



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 09:27 PM EDT

PDB ID : 6ZT7  
Title : X-ray structure of mutated arabinofuranosidase  
Authors : Tandrup, T.; Lo Leggio, L.; Zhao, J.; Bissaro, B.; Barbe, S.; Andre, I.; Dumon, C.; O'Donohue, M.J.; Faure, R.  
Deposited on : 2020-07-17  
Resolution : 1.85 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) 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

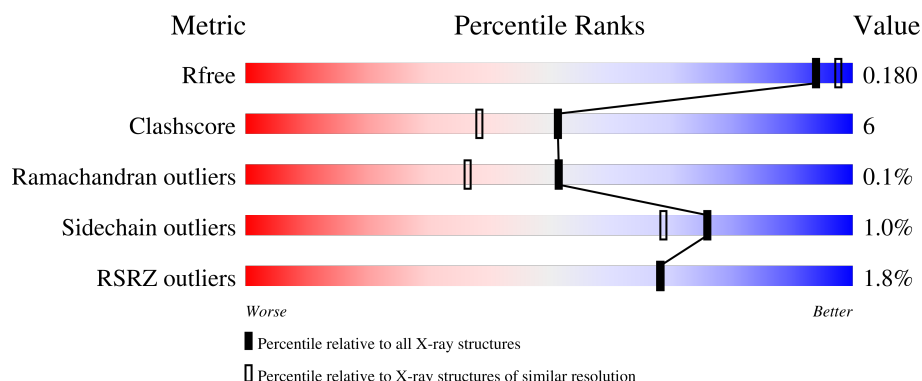
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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	496	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	B	496	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>..</div> </div> </div>
1	C	496	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>

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
2	ACT	B	503	-	-	X	-
2	ACT	B	505	-	-	X	-
2	ACT	C	501	-	-	X	-
2	ACT	C	505	-	-	-	X
2	ACT	C	506	-	-	-	X
3	MPD	A	513	-	-	-	X
3	MPD	A	514	-	-	-	X
3	MPD	A	515	-	-	-	X
3	MPD	A	516	-	-	-	X
3	MPD	B	515	-	-	-	X
3	MPD	C	510	-	-	-	X
3	MPD	C	511	-	-	-	X
3	MPD	C	512	-	-	-	X
3	MPD	C	514	-	-	-	X
3	MPD	C	515	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13895 atoms, of which 154 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	491	Total	C	N	O	S	0	21	0
			4020	2561	696	738	25			
1	B	491	Total	C	N	O	S	0	19	0
			4006	2546	695	739	26			
1	C	491	Total	C	N	O	S	0	19	0
			4006	2550	695	735	26			

There are 9 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



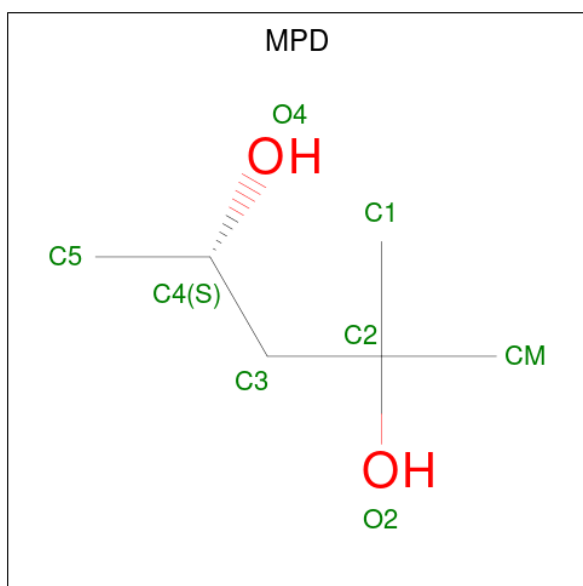
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total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

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

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



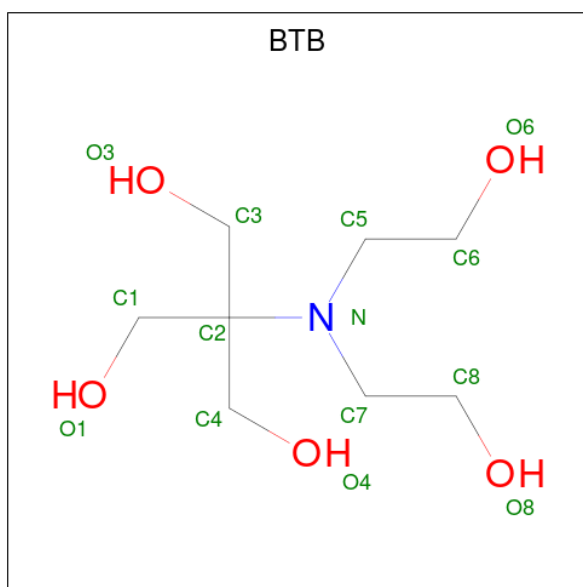
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 8	C 6	O 2	0	0	
3	A	1	Total 8	C 6	O 2	0	0	
3	A	1	Total 8	C 6	O 2	0	0	
3	A	1	Total 8	C 6	O 2	0	0	
3	A	1	Total 8	C 6	O 2	0	0	
3	A	1	Total 8	C 6	O 2	0	0	
3	A	1	Total 8	C 6	O 2	0	0	
3	A	1	Total 22	C 6	H 14	O 2	0	0
3	A	1	Total 22	C 6	H 14	O 2	0	0

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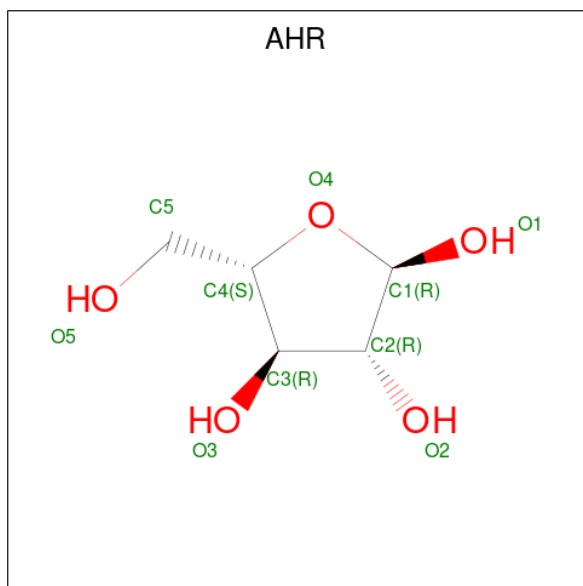
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O 22 6 14 2	0	0
3	A	1	Total C H O 22 6 14 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	B	1	Total C H O 22 6 14 2	0	0
3	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
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
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 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C<sub>8</sub>H<sub>19</sub>NO<sub>5</sub>).



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

- Molecule 5 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
5	A	1	Total	C	O	0	1
			20	10	10		
5	B	1	Total	C	O	0	1
			20	10	10		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	1
			20	10	10		

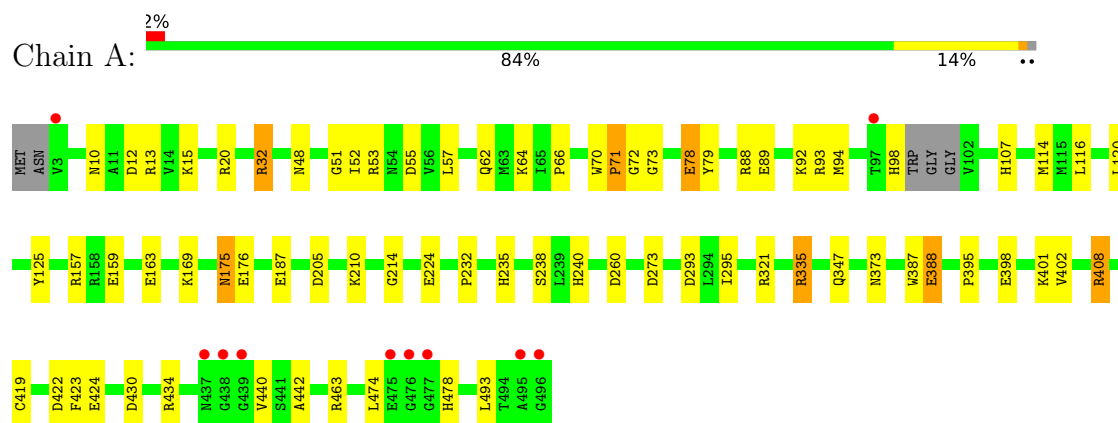
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	473	Total	O	0	0
			473	473		
6	B	452	Total	O	0	3
			452	452		
6	C	418	Total	O	0	0
			418	418		

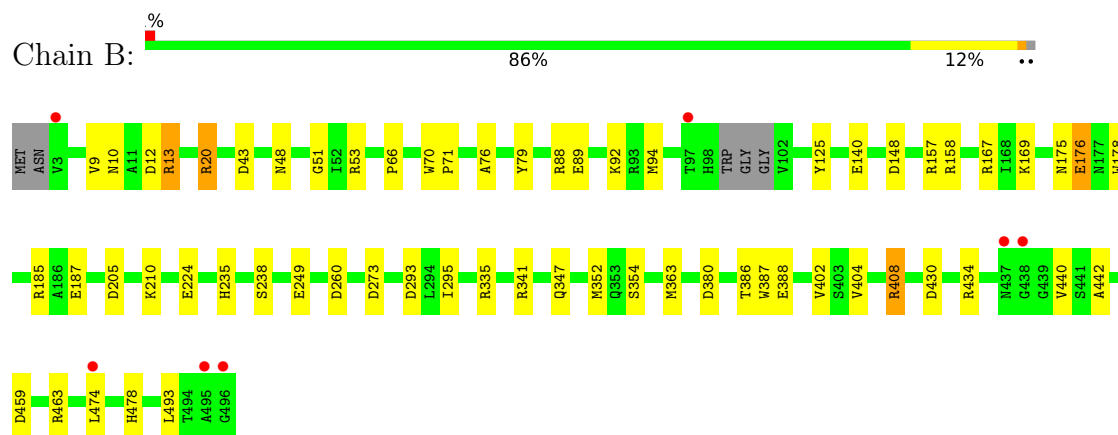
### 3 Residue-property plots

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.

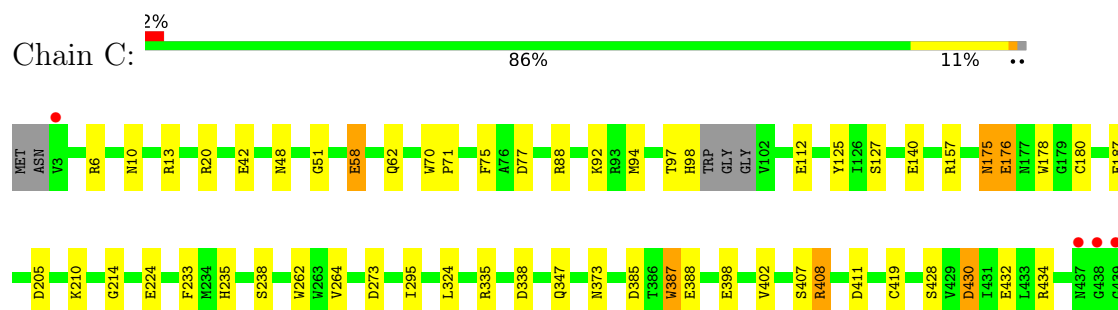
#### • Molecule 1: Alpha-L-arabinofuranosidase

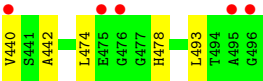


#### • Molecule 1: Alpha-L-arabinofuranosidase



#### • Molecule 1: Alpha-L-arabinofuranosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	156.79Å 156.79Å 378.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	135.79 – 1.85 49.53 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (135.79-1.85) 99.7 (49.53-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.144 , 0.166 0.162 , 0.180	Depositor DCC
$R_{free}$ test set	2315 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13895	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BTB, ACT, AHR, MPD

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	1.20	10/4186 (0.2%)	1.09	23/5680 (0.4%)
1	B	1.18	8/4169 (0.2%)	1.08	27/5656 (0.5%)
1	C	1.22	12/4169 (0.3%)	1.07	19/5655 (0.3%)
All	All	1.20	30/12524 (0.2%)	1.08	69/16991 (0.4%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	176[A]	GLU	CD-OE1	10.40	1.37	1.25
1	C	176[B]	GLU	CD-OE1	10.40	1.37	1.25
1	B	176	GLU	CD-OE1	9.96	1.36	1.25
1	A	176	GLU	CD-OE1	8.02	1.34	1.25
1	A	176	GLU	CD-OE2	7.92	1.34	1.25
1	B	176	GLU	CD-OE2	7.58	1.33	1.25
1	B	176	GLU	CB-CG	7.56	1.66	1.52
1	C	176[A]	GLU	CD-OE2	7.11	1.33	1.25
1	C	176[B]	GLU	CD-OE2	7.11	1.33	1.25
1	C	140	GLU	CD-OE2	-6.90	1.18	1.25
1	A	224	GLU	CD-OE2	-6.80	1.18	1.25
1	B	187	GLU	CD-OE1	6.25	1.32	1.25
1	B	249	GLU	CD-OE1	6.15	1.32	1.25
1	A	89	GLU	CD-OE2	5.90	1.32	1.25
1	A	79	TYR	CG-CD2	-5.82	1.31	1.39
1	B	224	GLU	CD-OE1	-5.72	1.19	1.25
1	C	187	GLU	CD-OE1	5.70	1.31	1.25
1	A	72	GLY	N-CA	5.69	1.54	1.46
1	C	407	SER	CA-CB	5.60	1.61	1.52
1	A	187	GLU	CD-OE1	5.54	1.31	1.25
1	C	58	GLU	CD-OE2	5.52	1.31	1.25
1	A	71	PRO	C-O	5.41	1.34	1.23
1	C	224	GLU	CD-OE1	-5.41	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	GLU	CD-OE2	-5.36	1.19	1.25
1	C	112	GLU	CD-OE1	5.36	1.31	1.25
1	C	387	TRP	CB-CG	-5.35	1.40	1.50
1	B	79	TYR	CE1-CZ	-5.29	1.31	1.38
1	C	224	GLU	CD-OE2	-5.12	1.20	1.25
1	A	388[A]	GLU	CD-OE2	-5.05	1.20	1.25
1	A	388[B]	GLU	CD-OE2	-5.05	1.20	1.25

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	408	ARG	NE-CZ-NH1	11.85	126.23	120.30
1	B	408	ARG	NE-CZ-NH1	11.29	125.95	120.30
1	C	408	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	B	408	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	A	408	ARG	NE-CZ-NH2	-10.17	115.21	120.30
1	A	273	ASP	CB-CG-OD1	9.74	127.07	118.30
1	C	408	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	C	434	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	A	434	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	A	422	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	B	434	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	C	20[A]	ARG	NE-CZ-NH1	-7.91	116.34	120.30
1	C	20[B]	ARG	NE-CZ-NH1	-7.91	116.34	120.30
1	A	53	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	157	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	459	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	20[A]	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	A	20[B]	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	B	434	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	B	13[A]	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	B	13[B]	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	B	88	ARG	CG-CD-NE	-6.96	97.18	111.80
1	C	273	ASP	CB-CG-OD1	6.75	124.37	118.30
1	B	205	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	157	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	B	352	MET	CG-SD-CE	-6.70	89.48	100.20
1	B	205	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	C	20[A]	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	C	20[B]	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	A	20[A]	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	20[B]	ARG	NE-CZ-NH2	6.52	123.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	A	434	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	12	ASP	CB-CG-OD1	6.17	123.85	118.30
1	B	187	GLU	OE1-CD-OE2	-5.96	116.15	123.30
1	B	20[A]	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	B	20[B]	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	293	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	273[A]	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	B	273[B]	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	B	167	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	176	GLU	OE1-CD-OE2	5.77	130.23	123.30
1	C	157	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	273	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	A	205	ASP	CB-CG-OD1	5.75	123.48	118.30
1	C	205	ASP	CB-CG-OD1	5.74	123.46	118.30
1	B	12	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	335	ARG	CG-CD-NE	-5.60	100.05	111.80
1	A	335	ARG	CG-CD-NE	-5.49	100.26	111.80
1	B	363	MET	CG-SD-CE	-5.47	91.45	100.20
1	C	180	CYS	CA-CB-SG	-5.45	104.19	114.00
1	A	32	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	273[A]	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	273[B]	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	430	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	176	GLU	OE1-CD-OE2	5.30	129.66	123.30
1	C	6	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	B	335	ARG	CG-CD-NE	-5.26	100.76	111.80
1	A	321	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	335	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	338	ASP	CB-CG-OD1	5.24	123.02	118.30
1	C	77	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	114	MET	CG-SD-CE	5.18	108.48	100.20
1	B	260	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	C	411	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	260	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	C	434	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	55	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	185	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	4020	0	3944	53	0
1	B	4006	0	3912	29	0
1	C	4006	0	3926	38	0
2	A	24	0	18	2	0
2	B	20	0	15	3	0
2	C	24	0	18	6	0
3	A	80	56	140	7	2
3	B	72	14	126	7	0
3	C	72	84	126	5	0
4	A	14	0	19	0	0
5	A	20	0	0	1	0
5	B	20	0	0	1	0
5	C	20	0	0	2	0
6	A	473	0	0	28	0
6	B	452	0	0	16	3
6	C	418	0	0	15	2
All	All	13741	154	12244	139	5

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

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:LYS:HE2	1:C:94:MET:SD	1.84	1.15
3:B:507:MPD:HM2	6:B:681:HOH:O	1.52	1.07
1:A:13[A]:ARG:NH1	6:A:602:HOH:O	1.95	0.99
1:A:163:GLU:OE1	6:A:601:HOH:O	1.88	0.92
1:A:57[B]:LEU:HD23	2:A:503:ACT:H1	1.49	0.91
3:C:511:MPD:HM2	6:C:816:HOH:O	1.71	0.90
1:A:62:GLN:NE2	6:A:603:HOH:O	2.07	0.86
1:A:335:ARG:HD2	6:A:890:HOH:O	1.74	0.86
2:B:503:ACT:H1	2:B:505:ACT:H2	1.60	0.84
1:A:210:LYS:H	1:A:235:HIS:HD2	1.28	0.81
1:B:210:LYS:H	1:B:235:HIS:HD2	1.26	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:514:MPD:H53	6:B:680:HOH:O	1.81	0.80
1:C:408:ARG:HD3	6:C:681:HOH:O	1.79	0.80
1:A:408:ARG:HD3	6:A:698:HOH:O	1.81	0.80
1:C:210:LYS:H	1:C:235:HIS:HD2	1.28	0.80
3:A:507:MPD:O4	3:A:507:MPD:HM1	1.83	0.78
2:C:501:ACT:H2	6:C:710:HOH:O	1.82	0.78
1:A:398:GLU:HB2	6:A:604:HOH:O	1.86	0.75
2:C:504:ACT:H3	6:C:900:HOH:O	1.86	0.74
1:C:42:GLU:HG3	2:C:501:ACT:OXT	1.89	0.72
1:A:93:ARG:HD2	6:A:864:HOH:O	1.89	0.71
1:B:13[A]:ARG:NH1	6:B:604:HOH:O	2.24	0.70
1:A:94:MET:HB3	6:A:1001:HOH:O	1.91	0.70
1:A:15:LYS:HB3	3:A:507:MPD:HM2	1.72	0.69
1:B:408:ARG:HD3	6:B:805:HOH:O	1.92	0.69
1:B:210:LYS:H	1:B:235:HIS:CD2	2.12	0.68
1:A:401:LYS:NZ	6:A:609:HOH:O	2.26	0.68
1:C:432:GLU:OE1	2:C:505:ACT:H3	1.95	0.67
1:C:94:MET:HB3	6:C:956:HOH:O	1.96	0.66
1:C:210:LYS:H	1:C:235:HIS:CD2	2.11	0.65
1:A:210:LYS:H	1:A:235:HIS:CD2	2.11	0.64
1:C:127[A]:SER:OG	6:C:601:HOH:O	2.15	0.64
1:C:58:GLU:HG3	6:C:974:HOH:O	1.98	0.64
1:B:20[B]:ARG:HG3	1:B:380:ASP:OD2	1.98	0.63
1:B:148:ASP:OD1	6:B:601:HOH:O	2.15	0.63
2:B:503:ACT:CH3	2:B:505:ACT:H2	2.28	0.62
1:C:13[B]:ARG:HG2	1:C:385:ASP:HB2	1.80	0.62
1:B:463:ARG:HD3	2:B:506:ACT:H3	1.80	0.61
1:A:169[B]:LYS:NZ	6:A:616:HOH:O	2.34	0.60
3:B:514:MPD:H51	6:B:652:HOH:O	2.02	0.60
1:B:20[B]:ARG:HG3	1:B:380:ASP:CG	2.21	0.60
1:A:395:PRO:O	6:A:604:HOH:O	2.17	0.59
1:B:48:ASN:HD22	1:B:51:GLY:H	1.49	0.59
1:B:402:VAL:HG12	1:B:404[B]:VAL:HG23	1.86	0.57
5:B:501[B]:AHR:O2	5:B:501[B]:AHR:C5	2.53	0.56
1:A:430:ASP:OD1	1:A:478:HIS:HD2	1.88	0.56
1:A:48:ASN:HD22	1:A:51:GLY:H	1.52	0.55
1:A:98:HIS:HE1	6:A:989:HOH:O	1.87	0.55
1:A:401:LYS:CE	6:A:609:HOH:O	2.53	0.55
1:C:10:ASN:ND2	1:C:387:TRP:CZ3	2.74	0.55
1:C:430:ASP:OD1	1:C:478:HIS:HD2	1.89	0.55
3:B:507:MPD:HM3	6:B:1037:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:440:VAL:HG23	1:C:474:LEU:HD21	1.90	0.54
2:C:503:ACT:H2	6:C:985:HOH:O	2.06	0.54
3:B:511:MPD:HM3	6:B:790:HOH:O	2.07	0.53
1:A:10:ASN:ND2	1:A:387:TRP:CZ3	2.76	0.53
1:A:232:PRO:O	3:A:515:MPD:HM3	2.08	0.53
1:B:10:ASN:ND2	1:B:387:TRP:CZ3	2.77	0.53
1:B:430:ASP:OD1	1:B:478:HIS:HD2	1.92	0.53
1:A:440:VAL:HG23	1:A:474:LEU:HD21	1.91	0.53
1:C:176[B]:GLU:HB2	6:C:602:HOH:O	2.07	0.53
1:B:92:LYS:HE2	1:B:94:MET:SD	2.49	0.52
1:C:13[B]:ARG:HG2	1:C:385:ASP:CB	2.39	0.52
1:A:92:LYS:HE2	1:A:94:MET:SD	2.50	0.52
1:C:92:LYS:CE	1:C:94:MET:SD	2.78	0.52
1:A:463:ARG:NE	6:A:626:HOH:O	2.44	0.51
1:C:88:ARG:HD2	2:C:501:ACT:O	2.10	0.51
1:C:48:ASN:HD22	1:C:51:GLY:H	1.59	0.51
3:B:509:MPD:O4	3:B:509:MPD:H12	2.10	0.50
1:C:176[B]:GLU:OE1	6:C:602:HOH:O	2.19	0.50
1:C:176[B]:GLU:HG2	1:C:178:TRP:CH2	2.46	0.50
2:A:501:ACT:H3	6:A:603:HOH:O	2.10	0.50
1:A:347:GLN:HE21	5:A:518[B]:AHR:C5	2.23	0.50
1:B:235:HIS:HE1	6:B:987:HOH:O	1.93	0.50
1:C:262:TRP:CH2	1:C:324[B]:LEU:HD12	2.46	0.50
1:A:52[A]:ILE:HD13	1:A:116:LEU:HD13	1.93	0.49
1:B:440:VAL:HG23	1:B:474:LEU:HD21	1.93	0.49
1:B:92:LYS:HD3	1:B:94:MET:HE1	1.94	0.49
1:A:175:ASN:ND2	6:A:613:HOH:O	2.45	0.49
3:B:511:MPD:H13	6:B:790:HOH:O	2.12	0.49
1:C:264:VAL:HG23	3:C:512:MPD:H13	1.95	0.49
1:A:32:ARG:HD3	3:A:513:MPD:H53	1.95	0.48
1:C:62:GLN:CD	6:C:636:HOH:O	2.51	0.48
1:A:62:GLN:HB2	6:A:854:HOH:O	2.14	0.48
1:A:423:PHE:CE1	1:A:424:GLU:HG3	2.48	0.48
1:A:463:ARG:HG3	6:A:626:HOH:O	2.12	0.47
1:B:43:ASP:HB2	6:B:782:HOH:O	2.14	0.47
1:C:75:PHE:CD1	6:C:952:HOH:O	2.68	0.47
1:C:235:HIS:HE1	6:C:958:HOH:O	1.98	0.46
1:B:176:GLU:HG3	6:B:696:HOH:O	2.15	0.46
1:A:57[B]:LEU:HD12	1:A:120:LEU:HD23	1.98	0.46
1:A:235:HIS:HE1	6:A:997:HOH:O	1.98	0.46
1:A:92:LYS:HD3	1:A:94:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:GLN:O	1:B:354:SER:HA	2.17	0.45
1:C:58:GLU:CG	6:C:974:HOH:O	2.61	0.45
1:A:62:GLN:HE21	1:A:373:ASN:HD21	1.64	0.44
1:B:158:ARG:HD2	6:B:821:HOH:O	2.16	0.44
1:B:238:SER:HA	1:B:295:ILE:O	2.18	0.44
1:B:442:ALA:HB2	1:B:493:LEU:HD22	1.99	0.44
1:A:10:ASN:OD1	6:A:605:HOH:O	2.21	0.44
1:A:48:ASN:ND2	1:A:51:GLY:H	2.16	0.44
1:C:92:LYS:HE2	1:C:94:MET:CE	2.46	0.44
1:A:240:HIS:CD2	6:A:843:HOH:O	2.70	0.44
1:A:64:LYS:HG3	3:A:509:MPD:C5	2.48	0.43
3:A:513:MPD:HM3	6:A:1024:HOH:O	2.17	0.43
5:C:516[B]:AHR:O2	5:C:516[B]:AHR:C5	2.64	0.43
1:A:78:GLU:OE1	6:A:606:HOH:O	2.21	0.43
1:B:293:ASP:OD1	1:B:341:ARG:HD2	2.19	0.43
1:C:70:TRP:CD1	1:C:71:PRO:HA	2.53	0.43
1:C:233:PHE:HA	3:C:511:MPD:H13	2.00	0.43
1:A:73:GLY:C	6:A:779:HOH:O	2.57	0.42
1:A:70:TRP:CD1	1:A:71:PRO:HA	2.55	0.42
1:A:442:ALA:HB2	1:A:493:LEU:HD22	2.01	0.42
1:C:238:SER:HA	1:C:295:ILE:O	2.18	0.42
1:A:175:ASN:HB3	6:A:779:HOH:O	2.20	0.42
1:A:238:SER:HA	1:A:295:ILE:O	2.20	0.42
1:A:88:ARG:NH1	6:A:624:HOH:O	2.43	0.42
1:A:395:PRO:HA	6:A:612:HOH:O	2.20	0.42
1:A:98:HIS:CE1	6:A:989:HOH:O	2.68	0.42
1:B:76:ALA:HB1	6:B:625:HOH:O	2.20	0.42
1:B:169[A]:LYS:HE2	6:B:986:HOH:O	2.19	0.42
1:C:62:GLN:HE21	1:C:373:ASN:HD21	1.67	0.41
1:A:88:ARG:HG3	1:A:107:HIS:CD2	2.55	0.41
1:C:347:GLN:HE21	5:C:516[B]:AHR:C5	2.34	0.41
1:A:88:ARG:HD3	1:A:107:HIS:CE1	2.55	0.41
1:B:70:TRP:CD1	1:B:71:PRO:HA	2.55	0.41
1:C:442:ALA:HB2	1:C:493:LEU:HD22	2.01	0.41
1:A:214:GLY:HA3	1:A:238:SER:O	2.21	0.41
1:C:175:ASN:ND2	6:C:601:HOH:O	2.53	0.41
1:C:402[A]:VAL:HA	1:C:419:CYS:O	2.21	0.41
1:A:402[A]:VAL:HA	1:A:419:CYS:O	2.21	0.40
1:A:159:GLU:CD	3:A:516:MPD:H51	2.41	0.40
1:B:48:ASN:ND2	1:B:51:GLY:H	2.16	0.40
1:C:398:GLU:OE2	3:C:512:MPD:H51	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:THR:O	1:C:98:HIS:C	2.59	0.40
3:C:513:MPD:HM1	3:C:513:MPD:H52	2.02	0.40
1:B:9:VAL:HG22	1:B:386[A]:THR:HG22	2.04	0.40
1:B:176:GLU:CG	6:B:696:HOH:O	2.69	0.40
1:C:214:GLY:HA3	1:C:238:SER:O	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:639:HOH:O	6:B:639:HOH:O[9_555]	0.69	1.51
6:B:726:HOH:O	6:B:726:HOH:O[9_555]	1.24	0.96
6:B:611:HOH:O	6:B:611:HOH:O[9_555]	1.53	0.67
3:A:514:MPD:C5	6:C:659:HOH:O[9_555]	2.13	0.07
3:A:514:MPD:H53	6:C:659:HOH:O[9_555]	1.54	0.06

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	508/496 (102%)	491 (97%)	16 (3%)	1 (0%)	47	33
1	B	506/496 (102%)	486 (96%)	19 (4%)	1 (0%)	47	33
1	C	506/496 (102%)	487 (96%)	19 (4%)	0	100	100
All	All	1520/1488 (102%)	1464 (96%)	54 (4%)	2 (0%)	51	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	66	PRO
1	A	66	PRO

### 5.3.2 Protein sidechains ⓘ

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	437/419 (104%)	432 (99%)	5 (1%)	73	65
1	B	435/419 (104%)	429 (99%)	6 (1%)	67	55
1	C	435/419 (104%)	430 (99%)	5 (1%)	73	65
All	All	1307/1257 (104%)	1291 (99%)	16 (1%)	76	62

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	GLU
1	A	125	TYR
1	A	175	ASN
1	A	388[A]	GLU
1	A	388[B]	GLU
1	B	89	GLU
1	B	125	TYR
1	B	175	ASN
1	B	178	TRP
1	B	388[A]	GLU
1	B	388[B]	GLU
1	C	125	TYR
1	C	175	ASN
1	C	388	GLU
1	C	428[A]	SER
1	C	428[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	62	GLN
1	A	175	ASN
1	A	183	ASN
1	A	235	HIS

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Mol	Chain	Res	Type
1	A	240	HIS
1	A	478	HIS
1	B	48	ASN
1	B	62	GLN
1	B	175	ASN
1	B	183	ASN
1	B	235	HIS
1	B	240	HIS
1	B	478	HIS
1	C	48	ASN
1	C	62	GLN
1	C	106	ASN
1	C	175	ASN
1	C	235	HIS
1	C	240	HIS
1	C	478	HIS

### 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](#)

52 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	ACT	A	505	-	3,3,3	0.95	0	3,3,3	0.36	0
2	ACT	B	505	-	3,3,3	0.62	0	3,3,3	1.73	2 (66%)
2	ACT	A	506	-	3,3,3	1.37	0	3,3,3	1.67	1 (33%)
5	AHR	A	518[A]	-	10,10,10	1.69	2 (20%)	13,14,14	2.26	5 (38%)
3	MPD	A	507	-	7,7,7	0.33	0	9,10,10	1.60	3 (33%)
2	ACT	C	502	-	3,3,3	0.82	0	3,3,3	1.58	1 (33%)
2	ACT	B	506	-	3,3,3	1.52	0	3,3,3	0.84	0
3	MPD	C	513	-	7,7,7	0.10	0	9,10,10	0.61	0
3	MPD	C	508	-	7,7,7	0.61	0	9,10,10	0.87	0
5	AHR	C	516[B]	-	10,10,10	1.06	0	13,14,14	1.94	3 (23%)
2	ACT	B	504	-	3,3,3	0.79	0	3,3,3	0.76	0
2	ACT	C	504	-	3,3,3	1.04	0	3,3,3	0.48	0
3	MPD	B	510	-	7,7,7	0.55	0	9,10,10	1.46	1 (11%)
4	BTB	A	517	-	13,13,13	1.84	5 (38%)	7,16,16	0.86	0
2	ACT	C	501	-	3,3,3	1.07	0	3,3,3	1.78	1 (33%)
3	MPD	B	511	-	7,7,7	0.75	0	9,10,10	0.83	0
2	ACT	B	502	-	3,3,3	0.71	0	3,3,3	1.14	0
3	MPD	A	515	-	7,7,7	0.12	0	9,10,10	0.40	0
3	MPD	C	507	-	7,7,7	1.05	1 (14%)	9,10,10	2.22	3 (33%)
3	MPD	B	515	-	7,7,7	0.14	0	9,10,10	0.27	0
2	ACT	C	505	-	3,3,3	1.05	0	3,3,3	0.45	0
3	MPD	C	509	-	7,7,7	0.54	0	9,10,10	0.61	0
2	ACT	C	503	-	3,3,3	0.77	0	3,3,3	1.26	0
3	MPD	A	513	-	7,7,7	0.12	0	9,10,10	0.25	0
3	MPD	A	511	-	7,7,7	0.75	0	9,10,10	1.45	2 (22%)
3	MPD	A	510	-	7,7,7	1.03	0	9,10,10	1.00	0
3	MPD	C	514	-	7,7,7	0.12	0	9,10,10	0.47	0
3	MPD	A	514	-	7,7,7	0.14	0	9,10,10	0.29	0
3	MPD	B	514	-	7,7,7	1.02	0	9,10,10	1.80	4 (44%)
2	ACT	A	504	-	3,3,3	0.80	0	3,3,3	1.50	1 (33%)
2	ACT	C	506	-	3,3,3	1.12	0	3,3,3	0.78	0
3	MPD	A	516	-	7,7,7	0.10	0	9,10,10	0.35	0
3	MPD	A	512	-	7,7,7	1.03	0	9,10,10	1.32	0
2	ACT	A	503	-	3,3,3	0.50	0	3,3,3	1.79	1 (33%)
3	MPD	A	508	-	7,7,7	0.78	0	9,10,10	1.06	0
3	MPD	B	509	-	7,7,7	0.43	0	9,10,10	0.64	0
3	MPD	C	510	-	7,7,7	0.11	0	9,10,10	0.23	0
3	MPD	C	511	-	7,7,7	0.14	0	9,10,10	0.25	0
3	MPD	C	512	-	7,7,7	0.11	0	9,10,10	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	AHR	B	501[B]	-	10,10,10	2.40	2 (20%)	13,14,14	4.17	9 (69%)
5	AHR	A	518[B]	-	10,10,10	1.29	1 (10%)	13,14,14	2.24	4 (30%)
5	AHR	C	516[A]	-	10,10,10	1.65	2 (20%)	13,14,14	2.33	5 (38%)
2	ACT	A	502	-	3,3,3	0.97	0	3,3,3	0.82	0
3	MPD	A	509	-	7,7,7	0.60	0	9,10,10	1.31	1 (11%)
2	ACT	A	501	-	3,3,3	1.07	0	3,3,3	0.32	0
3	MPD	B	512	-	7,7,7	0.77	0	9,10,10	1.63	2 (22%)
3	MPD	B	508	-	7,7,7	0.45	0	9,10,10	0.79	0
3	MPD	B	513	-	7,7,7	0.97	0	9,10,10	2.05	5 (55%)
2	ACT	B	503	-	3,3,3	1.00	0	3,3,3	0.89	0
3	MPD	C	515	-	7,7,7	0.12	0	9,10,10	0.28	0
3	MPD	B	507	-	7,7,7	0.53	0	9,10,10	1.23	0
5	AHR	B	501[A]	-	10,10,10	1.82	3 (30%)	13,14,14	1.62	5 (38%)

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
5	AHR	A	518[A]	-	-	2/2/18/18	0/1/1/1
3	MPD	A	507	-	-	3/5/5/5	-
3	MPD	C	513	-	-	1/5/5/5	-
3	MPD	C	508	-	-	2/5/5/5	-
5	AHR	C	516[B]	-	-	0/2/18/18	0/1/1/1
3	MPD	B	510	-	-	0/5/5/5	-
4	BTB	A	517	-	-	2/21/21/21	-
3	MPD	C	507	-	-	3/5/5/5	-
3	MPD	B	511	-	-	5/5/5/5	-
3	MPD	A	515	-	-	2/5/5/5	-
3	MPD	C	509	-	-	0/5/5/5	-
3	MPD	B	515	-	-	0/5/5/5	-
3	MPD	A	513	-	-	0/5/5/5	-
3	MPD	A	511	-	-	0/5/5/5	-
3	MPD	A	510	-	-	1/5/5/5	-
3	MPD	C	514	-	-	2/5/5/5	-
3	MPD	A	514	-	-	1/5/5/5	-
3	MPD	B	514	-	-	2/5/5/5	-
3	MPD	C	510	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	B	509	-	-	2/5/5/5	-
3	MPD	A	516	-	-	2/5/5/5	-
3	MPD	A	512	-	-	2/5/5/5	-
3	MPD	C	512	-	-	1/5/5/5	-
3	MPD	A	508	-	-	2/5/5/5	-
5	AHR	B	501[B]	-	-	2/2/18/18	0/1/1/1
3	MPD	C	511	-	-	0/5/5/5	-
5	AHR	A	518[B]	-	-	2/2/18/18	0/1/1/1
5	AHR	C	516[A]	-	-	0/2/18/18	0/1/1/1
3	MPD	A	509	-	-	0/5/5/5	-
3	MPD	B	512	-	-	0/5/5/5	-
3	MPD	B	508	-	-	0/5/5/5	-
3	MPD	B	513	-	-	1/5/5/5	-
3	MPD	C	515	-	-	1/5/5/5	-
3	MPD	B	507	-	-	0/5/5/5	-
5	AHR	B	501[A]	-	-	1/2/18/18	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501[B]	AHR	C1-C2	5.67	1.59	1.52
5	B	501[B]	AHR	O1-C1	4.48	1.53	1.39
5	A	518[A]	AHR	O4-C1	4.26	1.48	1.43
4	A	517	BTB	C2-N	3.85	1.56	1.48
5	C	516[A]	AHR	O4-C1	3.72	1.47	1.43
5	B	501[A]	AHR	O4-C1	3.56	1.47	1.43
5	B	501[A]	AHR	O1-C1	3.27	1.50	1.39
5	B	501[A]	AHR	C1-C2	2.99	1.56	1.52
5	C	516[A]	AHR	C1-C2	2.81	1.56	1.52
4	A	517	BTB	C5-N	2.33	1.51	1.48
5	A	518[A]	AHR	O1-C1	2.32	1.47	1.39
4	A	517	BTB	C4-C2	2.32	1.56	1.53
3	C	507	MPD	CM-C2	-2.23	1.45	1.52
5	A	518[B]	AHR	C1-C2	2.19	1.55	1.52
4	A	517	BTB	O3-C3	2.17	1.49	1.42
4	A	517	BTB	C3-C2	2.14	1.56	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501[B]	AHR	C1-C2-C3	8.64	113.11	102.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501[B]	AHR	C5-C4-C3	-7.12	97.93	115.09
5	C	516[A]	AHR	O4-C4-C5	5.48	121.06	109.21
5	A	518[B]	AHR	C5-C4-C3	-5.04	102.94	115.09
5	A	518[A]	AHR	O4-C4-C5	4.85	119.69	109.21
5	B	501[B]	AHR	O4-C1-C2	-4.81	98.55	104.46
5	B	501[B]	AHR	O2-C2-C3	-4.66	96.75	111.82
5	A	518[A]	AHR	O1-C1-O4	4.31	116.65	111.13
5	B	501[B]	AHR	C2-C3-C4	-3.74	95.38	102.64
5	B	501[B]	AHR	O4-C4-C3	3.70	112.44	105.11
5	C	516[B]	AHR	O4-C4-C5	-3.68	101.27	109.21
3	B	513	MPD	CM-C2-C1	3.67	118.22	110.57
3	C	507	MPD	O4-C4-C3	-3.60	96.84	111.36
5	C	516[B]	AHR	C2-C3-C4	-3.59	95.66	102.64
3	C	507	MPD	C1-C2-C3	3.59	126.67	109.96
5	A	518[B]	AHR	O1-C1-O4	-3.45	106.71	111.13
5	A	518[B]	AHR	C1-C2-C3	3.22	106.33	102.30
5	A	518[A]	AHR	C1-C2-C3	3.21	106.32	102.30
3	B	512	MPD	CM-C2-C1	3.18	117.21	110.57
5	B	501[A]	AHR	C1-C2-C3	3.15	106.24	102.30
3	B	512	MPD	O2-C2-C1	-3.13	98.03	108.08
5	C	516[B]	AHR	C5-C4-C3	-3.05	107.74	115.09
5	C	516[A]	AHR	O5-C5-C4	-3.04	100.85	111.29
3	C	507	MPD	O2-C2-C1	-3.03	98.37	108.08
3	A	507	MPD	CM-C2-C1	-2.93	104.47	110.57
3	B	514	MPD	C5-C4-C3	-2.93	97.89	111.69
5	B	501[B]	AHR	O5-C5-C4	-2.83	101.58	111.29
5	C	516[A]	AHR	O3-C3-C4	2.78	119.10	111.05
3	A	511	MPD	O4-C4-C5	-2.77	97.39	109.38
3	B	513	MPD	O2-C2-C1	-2.65	99.58	108.08
3	B	514	MPD	O2-C2-C3	-2.54	100.27	109.80
2	C	501	ACT	O-C-CH3	-2.48	112.67	122.33
5	A	518[B]	AHR	O3-C3-C2	2.48	119.84	111.82
3	A	509	MPD	CM-C2-C1	2.48	115.74	110.57
2	A	503	ACT	O-C-CH3	-2.48	112.69	122.33
5	B	501[B]	AHR	O1-C1-C2	2.45	122.09	110.39
5	C	516[A]	AHR	O2-C2-C3	-2.41	104.02	111.82
3	A	511	MPD	CM-C2-C1	-2.41	105.56	110.57
3	B	513	MPD	O4-C4-C5	-2.38	99.08	109.38
2	A	506	ACT	OXT-C-O	-2.33	113.45	122.05
3	B	510	MPD	O4-C4-C3	-2.32	101.98	111.36
5	C	516[A]	AHR	O2-C2-C1	2.29	118.15	111.82
5	B	501[A]	AHR	O4-C4-C5	2.26	114.09	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	507	MPD	C1-C2-C3	2.23	120.36	109.96
3	B	514	MPD	O4-C4-C5	2.23	119.03	109.38
3	A	507	MPD	O2-C2-CM	2.22	115.22	108.08
3	B	513	MPD	O2-C2-C3	2.20	118.06	109.80
5	B	501[B]	AHR	O3-C3-C2	2.20	118.93	111.82
5	B	501[A]	AHR	O1-C1-O4	2.20	113.94	111.13
2	B	505	ACT	O-C-CH3	-2.15	113.98	122.33
5	A	518[A]	AHR	C5-C4-C3	-2.14	109.92	115.09
3	B	514	MPD	CM-C2-C1	2.13	115.02	110.57
5	A	518[A]	AHR	O5-C5-C4	-2.10	104.07	111.29
2	A	504	ACT	OXT-C-CH3	2.09	123.82	115.18
2	B	505	ACT	OXT-C-CH3	2.08	123.78	115.18
2	C	502	ACT	OXT-C-CH3	2.07	123.74	115.18
5	B	501[A]	AHR	O5-C5-C4	-2.05	104.27	111.29
3	B	513	MPD	O2-C2-CM	-2.03	101.55	108.08
5	B	501[A]	AHR	O2-C2-C1	2.03	117.41	111.82

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	507	MPD	O2-C2-C3-C4
3	A	507	MPD	CM-C2-C3-C4
3	A	508	MPD	C1-C2-C3-C4
3	A	508	MPD	O2-C2-C3-C4
3	A	510	MPD	C2-C3-C4-O4
3	B	511	MPD	C1-C2-C3-C4
3	B	511	MPD	O2-C2-C3-C4
3	C	507	MPD	C1-C2-C3-C4
3	C	507	MPD	O2-C2-C3-C4
3	C	508	MPD	C1-C2-C3-C4
3	C	508	MPD	O2-C2-C3-C4
3	C	513	MPD	C2-C3-C4-O4
5	A	518[B]	AHR	C3-C4-C5-O5
5	A	518[A]	AHR	O4-C4-C5-O5
5	A	518[B]	AHR	O4-C4-C5-O5
4	A	517	BTB	N-C7-C8-O8
5	B	501[B]	AHR	C3-C4-C5-O5
3	A	514	MPD	O2-C2-C3-C4
5	B	501[B]	AHR	O4-C4-C5-O5
3	A	515	MPD	C2-C3-C4-C5
3	A	516	MPD	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	514	MPD	C2-C3-C4-C5
3	C	514	MPD	C2-C3-C4-C5
3	C	514	MPD	C2-C3-C4-O4
5	B	501[A]	AHR	O4-C4-C5-O5
3	A	512	MPD	C1-C2-C3-C4
3	B	509	MPD	C1-C2-C3-C4
3	B	511	MPD	CM-C2-C3-C4
3	C	507	MPD	CM-C2-C3-C4
5	A	518[A]	AHR	C3-C4-C5-O5
3	C	510	MPD	O2-C2-C3-C4
3	C	512	MPD	O2-C2-C3-C4
3	C	515	MPD	O2-C2-C3-C4
3	B	511	MPD	C2-C3-C4-C5
3	B	513	MPD	C2-C3-C4-C5
4	A	517	BTB	C3-C2-C4-O4
3	A	507	MPD	C2-C3-C4-O4
3	A	512	MPD	C2-C3-C4-O4
3	A	515	MPD	C2-C3-C4-O4
3	A	516	MPD	C2-C3-C4-O4
3	B	509	MPD	C2-C3-C4-O4
3	B	511	MPD	C2-C3-C4-O4
3	B	514	MPD	C2-C3-C4-O4

There are no ring outliers.

25 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	ACT	2	0
3	A	507	MPD	2	0
2	B	506	ACT	1	0
3	C	513	MPD	1	0
5	C	516[B]	AHR	2	0
2	C	504	ACT	1	0
2	C	501	ACT	3	0
3	B	511	MPD	2	0
3	A	515	MPD	1	0
2	C	505	ACT	1	0
2	C	503	ACT	1	0
3	A	513	MPD	2	0
3	A	514	MPD	0	2
3	B	514	MPD	2	0
3	A	516	MPD	1	0

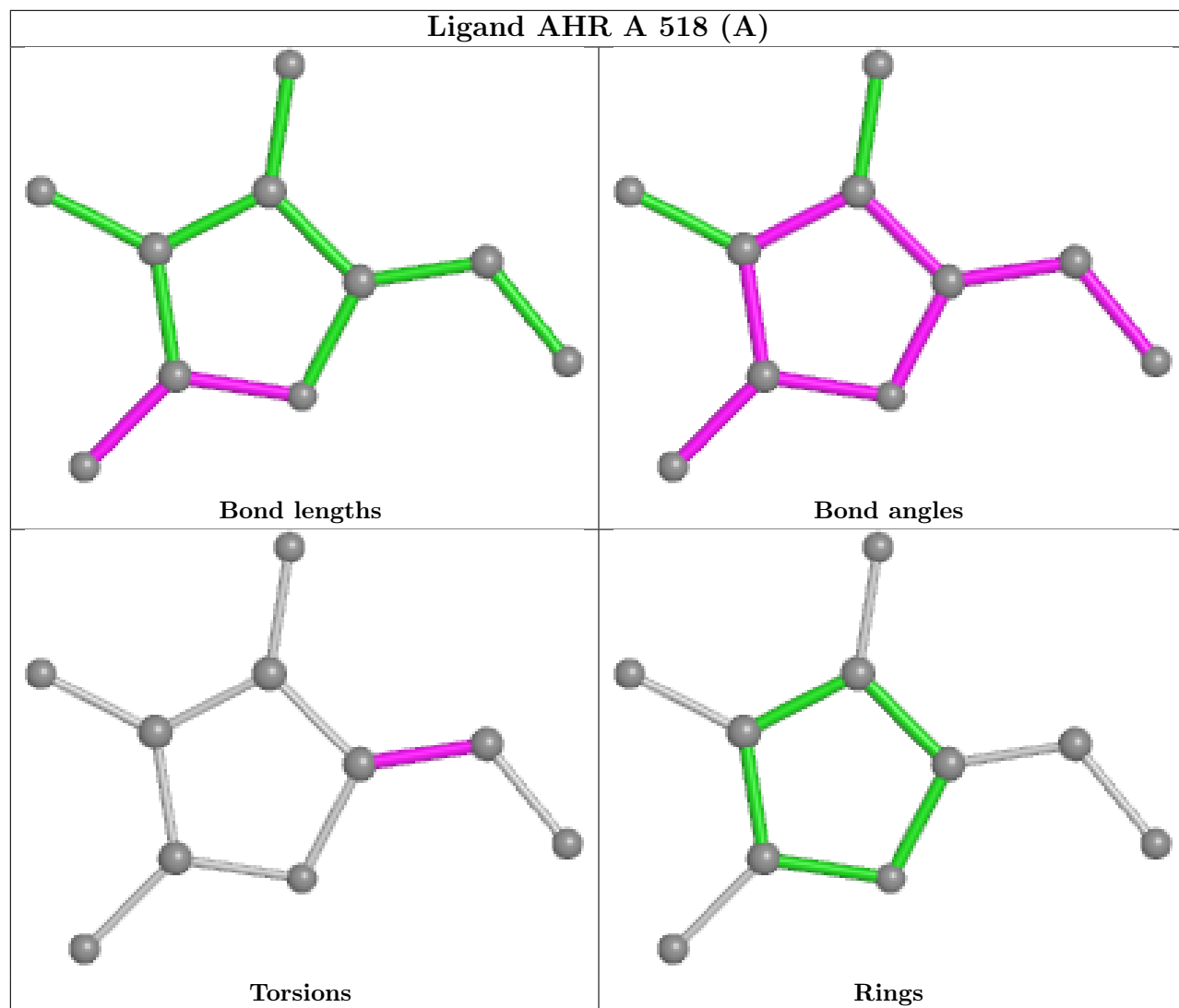
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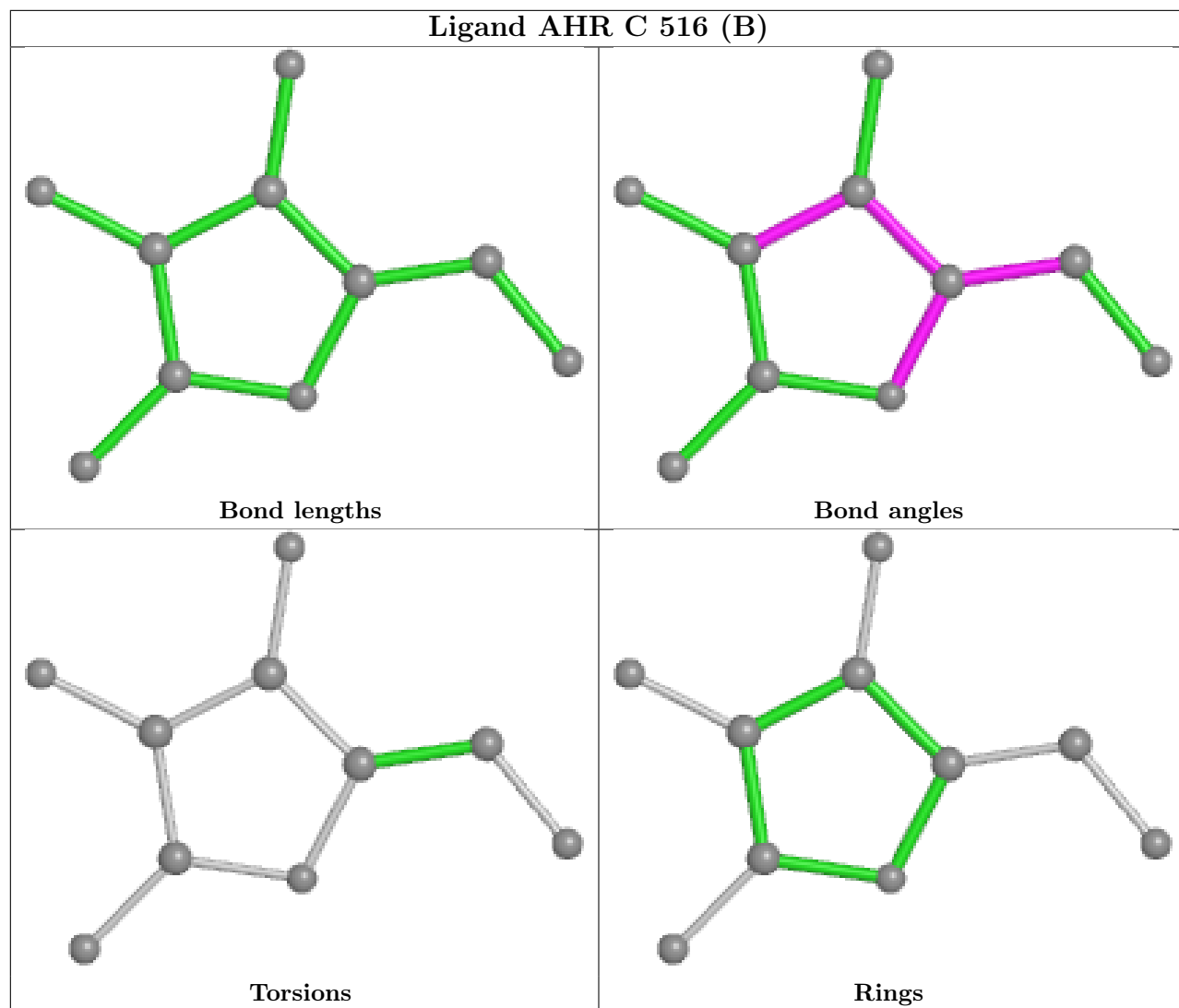
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	ACT	1	0
3	B	509	MPD	1	0
3	C	511	MPD	2	0
3	C	512	MPD	2	0
5	B	501[B]	AHR	1	0
5	A	518[B]	AHR	1	0
3	A	509	MPD	1	0
2	A	501	ACT	1	0
2	B	503	ACT	2	0
3	B	507	MPD	2	0

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.

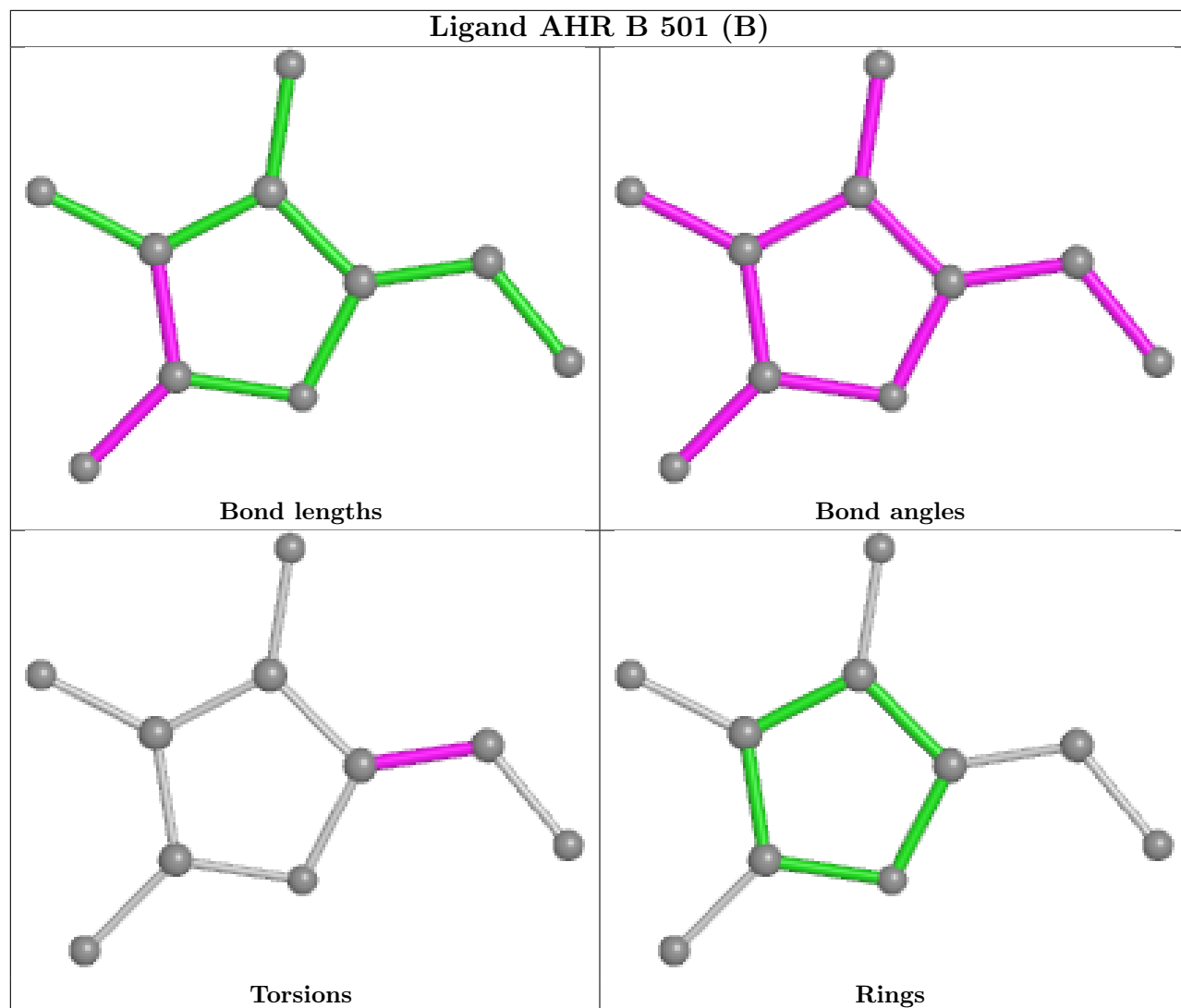
## Ligand AHR A 518 (A)



## Ligand AHR C 516 (B)

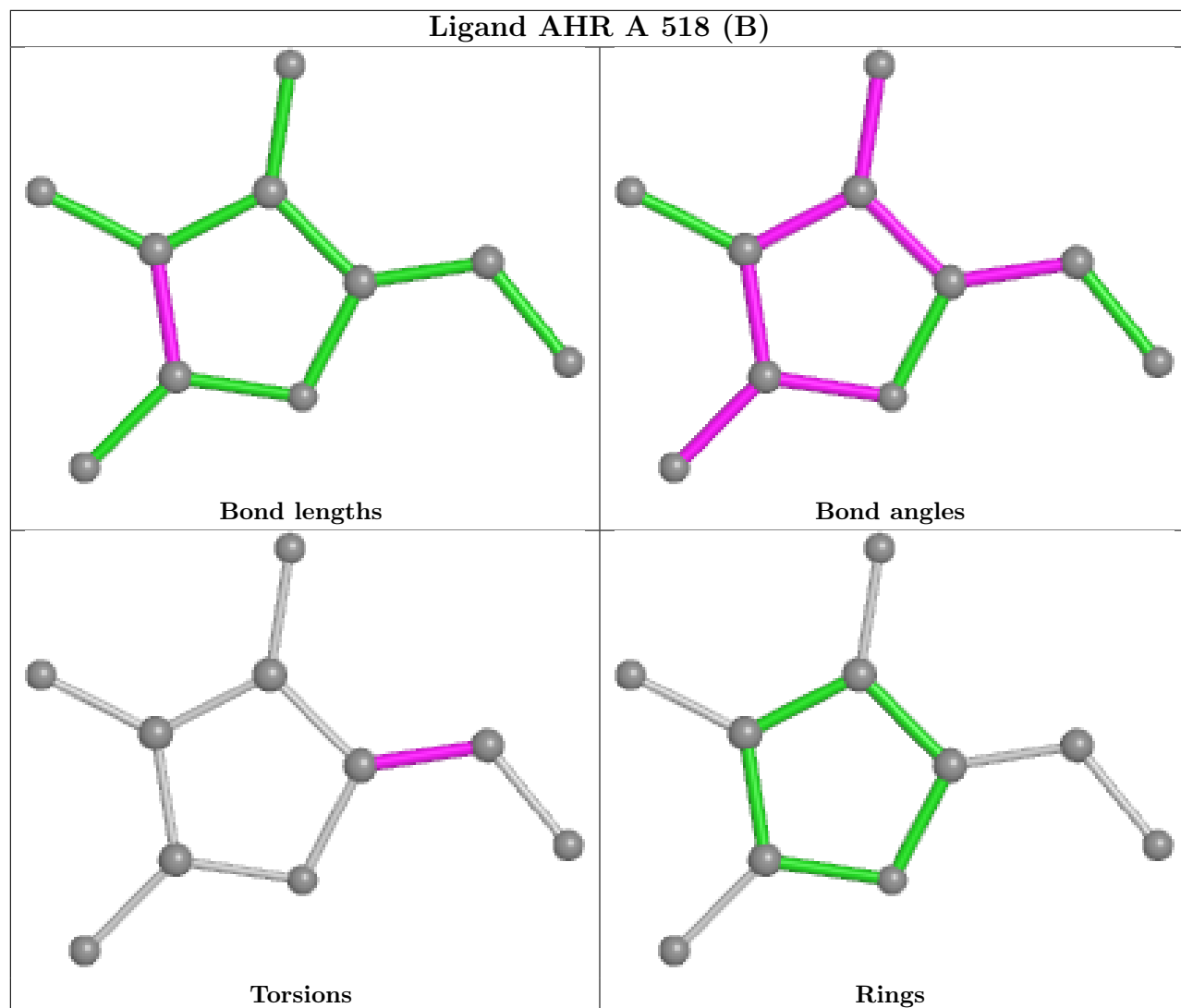


## Ligand AHR B 501 (B)

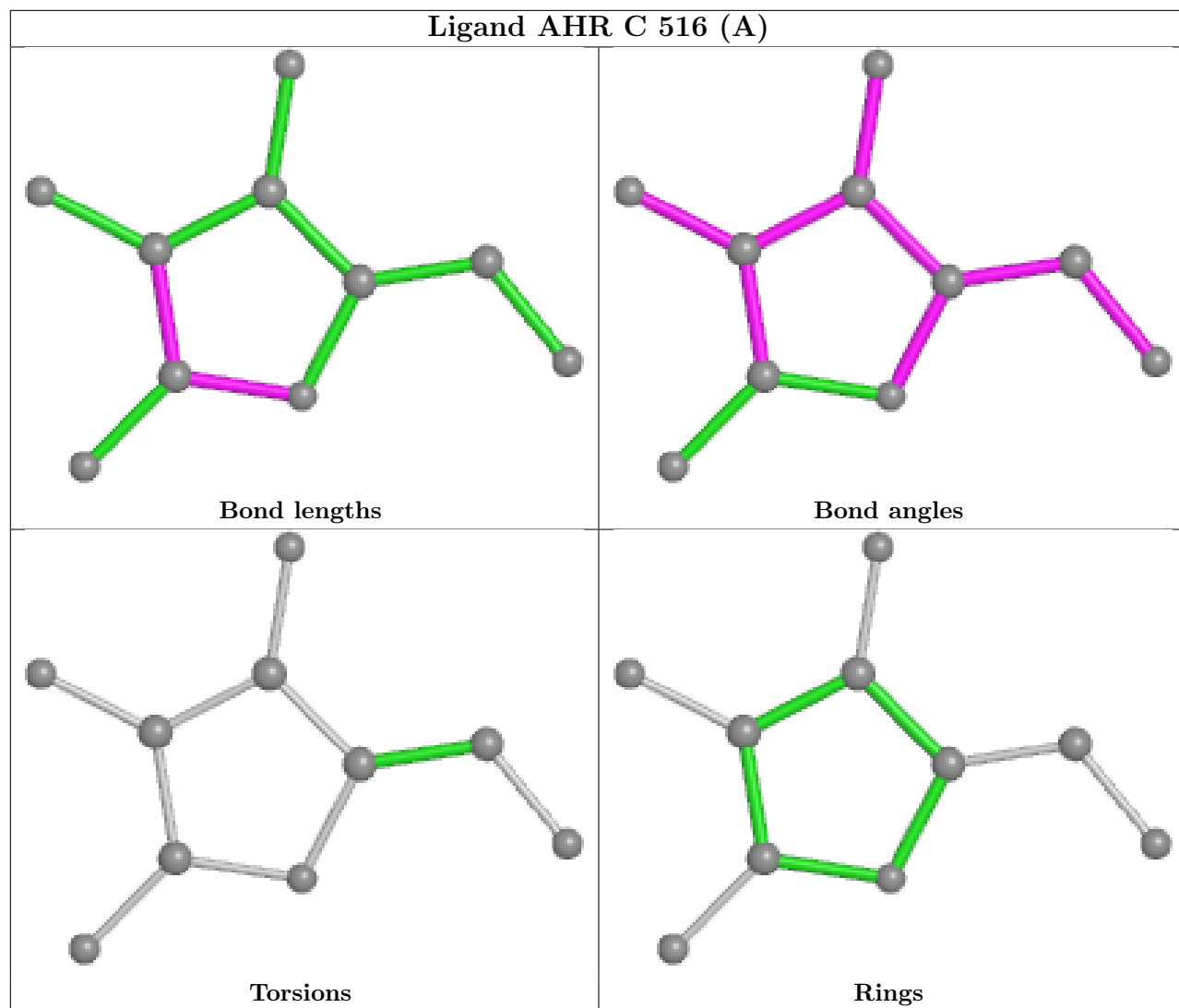


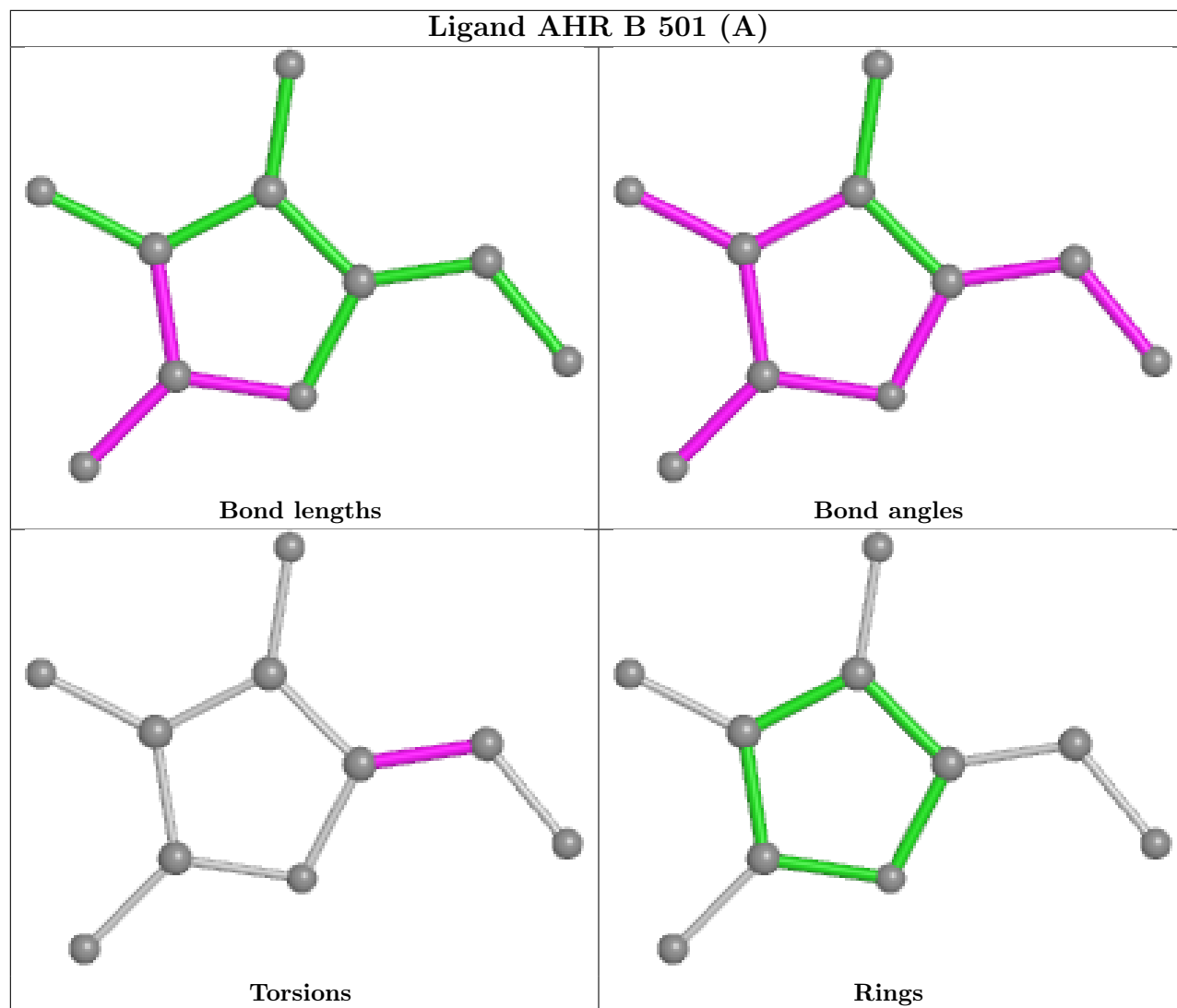


## Ligand AHR A 518 (B)



## Ligand AHR C 516 (A)





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	491/496 (98%)	-0.59	10 (2%) 65 64	17, 26, 53, 114	0
1	B	491/496 (98%)	-0.40	7 (1%) 75 76	18, 29, 61, 130	0
1	C	491/496 (98%)	-0.45	9 (1%) 68 68	18, 30, 60, 132	0
All	All	1473/1488 (98%)	-0.48	26 (1%) 68 68	17, 28, 58, 132	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	GLY	10.9
1	C	496	GLY	9.9
1	A	496	GLY	7.1
1	A	3	VAL	6.4
1	B	3	VAL	5.7
1	C	437	ASN	5.0
1	C	476	GLY	4.0
1	C	3	VAL	3.9
1	B	437	ASN	3.9
1	A	437	ASN	3.7
1	A	495	ALA	3.2
1	C	439	GLY	3.2
1	A	477	GLY	2.9
1	B	495	ALA	2.9
1	A	476	GLY	2.7
1	A	438	GLY	2.7
1	A	97	THR	2.6
1	B	438	GLY	2.4
1	C	440	VAL	2.4
1	C	495	ALA	2.4
1	B	97	THR	2.3
1	A	475	GLU	2.3
1	B	474	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	439	GLY	2.2
1	C	475	GLU	2.2
1	C	438	GLY	2.2

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	ACT	C	503	4/4	0.23	0.35	61,64,80,84	0
2	ACT	C	506	4/4	0.31	0.46	70,71,92,97	0
2	ACT	C	505	4/4	0.55	0.44	74,90,105,123	0
3	MPD	A	512	8/8	0.57	0.26	74,87,99,107	0
3	MPD	C	511	8/8	0.61	0.69	20,20,20,20	0
3	MPD	A	510	8/8	0.63	0.37	77,91,95,97	0
3	MPD	C	515	8/8	0.64	0.53	20,20,20,20	0
2	ACT	A	502	4/4	0.67	0.21	61,70,78,87	0
3	MPD	A	514	8/8	0.68	0.43	20,20,20,20	0
3	MPD	A	515	8/8	0.68	0.55	20,20,20,20	0
3	MPD	C	514	8/8	0.69	0.67	20,20,20,20	0
3	MPD	B	511	8/8	0.70	0.28	70,85,91,97	0
2	ACT	B	505	4/4	0.70	0.34	75,95,101,104	0
3	MPD	B	512	8/8	0.73	0.37	83,91,97,97	0
2	ACT	A	506	4/4	0.73	0.23	57,58,64,75	0
3	MPD	A	511	8/8	0.75	0.31	69,80,82,85	0
3	MPD	C	512	8/8	0.75	0.67	20,20,20,20	0
3	MPD	A	513	8/8	0.76	0.68	20,20,20,20	0
3	MPD	A	516	8/8	0.76	0.51	20,20,20,20	0
3	MPD	B	513	8/8	0.78	0.26	73,84,94,101	0

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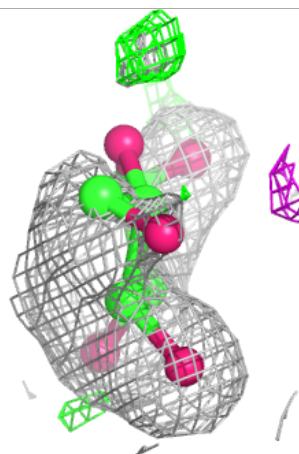
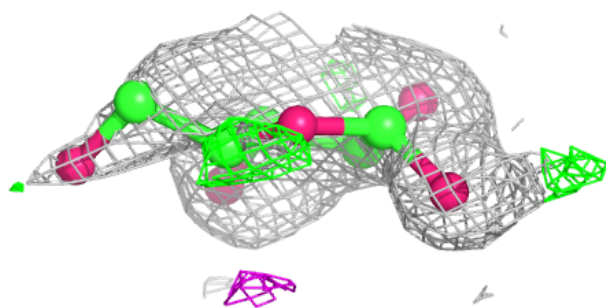
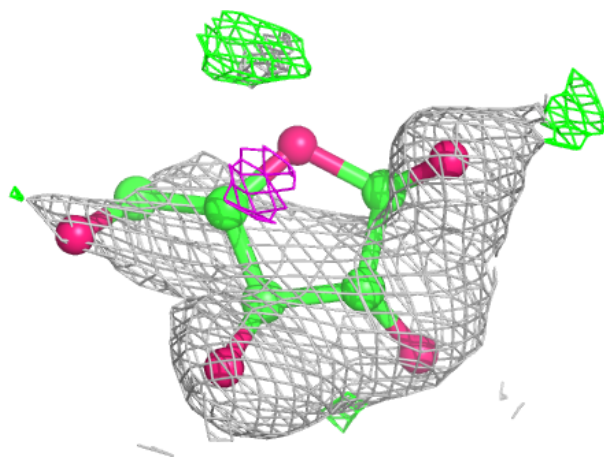
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MPD	B	515	8/8	0.78	0.56	20,20,20,20	0
2	ACT	B	503	4/4	0.78	0.24	74,76,76,82	0
3	MPD	C	510	8/8	0.79	0.71	20,20,20,20	0
2	ACT	A	501	4/4	0.80	0.18	73,75,75,86	0
3	MPD	C	513	8/8	0.80	0.62	20,20,20,20	0
3	MPD	A	508	8/8	0.81	0.15	51,56,67,68	0
2	ACT	C	502	4/4	0.82	0.19	63,73,79,83	0
3	MPD	C	508	8/8	0.82	0.21	51,65,71,75	0
5	AHR	A	518[A]	10/10	0.82	0.25	41,64,67,71	10
5	AHR	A	518[B]	10/10	0.82	0.25	35,50,59,59	10
2	ACT	B	506	4/4	0.83	0.24	54,66,68,72	0
3	MPD	B	510	8/8	0.83	0.24	77,86,92,96	0
3	MPD	A	509	8/8	0.83	0.22	59,77,79,83	0
3	MPD	B	508	8/8	0.85	0.16	74,83,96,99	0
5	AHR	B	501[A]	10/10	0.85	0.23	28,52,67,71	10
5	AHR	B	501[B]	10/10	0.85	0.23	29,53,60,68	10
2	ACT	C	504	4/4	0.86	0.21	73,77,78,78	0
5	AHR	C	516[A]	10/10	0.86	0.21	33,54,61,65	10
5	AHR	C	516[B]	10/10	0.86	0.21	33,54,59,60	10
2	ACT	A	504	4/4	0.87	0.37	88,92,92,99	0
3	MPD	C	509	8/8	0.87	0.17	77,81,91,94	0
3	MPD	B	514	8/8	0.89	0.15	46,58,71,76	0
2	ACT	B	502	4/4	0.89	0.23	81,83,83,90	0
3	MPD	C	507	8/8	0.89	0.16	48,68,71,74	0
4	BTB	A	517	14/14	0.89	0.18	41,46,49,54	0
3	MPD	B	509	8/8	0.89	0.14	70,78,89,93	0
2	ACT	A	503	4/4	0.90	0.14	63,68,71,72	0
2	ACT	B	504	4/4	0.91	0.17	74,77,78,79	0
3	MPD	B	507	8/8	0.91	0.12	46,62,76,76	0
2	ACT	A	505	4/4	0.92	0.24	62,65,73,76	0
3	MPD	A	507	8/8	0.93	0.13	51,64,66,66	0
2	ACT	C	501	4/4	0.96	0.30	35,35,56,76	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.

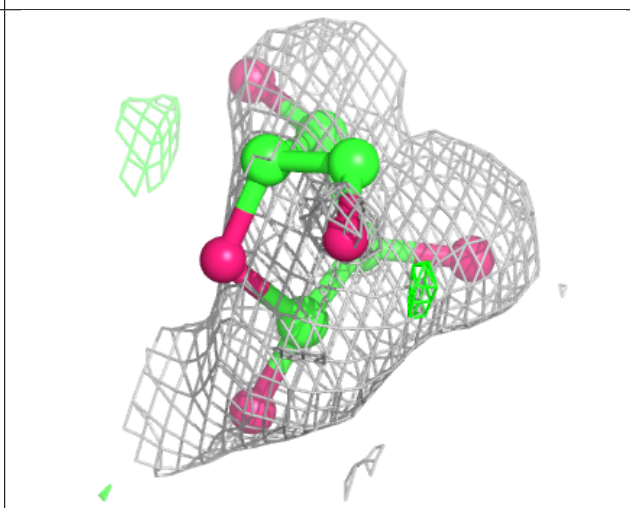
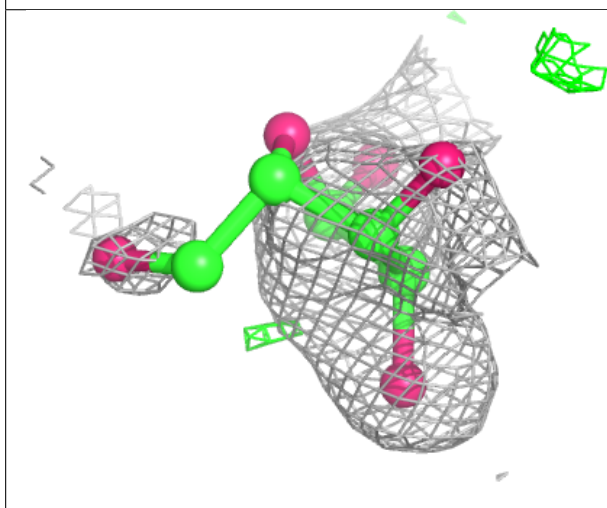
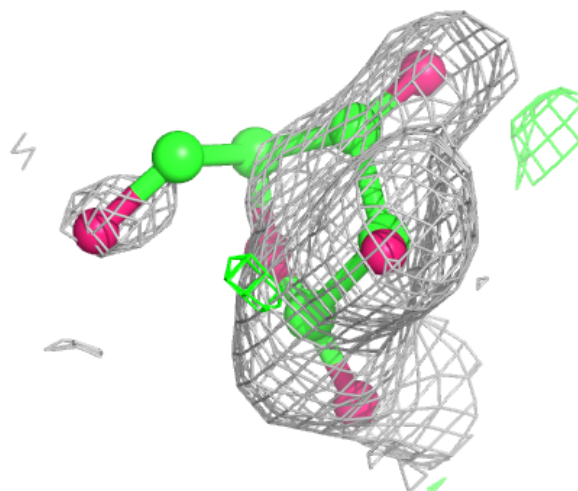
**Electron density around AHR A 518 (A):**

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



**Electron density around AHR A 518 (B):**

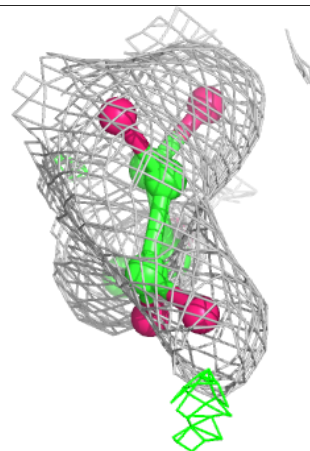
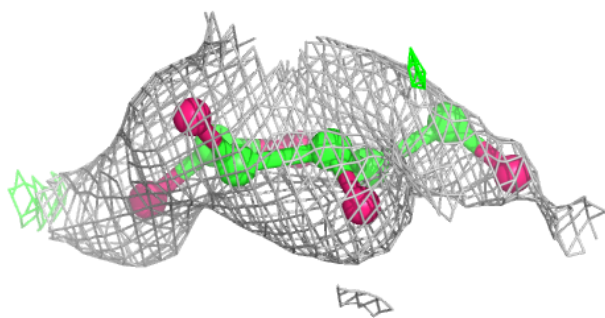
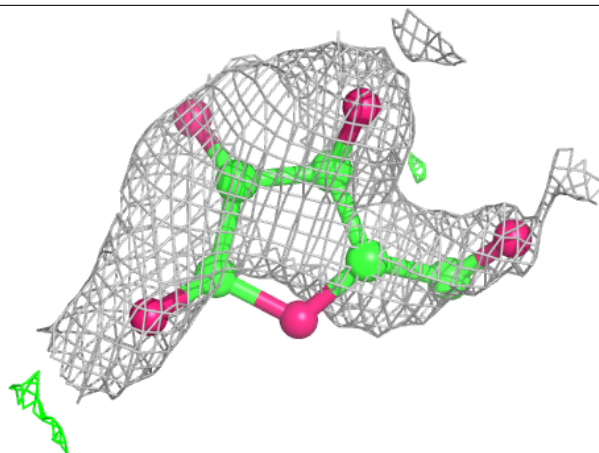
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





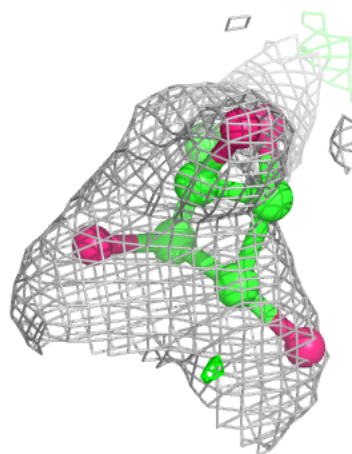
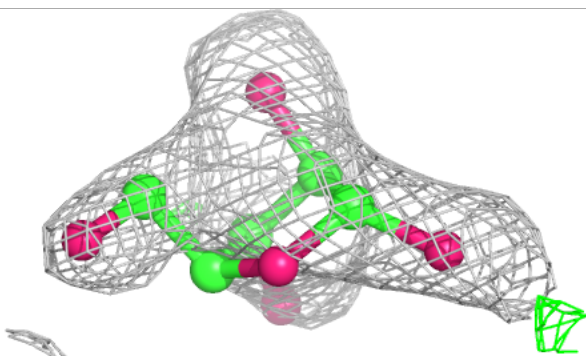
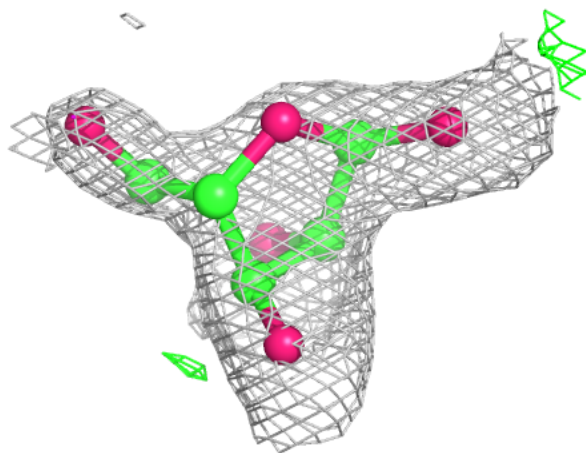
**Electron density around AHR B 501 (A):**

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



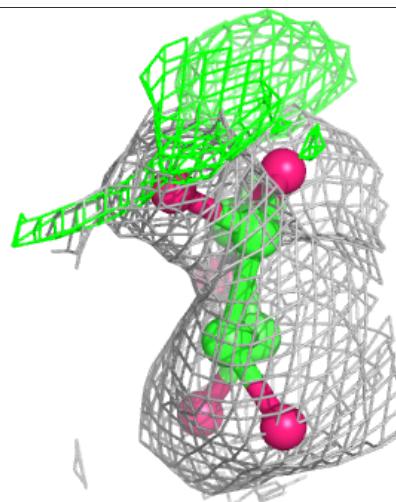
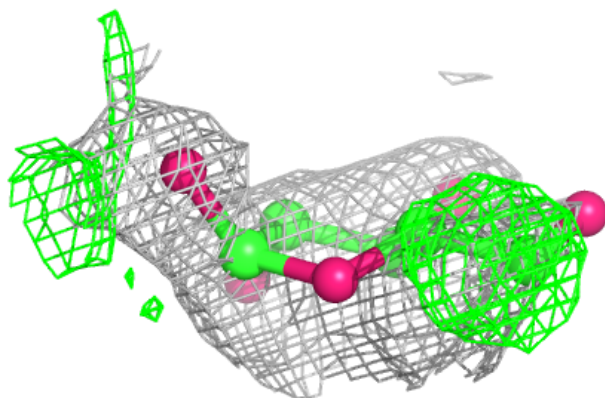
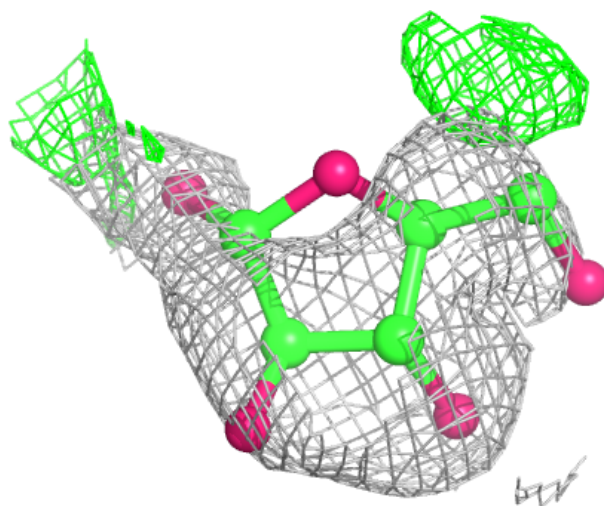
**Electron density around AHR B 501 (B):**

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



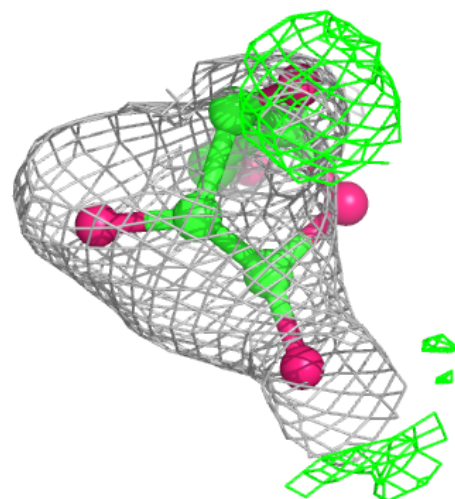
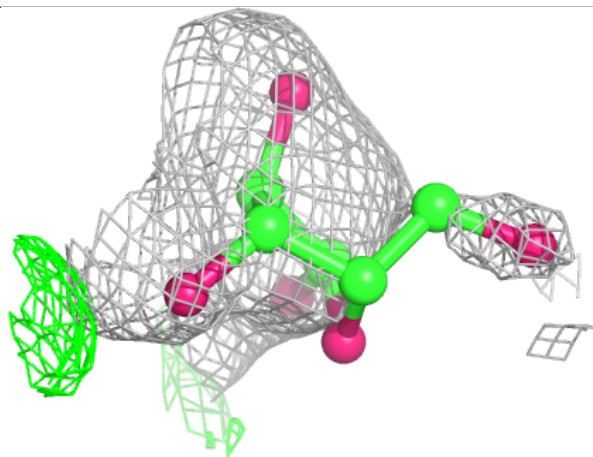
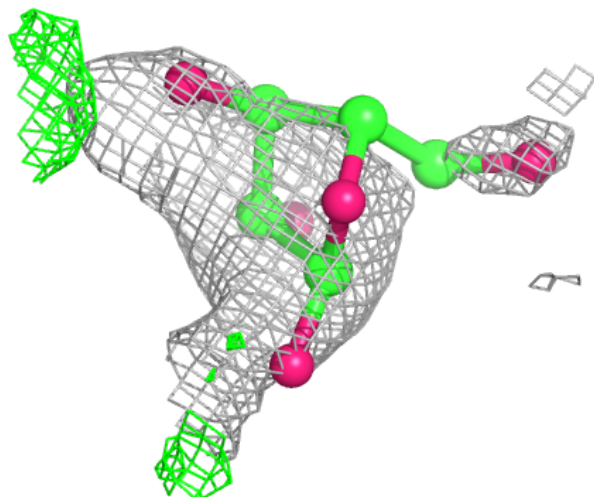
**Electron density around AHR C 516 (A):**

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



**Electron density around AHR C 516 (B):**

$2mF_o-DF_c$  (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.