.3
1	B	509	LEU	2.3
1	C	479	LEU	2.3
1	A	452	ILE	2.3
1	B	546	ALA	2.3
1	A	413	ASN	2.3
1	C	451	ILE	2.2
1	A	464	SER	2.2
1	D	510	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	525	LEU	2.1
1	D	397	GLU	2.1
1	B	460	THR	2.1
1	D	531	LYS	2.1
1	B	308	LEU	2.1
1	D	422	VAL	2.0
1	D	524	HIS	2.0
1	D	307	ALA	2.0
1	A	461	PHE	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)

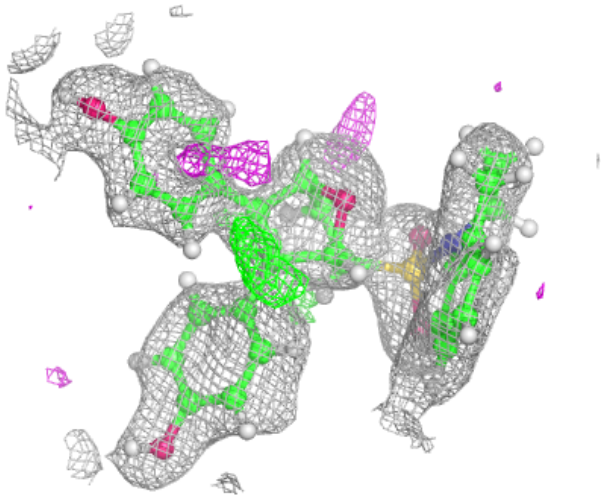
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

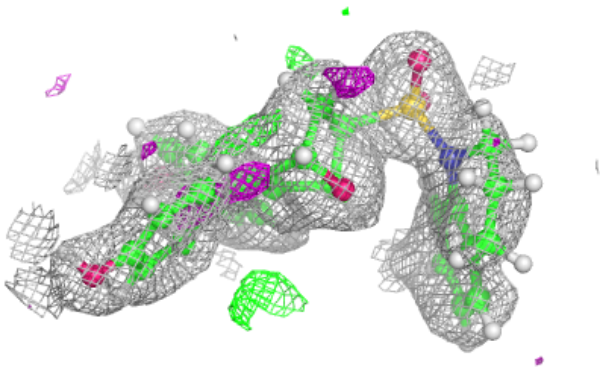
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1AHU	B	600	34/34	0.89	0.13	15,33,43,50	0
2	A1AHU	A	600	34/34	0.90	0.13	13,27,57,68	0
2	A1AHU	C	600	34/34	0.90	0.13	14,27,46,55	0
2	A1AHU	D	600	34/34	0.92	0.13	13,29,60,73	0

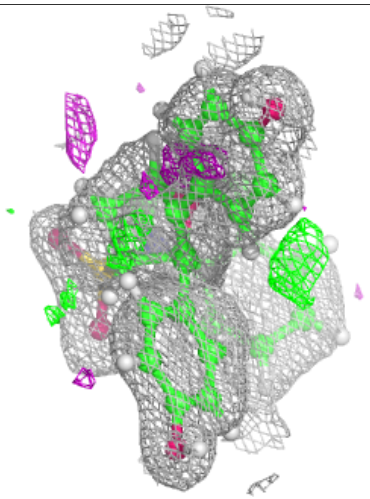
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AHU B 600:

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

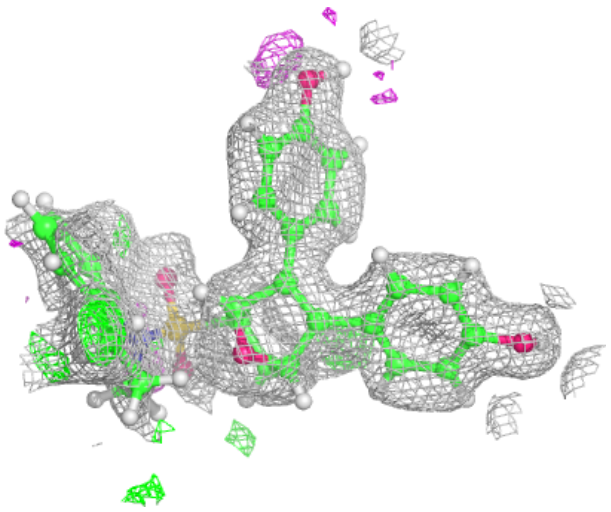


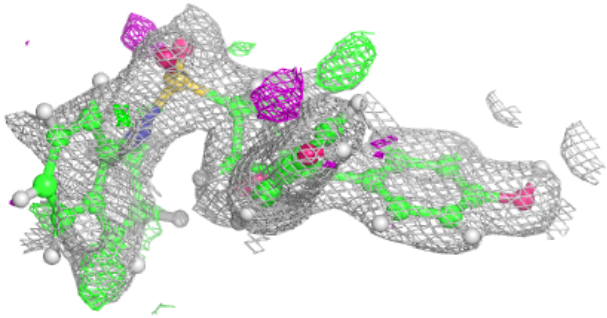


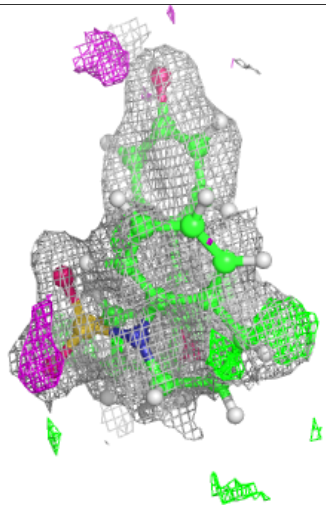


Electron density around A1AHU A 600:

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

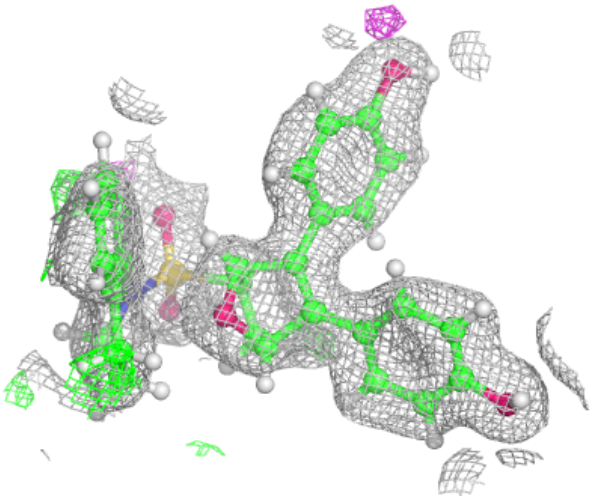


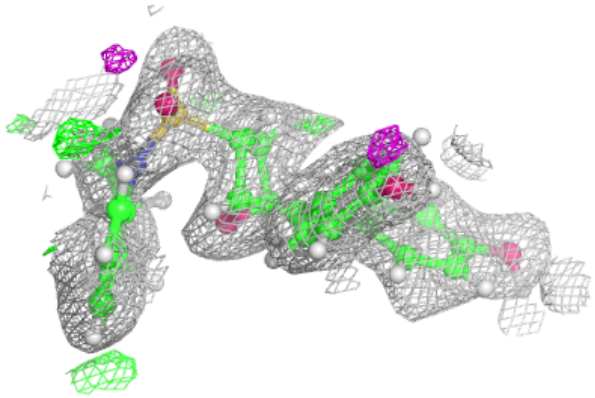


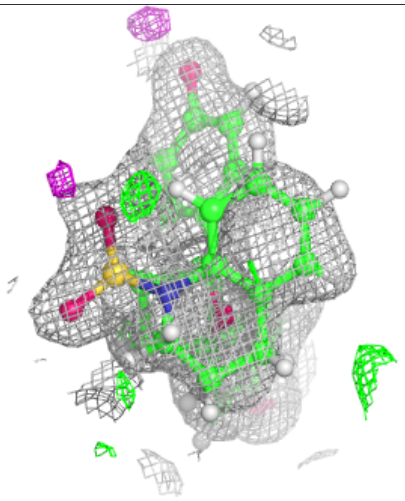


Electron density around A1AHU C 600:

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

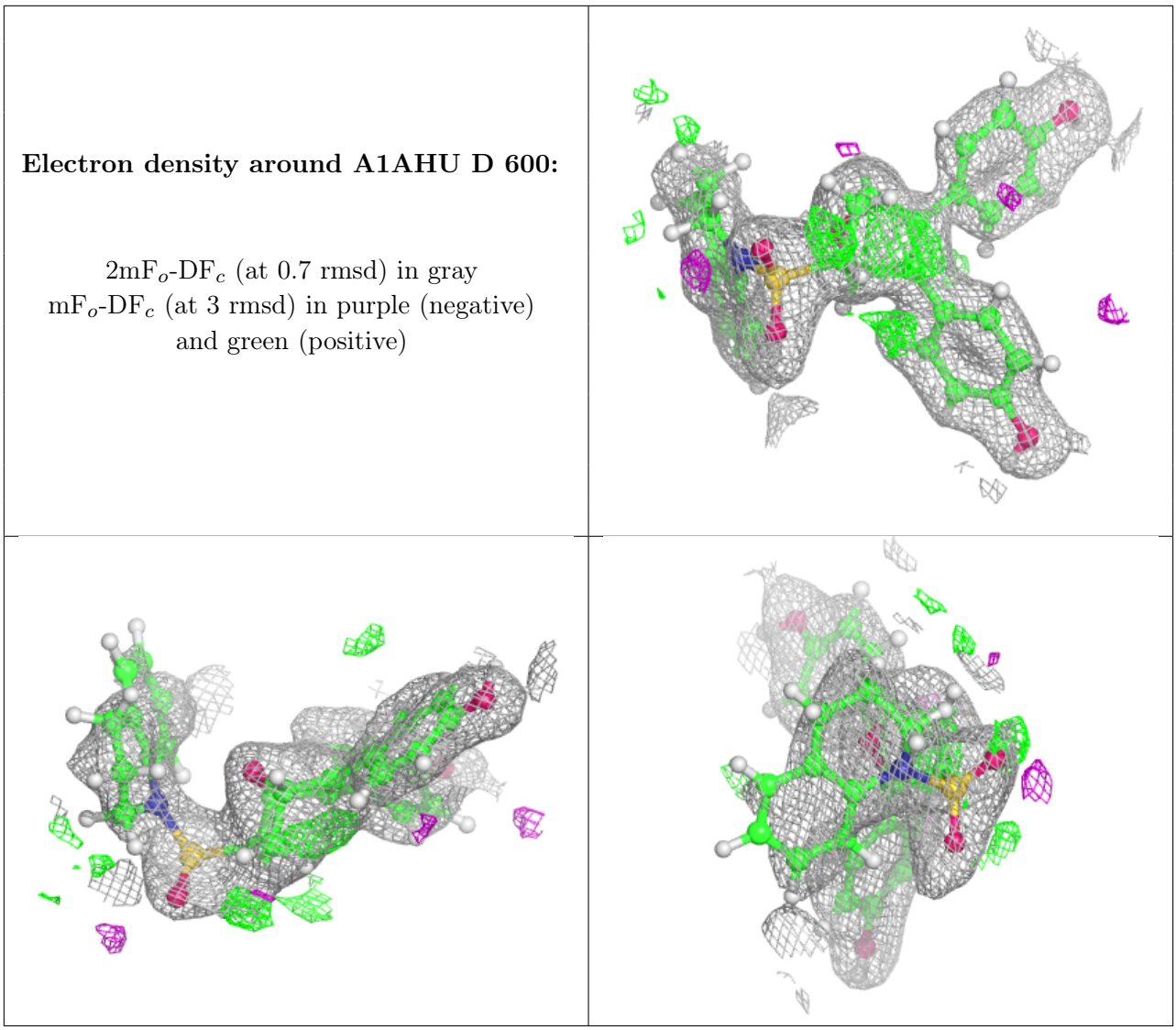






Electron density around A1AHU D 600:

$2mF_o$-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.