wwPDB X-ray Structure Validation Summary Report (i)

Jun 25, 2024 – 10:06 PM EDT

PDB ID	:	6ZT9
Title	:	X-ray structure of mutated arabinofuranosidase
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Deposited on	:	2020-07-17
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

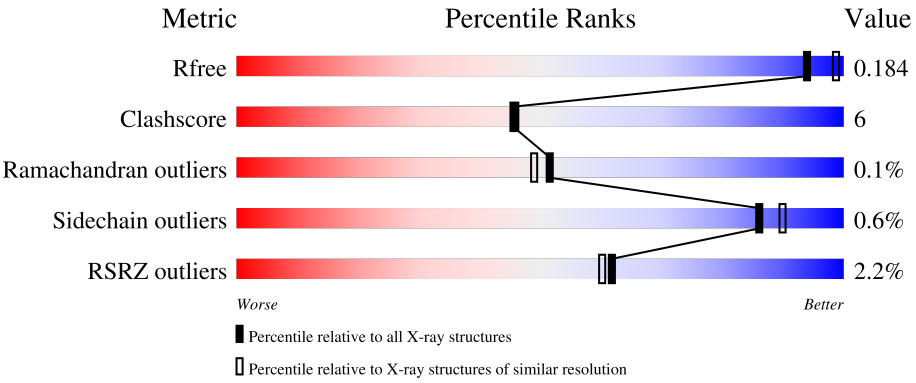
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	496	3% 89% 10%
1	B	496	2% 87% 10%
1	C	496	2% 88% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MPD	A	508	-	-	-	X
3	MPD	B	506	-	-	X	X
3	MPD	B	507	-	-	-	X
3	MPD	B	508	-	-	X	X
3	MPD	C	506	-	-	-	X
4	ACT	A	511	-	-	X	X
4	ACT	C	508	-	-	X	-
4	ACT	C	512	-	-	X	-
4	ACT	C	513	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13672 atoms, of which 98 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.

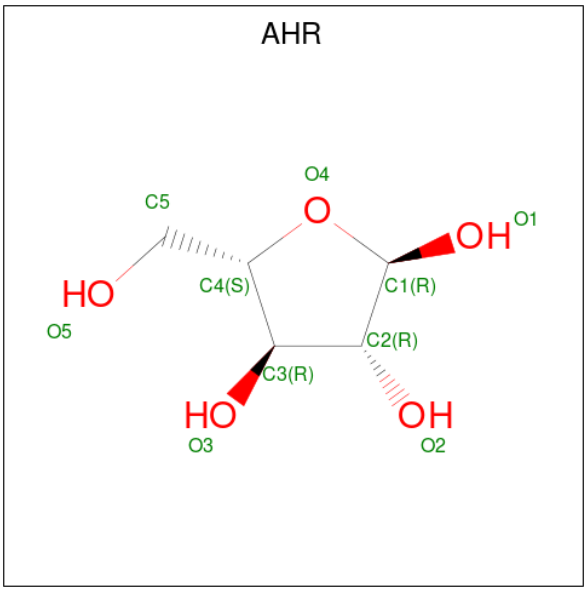
- Molecule 1 is a protein called Alpha-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	18	0
			4013	2556	695	735	27			
1	B	491	Total	C	N	O	S	0	17	0
			3998	2544	693	734	27			
1	C	492	Total	C	N	O	S	0	17	0
			4004	2550	693	733	28			

There are 12 discrepancies between the modelled and reference sequences:

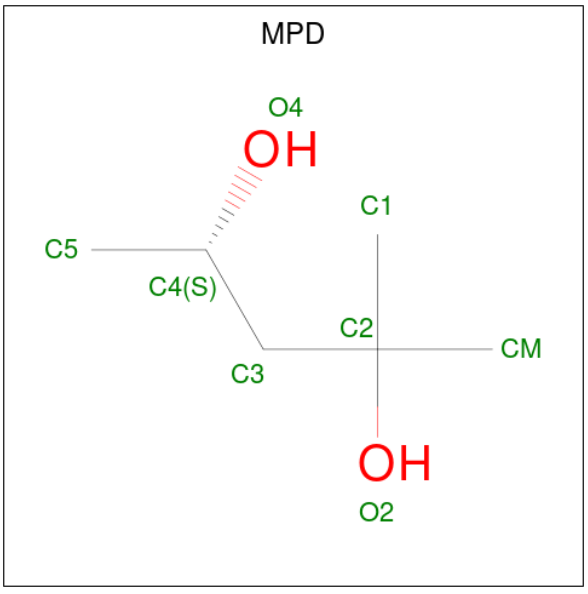
Chain	Residue	Modelled	Actual	Comment	Reference
A	69	HIS	ARG	conflict	UNP O69262
A	216	TRP	ASN	conflict	UNP O69262
A	274	GLU	ARG	conflict	UNP O69262
A	352	MET	LEU	conflict	UNP O69262
B	69	HIS	ARG	conflict	UNP O69262
B	216	TRP	ASN	conflict	UNP O69262
B	274	GLU	ARG	conflict	UNP O69262
B	352	MET	LEU	conflict	UNP O69262
C	69	HIS	ARG	conflict	UNP O69262
C	216	TRP	ASN	conflict	UNP O69262
C	274	GLU	ARG	conflict	UNP O69262
C	352	MET	LEU	conflict	UNP O69262

- Molecule 2 is alpha-L-arabinofuranose (three-letter code: AHR) (formula: $C_5H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



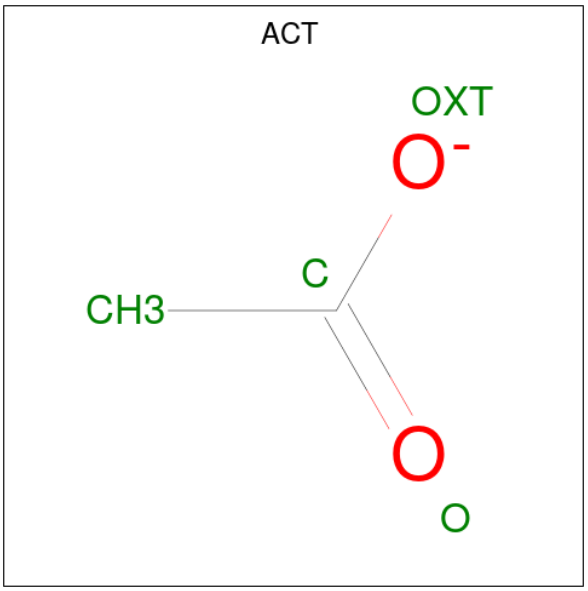
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0
2	B	1	Total C O 10 5 5	0	0
2	C	1	Total C O 10 5 5	0	0

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C O 8 6 2	0	0
3	A	1	Total C H O 22 6 14 2	0	0
3	A	1	Total C H O 22 6 14 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C H O 22 6 14 2	0	0
3	B	1	Total C H O 22 6 14 2	0	0
3	B	1	Total C H O 22 6 14 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	C	1	Total C O 8 6 2	0	0
3	C	1	Total C H O 22 6 14 2	0	0
3	C	1	Total C H O 22 6 14 2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

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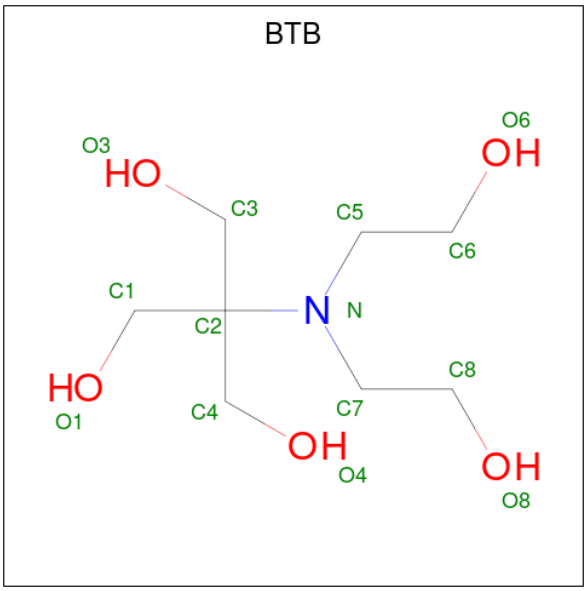
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

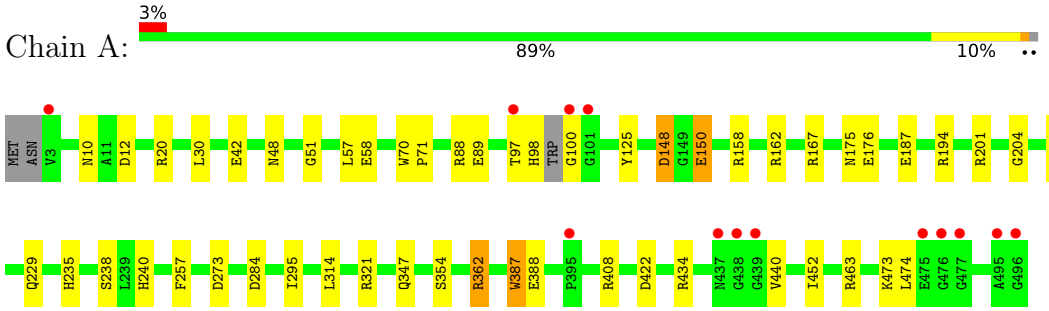
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	443	Total O 443 443	0	0
6	B	431	Total O 431 431	0	0
6	C	409	Total O 409 409	0	1

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.

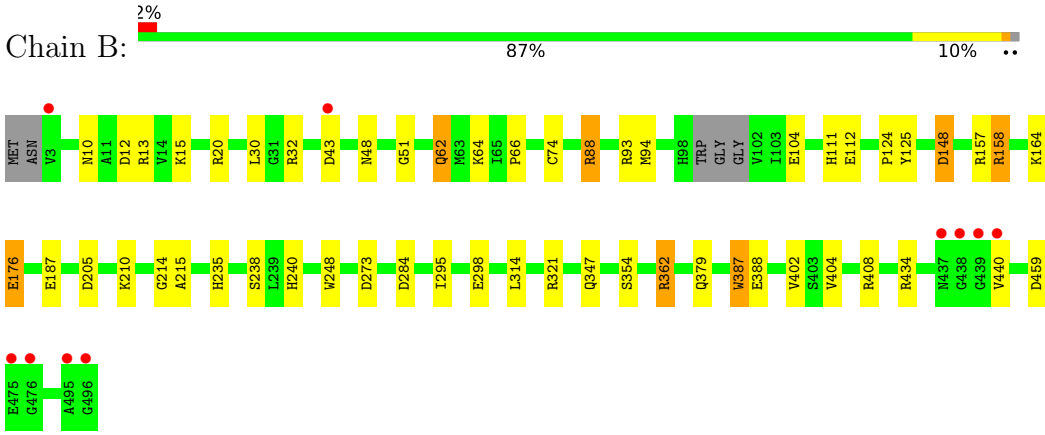
• Molecule 1: Alpha-L-arabinofuranosidase

Chain A:



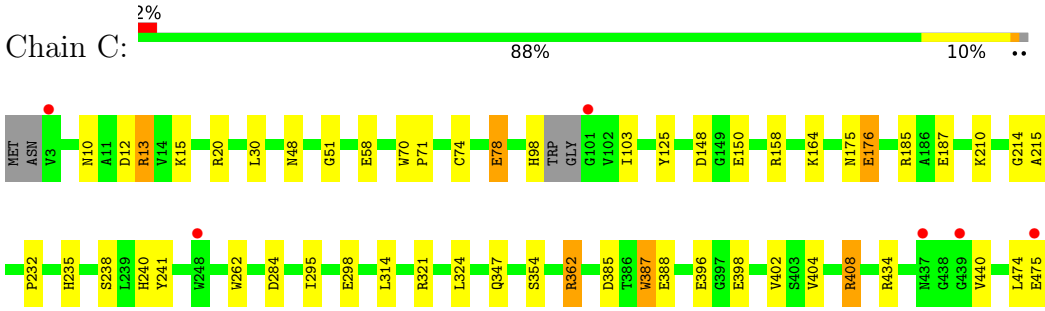
• Molecule 1: Alpha-L-arabinofuranosidase

Chain B:



• Molecule 1: Alpha-L-arabinofuranosidase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	157.06Å 157.06Å 379.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	136.02 – 2.00 49.27 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (136.02-2.00) 99.9 (49.27-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.147 , 0.173 0.163 , 0.184	Depositor DCC
R_{free} test set	1999 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13672	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 1.85% 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: AHR, MPD, ACT, BTB

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	1.00	6/4176 (0.1%)	1.02	22/5668 (0.4%)
1	B	0.96	8/4158 (0.2%)	1.01	26/5644 (0.5%)
1	C	0.99	7/4164 (0.2%)	0.99	16/5651 (0.3%)
All	All	0.98	21/12498 (0.2%)	1.01	64/16963 (0.4%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	GLU	CD-OE1	6.54	1.32	1.25
1	C	176[A]	GLU	CD-OE1	6.50	1.32	1.25
1	C	176[B]	GLU	CD-OE1	6.50	1.32	1.25
1	A	187	GLU	CG-CD	6.43	1.61	1.51
1	B	187	GLU	CG-CD	5.99	1.60	1.51

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	362	ARG	NE-CZ-NH1	12.74	126.67	120.30
1	A	362	ARG	NE-CZ-NH2	-12.09	114.25	120.30
1	A	434	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	C	434	ARG	NE-CZ-NH2	-10.57	115.02	120.30
1	B	362	ARG	NE-CZ-NH2	-9.97	115.31	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4013	0	3917	36	0
1	B	3998	0	3894	61	0
1	C	4004	0	3906	46	0
2	A	10	0	0	1	0
2	B	10	0	0	2	0
2	C	10	0	0	0	0
3	A	64	28	112	10	0
3	B	56	42	96	35	0
3	C	48	28	84	7	0
4	A	16	0	12	3	0
4	B	20	0	15	0	0
4	C	28	0	21	6	0
5	A	14	0	19	0	0
6	A	443	0	0	15	0
6	B	431	0	0	16	0
6	C	409	0	0	19	0
All	All	13574	98	12076	156	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 156 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:64:LYS:HD2	3:B:506:MPD:O2	1.45	1.17
1:B:64:LYS:HG3	3:B:506:MPD:HM1	1.33	1.11
1:B:379:GLN:HB2	3:B:506:MPD:H53	1.38	1.05
1:B:64:LYS:HE2	3:B:506:MPD:HM2	1.40	1.04
1:B:112:GLU:CD	3:B:508:MPD:H51	1.80	1.00

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/496 (102%)	489 (96%)	18 (4%)	0	100	100
1	B	504/496 (102%)	487 (97%)	16 (3%)	1 (0%)	47	44
1	C	505/496 (102%)	485 (96%)	20 (4%)	0	100	100
All	All	1516/1488 (102%)	1461 (96%)	54 (4%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	PRO

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	434/419 (104%)	432 (100%)	2 (0%)	88	92
1	B	433/419 (103%)	429 (99%)	4 (1%)	78	83
1	C	433/419 (103%)	432 (100%)	1 (0%)	93	95
All	All	1300/1257 (103%)	1293 (100%)	7 (0%)	86	92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	TYR
1	B	164	LYS

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Mol	Chain	Res	Type
1	C	125	TYR
1	B	463	ARG
1	B	62	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	235	HIS
1	C	183	ASN
1	B	235	HIS
1	C	175	ASN
1	B	183	ASN

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)

41 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	$\#\|Z\| > 2$
3	MPD	B	507	-	7,7,7	0.15	0	9,10,10	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ACT	B	512	-	3,3,3	1.14	0	3,3,3	1.29	0
3	MPD	C	503	-	7,7,7	0.85	0	9,10,10	1.34	1 (11%)
4	ACT	C	511	-	3,3,3	0.78	0	3,3,3	0.70	0
3	MPD	A	503	-	7,7,7	0.87	0	9,10,10	1.23	1 (11%)
3	MPD	B	504	-	7,7,7	1.10	0	9,10,10	1.19	1 (11%)
4	ACT	B	511	-	3,3,3	1.06	0	3,3,3	0.88	0
5	BTB	A	514	-	13,13,13	1.72	3 (23%)	7,16,16	1.67	2 (28%)
4	ACT	A	511	-	3,3,3	0.88	0	3,3,3	1.44	0
3	MPD	C	505	-	7,7,7	0.63	0	9,10,10	0.95	0
2	AHR	B	501	-	10,10,10	1.77	2 (20%)	13,14,14	3.00	8 (61%)
3	MPD	B	505	-	7,7,7	0.74	0	9,10,10	0.72	0
3	MPD	C	507	-	7,7,7	0.13	0	9,10,10	0.40	0
4	ACT	B	509	-	3,3,3	0.89	0	3,3,3	0.83	0
4	ACT	A	512	-	3,3,3	0.60	0	3,3,3	1.36	0
4	ACT	A	510	-	3,3,3	0.37	0	3,3,3	2.14	2 (66%)
4	ACT	C	513	-	3,3,3	0.53	0	3,3,3	1.09	0
4	ACT	C	508	-	3,3,3	0.98	0	3,3,3	1.39	0
4	ACT	B	513	-	3,3,3	1.05	0	3,3,3	1.27	0
4	ACT	C	510	-	3,3,3	0.61	0	3,3,3	1.17	0
2	AHR	C	501	-	10,10,10	1.09	0	13,14,14	1.80	5 (38%)
3	MPD	A	504	-	7,7,7	0.57	0	9,10,10	1.31	1 (11%)
3	MPD	B	506	1	7,7,7	0.10	0	9,10,10	0.32	0
3	MPD	A	508	-	7,7,7	0.13	0	9,10,10	0.28	0
3	MPD	C	502	-	7,7,7	0.92	0	9,10,10	2.14	3 (33%)
3	MPD	A	505	-	7,7,7	0.96	0	9,10,10	1.54	3 (33%)
3	MPD	B	508	-	7,7,7	0.10	0	9,10,10	0.32	0
3	MPD	B	502	-	7,7,7	0.85	0	9,10,10	1.55	2 (22%)
3	MPD	A	507	-	7,7,7	0.61	0	9,10,10	1.13	1 (11%)
3	MPD	B	503	-	7,7,7	0.51	0	9,10,10	1.12	1 (11%)
4	ACT	C	514	-	3,3,3	0.90	0	3,3,3	0.32	0
2	AHR	A	501	-	10,10,10	0.96	0	13,14,14	2.58	2 (15%)
4	ACT	A	513	-	3,3,3	0.94	0	3,3,3	0.22	0
3	MPD	C	506	-	7,7,7	0.13	0	9,10,10	0.29	0
4	ACT	C	509	-	3,3,3	0.84	0	3,3,3	0.71	0
4	ACT	B	510	-	3,3,3	0.64	0	3,3,3	1.51	0
4	ACT	C	512	-	3,3,3	0.98	0	3,3,3	0.65	0
3	MPD	A	506	-	7,7,7	0.92	0	9,10,10	1.26	1 (11%)
3	MPD	A	502	-	7,7,7	0.55	0	9,10,10	1.23	2 (22%)
3	MPD	A	509	-	7,7,7	0.16	0	9,10,10	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	MPD	C	504	-	7,7,7	1.00	1 (14%)	9,10,10	1.53	4 (44%)

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
3	MPD	B	507	-	-	0/5/5/5	-
3	MPD	C	503	-	-	1/5/5/5	-
3	MPD	A	503	-	-	2/5/5/5	-
3	MPD	B	504	-	-	2/5/5/5	-
5	BTB	A	514	-	-	7/21/21/21	-
3	MPD	C	505	-	-	2/5/5/5	-
2	AHR	B	501	-	-	0/2/18/18	0/1/1/1
3	MPD	B	505	-	-	2/5/5/5	-
3	MPD	C	507	-	-	2/5/5/5	-
2	AHR	C	501	-	-	2/2/18/18	0/1/1/1
3	MPD	A	504	-	-	1/5/5/5	-
3	MPD	B	506	1	-	0/5/5/5	-
3	MPD	A	508	-	-	0/5/5/5	-
3	MPD	C	502	-	-	2/5/5/5	-
3	MPD	A	505	-	-	0/5/5/5	-
3	MPD	B	508	-	-	0/5/5/5	-
3	MPD	B	502	-	-	2/5/5/5	-
3	MPD	A	507	-	-	3/5/5/5	-
3	MPD	B	503	-	-	0/5/5/5	-
2	AHR	A	501	-	-	2/2/18/18	0/1/1/1
3	MPD	C	506	-	-	0/5/5/5	-
3	MPD	A	506	-	-	5/5/5/5	-
3	MPD	A	502	-	-	1/5/5/5	-
3	MPD	A	509	-	-	0/5/5/5	-
3	MPD	C	504	-	-	3/5/5/5	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	AHR	O4-C1	-4.66	1.37	1.43
5	A	514	BTB	C2-N	3.72	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	514	BTB	C7-N	2.70	1.51	1.48
5	A	514	BTB	C3-C2	2.33	1.56	1.53
3	C	504	MPD	C3-C2	2.06	1.59	1.53

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	AHR	C1-C2-C3	5.86	109.64	102.30
2	A	501	AHR	O1-C1-O4	-5.83	103.66	111.13
2	B	501	AHR	O1-C1-O4	-4.88	104.88	111.13
2	B	501	AHR	C1-C2-C3	4.71	108.19	102.30
2	B	501	AHR	O4-C4-C5	-4.41	99.68	109.21

There are no chirality outliers.

5 of 39 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	MPD	C2-C3-C4-O4
3	A	506	MPD	C1-C2-C3-C4
3	A	507	MPD	C1-C2-C3-C4
3	A	507	MPD	O2-C2-C3-C4
3	B	504	MPD	C2-C3-C4-O4

There are no ring outliers.

22 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	507	MPD	1	0
3	B	504	MPD	2	0
4	A	511	ACT	2	0
3	C	505	MPD	2	0
2	B	501	AHR	2	0
3	C	507	MPD	3	0
4	A	510	ACT	1	0
4	C	513	ACT	2	0
4	C	508	ACT	2	0
3	A	504	MPD	1	0
3	B	506	MPD	18	0
3	A	508	MPD	5	0
3	C	502	MPD	1	0
3	B	508	MPD	11	0

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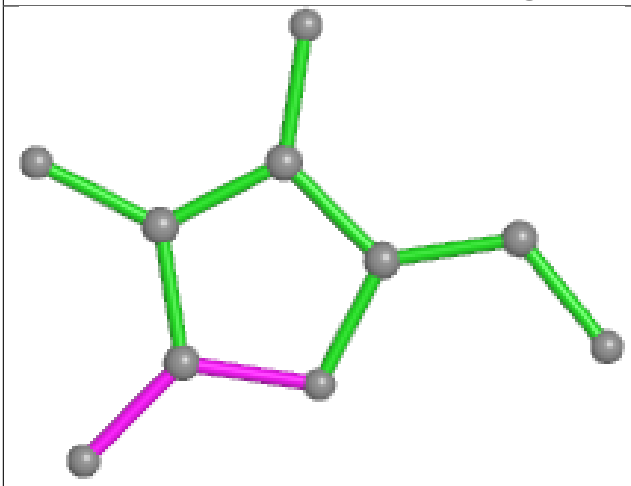
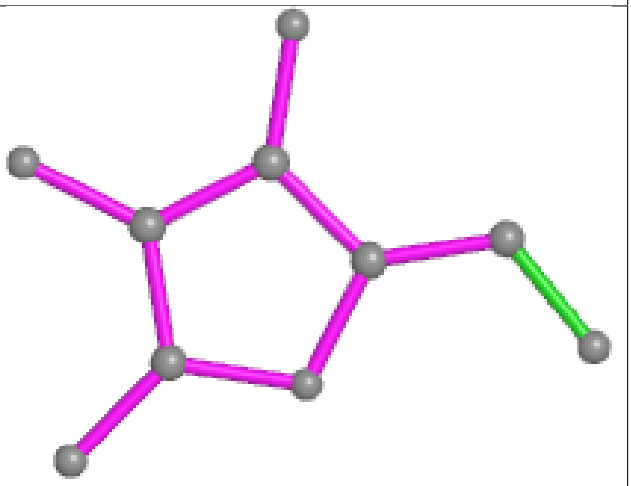
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	MPD	1	0
3	A	507	MPD	1	0
3	B	503	MPD	2	0
2	A	501	AHR	1	0
3	C	506	MPD	1	0
4	C	512	ACT	2	0
3	A	506	MPD	2	0
3	A	502	MPD	1	0

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.

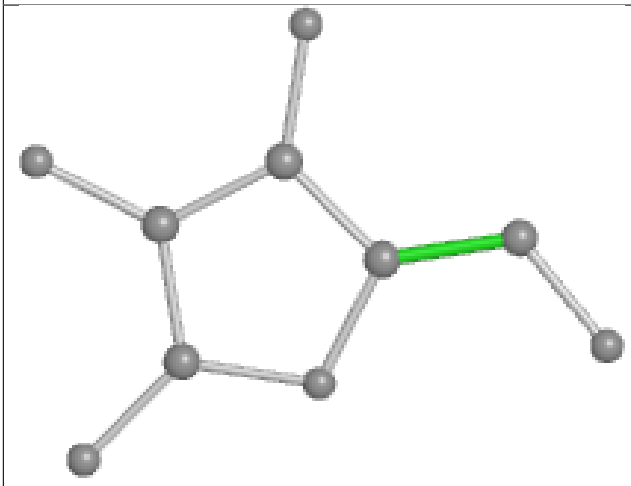
Ligand AHR B 501



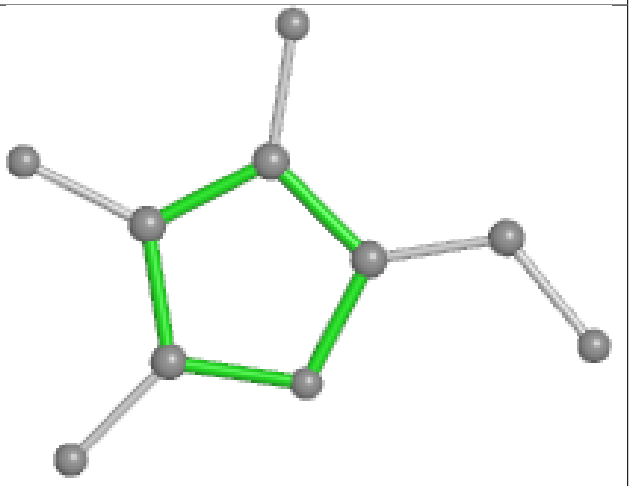
Bond lengths



Bond angles

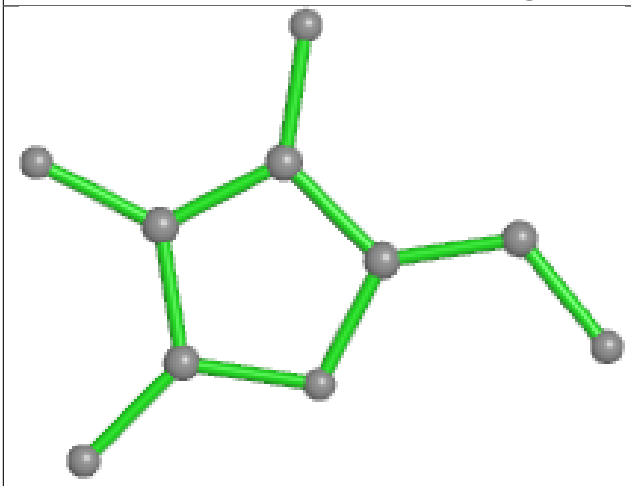


Torsions

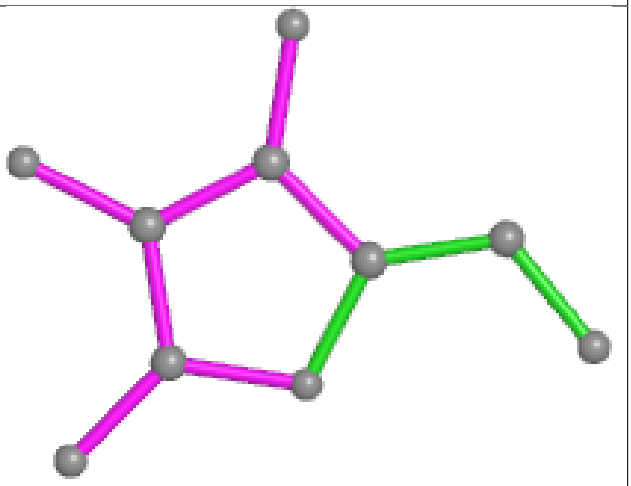


Rings

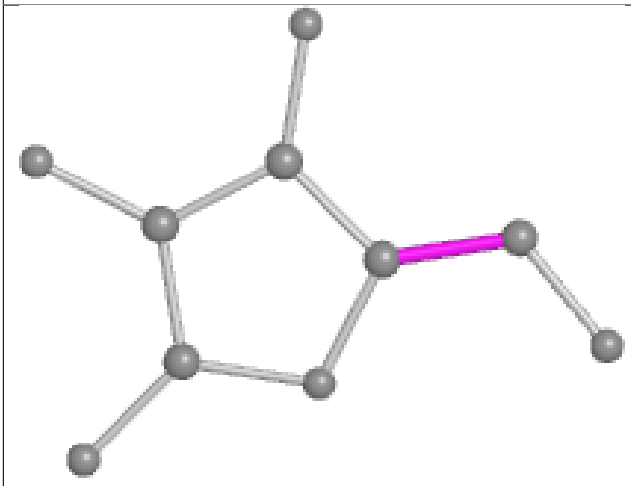
Ligand AHR C 501



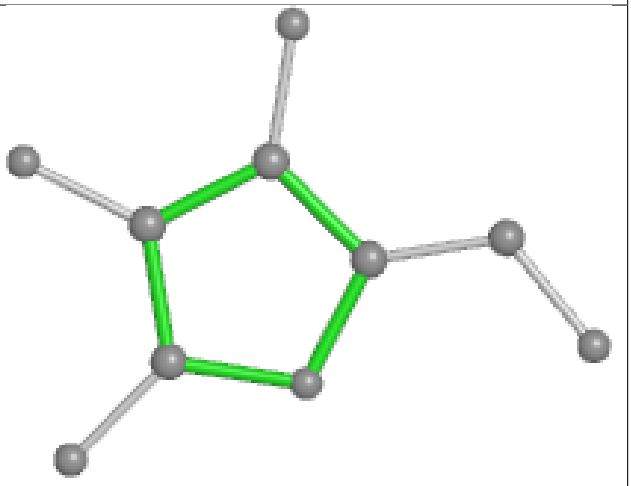
Bond lengths



Bond angles

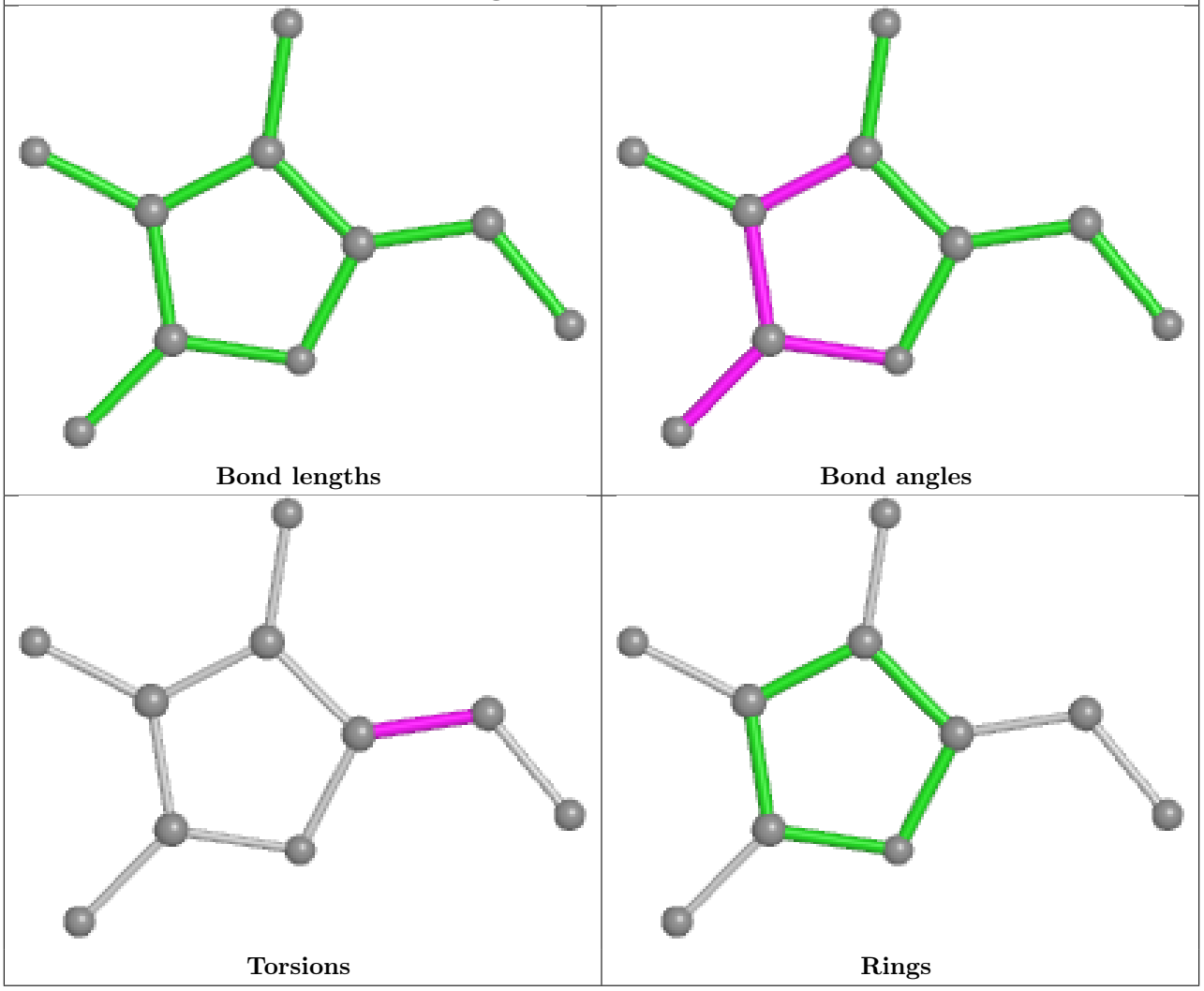


Torsions



Rings

Ligand AHR A 501



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	493/496 (99%)	-0.59	13 (2%) 56 54	23, 33, 62, 125	0
1	B	491/496 (98%)	-0.44	11 (2%) 62 60	24, 36, 67, 137	0
1	C	492/496 (99%)	-0.48	9 (1%) 68 66	24, 37, 71, 135	0
All	All	1476/1488 (99%)	-0.50	33 (2%) 62 60	23, 35, 67, 137	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	GLY	10.0
1	A	496	GLY	7.4
1	C	496	GLY	6.9
1	A	3	VAL	6.1
1	C	476	GLY	4.6

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 monosaccharides 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, 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.

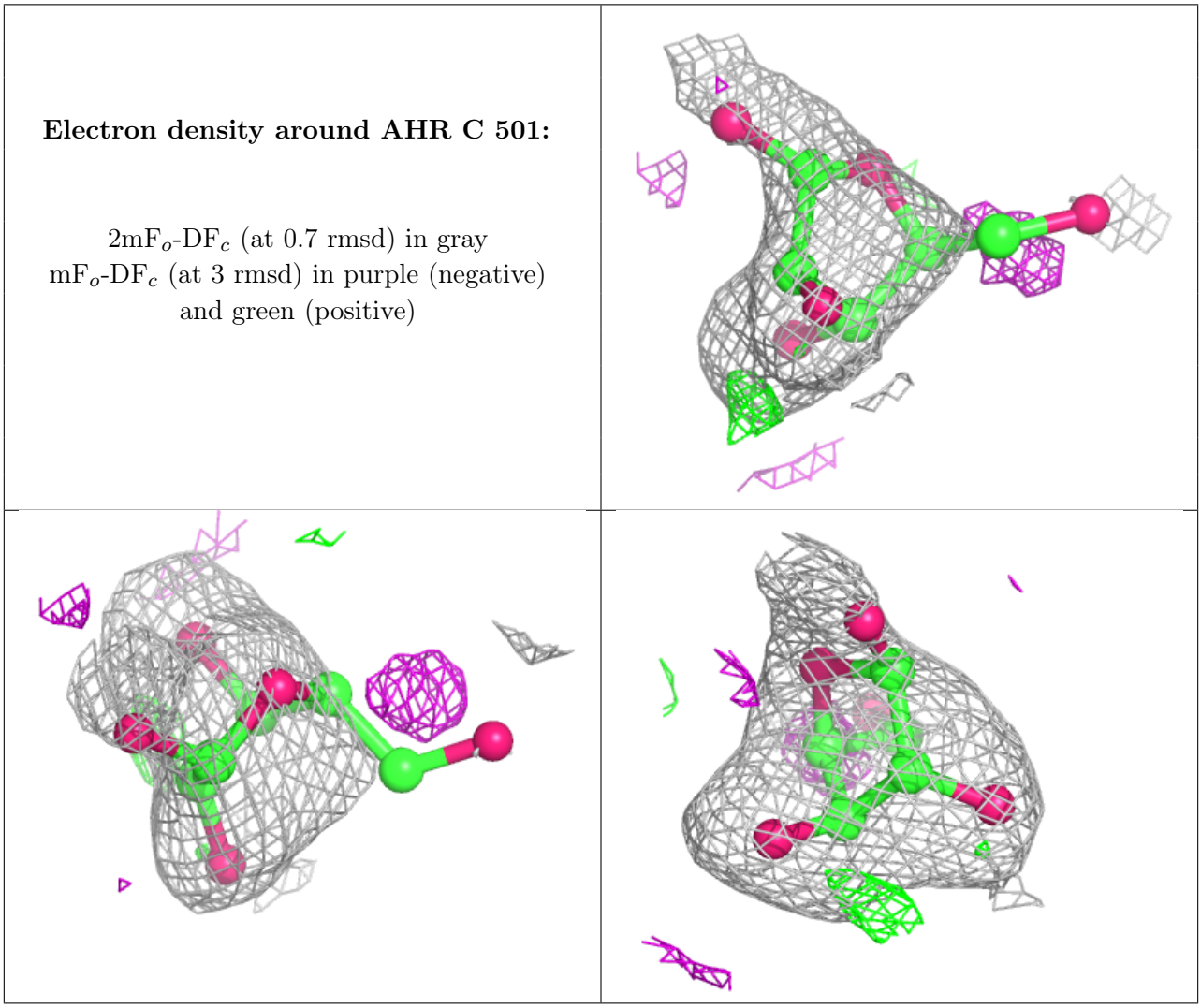
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MPD	B	506	8/8	0.33	0.95	20,20,20,20	0
3	MPD	B	508	8/8	0.49	0.88	20,20,20,20	0
3	MPD	B	504	8/8	0.67	0.25	73,88,99,103	0
3	MPD	B	507	8/8	0.71	0.50	20,20,20,20	0
3	MPD	C	505	8/8	0.73	0.30	83,101,112,113	0
3	MPD	C	506	8/8	0.73	0.67	20,20,20,20	0
3	MPD	A	506	8/8	0.76	0.22	83,90,99,99	0
3	MPD	A	508	8/8	0.76	0.61	20,20,20,20	0
4	ACT	A	511	4/4	0.79	0.41	89,90,93,99	0
2	AHR	C	501	10/10	0.80	0.23	60,93,102,106	0
3	MPD	C	507	8/8	0.81	0.48	20,20,20,20	0
3	MPD	C	503	8/8	0.81	0.43	82,109,133,138	0
4	ACT	A	513	4/4	0.81	0.20	80,82,86,94	0
4	ACT	B	509	4/4	0.82	0.25	79,81,91,101	0
3	MPD	B	505	8/8	0.83	0.34	85,96,100,102	0
3	MPD	A	505	8/8	0.84	0.38	73,85,89,97	0
4	ACT	B	512	4/4	0.84	0.16	69,80,83,88	0
4	ACT	C	509	4/4	0.84	0.29	78,84,90,107	0
3	MPD	A	503	8/8	0.85	0.15	64,66,76,78	0
2	AHR	A	501	10/10	0.85	0.27	52,101,124,126	0
3	MPD	A	502	8/8	0.86	0.18	64,70,78,86	0
4	ACT	C	513	4/4	0.86	0.25	76,79,83,96	0
3	MPD	A	504	8/8	0.87	0.29	72,81,89,98	0
3	MPD	A	507	8/8	0.87	0.19	63,84,88,88	0
4	ACT	C	512	4/4	0.88	0.16	59,82,91,91	0
4	ACT	A	512	4/4	0.89	0.23	75,82,86,87	0
2	AHR	B	501	10/10	0.89	0.18	50,81,88,88	0
4	ACT	C	511	4/4	0.89	0.23	91,99,101,101	0
3	MPD	C	504	8/8	0.89	0.37	90,98,111,111	0
4	ACT	B	511	4/4	0.89	0.37	86,89,92,99	0
5	BTB	A	514	14/14	0.89	0.17	49,61,67,67	0
4	ACT	A	510	4/4	0.91	0.15	75,81,84,92	0
3	MPD	A	509	8/8	0.91	0.49	20,20,20,20	0
3	MPD	B	503	8/8	0.91	0.16	62,74,90,92	0
4	ACT	B	513	4/4	0.92	0.15	80,83,86,89	0
4	ACT	B	510	4/4	0.92	0.11	74,76,80,88	0
4	ACT	C	514	4/4	0.93	0.17	87,90,91,92	0
4	ACT	C	510	4/4	0.95	0.08	74,77,79,83	0
3	MPD	C	502	8/8	0.96	0.13	58,68,76,78	0
3	MPD	B	502	8/8	0.96	0.18	55,65,79,86	0
4	ACT	C	508	4/4	0.97	0.24	42,59,65,84	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.

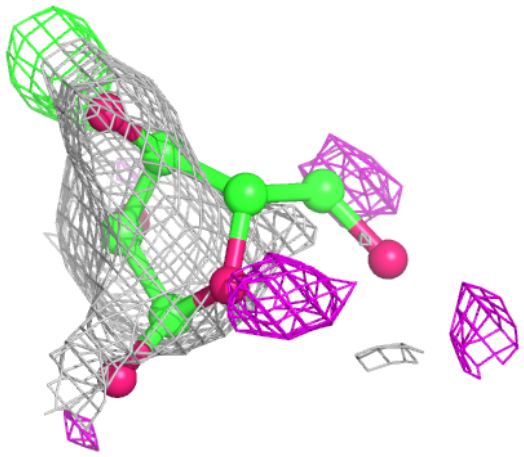
Electron density around AHR C 501:

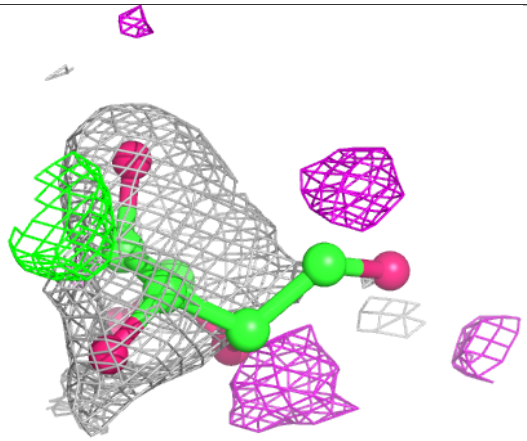
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

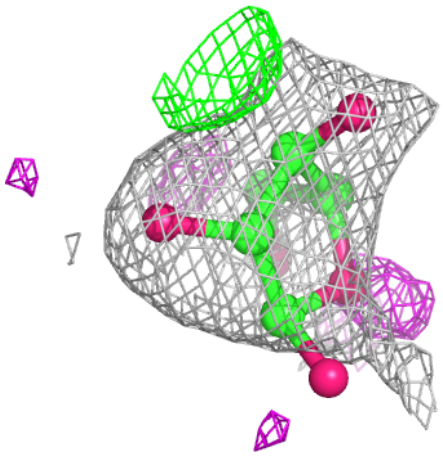


Electron density around AHR A 501:

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

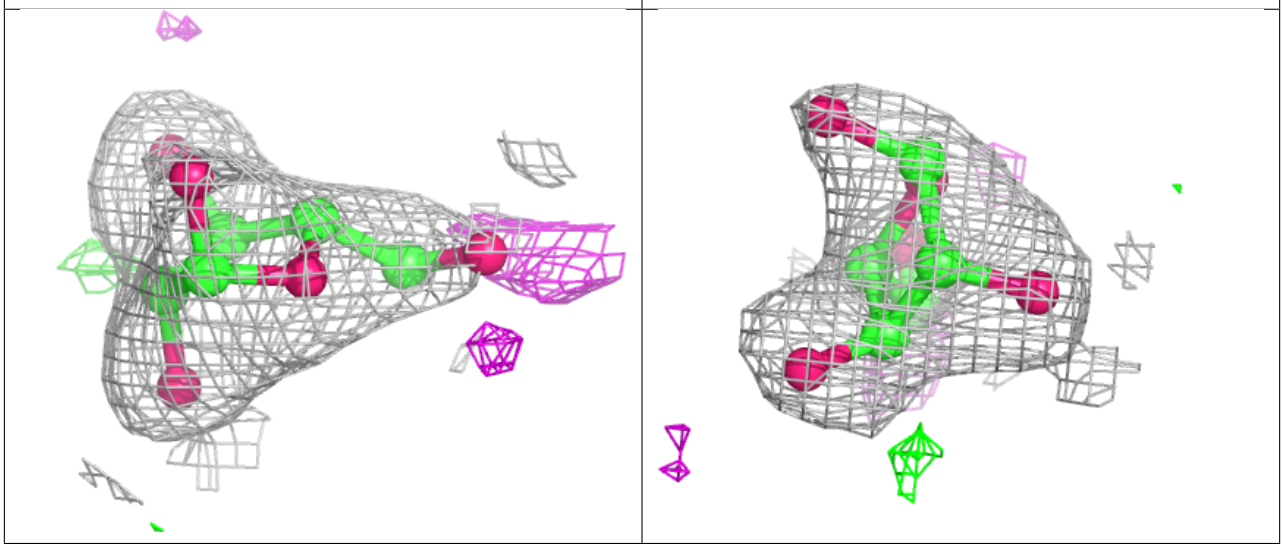






Electron density around AHR B 501:

$2mF_o$-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.