Full wwPDB X-ray Structure Validation Report

Jun 4, 2024 – 08:19 PM EDT

PDB ID	:	8VYT
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with k-411
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	:	1.61 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:

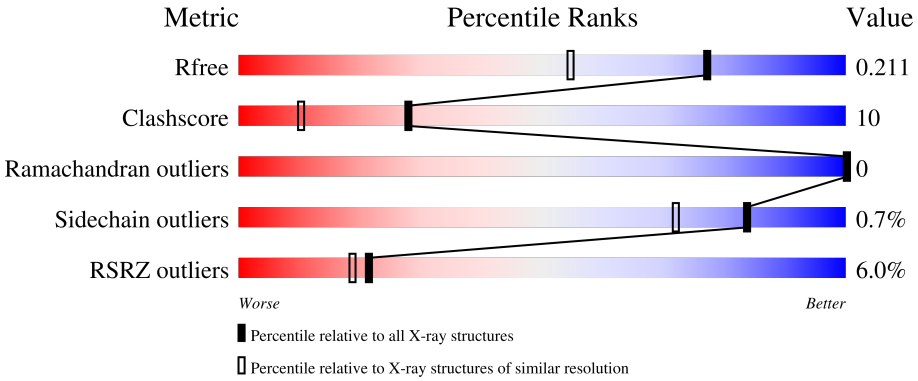
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.61 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	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	243	5% 82% 14% ••
1	B	243	6% 80% 8% •• 9%
1	C	243	5% 83% 13% ••
1	D	243	7% 76% 14% •• 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15510 atoms, of which 7493 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.

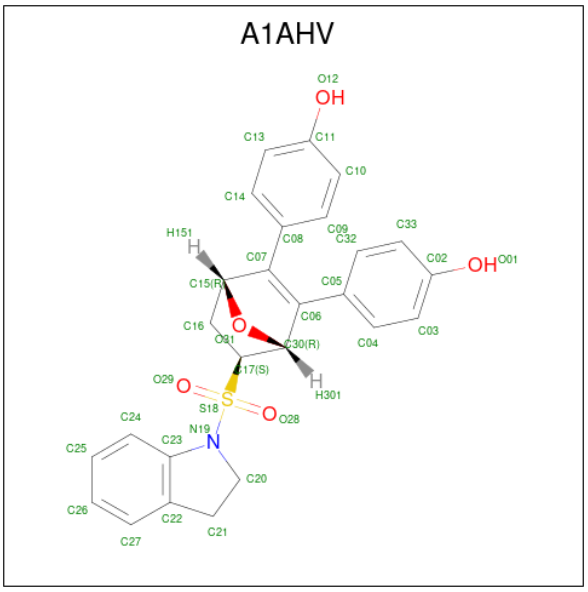
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	237	Total	C	H	N	O	S	0	0	0
			3771	1199	1896	317	341	18			
1	B	220	Total	C	H	N	O	S	0	1	0
			3557	1134	1792	300	314	17			
1	C	235	Total	C	H	N	O	S	0	0	0
			3751	1193	1891	315	334	18			
1	D	224	Total	C	H	N	O	S	0	0	0
			3601	1140	1822	302	321	16			

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'-[(1R,4R,5S)-5-(2,3-dihydro-1H-indole-1-sulfonyl)-7-oxabicyclo[2.2.1]hept-2-ene-2,3-diyl]diphenol (three-letter code: A1AHV) (formula: $C_{26}H_{23}NO_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			56	26	23	1	5	1		
2	B	1	Total	C	H	N	O	S	0	0
			56	26	23	1	5	1		
2	C	1	Total	C	H	N	O	S	0	0
			56	26	23	1	5	1		
2	D	1	Total	C	H	N	O	S	0	0
			56	26	23	1	5	1		

- Molecule 3 is water.

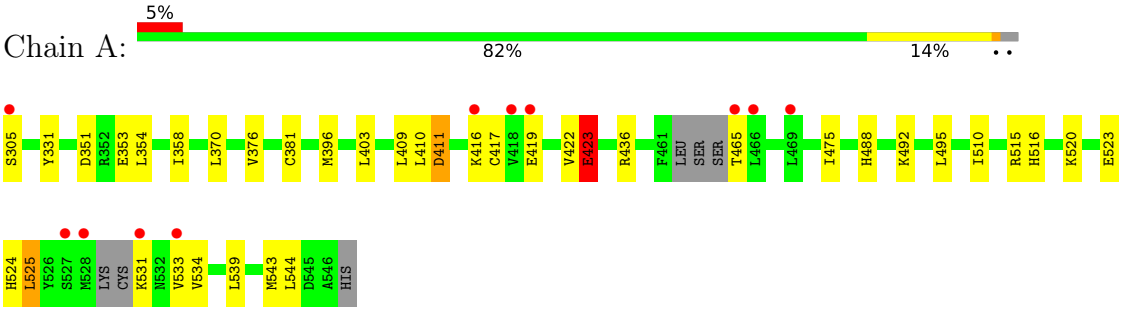
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total	O	0	0
			179	179		
3	B	144	Total	O	0	0
			144	144		
3	C	153	Total	O	0	0
			153	153		
3	D	130	Total	O	0	0
			130	130		

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.

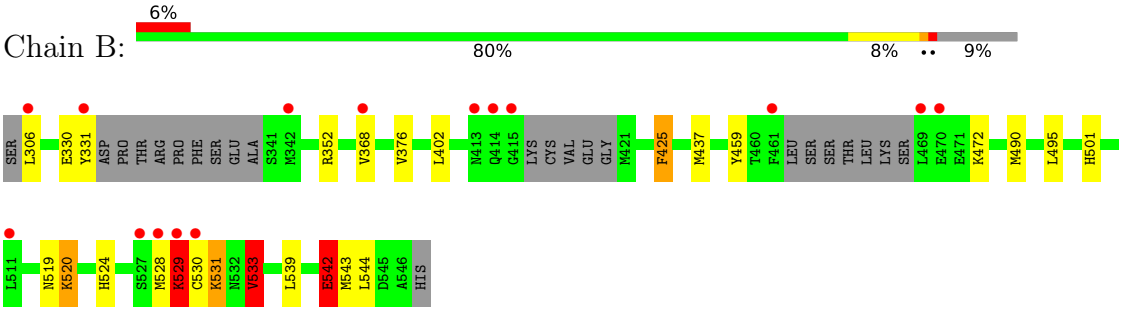
• Molecule 1: Estrogen receptor

Chain A:



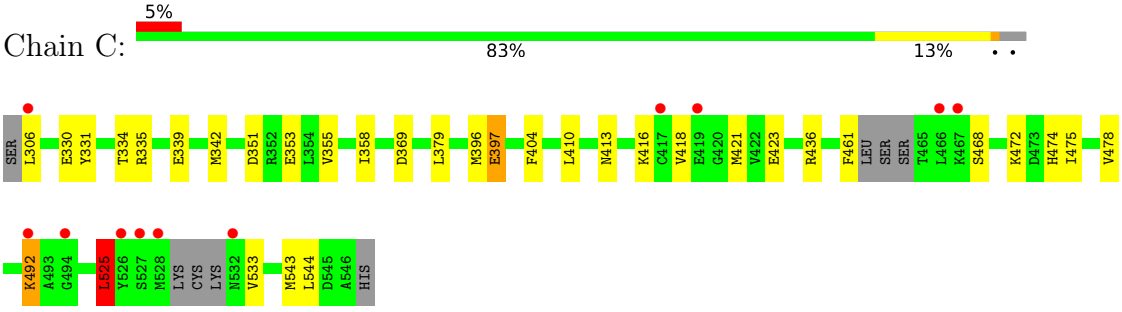
• Molecule 1: Estrogen receptor

Chain B:



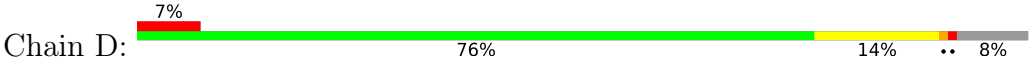
• Molecule 1: Estrogen receptor

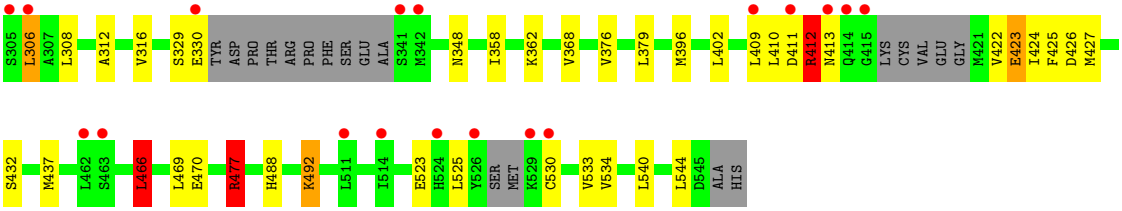
Chain C:



• Molecule 1: Estrogen receptor

Chain D:




S305 L306 A307 L308 A312 V316 S329 E330 TYR ASP PRO THR ARG PRO PHE SER GLU ALA S341 M342 N348 I358 K362 V368 V376 L379 M396 L402 L409 L410 D411 R412 N413 Q414 G415 LYS CYS VAL GLU GLY M421 V422 E423 I424 F425 D426 M427
S432 M437 L462 S463 L466 L469 E470 R477 H488 K492 L511 I514 E523 H524 L525 Y526 SER MET K529 C530 V533 V534 L540 L544 D545 ALA HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.39Å 58.70Å 93.36Å 86.88° 74.94° 63.05°	Depositor
Resolution (Å)	37.10 – 1.61 37.11 – 1.61	Depositor EDS
% Data completeness (in resolution range)	61.9 (37.10-1.61) 61.9 (37.11-1.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 1.62Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.180 , 0.212 0.180 , 0.211	Depositor DCC
R_{free} test set	3828 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.44 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.094 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15510	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.73% 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: A1AHV

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	0.67	2/1909 (0.1%)	1.44	12/2580 (0.5%)
1	B	1.12	7/1799 (0.4%)	1.04	17/2428 (0.7%)
1	C	0.60	1/1894 (0.1%)	0.75	3/2560 (0.1%)
1	D	0.92	3/1808 (0.2%)	1.33	14/2441 (0.6%)
All	All	0.85	13/7410 (0.2%)	1.17	46/10009 (0.5%)

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	3
1	B	0	2
1	D	0	1
All	All	0	6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	423	GLU	CD-OE2	-29.25	0.93	1.25
1	B	529	LYS	CE-NZ	25.69	2.13	1.49
1	B	529	LYS	CD-CE	25.61	2.15	1.51
1	B	529	LYS	CB-CG	9.49	1.78	1.52
1	B	529	LYS	CA-CB	7.19	1.69	1.53
1	A	423	GLU	CD-OE2	-6.99	1.18	1.25
1	D	423	GLU	CB-CG	6.69	1.64	1.52
1	B	529	LYS	CG-CD	6.64	1.75	1.52
1	D	534	VAL	CB-CG2	-5.62	1.41	1.52
1	B	520	LYS	N-CA	-5.40	1.35	1.46
1	A	411	ASP	CG-OD2	-5.36	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	397	GLU	CG-CD	-5.35	1.44	1.51
1	B	529	LYS	CA-C	5.18	1.66	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	411	ASP	CB-CG-OD1	48.92	162.33	118.30
1	D	423	GLU	OE1-CD-OE2	-35.21	81.05	123.30
1	D	423	GLU	CG-CD-OE1	25.61	169.52	118.30
1	A	411	ASP	OD1-CG-OD2	-24.41	76.92	123.30
1	D	466	LEU	CB-CG-CD2	17.91	141.44	111.00
1	A	534	VAL	CG1-CB-CG2	16.35	137.06	110.90
1	C	525	LEU	CB-CG-CD2	15.58	137.48	111.00
1	A	423	GLU	OE1-CD-OE2	-15.19	105.08	123.30
1	D	423	GLU	CG-CD-OE2	-14.89	88.52	118.30
1	B	533	VAL	CG1-CB-CG2	14.17	133.57	110.90
1	A	525	LEU	CB-CG-CD1	14.12	135.01	111.00
1	B	529	LYS	CB-CA-C	13.85	138.10	110.40
1	A	411	ASP	CB-CG-OD2	-13.04	106.57	118.30
1	B	542	GLU	OE1-CD-OE2	-12.05	108.84	123.30
1	B	437	MET	CB-CG-SD	-10.86	79.83	112.40
1	D	306	LEU	CB-CG-CD1	10.05	128.08	111.00
1	B	529	LYS	CD-CE-NZ	-9.87	89.00	111.70
1	A	423	GLU	CG-CD-OE1	9.57	137.44	118.30
1	D	306	LEU	CB-CG-CD2	-9.51	94.84	111.00
1	B	542	GLU	CG-CD-OE1	8.81	135.93	118.30
1	B	542	GLU	CG-CD-OE2	-8.18	101.94	118.30
1	A	423	GLU	CG-CD-OE2	-8.05	102.19	118.30
1	D	412	ARG	CB-CA-C	7.62	125.63	110.40
1	A	416	LYS	CD-CE-NZ	-7.36	94.76	111.70
1	D	534	VAL	CG1-CB-CG2	7.35	122.66	110.90
1	D	412	ARG	CA-CB-CG	7.16	129.14	113.40
1	B	529	LYS	CB-CG-CD	-6.87	93.75	111.60
1	C	492	LYS	CD-CE-NZ	6.85	127.45	111.70
1	A	411	ASP	CA-C-N	-6.37	103.20	117.20
1	D	492	LYS	CG-CD-CE	-6.14	93.48	111.90
1	B	472	LYS	CA-CB-CG	6.04	126.68	113.40
1	D	412	ARG	N-CA-CB	-6.01	99.79	110.60
1	B	519	ASN	O-C-N	5.80	131.98	122.70
1	D	412	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	423	GLU	N-CA-CB	5.58	120.64	110.60
1	B	528	MET	CA-C-N	5.46	129.21	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	411	ASP	CA-C-O	5.42	131.49	120.10
1	A	515	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	B	425	PHE	CB-CG-CD1	-5.36	117.05	120.80
1	B	529	LYS	CA-CB-CG	-5.35	101.63	113.40
1	C	492	LYS	CG-CD-CE	-5.35	95.85	111.90
1	B	472	LYS	CB-CG-CD	-5.33	97.73	111.60
1	B	501	HIS	N-CA-CB	5.31	120.15	110.60
1	B	529	LYS	O-C-N	-5.23	114.33	122.70
1	B	531	LYS	CD-CE-NZ	5.16	123.56	111.70
1	D	477	ARG	CD-NE-CZ	5.16	130.82	123.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	410	LEU	Peptide
1	A	411	ASP	Sidechain
1	A	423	GLU	Sidechain
1	B	529	LYS	Mainchain
1	B	542	GLU	Sidechain
1	D	477	ARG	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	1875	1896	1895	26	1
1	B	1765	1792	1805	30	0
1	C	1860	1891	1891	38	0
1	D	1779	1822	1821	39	1
2	A	33	23	0	4	0
2	B	33	23	0	4	0
2	C	33	23	0	5	0
2	D	33	23	0	7	0
3	A	179	0	0	10	4
3	B	144	0	0	6	4
3	C	153	0	0	15	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	130	0	0	7	2
All	All	8017	7493	7412	146	8

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 10.

All (146) 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:529:LYS:CB	1:B:529:LYS:CG	1.78	1.59
1:B:529:LYS:CG	1:B:529:LYS:CD	1.75	1.59
2:B:600:A1AHV:S18	2:B:600:A1AHV:C17	2.10	1.38
2:D:600:A1AHV:C17	2:D:600:A1AHV:S18	2.11	1.38
2:A:600:A1AHV:C17	2:A:600:A1AHV:S18	2.12	1.38
2:C:600:A1AHV:C17	2:C:600:A1AHV:S18	2.13	1.36
1:B:529:LYS:CD	1:B:529:LYS:CE	2.15	1.25
2:B:600:A1AHV:C15	2:B:600:A1AHV:O31	1.65	1.23
2:A:600:A1AHV:O31	2:A:600:A1AHV:C15	1.67	1.22
2:D:600:A1AHV:C15	2:D:600:A1AHV:O31	1.64	1.15
1:B:529:LYS:HD2	1:B:531:LYS:HZ2	1.11	1.15
2:C:600:A1AHV:C15	2:C:600:A1AHV:O31	1.65	1.15
1:B:529:LYS:CE	1:B:529:LYS:NZ	2.13	1.12
2:C:600:A1AHV:S18	2:C:600:A1AHV:C30	2.47	1.01
1:D:437:MET:SD	3:D:748:HOH:O	2.17	0.99
2:A:600:A1AHV:S18	2:A:600:A1AHV:C30	2.51	0.98
1:B:529:LYS:HD2	1:B:531:LYS:NZ	1.80	0.96
1:C:397:GLU:O	1:C:397:GLU:HG2	1.65	0.95
1:B:306:LEU:N	3:B:701:HOH:O	1.99	0.93
1:B:529:LYS:HD2	1:B:529:LYS:HA	1.52	0.92
1:D:348:ASN:ND2	3:D:701:HOH:O	2.01	0.92
1:A:419:GLU:OE1	3:A:701:HOH:O	1.88	0.92
1:B:529:LYS:CB	1:B:529:LYS:CD	2.57	0.82
1:D:362:LYS:HE3	1:D:544:LEU:HD12	1.60	0.82
2:B:600:A1AHV:S18	2:B:600:A1AHV:C30	2.66	0.82
1:D:470:GLU:HB2	3:D:757:HOH:O	1.78	0.82
1:C:369:ASP:OD1	3:C:701:HOH:O	1.98	0.80
1:A:403:LEU:HD13	1:A:409:LEU:HD13	1.64	0.78
1:A:331:TYR:O	3:A:702:HOH:O	2.01	0.78
1:A:305:SER:N	3:A:706:HOH:O	2.17	0.77
2:D:600:A1AHV:S18	2:D:600:A1AHV:C30	2.71	0.77
1:A:417:CYS:SG	3:A:856:HOH:O	2.42	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:LYS:CD	1:B:529:LYS:HA	2.16	0.76
1:C:306:LEU:N	3:C:705:HOH:O	2.18	0.76
1:C:331:TYR:O	3:C:702:HOH:O	2.05	0.75
1:A:351:ASP:OD2	3:A:703:HOH:O	2.02	0.75
1:A:354:LEU:O	1:A:358:ILE:HD12	1.86	0.74
1:C:358:ILE:HD12	1:C:379:LEU:HD13	1.72	0.72
1:B:331:TYR:O	3:B:702:HOH:O	2.06	0.72
1:B:529:LYS:CD	1:B:531:LYS:HZ2	1.99	0.72
1:D:523:GLU:OE2	3:D:702:HOH:O	2.07	0.71
1:B:529:LYS:CG	1:B:529:LYS:CA	2.69	0.70
1:C:355:VAL:HG22	1:C:543:MET:CE	2.23	0.68
1:B:529:LYS:CD	1:B:531:LYS:NZ	2.57	0.68
1:D:306:LEU:H	1:D:306:LEU:HD23	1.60	0.67
1:A:422:VAL:HG12	1:A:423:GLU:OE1	1.94	0.66
1:D:412:ARG:HH22	1:D:422:VAL:HG11	1.59	0.66
1:C:330:GLU:C	3:C:702:HOH:O	2.34	0.66
1:C:351:ASP:OD2	3:C:704:HOH:O	2.13	0.66
1:A:523:GLU:OE1	3:A:704:HOH:O	2.15	0.65
1:C:436:ARG:NH2	3:C:706:HOH:O	2.18	0.65
1:D:423:GLU:HG3	1:D:424:ILE:N	2.12	0.65
1:C:355:VAL:HG22	1:C:543:MET:HE2	1.79	0.64
2:D:600:A1AHV:S18	2:D:600:A1AHV:C16	2.83	0.64
1:D:533:VAL:HG22	1:D:533:VAL:O	1.99	0.63
1:C:413:ASN:HA	1:C:416:LYS:HE3	1.81	0.62
1:D:533:VAL:HG21	2:D:600:A1AHV:O01	1.99	0.62
1:A:525:LEU:HD12	1:A:533:VAL:HG11	1.80	0.61
1:C:468:SER:HB2	3:C:835:HOH:O	2.00	0.61
1:A:523:GLU:OE2	3:A:705:HOH:O	2.15	0.60
1:A:510:ILE:HD13	1:B:459:TYR:CZ	2.37	0.59
1:D:488:HIS:CE1	1:D:492:LYS:HE3	2.36	0.59
1:C:396:MET:O	1:C:436:ARG:NH1	2.32	0.58
1:D:530:CYS:O	1:D:533:VAL:HG12	2.03	0.58
1:A:381:CYS:SG	3:A:860:HOH:O	2.24	0.58
1:D:423:GLU:HG3	1:D:424:ILE:HG13	1.85	0.58
1:C:334:THR:HG23	3:C:716:HOH:O	2.03	0.57
1:B:531:LYS:HD3	1:B:531:LYS:H	1.68	0.57
1:B:529:LYS:HD2	1:B:529:LYS:CA	2.32	0.56
1:A:376:VAL:HG22	1:A:544:LEU:HD12	1.88	0.55
1:C:335:ARG:NH2	3:C:703:HOH:O	2.11	0.55
1:D:412:ARG:NH2	1:D:422:VAL:HG11	2.22	0.55
1:B:529:LYS:CD	1:B:529:LYS:CA	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:TYR:N	3:C:702:HOH:O	2.40	0.54
1:C:397:GLU:O	1:C:397:GLU:CG	2.44	0.54
1:D:525:LEU:HD23	2:D:600:A1AHV:C21	2.38	0.54
1:D:362:LYS:CE	1:D:544:LEU:HD12	2.37	0.53
2:B:600:A1AHV:S18	2:B:600:A1AHV:C16	2.87	0.53
1:B:330:GLU:HB2	3:B:746:HOH:O	2.08	0.53
1:A:539:LEU:HG	1:A:543:MET:CE	2.38	0.53
1:A:524:HIS:NE2	3:A:709:HOH:O	2.34	0.53
1:A:370:LEU:HD11	1:A:475:ILE:HD11	1.90	0.52
1:A:525:LEU:HD12	1:A:533:VAL:CG1	2.39	0.52
1:C:461:PHE:HE2	1:C:475:ILE:HD12	1.75	0.52
1:D:412:ARG:NH1	1:D:426:ASP:OD2	2.42	0.51
1:A:523:GLU:CD	3:A:705:HOH:O	2.48	0.51
1:B:490:MET:HB3	1:B:495:LEU:HD22	1.91	0.51
1:B:524[A]:HIS:CD2	3:B:709:HOH:O	2.62	0.51
1:C:355:VAL:HG22	1:C:543:MET:HE1	1.92	0.50
1:B:368:VAL:HG22	3:B:714:HOH:O	2.11	0.50
1:A:396:MET:O	1:A:436:ARG:HD3	2.11	0.50
2:C:600:A1AHV:O01	3:C:707:HOH:O	2.20	0.50
1:D:362:LYS:HE3	1:D:544:LEU:CD1	2.39	0.50
1:D:423:GLU:CG	1:D:424:ILE:N	2.74	0.50
1:B:330:GLU:OE1	1:B:352:ARG:NE	2.45	0.50
1:C:423:GLU:H	1:C:423:GLU:CD	2.14	0.49
1:C:525:LEU:HD22	1:C:533:VAL:HG11	1.93	0.49
1:B:542:GLU:CD	3:B:705:HOH:O	2.51	0.48
1:B:539:LEU:O	1:B:543:MET:HG3	2.14	0.48
1:C:331:TYR:C	3:C:702:HOH:O	2.49	0.48
1:C:492:LYS:HE2	1:C:492:LYS:CA	2.44	0.48
1:D:525:LEU:CD2	2:D:600:A1AHV:C21	2.92	0.48
1:B:530:CYS:O	1:B:533:VAL:HG22	2.14	0.47
1:A:370:LEU:HD21	1:A:475:ILE:HD11	1.95	0.47
1:C:525:LEU:HD22	1:C:533:VAL:CG1	2.44	0.47
1:C:339:GLU:HG3	1:C:418:VAL:HG22	1.96	0.47
1:C:358:ILE:CD1	1:C:379:LEU:HD13	2.41	0.47
1:D:409:LEU:C	1:D:410:LEU:HD23	2.36	0.45
1:D:466:LEU:O	1:D:466:LEU:HD12	2.15	0.45
1:D:423:GLU:O	1:D:427:MET:HG3	2.17	0.45
1:C:339:GLU:HG3	1:C:418:VAL:HA	1.97	0.44
1:C:492:LYS:HE2	1:C:492:LYS:N	2.32	0.44
1:D:368:VAL:HG22	3:D:727:HOH:O	2.19	0.43
1:C:334:THR:N	3:C:718:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:LEU:HD12	1:D:469:LEU:CD1	2.48	0.43
1:D:402:LEU:HD12	1:D:425:PHE:CE1	2.53	0.43
1:D:329:SER:O	1:D:330:GLU:C	2.57	0.43
1:D:396:MET:HA	1:D:432:SER:OG	2.19	0.42
1:D:477:ARG:NH2	3:D:711:HOH:O	2.51	0.42
1:A:488:HIS:O	1:A:492:LYS:HG2	2.19	0.42
1:C:342:MET:CE	1:C:421:MET:SD	3.07	0.42
1:D:376:VAL:HG23	1:D:544:LEU:HD23	2.01	0.42
1:C:492:LYS:HE2	1:C:492:LYS:HA	2.01	0.42
1:D:533:VAL:O	1:D:533:VAL:CG2	2.65	0.42
1:A:353:GLU:OE1	2:A:600:A1AHV:O12	2.38	0.42
1:A:516:HIS:CE1	1:A:520:LYS:HE2	2.54	0.42
1:D:411:ASP:OD1	1:D:411:ASP:C	2.58	0.42
1:C:358:ILE:HG23	1:C:544:LEU:HD13	2.02	0.41
1:B:531:LYS:HB2	1:B:531:LYS:HE2	1.71	0.41
1:D:470:GLU:CD	3:D:704:HOH:O	2.58	0.41
1:C:472:LYS:HE2	1:C:472:LYS:HB2	1.73	0.41
1:C:474:HIS:O	1:C:478:VAL:HG23	2.21	0.41
1:D:358:ILE:HD12	1:D:379:LEU:HD13	2.02	0.41
1:D:540:LEU:O	1:D:544:LEU:HB2	2.21	0.41
1:A:354:LEU:O	1:A:358:ILE:CD1	2.63	0.41
1:C:353:GLU:OE1	2:C:600:A1AHV:O12	2.39	0.41
1:D:308:LEU:HD11	1:D:477:ARG:HH11	1.86	0.41
1:D:312:ALA:O	1:D:316:VAL:HG23	2.21	0.41
1:B:306:LEU:HD12	1:B:306:LEU:O	2.20	0.40
1:B:402:LEU:HD12	1:B:425:PHE:CE1	2.55	0.40
1:D:308:LEU:HD11	1:D:477:ARG:NH1	2.36	0.40
1:C:461:PHE:HB2	3:C:840:HOH:O	2.21	0.40
1:D:358:ILE:O	1:D:362:LYS:HG2	2.20	0.40
1:B:376:VAL:HG22	1:B:544:LEU:HD12	2.03	0.40
1:C:330:GLU:HG3	3:C:770:HOH:O	2.22	0.40
1:C:404:PHE:CE2	1:C:410:LEU:HD12	2.56	0.40

All (8) 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:855:HOH:O	3:C:851:HOH:O[1_554]	1.74	0.46
3:B:704:HOH:O	3:B:777:HOH:O[1_455]	1.86	0.34
3:C:827:HOH:O	3:D:781:HOH:O[1_545]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:849:HOH:O	3:B:833:HOH:O[1_655]	1.97	0.23
3:A:863:HOH:O	3:B:768:HOH:O[1_655]	2.09	0.11
3:A:871:HOH:O	3:B:767:HOH:O[1_565]	2.11	0.09
3:C:718:HOH:O	3:D:784:HOH:O[1_545]	2.11	0.09
1:A:531:LYS:NZ	1:D:413:ASN:OD1[1_554]	2.16	0.04

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	231/243 (95%)	228 (99%)	3 (1%)	0	100	100
1	B	213/243 (88%)	209 (98%)	4 (2%)	0	100	100
1	C	229/243 (94%)	225 (98%)	4 (2%)	0	100	100
1	D	216/243 (89%)	213 (99%)	3 (1%)	0	100	100
All	All	889/972 (92%)	875 (98%)	14 (2%)	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	209/219 (95%)	208 (100%)	1 (0%)	88	80
1	B	198/219 (90%)	196 (99%)	2 (1%)	76	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	207/219 (94%)	206 (100%)	1 (0%)	88 80
1	D	201/219 (92%)	199 (99%)	2 (1%)	76 60
All	All	815/876 (93%)	809 (99%)	6 (1%)	84 72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	THR
1	B	520	LYS
1	B	533	VAL
1	C	525	LEU
1	D	412	ARG
1	D	466	LEU

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

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)

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	A1AHV	A	600	-	36,38,38	5.98	10 (27%)	47,58,58	4.08	16 (34%)
2	A1AHV	B	600	-	36,38,38	5.65	11 (30%)	47,58,58	3.72	13 (27%)
2	A1AHV	C	600	-	36,38,38	5.83	10 (27%)	47,58,58	4.01	16 (34%)
2	A1AHV	D	600	-	36,38,38	5.92	11 (30%)	47,58,58	4.67	19 (40%)

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	A1AHV	A	600	-	-	6/18/53/53	0/7/6/6
2	A1AHV	B	600	-	-	4/18/53/53	0/7/6/6
2	A1AHV	C	600	-	-	8/18/53/53	0/7/6/6
2	A1AHV	D	600	-	-	9/18/53/53	0/7/6/6

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	A1AHV	C16-C17	-19.59	1.29	1.54
2	D	600	A1AHV	C07-C06	19.50	1.73	1.34
2	D	600	A1AHV	C16-C17	-18.92	1.30	1.54
2	B	600	A1AHV	C07-C06	18.86	1.71	1.34
2	A	600	A1AHV	C16-C17	-18.83	1.30	1.54
2	B	600	A1AHV	C16-C17	-18.46	1.31	1.54
2	A	600	A1AHV	C07-C06	18.38	1.70	1.34
2	C	600	A1AHV	C07-C06	17.26	1.68	1.34
2	D	600	A1AHV	C16-C15	-13.75	1.23	1.53
2	A	600	A1AHV	C16-C15	-13.72	1.23	1.53
2	C	600	A1AHV	C16-C15	-13.71	1.23	1.53
2	B	600	A1AHV	C16-C15	-12.68	1.25	1.53
2	A	600	A1AHV	O31-C30	11.76	1.59	1.43
2	C	600	A1AHV	O31-C30	11.57	1.59	1.43
2	B	600	A1AHV	O31-C30	10.48	1.58	1.43
2	A	600	A1AHV	O31-C15	10.08	1.67	1.44
2	D	600	A1AHV	O31-C30	9.64	1.57	1.43
2	B	600	A1AHV	O31-C15	9.42	1.65	1.44
2	C	600	A1AHV	O31-C15	9.42	1.65	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	A1AHV	O31-C15	8.90	1.64	1.44
2	D	600	A1AHV	C20-N19	-6.78	1.43	1.50
2	A	600	A1AHV	O28-S18	6.28	1.48	1.43
2	A	600	A1AHV	O29-S18	5.89	1.48	1.43
2	D	600	A1AHV	O28-S18	5.81	1.48	1.43
2	A	600	A1AHV	C23-N19	5.73	1.49	1.43
2	D	600	A1AHV	C23-N19	5.61	1.49	1.43
2	B	600	A1AHV	C23-N19	5.09	1.48	1.43
2	C	600	A1AHV	O28-S18	5.07	1.47	1.43
2	C	600	A1AHV	C30-C06	-4.92	1.45	1.50
2	A	600	A1AHV	C30-C06	-4.77	1.45	1.50
2	C	600	A1AHV	C20-N19	-4.73	1.45	1.50
2	C	600	A1AHV	C23-N19	4.24	1.47	1.43
2	D	600	A1AHV	O29-S18	4.21	1.47	1.43
2	C	600	A1AHV	O29-S18	4.20	1.47	1.43
2	B	600	A1AHV	O28-S18	4.18	1.47	1.43
2	A	600	A1AHV	C20-N19	-3.60	1.46	1.50
2	B	600	A1AHV	O29-S18	3.60	1.46	1.43
2	B	600	A1AHV	C20-N19	-2.79	1.47	1.50
2	D	600	A1AHV	C05-C06	2.69	1.53	1.48
2	B	600	A1AHV	C30-C06	-2.30	1.48	1.50
2	D	600	A1AHV	C20-C21	-2.21	1.50	1.53
2	B	600	A1AHV	C05-C06	2.21	1.52	1.48

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	A1AHV	O29-S18-O28	-24.15	103.69	119.22
2	A	600	A1AHV	O29-S18-O28	-20.09	106.30	119.22
2	C	600	A1AHV	O29-S18-O28	-18.59	107.27	119.22
2	B	600	A1AHV	O29-S18-O28	-17.96	107.68	119.22
2	C	600	A1AHV	C15-C16-C17	13.58	112.61	100.61
2	A	600	A1AHV	C15-C16-C17	12.29	111.47	100.61
2	B	600	A1AHV	C15-C16-C17	10.84	110.19	100.61
2	B	600	A1AHV	O29-S18-N19	9.59	119.30	107.56
2	D	600	A1AHV	C15-C16-C17	9.42	108.93	100.61
2	C	600	A1AHV	O28-S18-N19	7.97	117.33	107.56
2	D	600	A1AHV	O28-S18-N19	7.86	117.18	107.56
2	A	600	A1AHV	O28-S18-N19	7.27	116.46	107.56
2	D	600	A1AHV	C22-C23-N19	-6.72	106.03	110.09
2	D	600	A1AHV	O29-S18-N19	6.02	114.93	107.56
2	D	600	A1AHV	C24-C23-N19	5.77	134.54	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	A1AHV	O31-C15-C07	-5.35	94.54	101.99
2	D	600	A1AHV	C32-C05-C06	-5.32	114.03	120.91
2	D	600	A1AHV	C08-C07-C06	-4.70	116.64	128.81
2	C	600	A1AHV	C08-C07-C15	4.40	128.61	121.44
2	C	600	A1AHV	O31-C15-C16	-4.32	96.14	104.64
2	A	600	A1AHV	C04-C05-C06	-4.31	115.33	120.91
2	A	600	A1AHV	O31-C15-C16	-4.14	96.50	104.64
2	D	600	A1AHV	O31-C15-C16	-3.87	97.03	104.64
2	C	600	A1AHV	C32-C05-C06	-3.75	116.05	120.91
2	A	600	A1AHV	C22-C23-N19	-3.73	107.84	110.09
2	D	600	A1AHV	C05-C06-C07	-3.72	119.18	128.81
2	B	600	A1AHV	O31-C15-C16	-3.56	97.64	104.64
2	B	600	A1AHV	O31-C15-C07	-3.53	97.09	101.99
2	C	600	A1AHV	O31-C15-C07	-3.52	97.10	101.99
2	C	600	A1AHV	C32-C05-C04	3.46	123.51	118.59
2	A	600	A1AHV	C08-C07-C15	3.40	126.98	121.44
2	B	600	A1AHV	C21-C20-N19	3.33	107.97	105.21
2	B	600	A1AHV	C08-C07-C15	3.29	126.80	121.44
2	A	600	A1AHV	C24-C23-N19	3.24	131.53	127.66
2	C	600	A1AHV	C22-C23-N19	-3.24	108.14	110.09
2	D	600	A1AHV	C14-C08-C07	-3.23	116.73	120.91
2	D	600	A1AHV	C04-C05-C06	3.11	124.94	120.91
2	B	600	A1AHV	C05-C06-C30	3.07	126.32	121.27
2	C	600	A1AHV	C15-C07-C06	-3.05	100.57	106.97
2	C	600	A1AHV	C05-C06-C07	3.00	136.58	128.81
2	D	600	A1AHV	C21-C20-N19	-2.93	102.79	105.21
2	A	600	A1AHV	C15-C07-C06	-2.90	100.88	106.97
2	A	600	A1AHV	C32-C05-C04	2.78	122.55	118.59
2	C	600	A1AHV	C24-C23-N19	2.71	130.90	127.66
2	D	600	A1AHV	C27-C22-C23	2.64	121.73	119.80
2	C	600	A1AHV	C14-C08-C07	-2.62	117.52	120.91
2	B	600	A1AHV	O28-S18-N19	2.61	110.76	107.56
2	C	600	A1AHV	C03-C04-C05	-2.53	117.84	120.78
2	B	600	A1AHV	C15-C07-C06	-2.51	101.69	106.97
2	D	600	A1AHV	C05-C06-C30	2.50	125.39	121.27
2	D	600	A1AHV	C15-C07-C06	-2.48	101.77	106.97
2	D	600	A1AHV	C23-N19-S18	2.45	129.42	123.42
2	A	600	A1AHV	C14-C08-C09	2.39	122.00	118.59
2	C	600	A1AHV	C33-C32-C05	-2.37	118.02	120.78
2	A	600	A1AHV	C21-C20-N19	-2.36	103.27	105.21
2	C	600	A1AHV	C30-O31-C15	-2.34	87.06	100.08
2	A	600	A1AHV	C30-O31-C15	-2.29	87.31	100.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	600	A1AHV	C20-N19-C23	2.23	110.14	105.90
2	B	600	A1AHV	C05-C06-C07	2.23	134.59	128.81
2	A	600	A1AHV	C33-C32-C05	-2.18	118.24	120.78
2	B	600	A1AHV	C30-O31-C15	-2.18	87.96	100.08
2	D	600	A1AHV	C24-C23-C22	-2.14	119.40	121.60
2	B	600	A1AHV	C24-C23-N19	2.07	130.13	127.66
2	A	600	A1AHV	C20-C21-C22	2.03	105.58	103.65

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	A1AHV	C30-C17-S18-O28
2	C	600	A1AHV	C30-C17-S18-O28
2	D	600	A1AHV	C30-C17-S18-O28
2	D	600	A1AHV	C30-C17-S18-O29
2	D	600	A1AHV	C23-N19-S18-C17
2	D	600	A1AHV	C16-C17-S18-O29
2	A	600	A1AHV	C23-N19-S18-O29
2	C	600	A1AHV	C23-N19-S18-O28
2	C	600	A1AHV	C23-N19-S18-O29
2	D	600	A1AHV	C23-N19-S18-O29
2	B	600	A1AHV	C06-C07-C08-C14
2	A	600	A1AHV	C32-C05-C06-C30
2	B	600	A1AHV	C06-C07-C08-C09
2	D	600	A1AHV	C06-C07-C08-C09
2	C	600	A1AHV	C04-C05-C06-C07
2	A	600	A1AHV	C23-N19-S18-C17
2	C	600	A1AHV	C23-N19-S18-C17
2	D	600	A1AHV	C16-C17-S18-O28
2	C	600	A1AHV	C32-C05-C06-C07
2	D	600	A1AHV	C06-C07-C08-C14
2	A	600	A1AHV	C04-C05-C06-C30
2	B	600	A1AHV	C04-C05-C06-C30
2	C	600	A1AHV	C32-C05-C06-C30
2	D	600	A1AHV	C20-N19-S18-O29
2	A	600	A1AHV	C23-N19-S18-O28
2	B	600	A1AHV	C32-C05-C06-C30
2	C	600	A1AHV	C04-C05-C06-C30

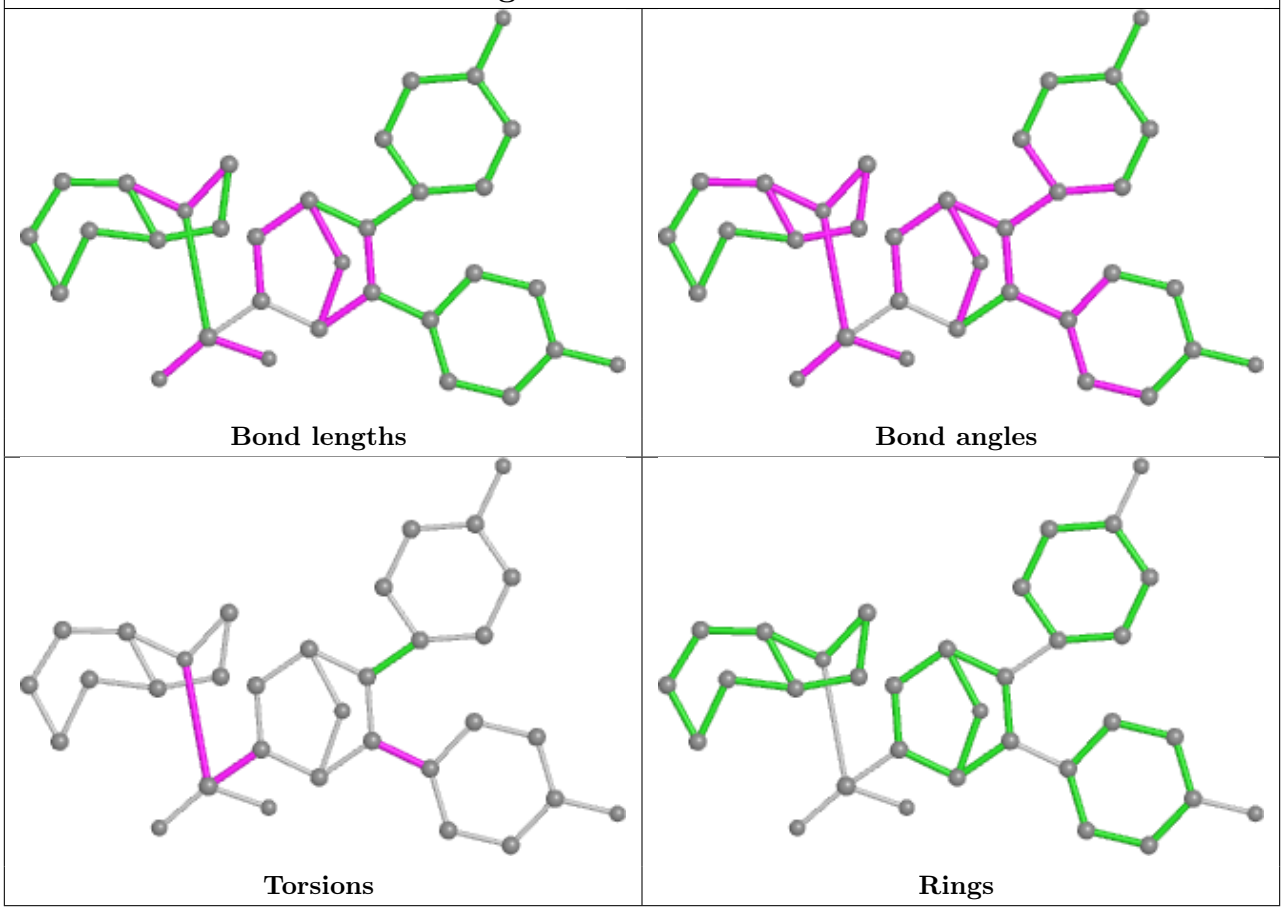
There are no ring outliers.

4 monomers are involved in 20 short contacts:

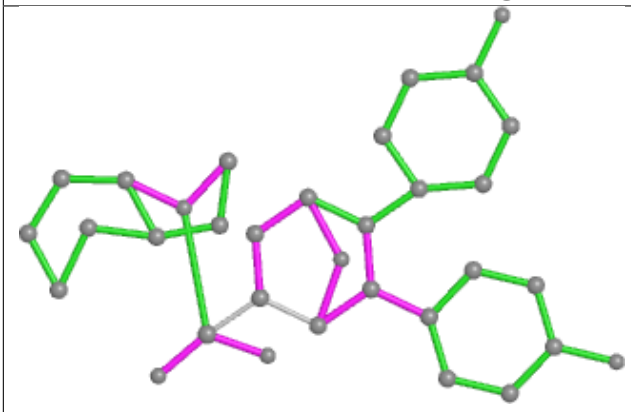
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	A1AHV	4	0
2	B	600	A1AHV	4	0
2	C	600	A1AHV	5	0
2	D	600	A1AHV	7	0

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.

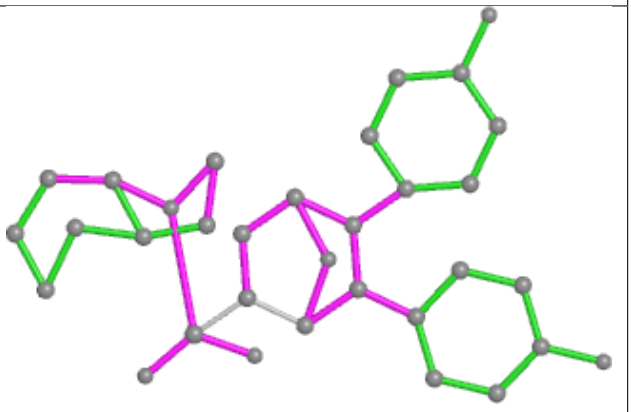
Ligand A1AHV A 600



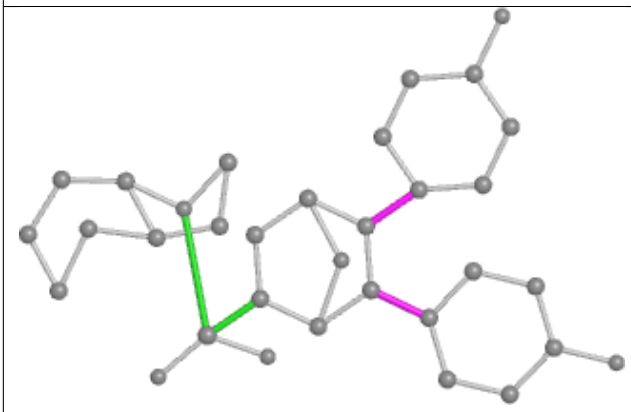
Ligand A1AHV B 600



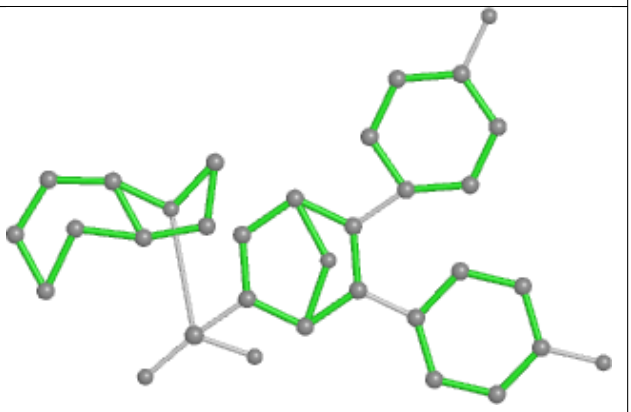
Bond lengths



Bond angles

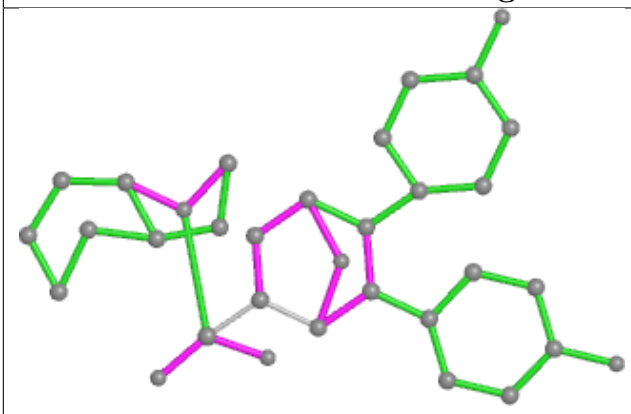


Torsions

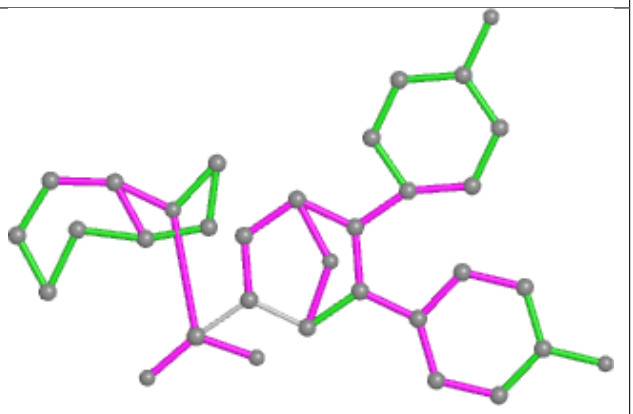


Rings

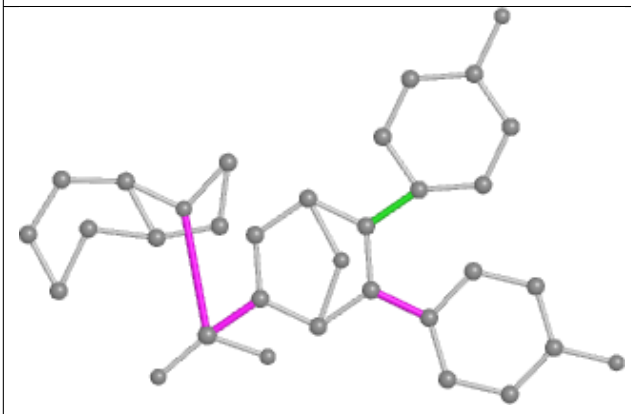
Ligand A1AHV C 600



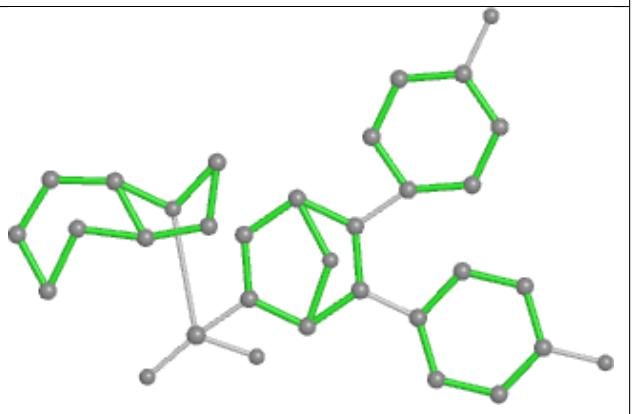
Bond lengths



Bond angles

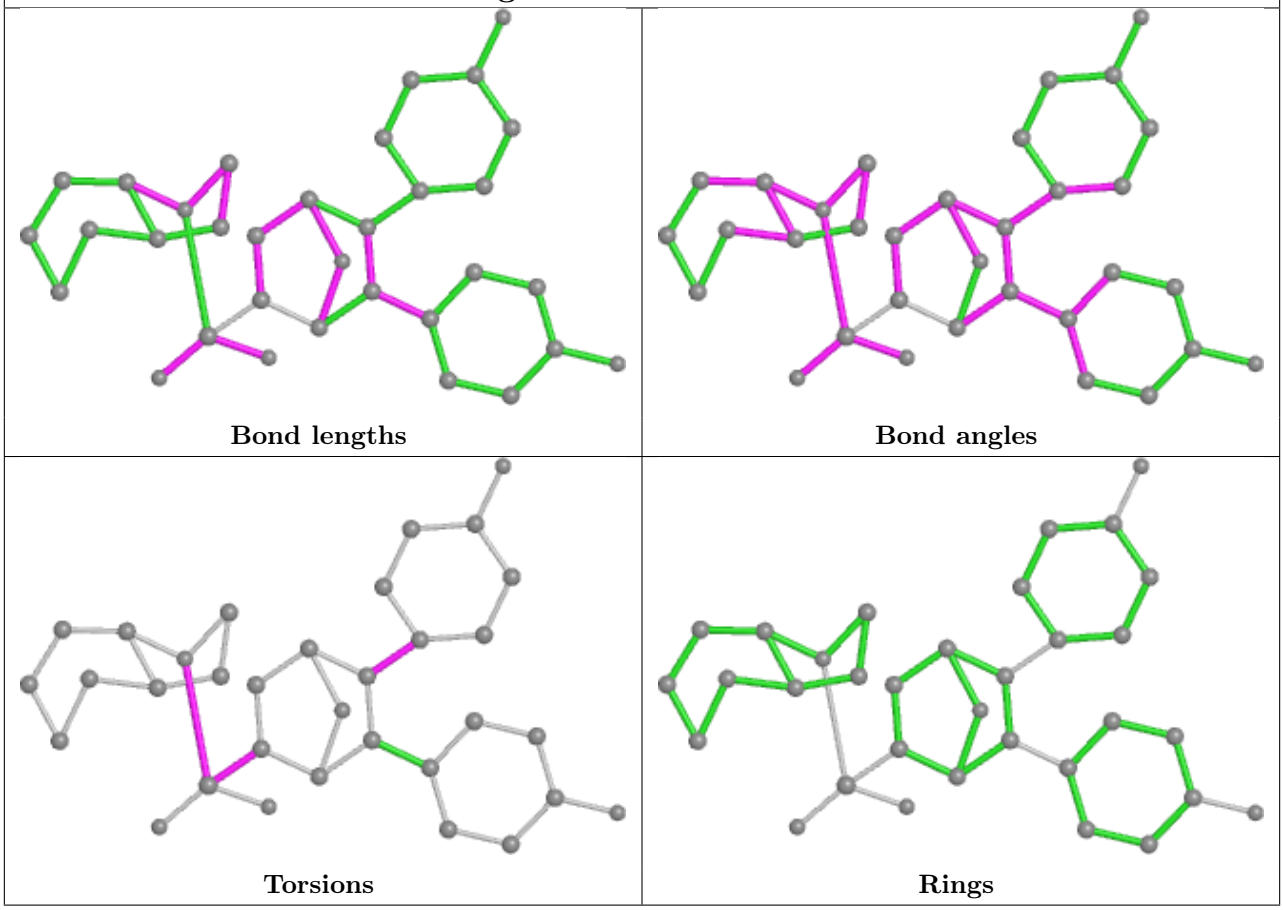


Torsions



Rings

Ligand A1AHV D 600



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	237/243 (97%)	0.02	11 (4%)	32	29	12, 25, 51, 77	0
1	B	220/243 (90%)	0.30	15 (6%)	17	15	13, 26, 52, 73	0
1	C	235/243 (96%)	0.18	11 (4%)	31	28	12, 28, 52, 68	0
1	D	224/243 (92%)	0.22	18 (8%)	12	10	12, 25, 51, 65	0
All	All	916/972 (94%)	0.18	55 (6%)	21	19	12, 26, 52, 77	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	306	LEU	7.1
1	B	414	GLN	5.6
1	D	306	LEU	5.4
1	A	531	LYS	4.8
1	B	331	TYR	4.5
1	D	462	LEU	4.4
1	B	528	MET	4.0
1	C	532	ASN	4.0
1	B	527	SER	4.0
1	D	530	CYS	3.9
1	B	413	ASN	3.8
1	A	466	LEU	3.7
1	D	342	MET	3.6
1	C	467	LYS	3.5
1	B	415	GLY	3.4
1	C	527	SER	3.4
1	B	306	LEU	3.3
1	C	526	TYR	3.3
1	C	419	GLU	3.3
1	D	415	GLY	3.3
1	C	466	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	414	GLN	3.2
1	D	524	HIS	3.2
1	C	417	CYS	3.1
1	B	529	LYS	3.1
1	B	470	GLU	3.1
1	B	342	MET	3.0
1	B	368	VAL	3.0
1	D	511	LEU	3.0
1	A	465	THR	3.0
1	C	492	LYS	2.9
1	A	305	SER	2.9
1	D	409	LEU	2.6
1	B	511	LEU	2.6
1	D	341	SER	2.5
1	B	461	PHE	2.5
1	A	419	GLU	2.4
1	D	305	SER	2.4
1	A	527	SER	2.4
1	D	463	SER	2.4
1	A	416	LYS	2.4
1	B	469	LEU	2.4
1	C	494	GLY	2.4
1	C	528	MET	2.3
1	A	469	LEU	2.3
1	B	530	CYS	2.3
1	A	528	MET	2.2
1	A	533	VAL	2.2
1	D	413	ASN	2.1
1	A	418	VAL	2.1
1	D	529	LYS	2.1
1	D	514	ILE	2.1
1	D	411	ASP	2.1
1	D	330	GLU	2.0
1	D	526	TYR	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)

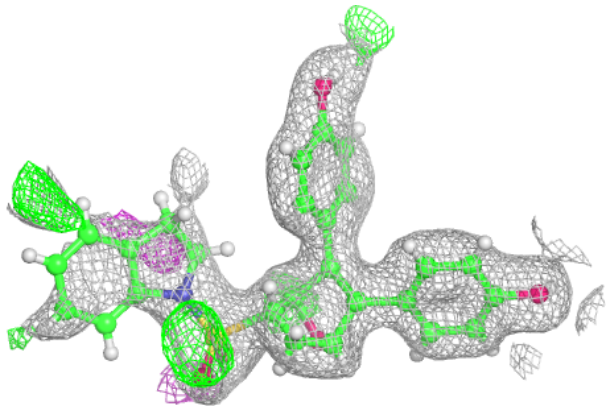
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

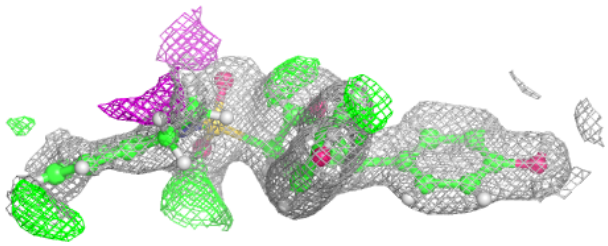
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1AHV	D	600	33/33	0.89	0.14	17,36,67,81	0
2	A1AHV	B	600	33/33	0.92	0.14	16,34,60,69	0
2	A1AHV	A	600	33/33	0.93	0.11	15,25,46,56	0
2	A1AHV	C	600	33/33	0.94	0.10	18,27,65,72	0

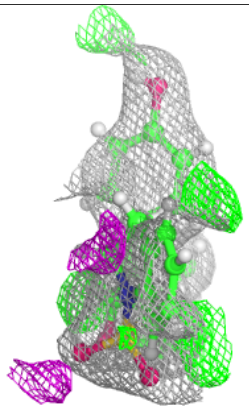
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AHV 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)

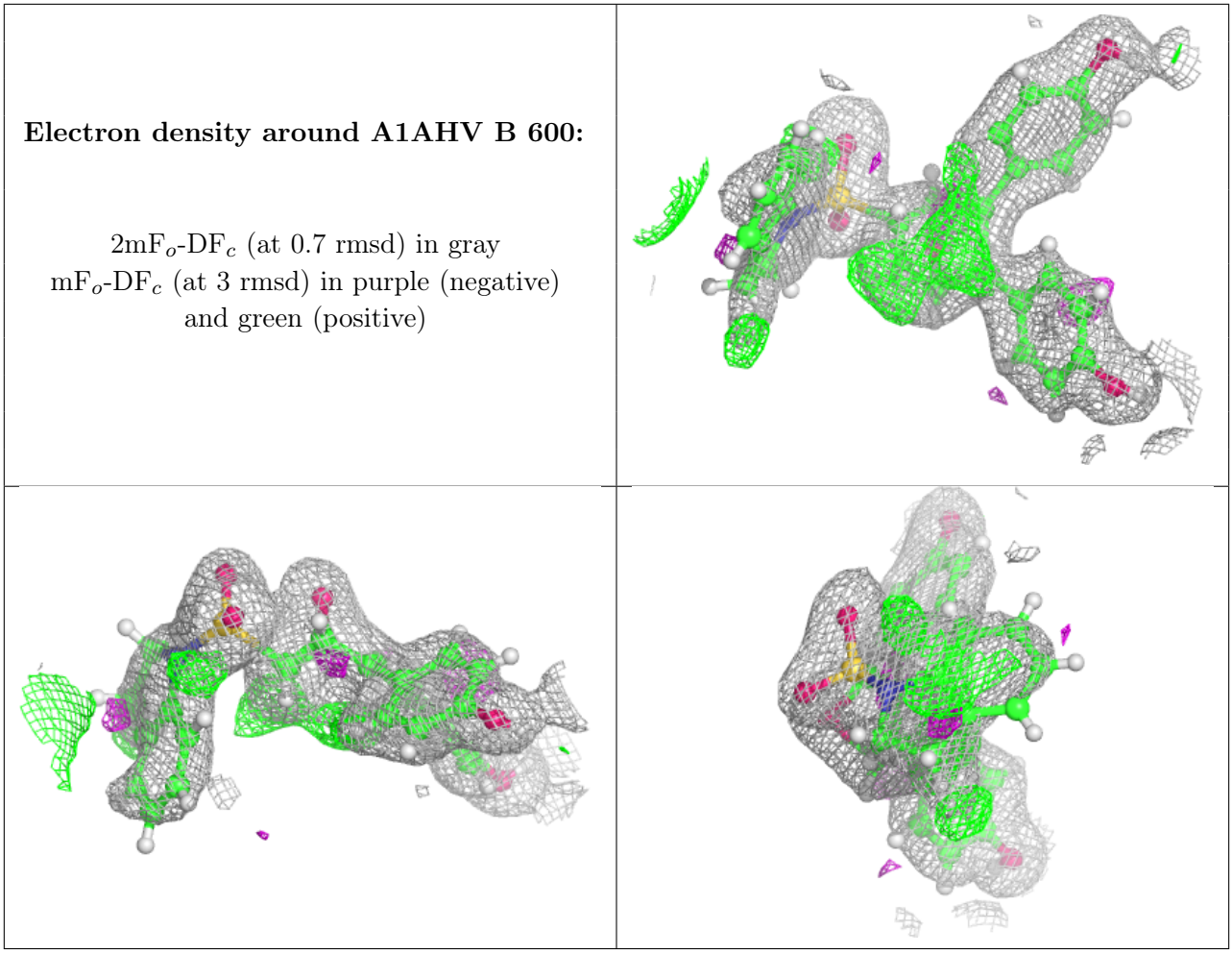






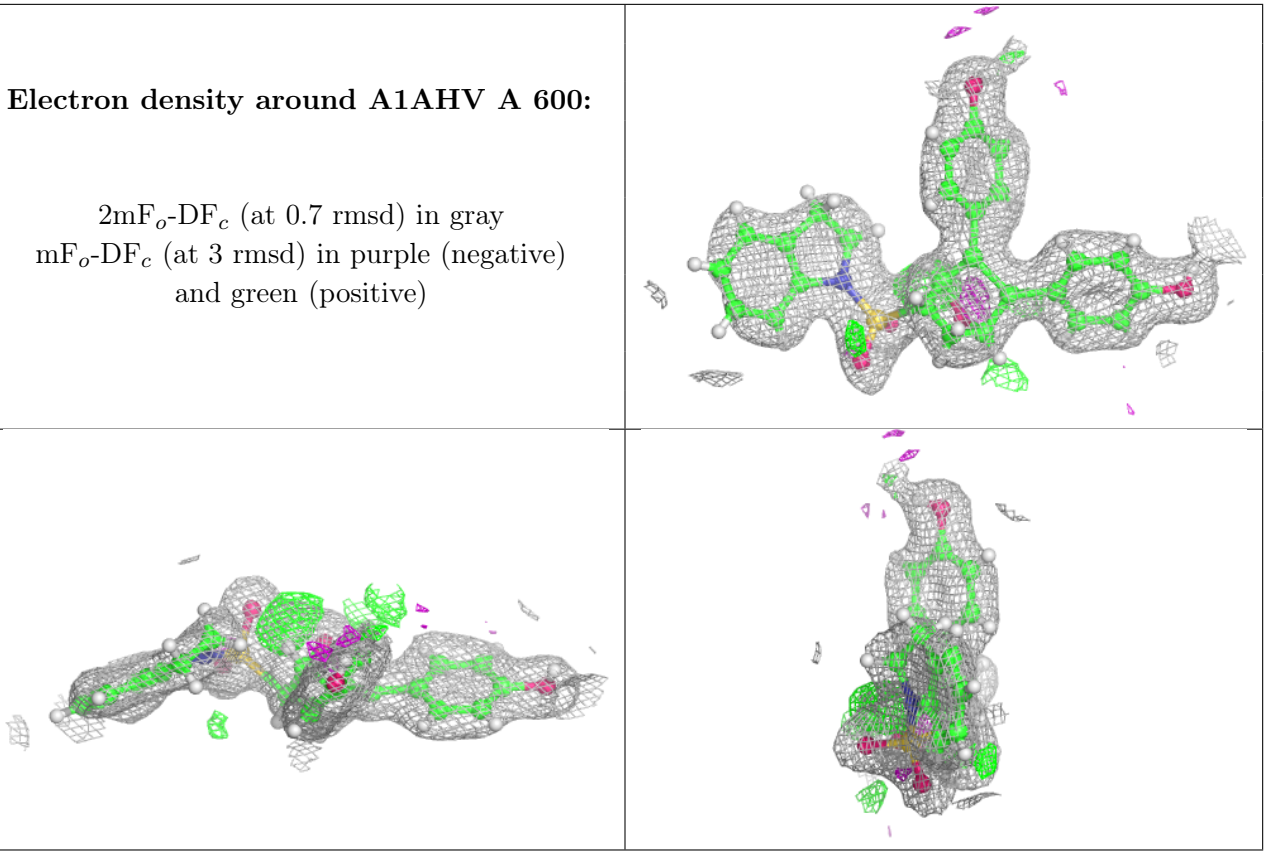
Electron density around A1AHV B 600:

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



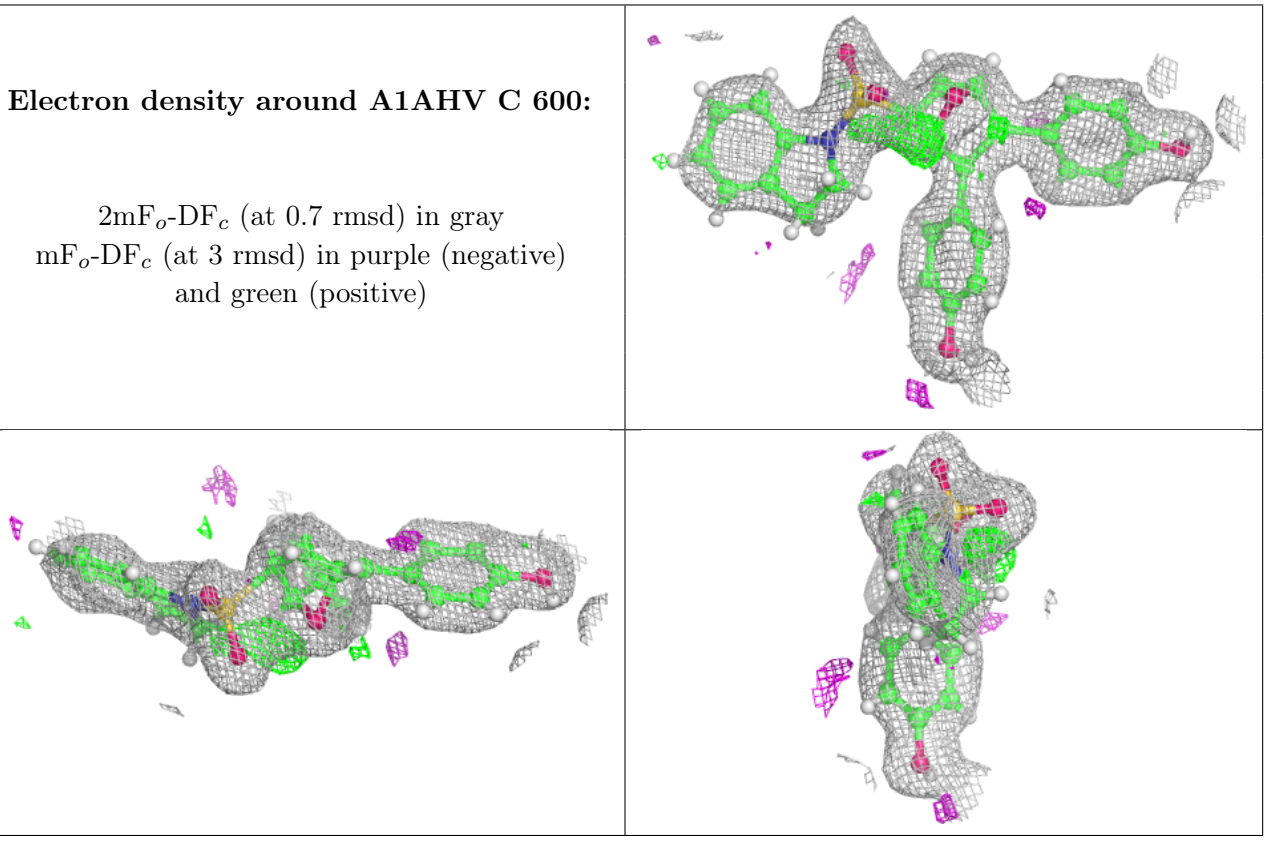
Electron density around A1AHV A 600:

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



Electron density around A1AHV 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)



6.5 Other polymers (i)

There are no such residues in this entry.