



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:44 PM UTC

PDB ID : 8VZP / pdb_00008vzp
Title : Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with k-403
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 : 2024-02-12
Resolution : 1.72 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

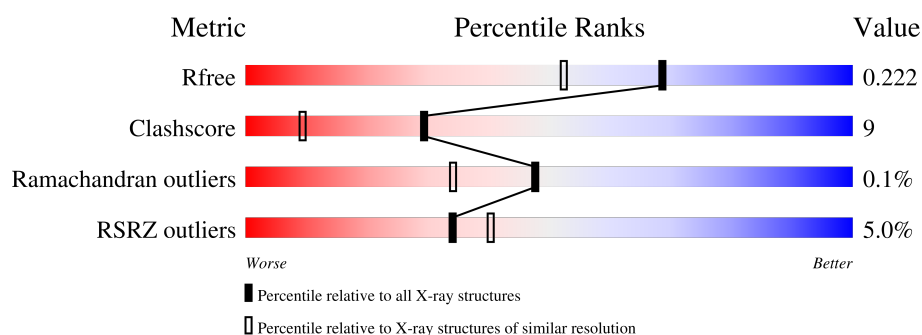
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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

Mol	Chain	Length	Quality of chain
1	A	242	5% 82% 13% • •
1	B	242	4% 81% 12% • 6%
1	C	242	5% 74% 20% • •
1	D	242	5% 73% 15% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14774 atoms, of which 7237 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.

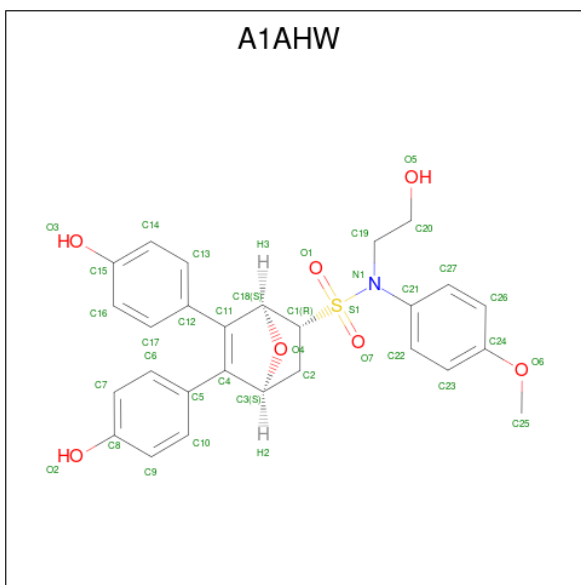
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	234	Total	C	H	N	O	S	0	1	0
			3611	1158	1805	311	320	17			
1	B	227	Total	C	H	N	O	S	0	0	0
			3541	1130	1777	302	316	16			
1	C	235	Total	C	H	N	O	S	0	1	0
			3668	1175	1832	313	331	17			
1	D	217	Total	C	H	N	O	S	0	0	0
			3419	1089	1722	291	301	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 (1S,2R,4S)-N-(2-hydroxyethyl)-5,6-bis(4-hydroxyphenyl)-N-(4-methoxyphenyl)-7-oxabicyclo[2.2.1]hept-5-ene-2-sulfonamide (CCD ID: A1AHW) (formula: C₂₇H₂₇NO₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 61	C 27	H 26	N 1	O 6	S 1	0	0
2	B	1	Total 58	C 26	H 24	N 1	O 6	S 1	0	0
2	C	1	Total 58	C 26	H 24	N 1	O 6	S 1	0	0
2	D	1	Total 63	C 27	H 27	N 1	O 7	S 1	0	0

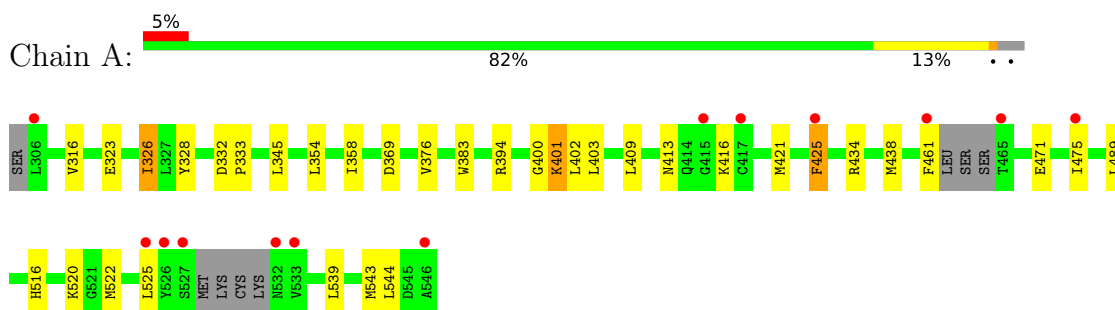
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	76	Total O 76 76	0	0
3	B	64	Total O 64 64	0	0
3	C	85	Total O 85 85	0	0
3	D	70	Total O 70 70	0	0

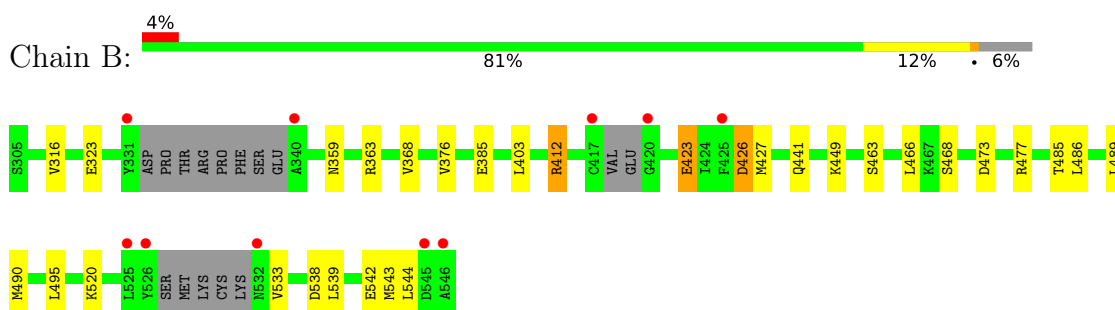
3 Residue-property plots [i](#)

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.

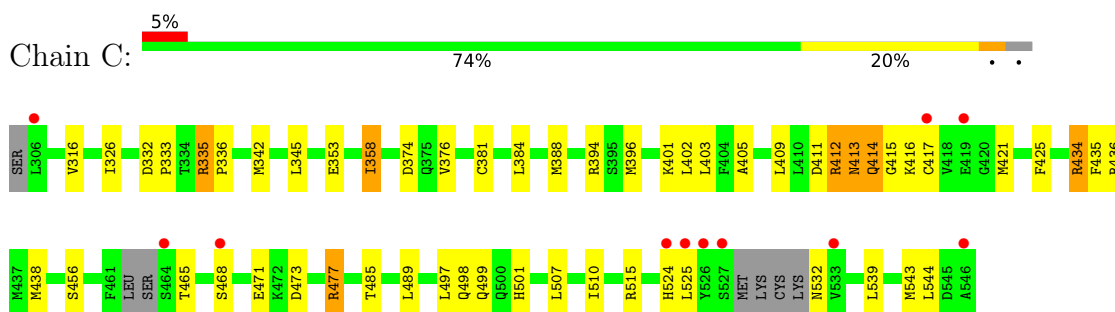
- Molecule 1: Estrogen receptor



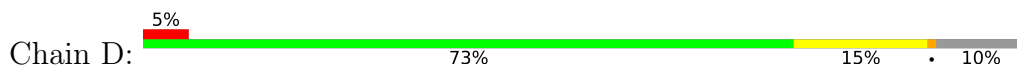
- Molecule 1: Estrogen receptor

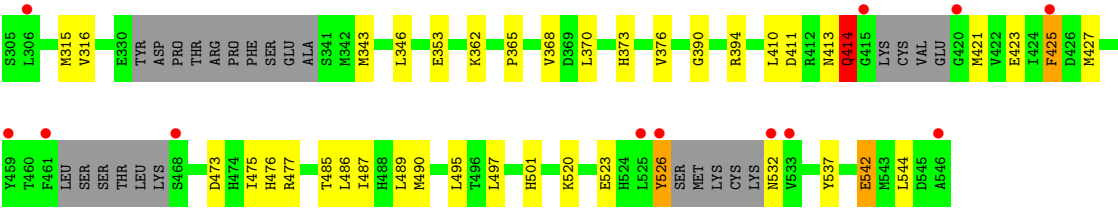


- Molecule 1: Estrogen receptor



- Molecule 1: Estrogen receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.56Å 58.91Å 93.24Å 86.76° 74.95° 63.05°	Depositor
Resolution (Å)	37.20 – 1.72 37.20 – 1.72	Depositor EDS
% Data completeness (in resolution range)	59.3 (37.20-1.72) 59.7 (37.20-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.181 , 0.222 0.182 , 0.222	Depositor DCC
R_{free} test set	3104 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.117 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14774	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1AHW

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	0.44	2/1850 (0.1%)	0.72	7/2507 (0.3%)
1	B	0.43	1/1793 (0.1%)	0.62	3/2425 (0.1%)
1	C	0.73	11/1881 (0.6%)	1.53	29/2548 (1.1%)
1	D	0.43	1/1724 (0.1%)	1.05	10/2330 (0.4%)
All	All	0.53	15/7248 (0.2%)	1.05	49/9810 (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	C	0	2
1	D	0	5
All	All	0	7

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	498	GLN	CD-OE1	-9.39	1.05	1.23
1	C	498	GLN	CD-NE2	7.97	1.50	1.33
1	C	498	GLN	N-CA	-7.75	1.36	1.46
1	A	401	LYS	CD-CE	7.45	1.74	1.52
1	B	426	ASP	C-O	-7.41	1.15	1.24
1	A	332	ASP	C-O	7.27	1.27	1.23
1	C	332	ASP	C-O	7.23	1.27	1.23
1	C	477	ARG	CZ-NH1	-7.09	1.22	1.32
1	C	498	GLN	C-O	7.08	1.32	1.23
1	C	499	GLN	N-CA	6.41	1.54	1.46
1	D	425	PHE	CE1-CZ	-5.90	1.21	1.38
1	C	414	GLN	CD-OE1	-5.88	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	498	GLN	CA-CB	-5.69	1.44	1.53
1	C	414	GLN	C-N	-5.53	1.27	1.33
1	C	416	LYS	CG-CD	5.48	1.68	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	498	GLN	CG-CD-OE1	29.54	179.88	120.80
1	D	425	PHE	CB-CG-CD2	-24.31	79.37	120.70
1	C	498	GLN	OE1-CD-NE2	-24.24	98.36	122.60
1	C	498	GLN	CG-CD-NE2	-23.18	81.64	116.40
1	C	414	GLN	CG-CD-NE2	-21.26	84.52	116.40
1	D	425	PHE	CB-CG-CD1	20.17	154.99	120.70
1	C	498	GLN	N-CA-CB	17.92	137.97	110.19
1	C	414	GLN	CG-CD-OE1	15.77	152.34	120.80
1	D	425	PHE	CD1-CG-CD2	-15.69	95.06	118.60
1	C	498	GLN	N-CA-C	-15.36	89.92	112.04
1	C	498	GLN	CB-CA-C	-15.14	82.85	110.56
1	C	477	ARG	CD-NE-CZ	13.83	143.76	124.40
1	C	414	GLN	OE1-CD-NE2	-13.76	108.84	122.60
1	C	498	GLN	CA-C-O	11.66	134.89	120.31
1	C	416	LYS	CG-CD-CE	11.18	137.01	111.30
1	D	542	GLU	CA-CB-CG	-10.54	93.03	114.10
1	B	423	GLU	N-CA-C	-8.49	102.10	111.36
1	B	423	GLU	CB-CA-C	-7.92	97.39	110.85
1	C	414	GLN	O-C-N	7.88	131.19	122.20
1	A	425	PHE	N-CA-C	-7.59	102.35	111.69
1	A	401	LYS	CB-CG-CD	-7.59	93.84	111.30
1	D	414	GLN	CG-CD-NE2	-7.34	105.39	116.40
1	C	414	GLN	CA-C-O	-7.17	112.17	120.20
1	C	477	ARG	N-CA-C	6.90	119.39	111.11
1	C	477	ARG	NE-CZ-NH2	-6.80	113.08	119.20
1	C	412	ARG	CB-CA-C	-6.71	100.24	110.92
1	D	526	TYR	N-CA-CB	6.35	121.29	110.50
1	D	542	GLU	CB-CG-CD	6.34	123.38	112.60
1	C	412	ARG	NE-CZ-NH2	-6.33	113.50	119.20
1	C	434	ARG	CA-CB-CG	-6.23	101.65	114.10
1	C	477	ARG	CG-CD-NE	-6.21	98.34	112.00
1	C	498	GLN	CA-C-N	5.96	128.27	120.28
1	C	498	GLN	C-N-CA	5.96	128.27	120.28
1	C	413	ASN	O-C-N	-5.91	115.31	122.11
1	A	401	LYS	N-CA-CB	-5.86	100.53	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	412	ARG	N-CA-C	5.76	118.33	111.71
1	C	335	ARG	CB-CG-CD	-5.76	98.06	111.30
1	A	326	ILE	CA-CB-CG1	-5.74	100.64	110.40
1	A	323	GLU	CA-CB-CG	5.71	125.53	114.10
1	C	412	ARG	CD-NE-CZ	5.64	132.29	124.40
1	C	498	GLN	O-C-N	-5.56	114.80	122.30
1	A	326	ILE	CG1-CB-CG2	5.51	127.24	110.70
1	A	425	PHE	CB-CG-CD1	-5.49	111.37	120.70
1	D	542	GLU	CG-CD-OE2	-5.43	105.92	118.40
1	C	358	ILE	CB-CG1-CD1	5.40	125.13	113.80
1	D	425	PHE	CG-CD1-CE1	5.35	129.80	120.70
1	C	335	ARG	CG-CD-NE	5.26	123.57	112.00
1	C	414	GLN	CB-CA-C	5.21	120.58	110.46
1	D	497	LEU	CD1-CG-CD2	-5.09	99.60	110.80

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	414	GLN	Sidechain
1	C	497	LEU	Peptide
1	D	413	ASN	Peptide
1	D	414	GLN	Sidechain
1	D	425	PHE	Sidechain
1	D	526	TYR	Sidechain
1	D	542	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	1805	1796	32	2
1	B	1764	1777	1777	21	2
1	C	1836	1832	1823	46	0
1	D	1697	1722	1722	27	0
2	A	35	26	0	4	0
2	B	34	24	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	34	24	0	2	0
2	D	36	27	0	3	0
3	A	76	0	0	4	0
3	B	64	0	0	4	0
3	C	85	0	0	3	2
3	D	70	0	0	5	2
All	All	7537	7237	7118	123	4

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 9.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LYS:CD	1:A:401:LYS:CE	1.74	1.57
1:B:473:ASP:OD1	1:B:477:ARG:NH1	1.82	1.10
1:D:411:ASP:N	1:D:414:GLN:OE1	2.04	0.90
1:D:532:ASN:N	3:D:702:HOH:O	2.05	0.89
1:C:381:CYS:SG	3:D:766:HOH:O	2.32	0.86
1:D:370:LEU:HD11	1:D:475:ILE:HD11	1.58	0.86
1:D:520:LYS:NZ	1:D:523:GLU:OE2	2.11	0.83
1:C:539:LEU:HD11	1:C:543:MET:HE2	1.62	0.82
1:B:412:ARG:NH1	1:B:426:ASP:OD1	2.16	0.79
1:A:401:LYS:CE	1:A:401:LYS:CG	2.61	0.78
1:A:401:LYS:CD	1:A:401:LYS:NZ	2.47	0.78
1:C:485:THR:O	1:C:489:LEU:HD13	1.85	0.76
1:C:473:ASP:OD1	1:C:477:ARG:NH1	2.18	0.76
1:C:316:VAL:HG21	1:C:489:LEU:HD11	1.68	0.75
1:C:525:LEU:HD12	2:C:601:A1AHW:C24	2.17	0.75
1:C:401:LYS:HE2	1:C:411:ASP:OD1	1.91	0.71
1:C:501:HIS:CD2	1:D:501:HIS:CE1	2.80	0.70
1:B:441:GLN:OE1	3:B:701:HOH:O	2.08	0.69
1:C:539:LEU:CD1	1:C:543:MET:HE2	2.22	0.69
1:A:354:LEU:O	1:A:358:ILE:HD12	1.93	0.69
1:D:353:GLU:OE1	3:D:703:HOH:O	2.10	0.67
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.78	0.66
1:D:362:LYS:NZ	3:D:701:HOH:O	2.03	0.65
1:A:403:LEU:HD13	1:A:409:LEU:HD13	1.79	0.64
1:C:532:ASN:N	3:C:703:HOH:O	2.30	0.64
1:C:438:MET:HE1	1:C:507:LEU:HD23	1.80	0.64
1:A:461:PHE:O	3:A:701:HOH:O	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:HIS:NE2	1:D:501:HIS:CE1	2.67	0.63
1:D:343:MET:HA	1:D:343:MET:HE2	1.81	0.62
1:D:485:THR:O	1:D:489:LEU:HD13	1.99	0.62
1:B:485:THR:O	1:B:489:LEU:HD23	1.99	0.62
1:C:342:MET:HE1	1:C:417:CYS:HB2	1.80	0.62
1:B:363:ARG:NH1	3:B:703:HOH:O	2.26	0.62
1:A:525:LEU:HD22	2:A:601:A1AHW:C24	2.30	0.61
1:A:369:ASP:OD2	3:A:702:HOH:O	2.16	0.61
1:B:385:GLU:HG3	3:B:731:HOH:O	1.98	0.60
1:C:413:ASN:N	1:C:413:ASN:OD1	2.32	0.60
1:C:326:ILE:HD12	1:C:394:ARG:HD3	1.83	0.60
1:C:412:ARG:HA	1:C:425:PHE:CE1	2.36	0.60
1:A:525:LEU:HD22	2:A:601:A1AHW:O6	2.02	0.60
1:A:326:ILE:HD13	3:A:737:HOH:O	2.01	0.59
1:C:376:VAL:HG22	1:C:544:LEU:HD12	1.85	0.59
1:C:342:MET:CE	1:C:417:CYS:HB2	2.33	0.59
1:C:411:ASP:HB3	1:C:413:ASN:OD1	2.03	0.58
1:A:376:VAL:HG22	1:A:544:LEU:HD12	1.86	0.58
1:C:415:GLY:O	1:C:421:MET:HB2	2.04	0.57
1:B:427:MET:HE1	1:B:520:LYS:HG3	1.87	0.57
1:A:421:MET:O	1:A:425:PHE:HB2	2.05	0.56
1:B:368:VAL:HG22	3:B:710:HOH:O	2.05	0.56
1:B:486:LEU:O	1:B:490:MET:HG3	2.05	0.56
1:D:476:HIS:HB3	1:D:477:ARG:HH21	1.70	0.56
1:C:374:ASP:OD1	1:C:471:GLU:OE1	2.23	0.55
1:A:520:LYS:NZ	3:A:703:HOH:O	2.38	0.55
1:B:466:LEU:C	1:B:466:LEU:HD23	2.31	0.55
1:A:413:ASN:HA	1:A:416:LYS:NZ	2.22	0.54
1:C:501:HIS:CD2	1:D:501:HIS:ND1	2.76	0.54
1:D:316:VAL:HG21	1:D:489:LEU:HD11	1.91	0.53
1:C:316:VAL:CG2	1:C:489:LEU:HD11	2.39	0.51
1:A:358:ILE:HG23	1:A:544:LEU:HD23	1.91	0.51
1:D:410:LEU:HA	1:D:414:GLN:OE1	2.11	0.51
1:D:490:MET:HB3	1:D:495:LEU:HD22	1.92	0.51
1:A:539:LEU:HG	1:A:543:MET:HE3	1.93	0.51
1:D:423:GLU:O	1:D:427:MET:HG3	2.12	0.50
1:C:438:MET:HE1	1:C:507:LEU:CD2	2.41	0.49
1:B:403:LEU:O	1:B:403:LEU:HD23	2.13	0.49
1:C:501:HIS:CE1	1:D:487:ILE:HG21	2.47	0.49
1:C:473:ASP:CG	1:C:477:ARG:NH1	2.69	0.49
1:C:326:ILE:HD13	3:C:750:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:HIS:ND1	1:D:537:TYR:OH	2.45	0.49
1:A:326:ILE:HD12	1:A:394:ARG:HD3	1.96	0.48
1:B:412:ARG:NH1	1:B:426:ASP:CG	2.70	0.48
1:B:538:ASP:O	1:B:542:GLU:HG3	2.14	0.47
1:A:400:GLY:C	1:A:401:LYS:HG3	2.38	0.47
1:B:490:MET:HB3	1:B:495:LEU:HD22	1.97	0.47
1:C:335:ARG:HA	1:C:336:PRO:C	2.40	0.47
1:B:323:GLU:OE1	1:B:449:LYS:NZ	2.37	0.47
1:A:333:PRO:HB3	1:A:345:LEU:HD21	1.97	0.46
1:A:516:HIS:O	1:A:520:LYS:HG2	2.14	0.46
1:A:421:MET:SD	2:A:601:A1AHW:C19	3.04	0.46
1:A:403:LEU:CD1	1:A:409:LEU:HD13	2.46	0.45
1:C:465:THR:HG23	1:C:468:SER:H	1.81	0.45
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.97	0.45
1:C:384:LEU:O	1:C:388:MET:HG3	2.17	0.45
1:C:402:LEU:HD12	1:C:425:PHE:CE2	2.51	0.45
2:D:601:A1AHW:O5	2:D:601:A1AHW:O7	2.35	0.45
1:A:383:TRP:CZ2	1:A:522:MET:HE1	2.51	0.45
1:C:403:LEU:HD12	1:C:405:ALA:O	2.16	0.45
1:D:421:MET:HG2	2:D:601:A1AHW:C20	2.46	0.45
1:A:421:MET:SD	2:A:601:A1AHW:O1	2.75	0.45
1:A:402:LEU:HD12	1:A:425:PHE:CE2	2.52	0.45
1:C:524:HIS:O	1:C:525:LEU:C	2.60	0.44
1:C:403:LEU:HD13	1:C:409:LEU:HD13	2.00	0.44
2:D:601:A1AHW:O7	2:D:601:A1AHW:C20	2.66	0.44
1:C:525:LEU:C	1:C:525:LEU:HD23	2.43	0.44
1:B:463:SER:HB3	1:B:468:SER:OG	2.18	0.43
1:B:423:GLU:OE2	1:B:520:LYS:HE3	2.18	0.43
1:B:533:VAL:O	1:B:533:VAL:HG12	2.17	0.43
1:C:456:SER:HA	1:C:515:ARG:NH2	2.33	0.43
1:C:358:ILE:HG23	1:C:544:LEU:HD23	2.01	0.43
1:A:401:LYS:CD	1:A:401:LYS:HZ2	2.30	0.43
1:C:435:PHE:HE1	1:C:510:ILE:HG21	1.83	0.43
1:C:353:GLU:OE1	2:C:601:A1AHW:O2	2.37	0.43
1:C:434:ARG:O	1:C:434:ARG:HG3	2.18	0.43
1:A:326:ILE:HD13	1:A:326:ILE:HA	1.75	0.42
1:C:434:ARG:NH1	3:C:701:HOH:O	2.18	0.42
1:A:471:GLU:O	1:A:475:ILE:HG13	2.19	0.42
1:C:411:ASP:CB	1:C:413:ASN:OD1	2.66	0.42
1:A:413:ASN:HA	1:A:416:LYS:HZ2	1.84	0.42
1:B:376:VAL:CG2	1:B:544:LEU:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:VAL:HG22	3:D:722:HOH:O	2.19	0.42
1:C:396:MET:O	1:C:436:ARG:HD3	2.20	0.42
1:D:486:LEU:O	1:D:490:MET:HG3	2.19	0.42
1:D:343:MET:CE	1:D:346:LEU:HD12	2.50	0.41
1:C:376:VAL:HG22	1:C:544:LEU:CD1	2.49	0.41
1:D:315:MET:SD	1:D:365:PRO:HG2	2.60	0.41
1:B:539:LEU:O	1:B:543:MET:HG3	2.20	0.41
1:C:333:PRO:HG3	1:C:345:LEU:HD11	2.02	0.41
1:C:501:HIS:HD2	1:D:501:HIS:ND1	2.16	0.40
1:A:434:ARG:O	1:A:438:MET:HG3	2.21	0.40
1:D:390:GLY:O	1:D:394:ARG:HG3	2.21	0.40
1:D:473:ASP:O	1:D:477:ARG:HG2	2.21	0.40
1:A:316:VAL:HG21	1:A:489:LEU:HD21	2.03	0.40
1:A:401:LYS:CG	1:A:401:LYS:NZ	2.84	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TYR:OH	1:B:359:ASN:ND2[1_645]	1.81	0.39
1:A:328:TYR:OH	1:B:359:ASN:HD21[1_645]	1.54	0.06
3:C:774:HOH:O	3:D:760:HOH:O[1_655]	2.14	0.06
3:C:774:HOH:O	3:D:719:HOH:O[1_655]	2.17	0.03

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	229/242 (95%)	227 (99%)	2 (1%)	0	100	100
1	B	219/242 (90%)	217 (99%)	2 (1%)	0	100	100
1	C	230/242 (95%)	225 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	207/242 (86%)	205 (99%)	1 (0%)	1 (0%)	24	11
All	All	885/968 (91%)	874 (99%)	10 (1%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	414	GLN

5.3.2 Protein sidechains [i](#)

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

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 oligosaccharides 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	A1AHW	D	601	-	39,40,40	1.78	5 (12%)	48,59,59	1.27	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1AHW	A	601	-	38,39,40	1.78	6 (15%)	47,58,59	1.30	5 (10%)
2	A1AHW	B	601	-	36,38,40	1.90	5 (13%)	47,57,59	1.31	6 (12%)
2	A1AHW	C	601	-	36,38,40	1.97	5 (13%)	47,57,59	1.45	5 (10%)

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	A1AHW	D	601	-	-	8/27/53/53	0/6/5/5
2	A1AHW	A	601	-	-	6/26/52/53	0/6/5/5
2	A1AHW	B	601	-	-	10/24/50/53	0/6/5/5
2	A1AHW	C	601	-	-	5/24/50/53	0/6/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	A1AHW	C19-N1	-5.89	1.36	1.47
2	D	601	A1AHW	S1-N1	5.80	1.79	1.67
2	D	601	A1AHW	C1-S1	5.65	1.89	1.77
2	B	601	A1AHW	C19-N1	-5.65	1.36	1.47
2	C	601	A1AHW	O1-S1	5.40	1.48	1.43
2	C	601	A1AHW	C1-S1	5.30	1.88	1.77
2	B	601	A1AHW	C1-S1	5.26	1.88	1.77
2	A	601	A1AHW	C1-S1	5.26	1.88	1.77
2	B	601	A1AHW	O7-S1	5.17	1.47	1.43
2	A	601	A1AHW	S1-N1	5.09	1.78	1.67
2	A	601	A1AHW	O1-S1	5.05	1.47	1.43
2	D	601	A1AHW	O7-S1	4.95	1.47	1.43
2	B	601	A1AHW	S1-N1	4.26	1.76	1.67
2	A	601	A1AHW	O7-S1	4.14	1.47	1.43
2	C	601	A1AHW	O7-S1	4.14	1.47	1.43
2	C	601	A1AHW	S1-N1	3.99	1.75	1.67
2	B	601	A1AHW	O1-S1	3.74	1.46	1.43
2	D	601	A1AHW	O1-S1	3.37	1.46	1.43
2	A	601	A1AHW	C21-N1	-3.01	1.40	1.44
2	D	601	A1AHW	C21-N1	-2.41	1.41	1.44
2	A	601	A1AHW	O4-C18	-2.24	1.40	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	A1AHW	O7-S1-O1	5.50	123.32	119.17
2	A	601	A1AHW	O7-S1-O1	4.67	122.69	119.17
2	D	601	A1AHW	O4-C3-C2	-4.52	95.92	104.73
2	B	601	A1AHW	O4-C3-C2	-4.11	96.70	104.73
2	C	601	A1AHW	C19-N1-S1	-3.85	112.70	118.23
2	A	601	A1AHW	O4-C3-C2	-3.71	97.49	104.73
2	C	601	A1AHW	O4-C3-C2	-3.65	97.61	104.73
2	D	601	A1AHW	C10-C5-C4	-3.42	116.47	120.91
2	D	601	A1AHW	O7-S1-N1	3.08	111.06	107.39
2	A	601	A1AHW	C20-C19-N1	3.05	120.21	111.71
2	B	601	A1AHW	C10-C5-C4	-2.96	117.08	120.91
2	C	601	A1AHW	C10-C5-C4	-2.92	117.11	120.91
2	B	601	A1AHW	O7-S1-O1	2.77	121.26	119.17
2	B	601	A1AHW	C19-N1-S1	-2.65	114.42	118.23
2	B	601	A1AHW	O7-S1-C1	2.64	111.00	107.79
2	B	601	A1AHW	O1-S1-N1	2.40	109.88	107.14
2	D	601	A1AHW	C6-C5-C4	2.21	123.78	120.91
2	C	601	A1AHW	C3-C2-C1	-2.18	98.69	100.61
2	A	601	A1AHW	C3-C2-C1	-2.11	98.75	100.61
2	D	601	A1AHW	C3-C2-C1	-2.07	98.78	100.61
2	A	601	A1AHW	C17-C12-C11	-2.02	118.29	120.91

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	A1AHW	C19-N1-S1-O7
2	A	601	A1AHW	C21-N1-S1-O7
2	B	601	A1AHW	C19-N1-S1-C1
2	B	601	A1AHW	C19-N1-S1-O1
2	C	601	A1AHW	C19-N1-S1-C1
2	C	601	A1AHW	C19-N1-S1-O7
2	C	601	A1AHW	C21-N1-S1-C1
2	D	601	A1AHW	C20-C19-N1-C21
2	D	601	A1AHW	C20-C19-N1-S1
2	D	601	A1AHW	C19-N1-S1-O1
2	D	601	A1AHW	C19-N1-S1-O7
2	D	601	A1AHW	C21-N1-S1-O1
2	A	601	A1AHW	C20-C19-N1-C21
2	A	601	A1AHW	C22-C21-N1-S1
2	D	601	A1AHW	C22-C21-N1-S1
2	D	601	A1AHW	C27-C21-N1-S1
2	B	601	A1AHW	C23-C24-O6-C25

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Mol	Chain	Res	Type	Atoms
2	B	601	A1AHW	C26-C24-O6-C25
2	A	601	A1AHW	C19-N1-S1-C1
2	D	601	A1AHW	C19-N1-S1-C1
2	C	601	A1AHW	C21-N1-S1-O7
2	B	601	A1AHW	C19-N1-S1-O7
2	B	601	A1AHW	C27-C21-N1-S1
2	C	601	A1AHW	C22-C21-N1-S1
2	B	601	A1AHW	C21-N1-S1-O1
2	B	601	A1AHW	C18-C11-C12-C13
2	B	601	A1AHW	C18-C11-C12-C17
2	B	601	A1AHW	C22-C21-N1-S1
2	A	601	A1AHW	C27-C21-N1-S1

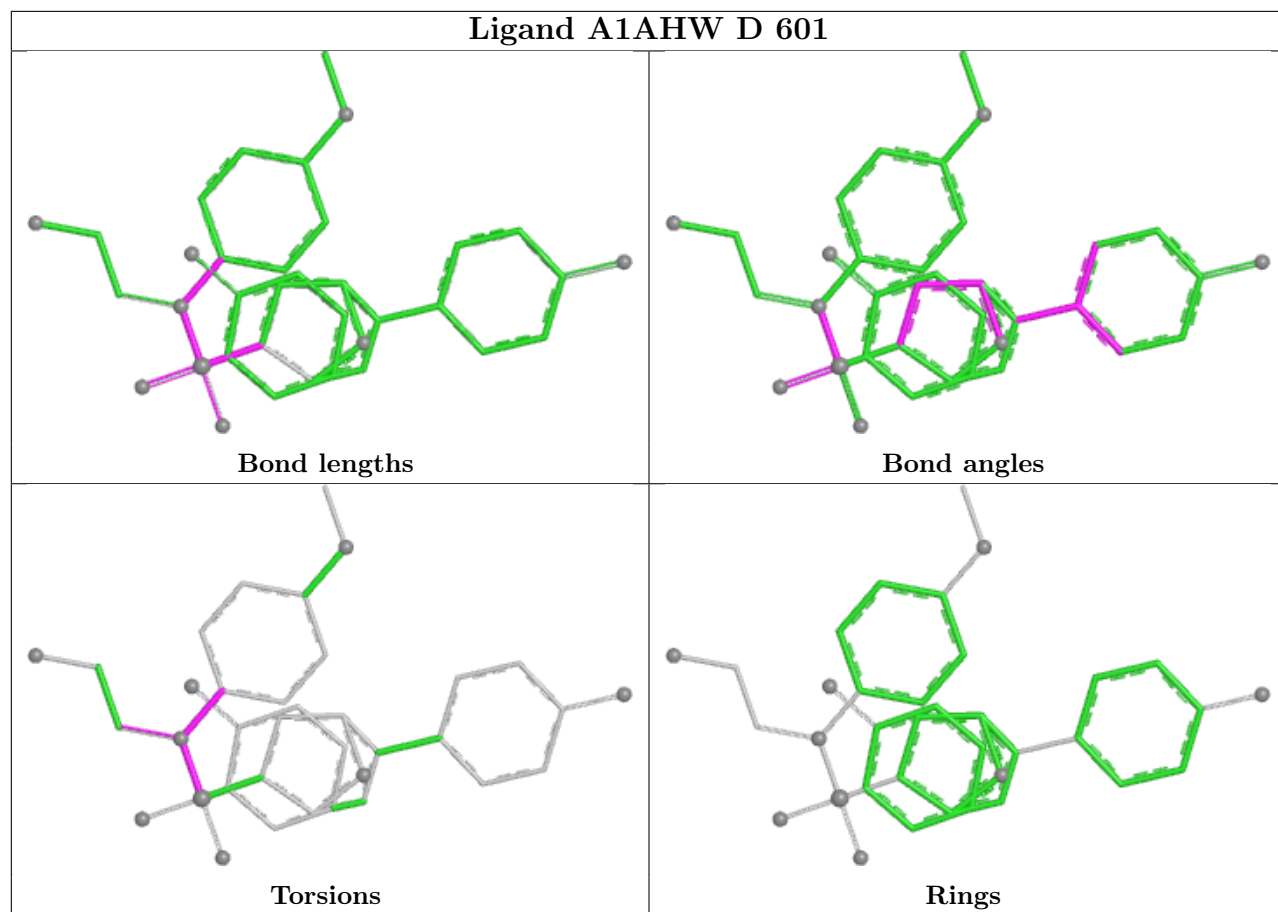
There are no ring outliers.

3 monomers are involved in 9 short contacts:

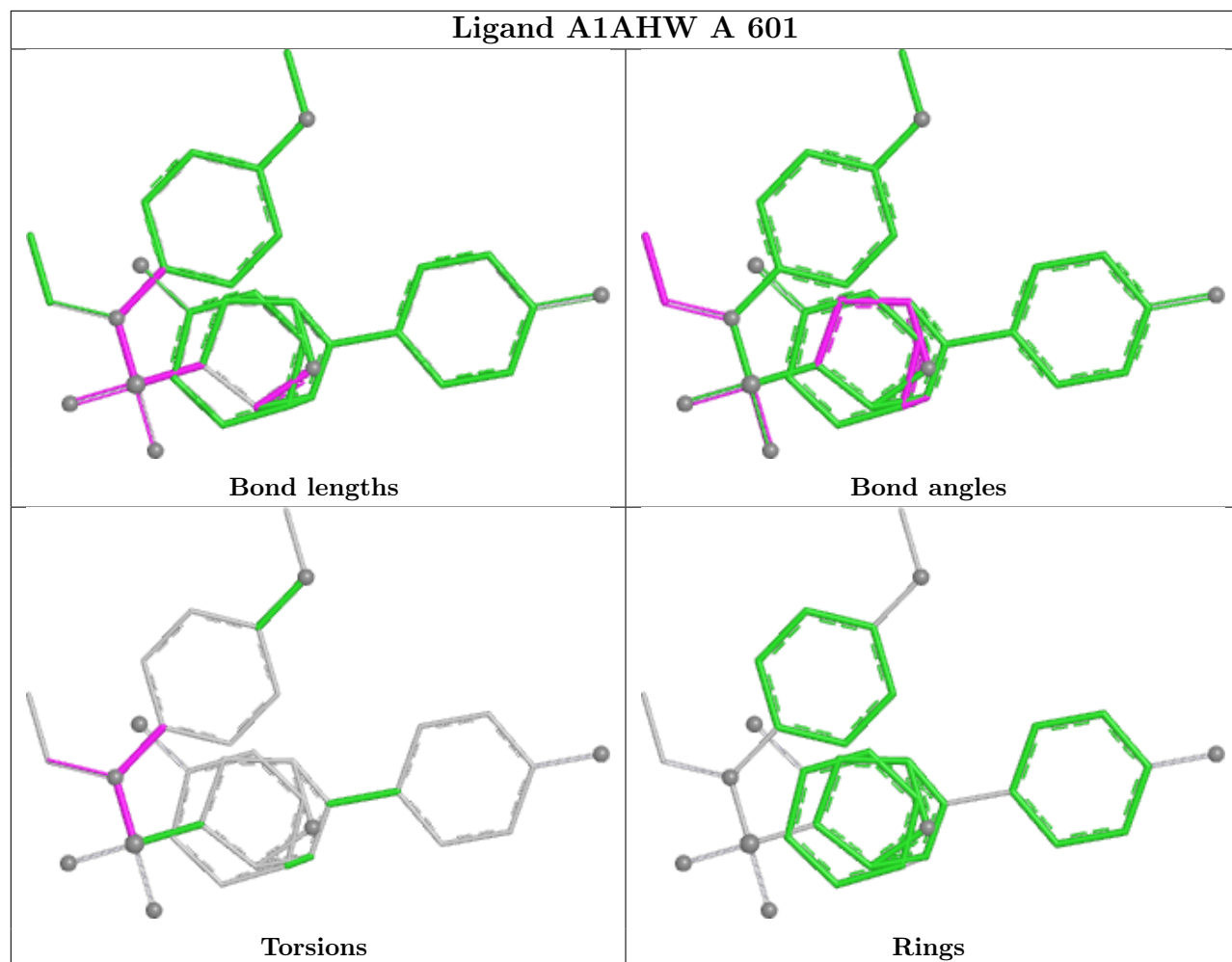
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	A1AHW	3	0
2	A	601	A1AHW	4	0
2	C	601	A1AHW	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

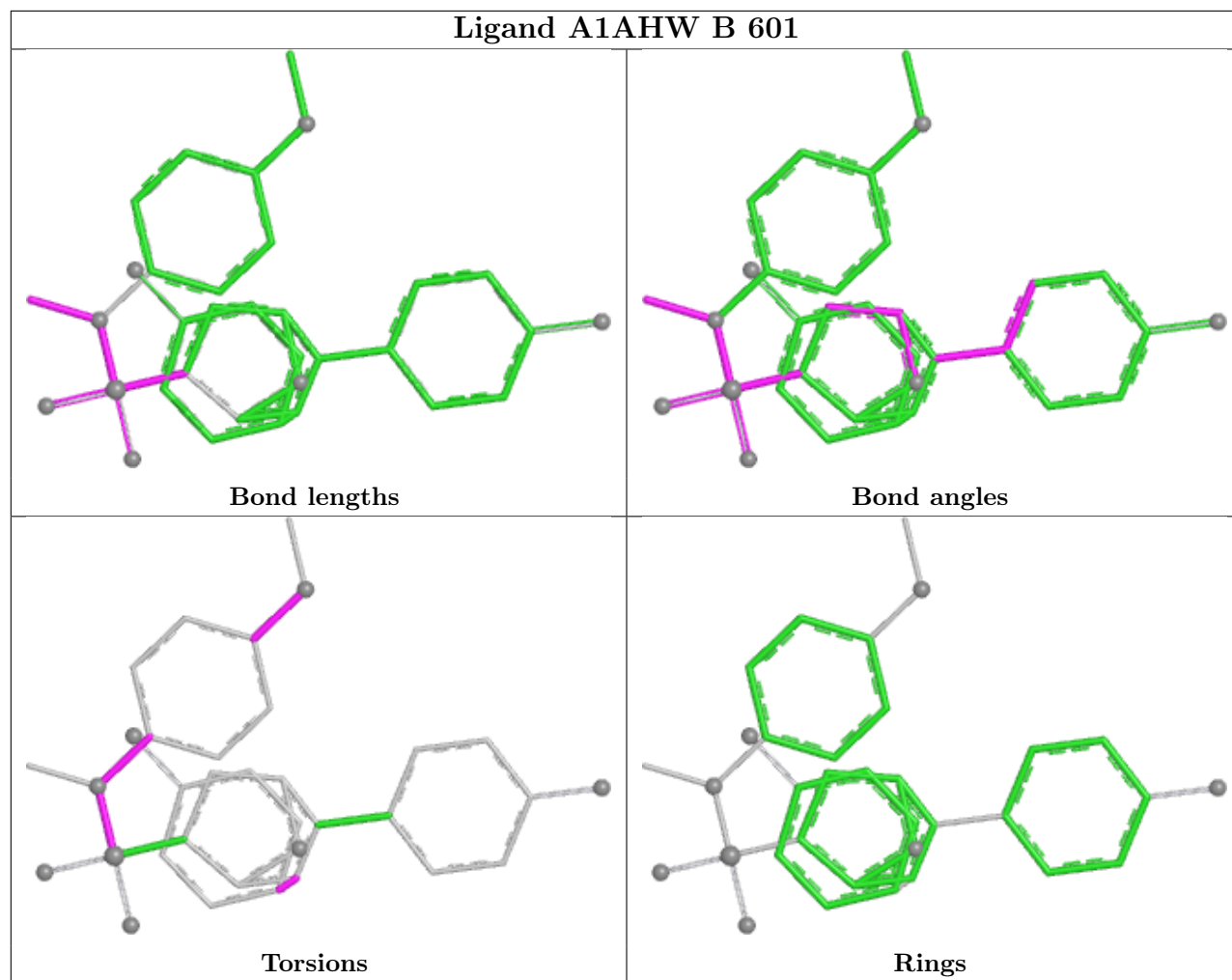
Ligand A1AHW D 601

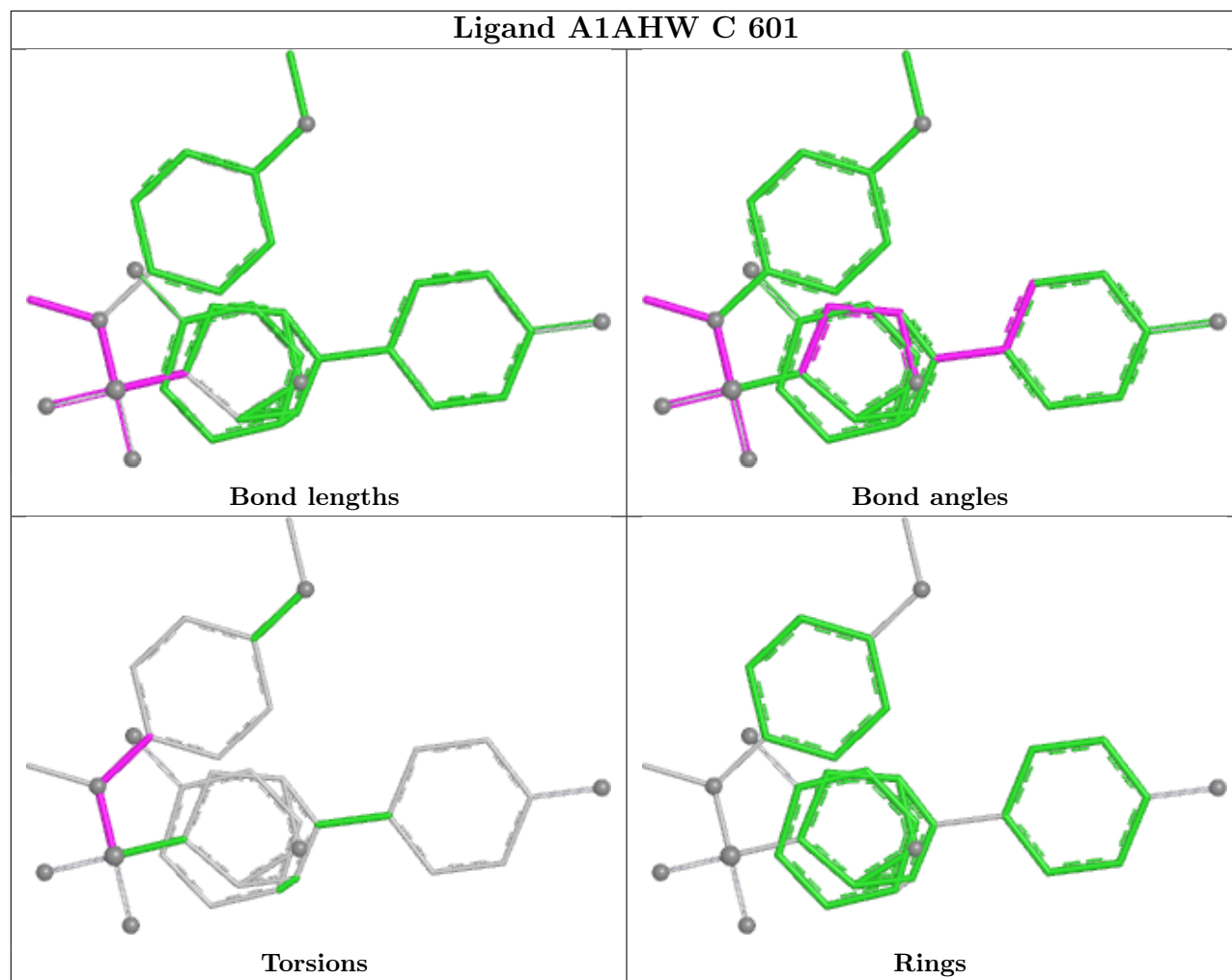


Ligand A1AHW A 601



Ligand A1AHW B 601





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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	234/242 (96%)	0.22	13 (5%) 30 36	23, 44, 74, 92	0
1	B	227/242 (93%)	0.09	10 (4%) 39 46	24, 40, 77, 104	0
1	C	235/242 (97%)	0.16	11 (4%) 36 42	23, 41, 76, 99	0
1	D	217/242 (89%)	0.18	12 (5%) 30 37	25, 41, 78, 103	0
All	All	913/968 (94%)	0.16	46 (5%) 34 40	23, 41, 77, 104	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	LEU	5.1
1	A	532	ASN	4.1
1	B	526	TYR	3.5
1	D	420	GLY	3.4
1	C	526	TYR	3.2
1	C	306	LEU	3.2
1	C	527	SER	3.1
1	C	533	VAL	3.1
1	B	425	PHE	3.0
1	D	461	PHE	3.0
1	D	459	TYR	3.0
1	A	425	PHE	2.9
1	B	532	ASN	2.8
1	B	420	GLY	2.8
1	D	468	SER	2.8
1	B	331	TYR	2.7
1	C	417	CYS	2.7
1	A	527	SER	2.6
1	A	415	GLY	2.6
1	A	525	LEU	2.6
1	B	546	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	417	CYS	2.6
1	C	468	SER	2.5
1	D	306	LEU	2.5
1	A	533	VAL	2.5
1	A	546	ALA	2.5
1	A	526	TYR	2.5
1	D	415	GLY	2.4
1	C	419	GLU	2.3
1	C	524	HIS	2.3
1	D	532	ASN	2.3
1	B	340	ALA	2.2
1	A	461	PHE	2.2
1	C	546	ALA	2.2
1	D	546	ALA	2.2
1	C	464	SER	2.2
1	B	545	ASP	2.1
1	D	533	VAL	2.1
1	A	417	CYS	2.1
1	C	525	LEU	2.1
1	D	525	LEU	2.1
1	D	526	TYR	2.1
1	A	475	ILE	2.1
1	B	525	LEU	2.0
1	A	465	THR	2.0
1	D	425	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

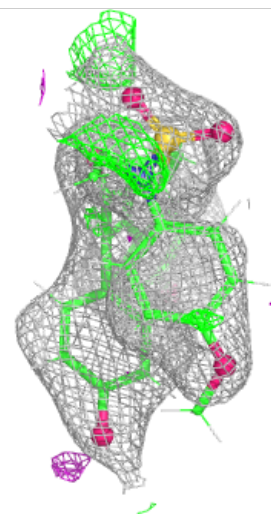
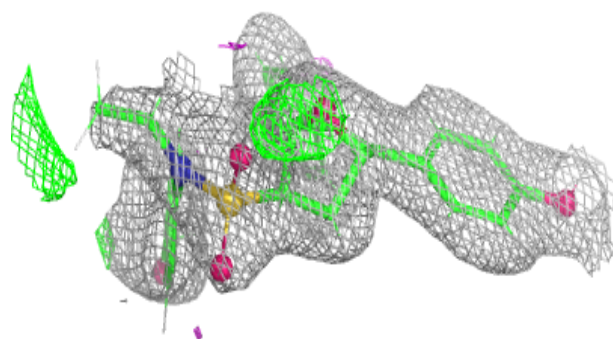
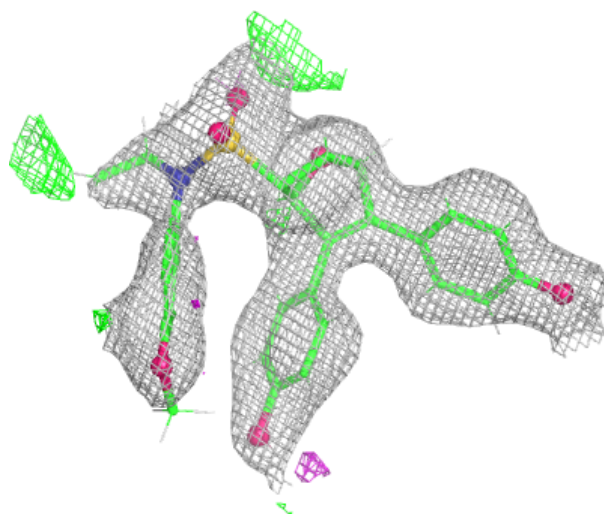
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1AHW	A	601	35/36	0.93	0.10	24,37,64,66	61
2	A1AHW	B	601	34/36	0.93	0.10	28,42,62,68	0
2	A1AHW	D	601	36/36	0.94	0.09	25,47,64,77	0
2	A1AHW	C	601	34/36	0.96	0.08	25,40,61,64	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.

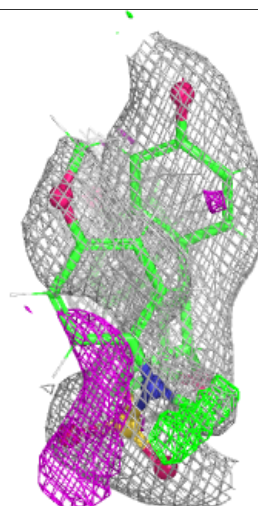
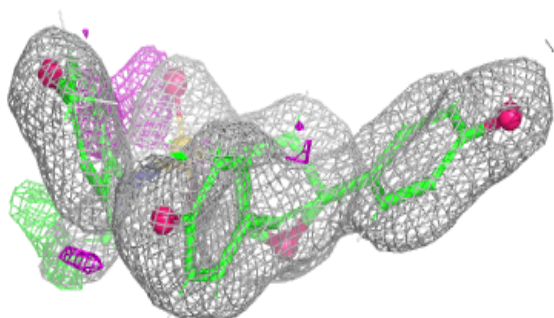
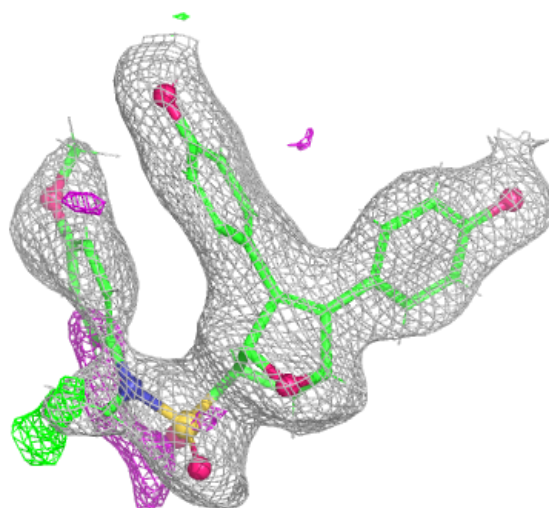
Electron density around A1AHW A 601:

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



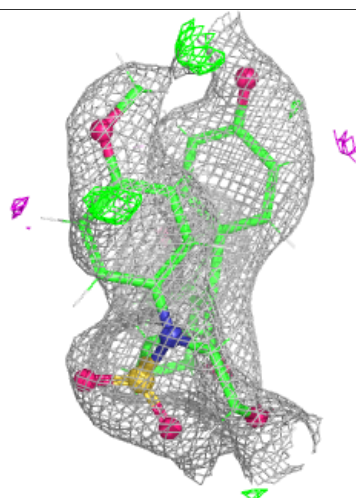
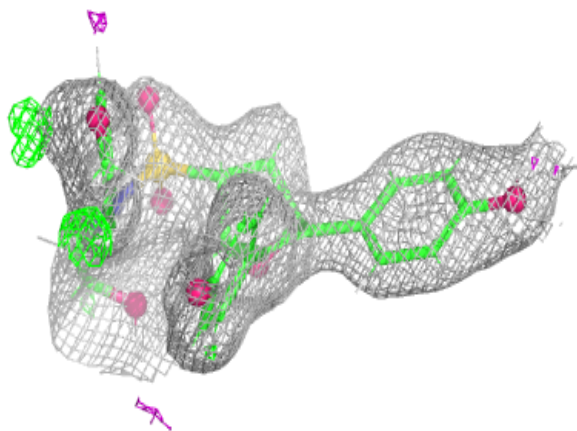
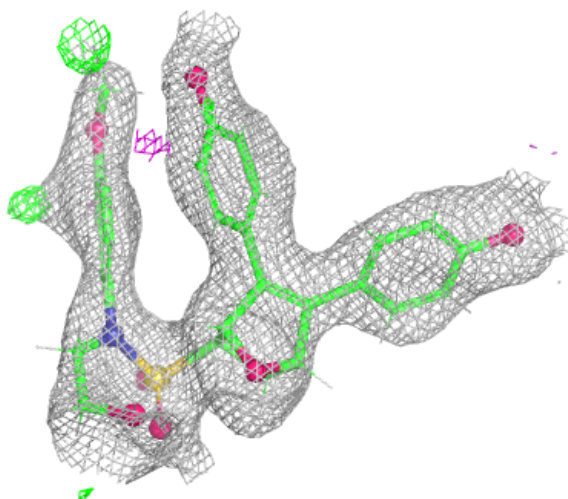
Electron density around A1AHW B 601:

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



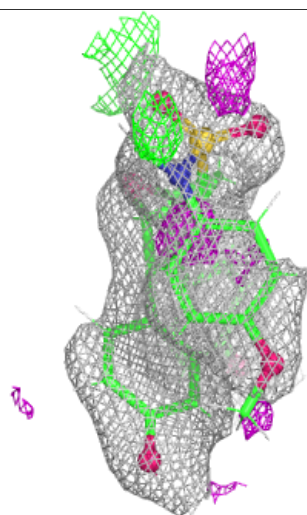
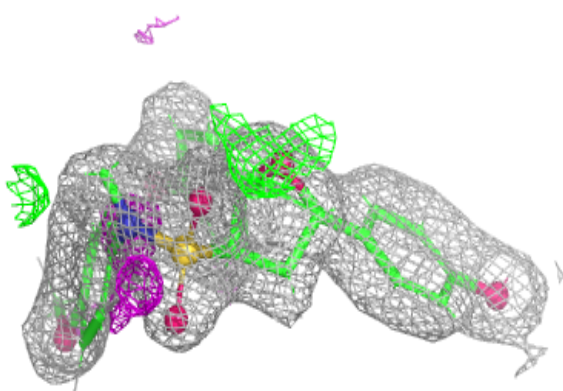
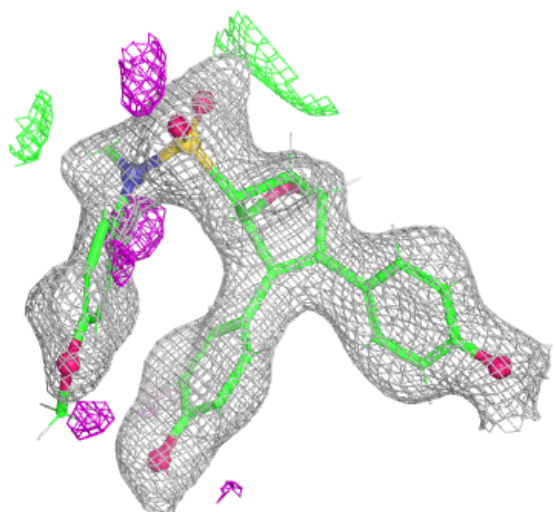
Electron density around A1AHW D 601:

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



Electron density around A1AHW C 601:

$2mF_o-DF_c$ (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.