Full wwPDB X-ray Structure Validation Report ⓘ

Jun 4, 2024 – 08:13 PM EDT

PDB ID	:	8VZ1
Title	:	Crystal Structure of the ER-alpha Ligand-binding Domain (L372S, L536S) in complex with k-409
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	:	1.82 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:

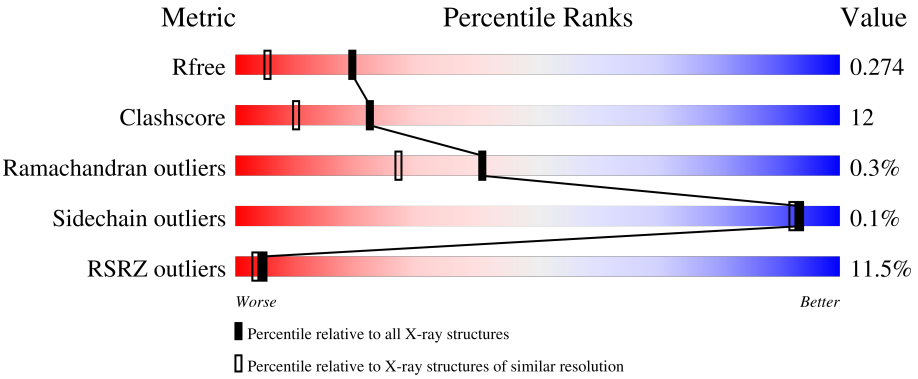
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.82 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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	12% 76% 21%
1	B	243	9% 74% 18% 8%
1	C	243	9% 78% 16%
1	D	243	14% 72% 19% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 14836 atoms, of which 7256 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.

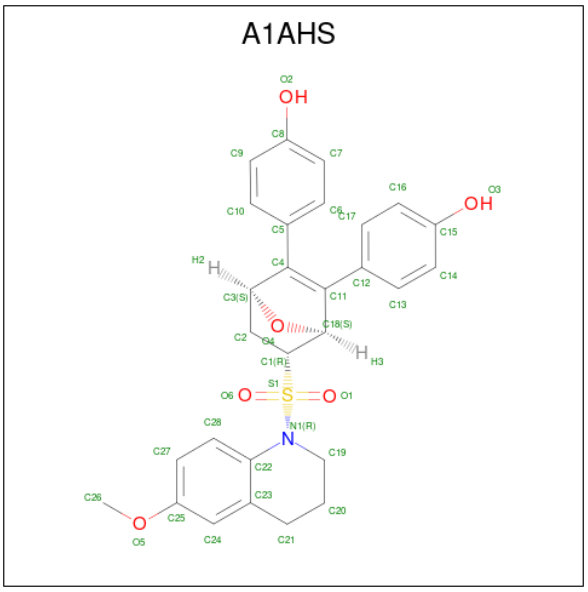
- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	239	Total	C	H	N	O	S	0	0	0
			3691	1184	1847	317	327	16			
1	B	224	Total	C	H	N	O	S	0	0	0
			3513	1121	1764	298	315	15			
1	C	233	Total	C	H	N	O	S	0	0	0
			3594	1161	1787	307	323	16			
1	D	224	Total	C	H	N	O	S	0	0	0
			3497	1119	1756	297	309	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'-[(1S,4S,5R)-5-(6-methoxy-3,4-dihydroquinoline-1(2H)-sulfonyl)-7-oxabicyclo[2.2.1]hept-2-ene-2,3-diyl]diphenol (three-letter code: A1AHS) (formula: $C_{28}H_{27}NO_6S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			63	28	27	1	6	1		
2	B	1	Total	C	H	N	O	S	0	0
			59	27	24	1	6	1		
2	C	1	Total	C	H	N	O	S	0	0
			63	28	27	1	6	1		
2	D	1	Total	C	H	N	O	S	0	0
			58	27	24	1	5	1		

- Molecule 3 is water.

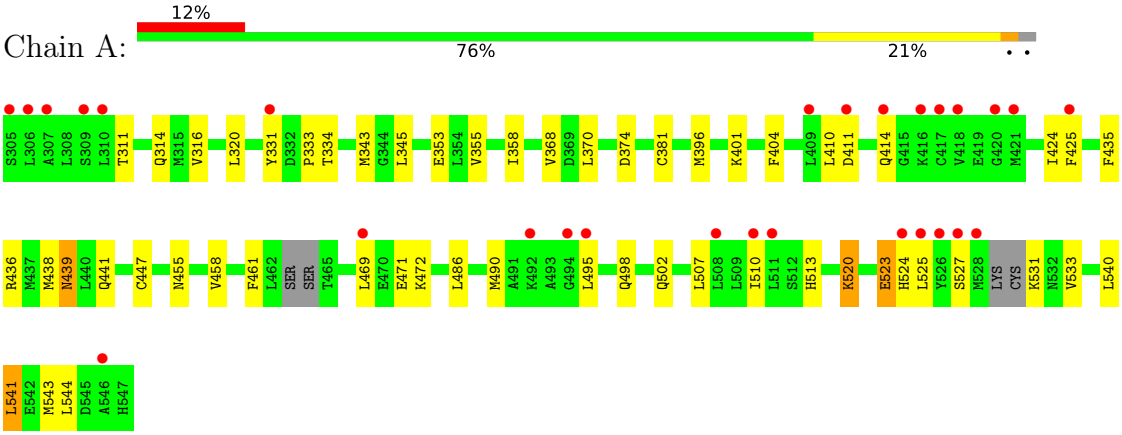
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	91	Total	O	0	0
			91	91		
3	B	70	Total	O	0	0
			70	70		
3	C	64	Total	O	0	0
			64	64		
3	D	73	Total	O	0	0
			73	73		

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.

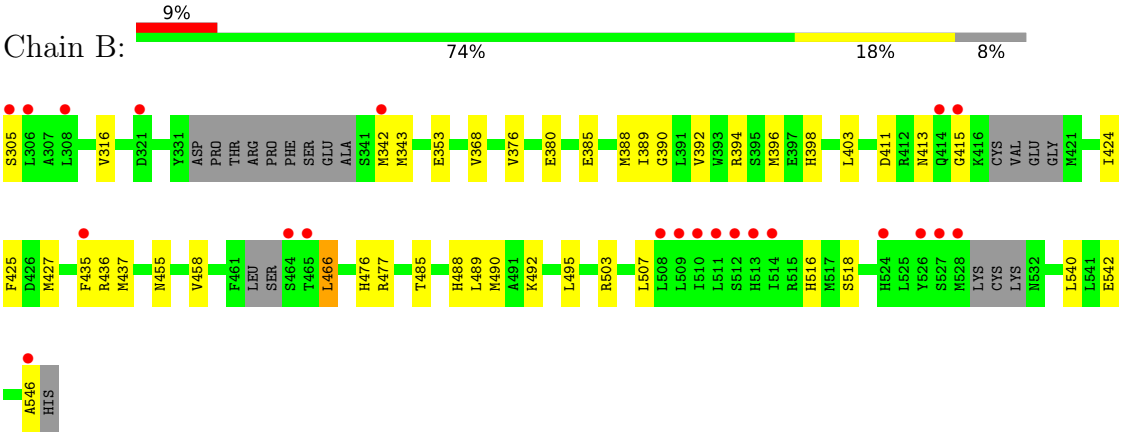
• Molecule 1: Estrogen receptor

Chain A:



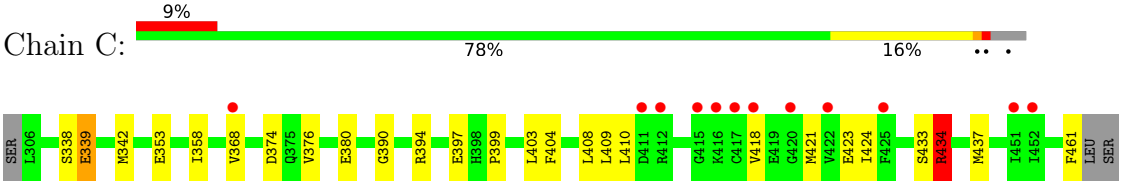
• Molecule 1: Estrogen receptor

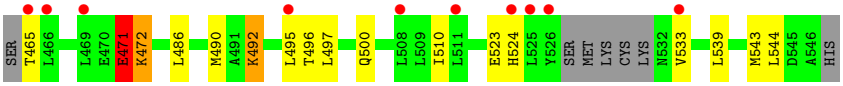
Chain B:



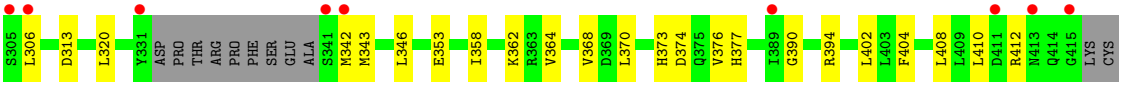
• Molecule 1: Estrogen receptor

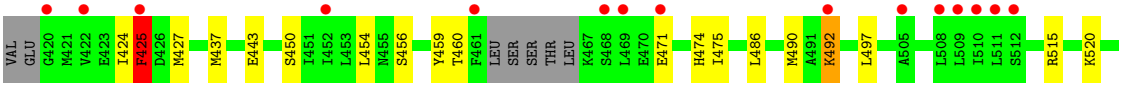
Chain C:

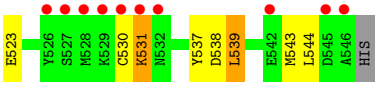




• Molecule 1: Estrogen receptor







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	53.53Å 58.97Å 93.75Å 86.51° 75.05° 63.02°	Depositor
Resolution (Å)	35.39 – 1.82 38.40 – 1.82	Depositor EDS
% Data completeness (in resolution range)	66.8 (35.39-1.82) 66.8 (38.40-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.225 , 0.275 0.225 , 0.274	Depositor DCC
R_{free} test set	2928 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.125 for h,h-k,h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14836	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.03% 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: A1AHS

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	0.82	6/1877 (0.3%)	0.91	7/2543 (0.3%)
1	B	0.52	0/1776	0.71	2/2399 (0.1%)
1	C	0.80	6/1840 (0.3%)	1.37	14/2494 (0.6%)
1	D	0.59	3/1769 (0.2%)	0.99	9/2390 (0.4%)
All	All	0.70	15/7262 (0.2%)	1.02	32/9826 (0.3%)

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	3
1	D	0	1
All	All	0	4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	520	LYS	CD-CE	-20.13	1.00	1.51
1	C	472	LYS	CE-NZ	16.01	1.89	1.49
1	C	472	LYS	CD-CE	10.35	1.77	1.51
1	A	541	LEU	CG-CD2	-9.28	1.17	1.51
1	A	520	LYS	CG-CD	8.60	1.81	1.52
1	D	539	LEU	CG-CD1	6.83	1.77	1.51
1	C	472	LYS	CB-CG	-6.73	1.34	1.52
1	C	471	GLU	CG-CD	6.26	1.61	1.51
1	D	492	LYS	CB-CG	-5.50	1.37	1.52
1	C	434	ARG	CD-NE	-5.23	1.37	1.46
1	A	523	GLU	CG-CD	5.21	1.59	1.51
1	C	339	GLU	CA-CB	5.17	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	541	LEU	CG-CD1	-5.14	1.32	1.51
1	A	520	LYS	CB-CG	-5.06	1.38	1.52
1	D	531	LYS	CB-CG	-5.02	1.39	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	471	GLU	OE1-CD-OE2	-38.75	76.81	123.30
1	D	539	LEU	CB-CG-CD2	24.69	152.97	111.00
1	C	471	GLU	CG-CD-OE2	-17.80	82.69	118.30
1	C	471	GLU	CG-CD-OE1	17.07	152.45	118.30
1	C	434	ARG	NE-CZ-NH1	-16.23	112.19	120.30
1	C	472	LYS	CD-CE-NZ	-15.84	75.28	111.70
1	A	469	LEU	CB-CG-CD1	15.40	137.17	111.00
1	C	434	ARG	NE-CZ-NH2	12.81	126.71	120.30
1	D	539	LEU	CA-CB-CG	-10.91	90.20	115.30
1	D	425	PHE	CB-CA-C	9.72	129.84	110.40
1	C	434	ARG	CG-CD-NE	9.69	132.14	111.80
1	B	466	LEU	CB-CG-CD1	9.33	126.86	111.00
1	A	520	LYS	CB-CG-CD	9.29	135.75	111.60
1	A	469	LEU	CA-CB-CG	-8.70	95.30	115.30
1	C	492	LYS	CD-CE-NZ	8.52	131.29	111.70
1	A	439	ASN	CB-CA-C	8.44	127.28	110.40
1	B	466	LEU	CB-CG-CD2	-7.50	98.25	111.00
1	C	338	SER	C-N-CA	-7.37	103.26	121.70
1	C	339	GLU	N-CA-CB	7.27	123.69	110.60
1	D	492	LYS	CG-CD-CE	-7.10	90.61	111.90
1	C	434	ARG	CB-CG-CD	7.01	129.83	111.60
1	A	523	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	C	461	PHE	CB-CG-CD2	-6.81	116.03	120.80
1	A	469	LEU	CB-CG-CD2	-6.58	99.81	111.00
1	C	461	PHE	CB-CG-CD1	6.33	125.23	120.80
1	D	531	LYS	CB-CG-CD	6.03	127.28	111.60
1	D	437	MET	CA-CB-CG	6.02	123.53	113.30
1	D	425	PHE	N-CA-CB	-5.55	100.61	110.60
1	C	492	LYS	CB-CG-CD	-5.54	97.19	111.60
1	D	539	LEU	CB-CG-CD1	-5.53	101.61	111.00
1	D	492	LYS	CD-CE-NZ	5.15	123.55	111.70
1	A	541	LEU	CB-CG-CD2	5.07	119.62	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	339	GLU	Mainchain
1	C	434	ARG	Sidechain
1	C	471	GLU	Sidechain
1	D	425	PHE	Mainchain

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	1844	1847	1846	52	0
1	B	1749	1764	1764	28	0
1	C	1807	1787	1814	40	0
1	D	1741	1756	1756	51	0
2	A	36	27	0	4	0
2	B	35	24	0	3	0
2	C	36	27	0	7	0
2	D	34	24	0	1	0
3	A	91	0	0	3	2
3	B	70	0	0	3	1
3	C	64	0	0	1	1
3	D	73	0	0	2	2
All	All	7580	7256	7180	169	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (169) 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:D:539:LEU:CG	1:D:539:LEU:CD1	1.77	1.62
1:C:472:LYS:CD	1:C:472:LYS:CE	1.77	1.59
1:A:520:LYS:CD	1:A:520:LYS:CG	1.81	1.58
1:C:472:LYS:CE	1:C:472:LYS:NZ	1.89	1.35
1:C:472:LYS:CD	1:C:472:LYS:NZ	2.23	1.01
1:D:539:LEU:HD22	1:D:543:MET:SD	2.05	0.95
1:B:305:SER:O	3:B:701:HOH:O	1.91	0.87
1:A:520:LYS:CG	1:A:520:LYS:CE	2.50	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:402:LEU:CD1	1:D:425:PHE:CD1	2.64	0.81
1:A:439:ASN:O	1:A:441:GLN:NE2	2.13	0.80
1:A:513:HIS:ND1	3:A:702:HOH:O	2.15	0.79
1:D:539:LEU:CD1	1:D:539:LEU:CB	2.60	0.79
1:D:370:LEU:HD21	1:D:475:ILE:HD11	1.65	0.78
1:D:539:LEU:CD1	1:D:539:LEU:CD2	2.62	0.78
1:C:380:GLU:OE1	3:C:701:HOH:O	2.02	0.77
1:D:313:ASP:OD1	3:D:701:HOH:O	2.04	0.74
1:D:402:LEU:HD12	1:D:425:PHE:CD1	2.23	0.74
1:A:334:THR:O	3:A:701:HOH:O	2.04	0.74
1:C:404:PHE:CE2	1:C:410:LEU:HD12	2.23	0.73
1:D:427:MET:HE1	1:D:520:LYS:HD3	1.71	0.72
1:D:539:LEU:CD2	1:D:543:MET:SD	2.77	0.72
1:A:358:ILE:HG23	1:A:544:LEU:HD23	1.72	0.71
1:B:342:MET:SD	1:B:343:MET:N	2.64	0.70
1:C:472:LYS:NZ	1:C:472:LYS:HD3	2.06	0.70
1:C:342:MET:HE3	2:C:600:A1AHS:C26	2.22	0.69
1:C:374:ASP:OD2	1:C:471:GLU:OE1	2.11	0.69
1:A:404:PHE:CE1	1:A:410:LEU:HD12	2.28	0.69
1:D:471:GLU:O	1:D:475:ILE:HD12	1.93	0.67
1:D:370:LEU:HD23	1:D:471:GLU:OE1	1.94	0.67
1:B:396:MET:O	1:B:436:ARG:NE	2.24	0.66
1:D:377:HIS:NE2	1:D:460:THR:HG23	2.11	0.64
1:D:450:SER:O	1:D:454:LEU:HD23	1.97	0.64
1:D:539:LEU:HD23	1:D:543:MET:HG3	1.79	0.63
1:A:424:ILE:HG21	2:A:600:A1AHS:O6	1.98	0.63
1:C:421:MET:CB	2:C:600:A1AHS:C25	2.77	0.63
1:B:490:MET:HB3	1:B:495:LEU:HD22	1.82	0.62
1:A:370:LEU:HA	1:A:471:GLU:OE1	2.00	0.61
1:A:438:MET:HE1	1:A:507:LEU:HD23	1.81	0.61
1:B:353:GLU:OE1	2:B:600:A1AHS:O2	2.19	0.60
1:B:503:ARG:O	1:B:507:LEU:HG	2.01	0.60
1:D:368:VAL:HG22	3:D:724:HOH:O	2.01	0.60
1:B:316:VAL:HG21	1:B:489:LEU:HD21	1.83	0.60
1:A:541:LEU:O	1:A:544:LEU:HB2	2.01	0.59
1:B:368:VAL:HG22	3:B:722:HOH:O	2.01	0.59
1:A:353:GLU:OE2	2:A:600:A1AHS:O2	2.21	0.58
1:A:525:LEU:O	1:A:531:LYS:N	2.36	0.58
1:D:373:HIS:HD1	1:D:537:TYR:HH	1.52	0.58
1:A:401:LYS:NZ	1:A:411:ASP:HB3	2.19	0.58
1:D:402:LEU:HD11	1:D:425:PHE:HD1	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:530:CYS:C	1:D:531:LYS:HG2	2.23	0.57
1:D:402:LEU:HD11	1:D:425:PHE:CD1	2.39	0.56
1:B:415:GLY:HA3	1:B:425:PHE:CE1	2.41	0.56
1:A:520:LYS:O	1:A:524:HIS:ND1	2.37	0.56
1:A:424:ILE:HD11	1:A:520:LYS:HB3	1.87	0.56
1:C:408:LEU:HD23	1:C:410:LEU:HG	1.87	0.56
1:A:461:PHE:HB2	1:A:472:LYS:HD2	1.87	0.56
1:A:425:PHE:HE2	2:A:600:A1AHS:C26	2.18	0.55
1:D:376:VAL:HG22	1:D:544:LEU:HD12	1.89	0.55
1:D:390:GLY:O	1:D:394:ARG:HG3	2.06	0.55
1:D:475:ILE:HD12	1:D:475:ILE:H	1.72	0.55
1:D:539:LEU:CD2	1:D:543:MET:HG3	2.37	0.54
1:C:472:LYS:CD	1:C:472:LYS:HZ2	2.20	0.54
1:A:438:MET:CE	1:A:507:LEU:HD23	2.37	0.54
1:C:403:LEU:HD13	1:C:409:LEU:HD13	1.90	0.54
1:C:418:VAL:HG23	1:C:421:MET:CB	2.38	0.53
1:A:331:TYR:C	1:A:333:PRO:HD3	2.29	0.53
1:A:490:MET:HB3	1:A:495:LEU:HD12	1.91	0.53
1:C:342:MET:CE	2:C:600:A1AHS:C26	2.87	0.52
1:C:433:SER:O	1:C:437:MET:HG3	2.10	0.52
1:D:424:ILE:HA	1:D:427:MET:HE3	1.91	0.52
1:A:435:PHE:CE2	1:A:510:ILE:HG21	2.45	0.51
1:C:510:ILE:HD13	1:D:459:TYR:CZ	2.46	0.51
1:A:447:CYS:HB2	1:A:486:LEU:HD21	1.92	0.51
1:A:358:ILE:HG23	1:A:544:LEU:CD2	2.41	0.51
1:D:402:LEU:HG	1:D:425:PHE:CE1	2.45	0.51
1:C:408:LEU:CD2	1:C:410:LEU:HG	2.42	0.50
1:A:374:ASP:OD2	1:A:471:GLU:OE2	2.29	0.50
1:C:404:PHE:HB2	1:C:408:LEU:HD22	1.93	0.50
1:B:398:HIS:CD2	1:B:403:LEU:HD12	2.46	0.49
1:C:533:VAL:CG1	2:C:600:A1AHS:O3	2.60	0.49
1:C:368:VAL:HG22	1:C:368:VAL:O	2.13	0.49
1:C:397:GLU:O	1:C:399:PRO:HD3	2.13	0.49
1:C:490:MET:HB3	1:C:495:LEU:HD12	1.93	0.49
1:B:380:GLU:HG2	1:B:540:LEU:HD12	1.94	0.49
1:A:411:ASP:OD1	1:A:414:GLN:HG3	2.13	0.49
1:B:488:HIS:NE2	1:B:492:LYS:HE2	2.27	0.49
1:C:472:LYS:CE	1:C:472:LYS:CG	2.81	0.49
1:C:408:LEU:HD21	1:C:410:LEU:HD11	1.94	0.49
1:A:316:VAL:HG13	1:A:320:LEU:HD11	1.95	0.48
1:A:410:LEU:CD2	1:A:414:GLN:OE1	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:GLU:H	1:C:423:GLU:CD	2.17	0.48
1:D:306:LEU:O	1:D:306:LEU:HD12	2.14	0.48
1:A:355:VAL:HG22	1:A:543:MET:CE	2.44	0.47
1:A:355:VAL:HG22	1:A:543:MET:HE1	1.96	0.47
1:D:492:LYS:HG2	1:D:492:LYS:O	2.14	0.47
1:C:533:VAL:HG11	2:C:600:A1AHS:O3	2.14	0.47
1:D:427:MET:CE	1:D:520:LYS:HD3	2.43	0.47
1:A:520:LYS:CG	1:A:520:LYS:NZ	2.77	0.47
1:B:427:MET:HE1	1:B:516:HIS:HD2	1.80	0.47
1:D:353:GLU:OE1	2:D:600:A1AHS:O2	2.33	0.47
1:C:486:LEU:O	1:C:490:MET:HG3	2.15	0.47
1:B:466:LEU:HB2	1:C:495:LEU:HD21	1.97	0.47
1:A:358:ILE:CG2	1:A:544:LEU:HD23	2.43	0.46
1:C:353:GLU:OE1	2:C:600:A1AHS:O2	2.33	0.46
1:D:404:PHE:CE2	1:D:410:LEU:HD12	2.50	0.46
1:A:396:MET:O	1:A:436:ARG:HD3	2.15	0.46
1:B:413:ASN:ND2	1:B:413:ASN:H	2.14	0.46
1:B:455:ASN:O	1:B:458:VAL:HG12	2.15	0.46
1:A:410:LEU:HD22	1:A:414:GLN:OE1	2.16	0.46
1:A:455:ASN:O	1:A:458:VAL:HG12	2.15	0.46
1:D:346:LEU:CD2	1:D:408:LEU:HD21	2.46	0.45
1:C:376:VAL:HG22	1:C:544:LEU:HD12	1.97	0.45
1:D:342:MET:HG2	1:D:343:MET:N	2.32	0.45
1:D:538:ASP:O	1:D:539:LEU:C	2.52	0.45
1:A:381:CYS:SG	3:B:764:HOH:O	2.58	0.45
1:D:456:SER:HA	1:D:515:ARG:NH2	2.31	0.45
1:D:492:LYS:HE3	1:D:492:LYS:HB2	1.69	0.45
1:A:316:VAL:HG12	1:A:320:LEU:HD12	1.97	0.45
1:B:424:ILE:HG21	2:B:600:A1AHS:O6	2.17	0.45
1:D:520:LYS:HA	1:D:523:GLU:HG2	1.99	0.45
1:C:492:LYS:HA	1:C:492:LYS:HD3	1.73	0.44
1:A:368:VAL:HG22	3:A:719:HOH:O	2.17	0.44
1:B:411:ASP:O	1:B:415:GLY:N	2.43	0.44
1:C:434:ARG:HG2	1:C:510:ILE:HD11	1.98	0.44
1:C:496:THR:O	1:C:500:GLN:HG3	2.17	0.44
1:A:533:VAL:CG1	2:A:600:A1AHS:O3	2.66	0.44
1:C:539:LEU:HG	1:C:543:MET:CE	2.48	0.44
1:D:530:CYS:O	1:D:531:LYS:C	2.56	0.44
1:D:320:LEU:HD11	1:D:443:GLU:HG3	2.00	0.44
1:D:374:ASP:OD2	1:D:471:GLU:HG3	2.18	0.44
1:D:486:LEU:O	1:D:490:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PHE:CD1	1:A:410:LEU:HD12	2.52	0.43
1:C:539:LEU:HG	1:C:543:MET:HE2	2.00	0.43
1:B:485:THR:O	1:B:489:LEU:HG	2.19	0.43
1:A:333:PRO:HB3	1:A:345:LEU:HD11	2.00	0.43
1:A:343:MET:HB2	1:A:343:MET:HE2	1.84	0.43
1:D:471:GLU:O	1:D:474:HIS:HB3	2.19	0.43
1:B:427:MET:HE1	1:B:516:HIS:CD2	2.53	0.42
1:C:497:LEU:HD21	1:D:497:LEU:HD13	1.99	0.42
1:B:476:HIS:HB3	1:B:477:ARG:HH21	1.84	0.42
1:B:376:VAL:HG13	1:B:540:LEU:HB2	2.02	0.42
1:D:364:VAL:HG11	1:D:454:LEU:HD21	2.01	0.42
1:A:498:GLN:O	1:A:502:GLN:HG3	2.20	0.42
1:B:389:ILE:HA	1:B:392:VAL:HG22	2.01	0.42
1:A:316:VAL:CG1	1:A:320:LEU:HD11	2.49	0.42
1:D:370:LEU:HD21	1:D:475:ILE:CD1	2.43	0.42
1:A:411:ASP:OD1	1:A:414:GLN:NE2	2.53	0.42
1:B:542:GLU:O	1:B:546:ALA:N	2.42	0.42
1:C:424:ILE:HG21	2:C:600:A1AHS:O6	2.19	0.42
1:D:539:LEU:CD2	1:D:543:MET:CG	2.98	0.42
1:D:346:LEU:N	1:D:346:LEU:HD23	2.35	0.41
1:D:358:ILE:HG22	1:D:362:LYS:HE3	2.00	0.41
1:B:396:MET:HE3	1:B:435:PHE:O	2.19	0.41
1:C:358:ILE:HG23	1:C:544:LEU:HD23	2.02	0.41
1:A:311:THR:OG1	1:A:314:GLN:HG3	2.20	0.41
1:A:331:TYR:O	1:A:331:TYR:CG	2.72	0.41
1:A:374:ASP:OD1	1:A:461:PHE:CE1	2.73	0.41
1:B:385:GLU:HG2	1:B:518:SER:HB2	2.03	0.41
1:B:390:GLY:O	1:B:394:ARG:HG3	2.21	0.41
1:D:539:LEU:HD23	1:D:539:LEU:O	2.20	0.41
1:A:435:PHE:HE2	1:A:510:ILE:HD13	1.85	0.41
1:A:540:LEU:O	1:A:541:LEU:C	2.57	0.41
1:A:523:GLU:O	1:A:527:SER:N	2.51	0.40
1:C:434:ARG:HD3	1:C:510:ILE:HD11	2.03	0.40
1:D:412:ARG:NH1	1:D:412:ARG:HG2	2.35	0.40
1:C:390:GLY:O	1:C:394:ARG:HG3	2.21	0.40
1:A:316:VAL:CG1	1:A:320:LEU:CD1	2.99	0.40
1:B:388:MET:O	1:B:392:VAL:HG13	2.22	0.40
2:B:600:A1AHS:C18	2:B:600:A1AHS:C28	2.99	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:709:HOH:O	3:B:731:HOH:O[1_655]	1.99	0.21
3:A:788:HOH:O	3:D:773:HOH:O[1_566]	2.14	0.06
3:C:753:HOH:O	3:D:731:HOH:O[1_565]	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	233/243 (96%)	225 (97%)	8 (3%)	0	100 100
1	B	214/243 (88%)	210 (98%)	3 (1%)	1 (0%)	29 15
1	C	227/243 (93%)	220 (97%)	5 (2%)	2 (1%)	17 6
1	D	216/243 (89%)	209 (97%)	7 (3%)	0	100 100
All	All	890/972 (92%)	864 (97%)	23 (3%)	3 (0%)	41 27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	524	HIS
1	B	437	MET
1	C	523	GLU

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	197/219 (90%)	197 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	191/219 (87%)	191 (100%)	0	100 100
1	C	196/219 (90%)	195 (100%)	1 (0%)	88 87
1	D	187/219 (85%)	187 (100%)	0	100 100
All	All	771/876 (88%)	770 (100%)	1 (0%)	93 92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	465	THR

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

Mol	Chain	Res	Type
1	A	441	GLN
1	B	413	ASN
1	B	513	HIS
1	B	524	HIS

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	A1AHS	B	600	-	38,40,41	1.38	4 (10%)	48,61,62	1.36	5 (10%)
2	A1AHS	A	600	-	39,41,41	1.37	2 (5%)	49,62,62	1.39	6 (12%)
2	A1AHS	D	600	-	37,39,41	1.65	5 (13%)	46,59,62	1.42	8 (17%)
2	A1AHS	C	600	-	39,41,41	1.46	7 (17%)	49,62,62	1.57	9 (18%)

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	A1AHS	B	600	-	-	4/18/54/56	0/7/6/6
2	A1AHS	A	600	-	-	8/20/56/56	0/7/6/6
2	A1AHS	D	600	-	-	10/18/54/56	0/7/6/6
2	A1AHS	C	600	-	-	8/20/56/56	0/7/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	A1AHS	S1-N1	6.37	1.80	1.67
2	D	600	A1AHS	S1-N1	6.28	1.80	1.67
2	B	600	A1AHS	S1-N1	5.70	1.78	1.67
2	C	600	A1AHS	S1-N1	5.58	1.78	1.67
2	D	600	A1AHS	O6-S1	4.39	1.47	1.43
2	A	600	A1AHS	O1-S1	3.04	1.46	1.43
2	C	600	A1AHS	C22-N1	-3.01	1.40	1.43
2	D	600	A1AHS	O1-S1	2.87	1.46	1.43
2	C	600	A1AHS	O1-S1	2.85	1.46	1.43
2	D	600	A1AHS	C19-N1	-2.83	1.46	1.48
2	B	600	A1AHS	C18-C11	2.76	1.53	1.50
2	B	600	A1AHS	O1-S1	2.66	1.45	1.43
2	C	600	A1AHS	C18-C11	2.66	1.53	1.50
2	D	600	A1AHS	C18-C11	2.20	1.53	1.50
2	C	600	A1AHS	O6-S1	2.20	1.45	1.43
2	C	600	A1AHS	O4-C3	-2.16	1.39	1.44
2	C	600	A1AHS	C19-N1	-2.09	1.47	1.48
2	B	600	A1AHS	O4-C3	-2.08	1.40	1.44

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	A1AHS	C19-N1-S1	-5.29	109.33	117.46
2	C	600	A1AHS	C23-C22-N1	5.17	122.38	118.31
2	B	600	A1AHS	C19-N1-S1	-5.08	109.65	117.46
2	C	600	A1AHS	O6-S1-O1	4.20	121.91	119.22
2	D	600	A1AHS	C19-N1-S1	-4.09	111.16	117.46
2	D	600	A1AHS	O6-S1-N1	-4.09	102.55	107.56
2	C	600	A1AHS	C28-C22-N1	-4.02	114.88	120.84
2	D	600	A1AHS	C20-C19-N1	-3.76	105.99	111.76
2	B	600	A1AHS	C23-C22-N1	3.30	120.91	118.31
2	B	600	A1AHS	C3-C2-C1	3.05	103.31	100.61
2	A	600	A1AHS	C17-C12-C11	-3.03	116.99	120.91
2	D	600	A1AHS	O4-C3-C2	-2.91	98.92	104.64
2	C	600	A1AHS	C3-C2-C1	2.75	103.04	100.61
2	B	600	A1AHS	O4-C3-C2	-2.72	99.29	104.64
2	A	600	A1AHS	O4-C3-C2	-2.59	99.54	104.64
2	D	600	A1AHS	C10-C5-C4	-2.59	117.56	120.91
2	C	600	A1AHS	O4-C3-C2	-2.55	99.62	104.64
2	C	600	A1AHS	C24-C23-C22	-2.38	116.77	118.95
2	A	600	A1AHS	C5-C4-C11	2.35	134.90	128.81
2	C	600	A1AHS	C19-N1-S1	2.21	120.86	117.46
2	D	600	A1AHS	C23-C22-N1	-2.17	116.60	118.31
2	C	600	A1AHS	O6-S1-N1	2.14	110.18	107.56
2	C	600	A1AHS	C5-C4-C11	2.12	134.30	128.81
2	D	600	A1AHS	C6-C5-C4	2.09	123.61	120.91
2	D	600	A1AHS	C28-C22-N1	2.08	123.93	120.84
2	A	600	A1AHS	C26-O5-C25	2.08	122.02	117.51
2	A	600	A1AHS	C20-C21-C23	-2.07	107.36	112.42
2	B	600	A1AHS	C10-C5-C4	-2.00	118.32	120.91

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	A1AHS	C18-C1-S1-O1
2	A	600	A1AHS	C18-C1-S1-O6
2	A	600	A1AHS	C2-C1-S1-O1
2	A	600	A1AHS	C2-C1-S1-O6
2	B	600	A1AHS	C18-C1-S1-O1
2	B	600	A1AHS	C2-C1-S1-O1
2	C	600	A1AHS	C18-C1-S1-O1
2	C	600	A1AHS	C18-C1-S1-O6

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Mol	Chain	Res	Type	Atoms
2	C	600	A1AHS	C2-C1-S1-O1
2	D	600	A1AHS	C22-N1-S1-C1
2	D	600	A1AHS	C18-C1-S1-O1
2	C	600	A1AHS	C24-C25-O5-C26
2	C	600	A1AHS	C27-C25-O5-C26
2	D	600	A1AHS	C19-N1-S1-O1
2	D	600	A1AHS	C22-N1-S1-O1
2	A	600	A1AHS	C22-N1-S1-O6
2	D	600	A1AHS	C2-C1-S1-O1
2	B	600	A1AHS	C18-C1-S1-O6
2	A	600	A1AHS	C22-N1-S1-C1
2	D	600	A1AHS	C19-N1-S1-C1
2	B	600	A1AHS	C2-C1-S1-O6
2	C	600	A1AHS	C2-C1-S1-O6
2	D	600	A1AHS	C2-C1-S1-O6
2	A	600	A1AHS	C19-N1-S1-O1
2	A	600	A1AHS	C19-N1-S1-O6
2	D	600	A1AHS	C18-C1-S1-O6
2	C	600	A1AHS	C18-C11-C12-C13
2	C	600	A1AHS	C18-C11-C12-C17
2	D	600	A1AHS	C22-N1-S1-O6
2	D	600	A1AHS	C11-C4-C5-C10

There are no ring outliers.

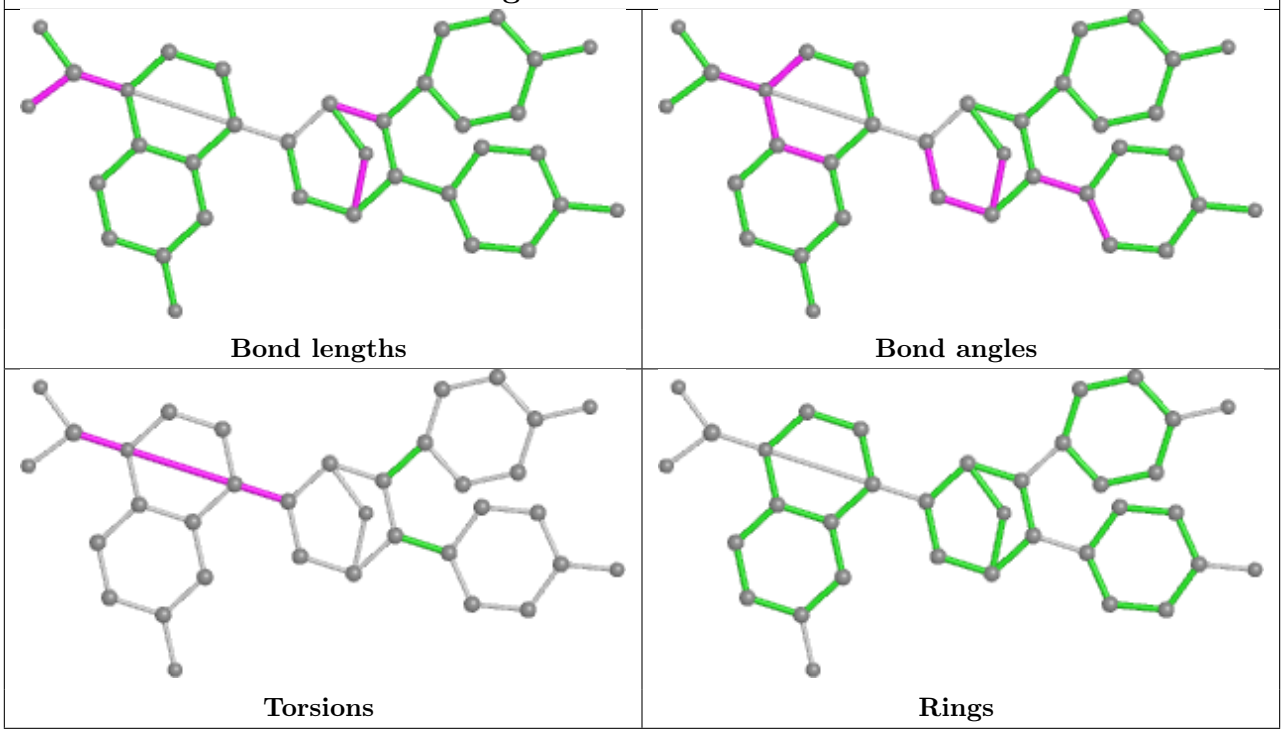
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	A1AHS	3	0
2	A	600	A1AHS	4	0
2	D	600	A1AHS	1	0
2	C	600	A1AHS	7	0

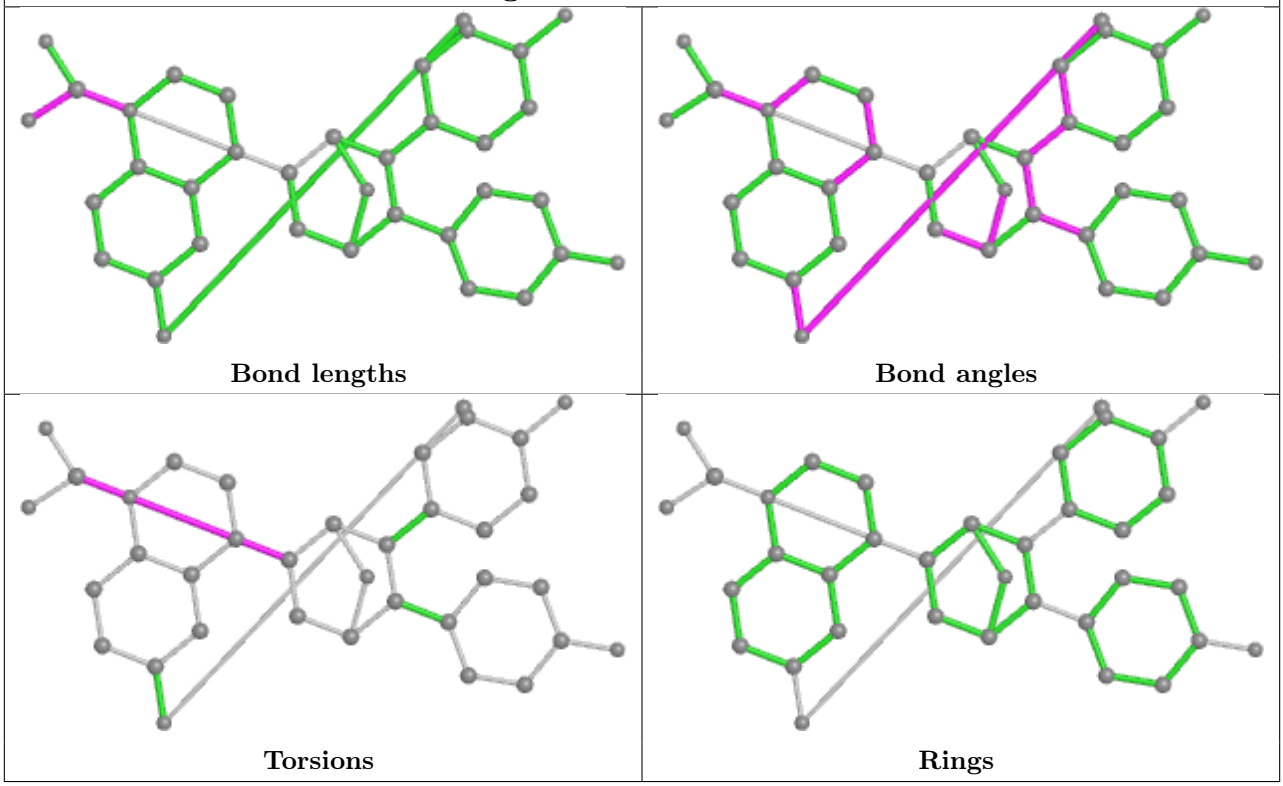
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

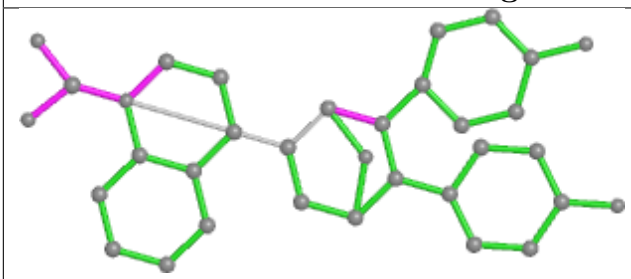
Ligand A1AHS B 600



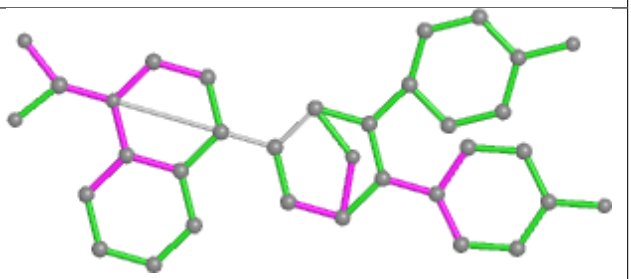
Ligand A1AHS A 600



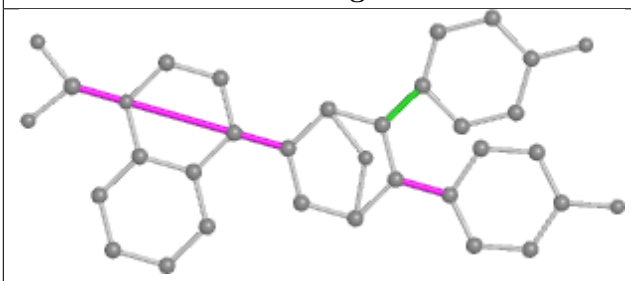
Ligand A1AHS D 600



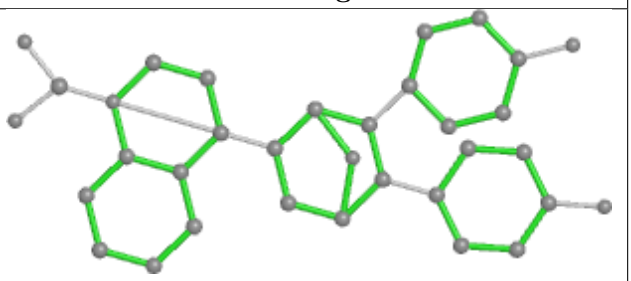
Bond lengths



Bond angles

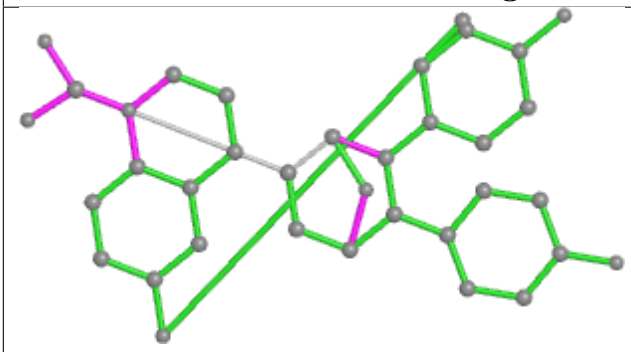


Torsions

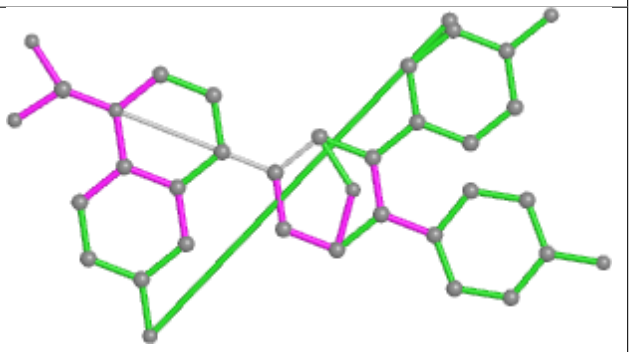


Rings

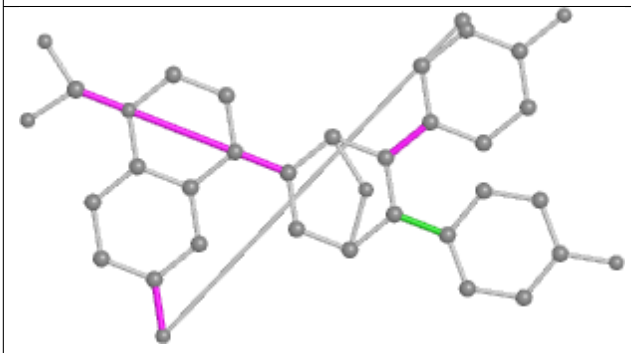
Ligand A1AHS C 600



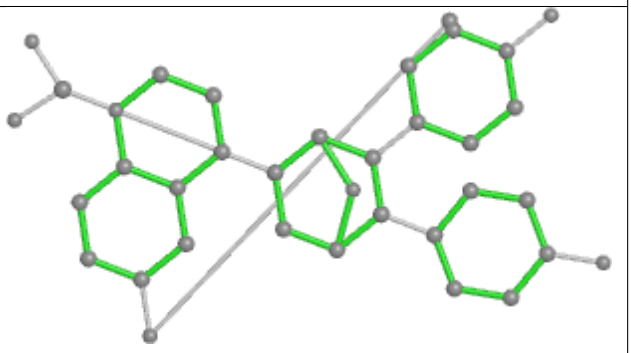
Bond lengths



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	239/243 (98%)	0.84	28 (11%) 4 3	18, 35, 66, 84	0
1	B	224/243 (92%)	0.79	22 (9%) 7 5	17, 33, 60, 99	0
1	C	233/243 (95%)	0.69	22 (9%) 8 6	16, 31, 62, 84	0
1	D	224/243 (92%)	1.00	34 (15%) 2 1	18, 33, 69, 99	0
All	All	920/972 (94%)	0.83	106 (11%) 4 3	16, 33, 67, 99	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	VAL	8.6
1	C	417	CYS	8.0
1	B	415	GLY	7.5
1	D	469	LEU	7.3
1	D	468	SER	6.9
1	A	306	LEU	5.9
1	D	530	CYS	5.8
1	D	527	SER	5.7
1	D	425	PHE	5.5
1	A	417	CYS	5.4
1	D	528	MET	5.2
1	D	532	ASN	5.0
1	C	418	VAL	4.8
1	B	306	LEU	4.6
1	B	527	SER	4.5
1	B	546	ALA	4.4
1	D	420	GLY	4.3
1	D	342	MET	4.2
1	D	511	LEU	4.2
1	A	494	GLY	4.2
1	D	546	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	533	VAL	4.1
1	A	528	MET	3.8
1	B	511	LEU	3.8
1	C	416	LYS	3.8
1	D	341	SER	3.7
1	C	525	LEU	3.7
1	A	425	PHE	3.7
1	B	526	TYR	3.6
1	A	526	TYR	3.6
1	D	415	GLY	3.5
1	D	305	SER	3.4
1	C	422	VAL	3.4
1	D	531	LYS	3.3
1	A	511	LEU	3.3
1	D	422	VAL	3.3
1	C	526	TYR	3.3
1	D	461	PHE	3.3
1	A	524	HIS	3.1
1	D	508	LEU	3.1
1	D	529	LYS	3.0
1	A	305	SER	3.0
1	A	411	ASP	3.0
1	C	466	LEU	3.0
1	A	546	ALA	2.9
1	A	495	LEU	2.9
1	B	342	MET	2.8
1	D	331	TYR	2.8
1	D	526	TYR	2.8
1	A	525	LEU	2.8
1	C	368	VAL	2.8
1	A	469	LEU	2.7
1	B	464	SER	2.7
1	A	421	MET	2.7
1	D	509	LEU	2.7
1	C	511	LEU	2.6
1	A	420	GLY	2.6
1	B	305	SER	2.6
1	D	492	LYS	2.6
1	D	510	ILE	2.6
1	B	414	GLN	2.6
1	D	411	ASP	2.6
1	A	527	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	307	ALA	2.5
1	B	524	HIS	2.5
1	A	510	ILE	2.5
1	C	452	ILE	2.5
1	C	425	PHE	2.5
1	C	469	LEU	2.5
1	A	414	GLN	2.4
1	B	510	ILE	2.4
1	C	420	GLY	2.4
1	C	411	ASP	2.4
1	B	512	SER	2.3
1	A	310	LEU	2.3
1	A	508	LEU	2.3
1	B	509	LEU	2.3
1	B	308	LEU	2.3
1	C	495	LEU	2.3
1	D	512	SER	2.3
1	C	451	ILE	2.3
1	B	528	MET	2.3
1	A	309	SER	2.3
1	D	542	GLU	2.3
1	D	505	ALA	2.2
1	B	435	PHE	2.2
1	B	514	ILE	2.2
1	C	415	GLY	2.2
1	B	321	ASP	2.2
1	B	513	HIS	2.2
1	C	508	LEU	2.2
1	B	465	THR	2.2
1	D	471	GLU	2.1
1	A	492	LYS	2.1
1	A	409	LEU	2.1
1	D	306	LEU	2.1
1	D	413	ASN	2.1
1	D	545	ASP	2.1
1	C	465	THR	2.1
1	C	412	ARG	2.1
1	A	331	TYR	2.1
1	C	524	HIS	2.1
1	B	508	LEU	2.1
1	D	452	ILE	2.0
1	A	416	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	389	ILE	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)

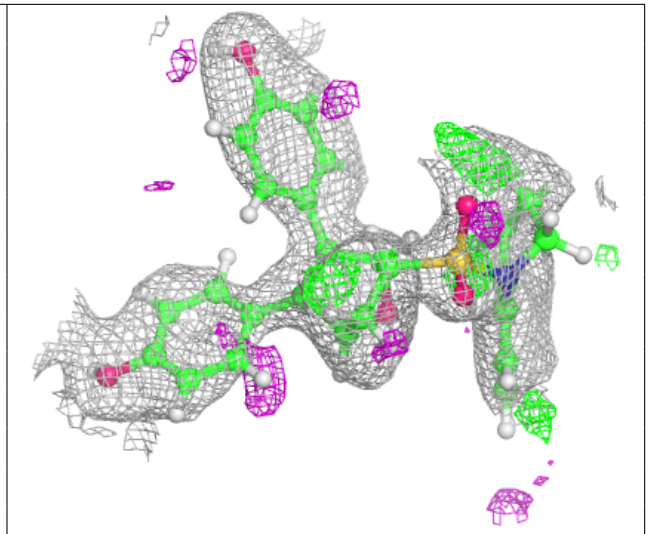
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

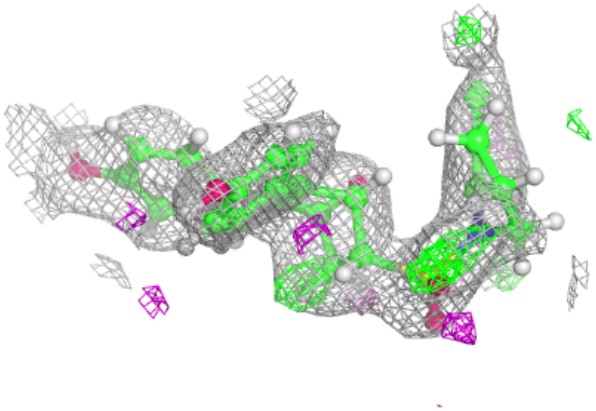
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1AHS	D	600	34/36	0.82	0.20	25,55,85,213	0
2	A1AHS	B	600	35/36	0.83	0.18	23,45,77,213	0
2	A1AHS	A	600	36/36	0.85	0.17	22,49,89,213	0
2	A1AHS	C	600	36/36	0.88	0.18	20,45,80,213	0

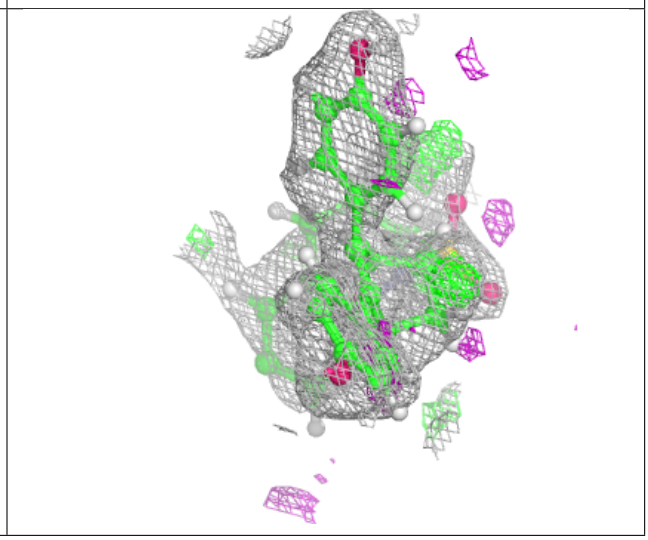
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AHS 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)

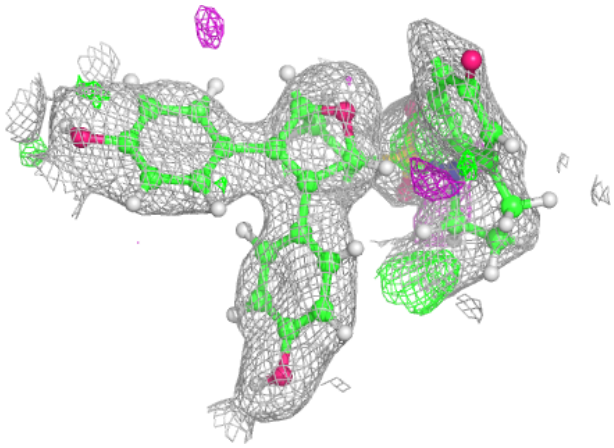


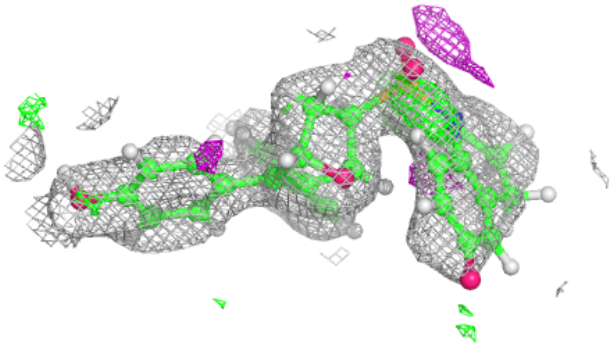


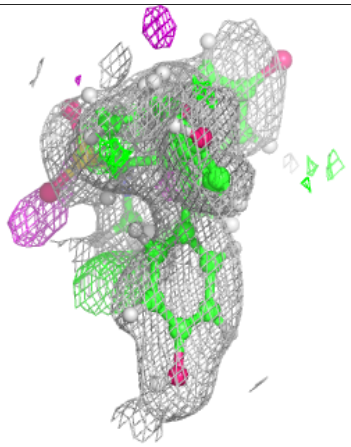


Electron density around A1AHS B 600:

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

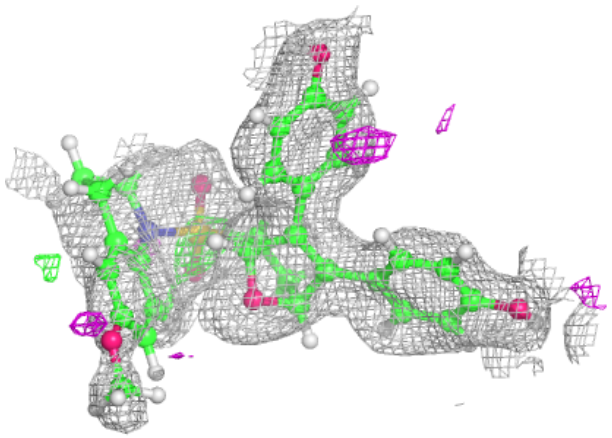


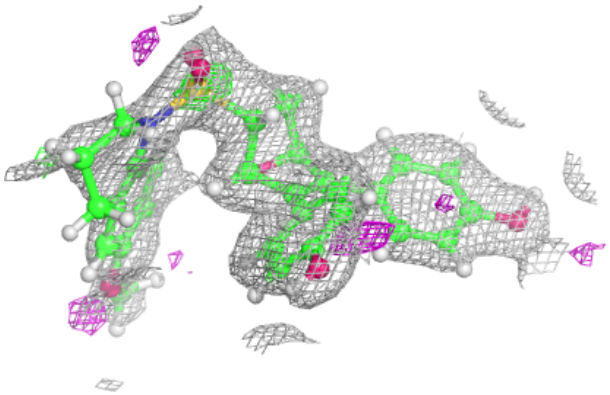


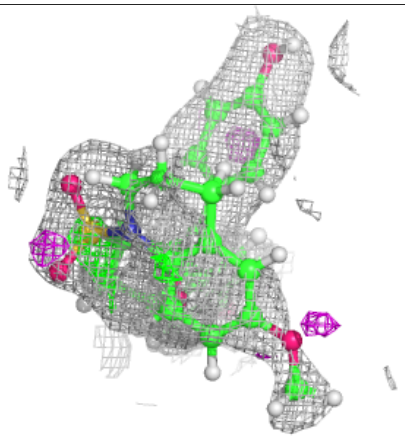


Electron density around A1AHS A 600:

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

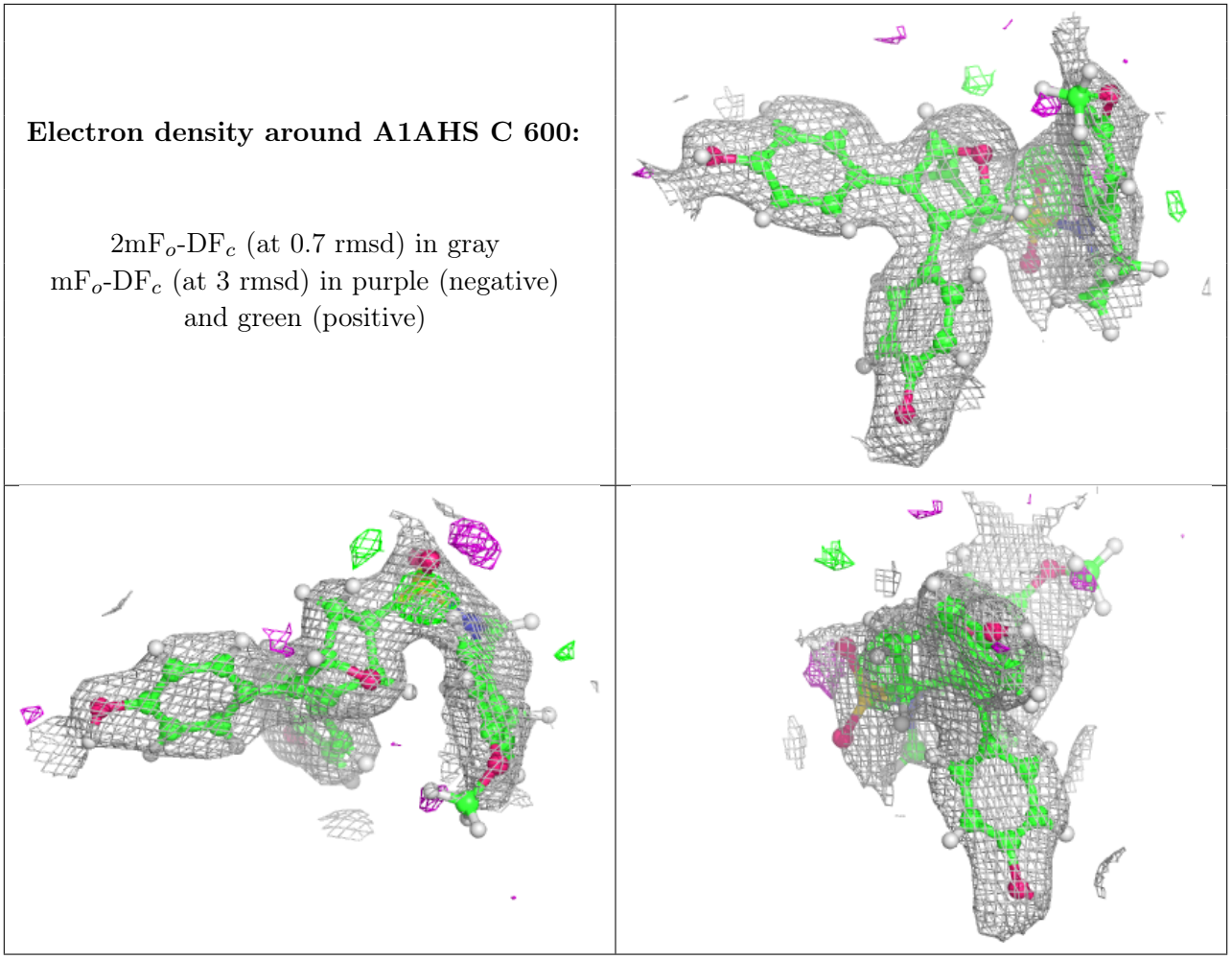






Electron density around A1AHS C 600:

$2mF_o$-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

There are no such residues in this entry.