W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Aug 10, 2020 – 04:47 AM BST

PDB ID : 2IUF

Title : The structures of Penicillium vitale catalase: resting state, oxidised state (compound I) and complex with aminotriazole

Authors : Murshudov, G.; Borovik, A.; Grebenko, A.; Barynin, V.; Vagin, A.; Melik-Adamyan, W.

Deposited on : 2006-06-02

Resolution : 1.71 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

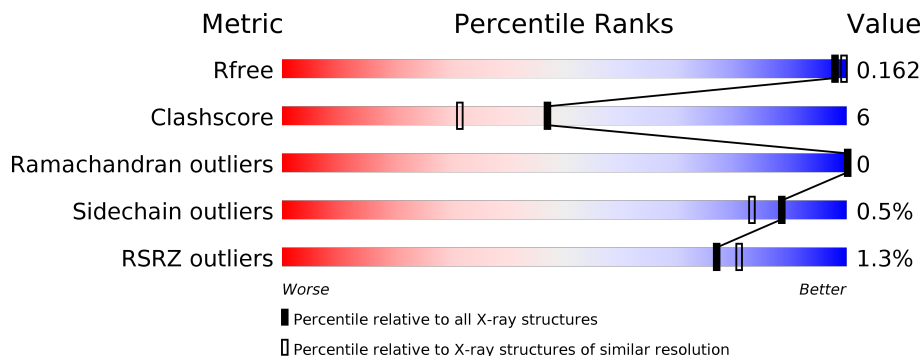|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 1.71 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	Percentile Ranks	Value
Rfree		0.162
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		0.5%
RSRZ outliers		1.3%

Worse　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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 on 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	688	%　90%　10%　•
1	E	688	%　91%　8%　•
2	B	2	100%

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
4	NAG	A	1693	-	-	X	-
4	NAG	A	1694	-	-	-	X
7	ACT	E	1701	-	-	X	-
7	ACT	E	1707	-	-	X	-
9	MPD	A	1704	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 12590 atoms, of which 0 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 CATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	688	Total 5429	C 3418	N 960	O 1041	S 10	0	11	0
1	E	688	Total 5402	C 3401	N 952	O 1039	S 10	0	8	0

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.
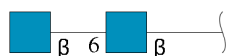
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).
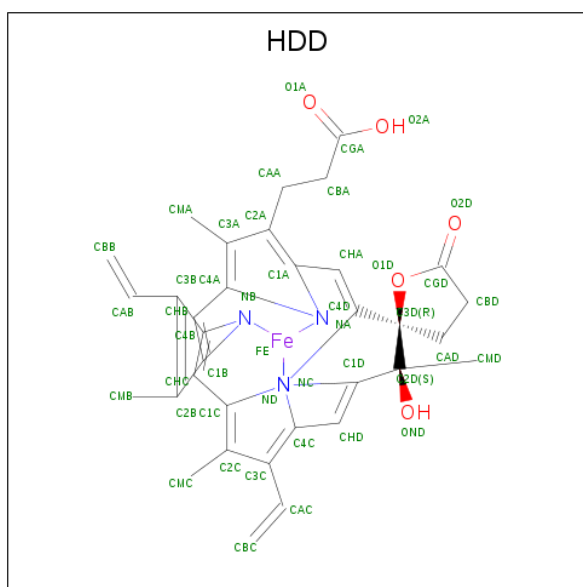
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
3	E	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	O 1	0	0
5	E	1	Total 1	O 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	Ca 2	0	0
6	E	4	Total 4	Ca 4	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
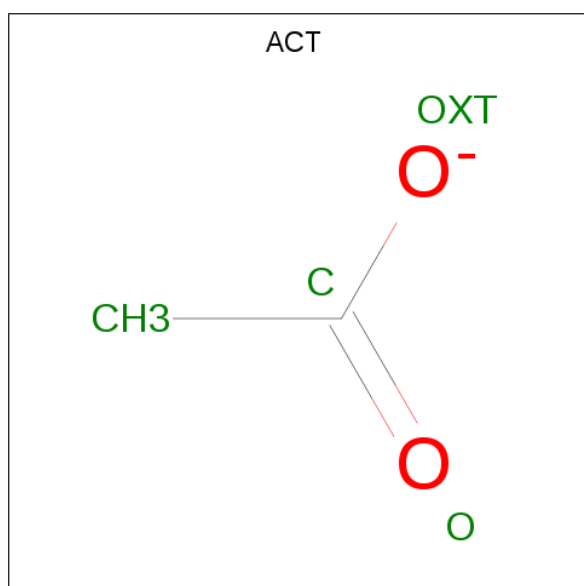
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	A	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0
7	E	1	Total 4	C 2	O 2	0	0

- Molecule 8 is ETHANEPEROXOIC ACID (three-letter code: F50) (formula: $C_2H_4O_3$).
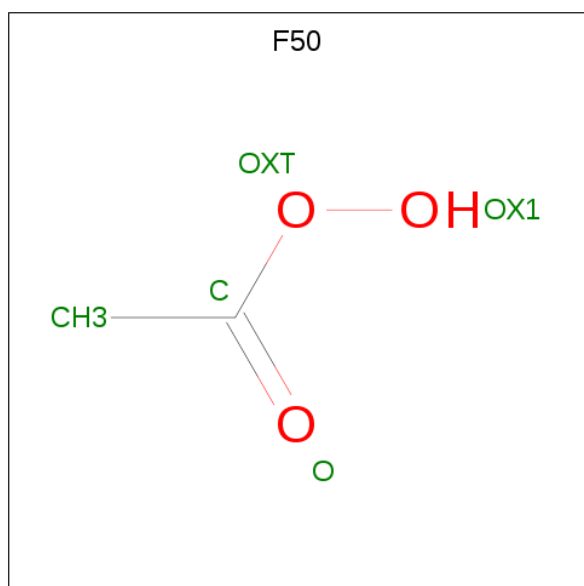
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 5	C 2	O 3	0	0
8	E	1	Total 5	C 2	O 3	0	0
8	E	1	Total 5	C 2	O 3	0	0

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).
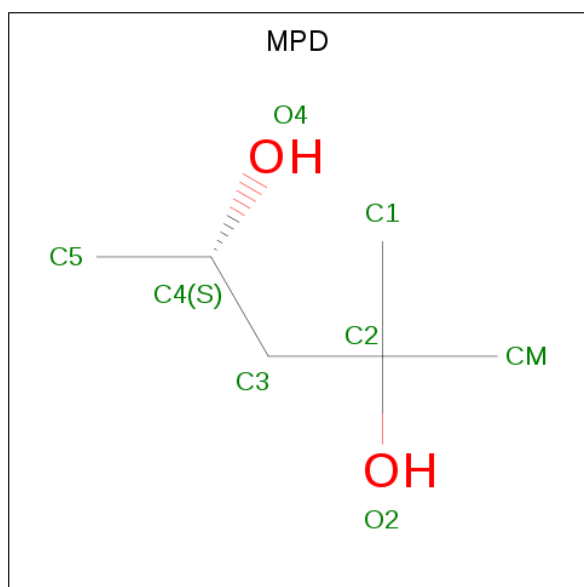
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 8	C 6	O 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	774	Total 774	O 774	0	0
10	E	716	Total 716	O 716	0	0

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, orang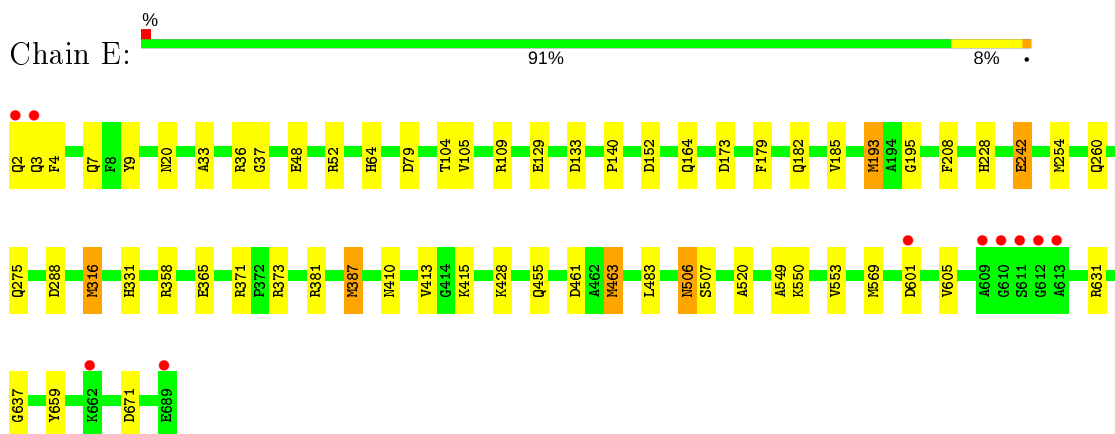e = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
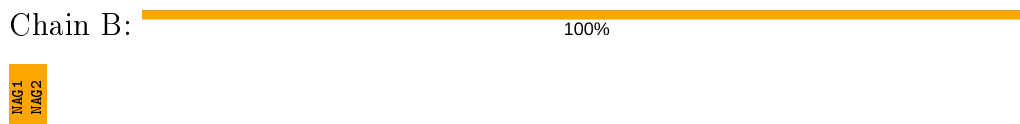
- Molecule 1: CATALASE
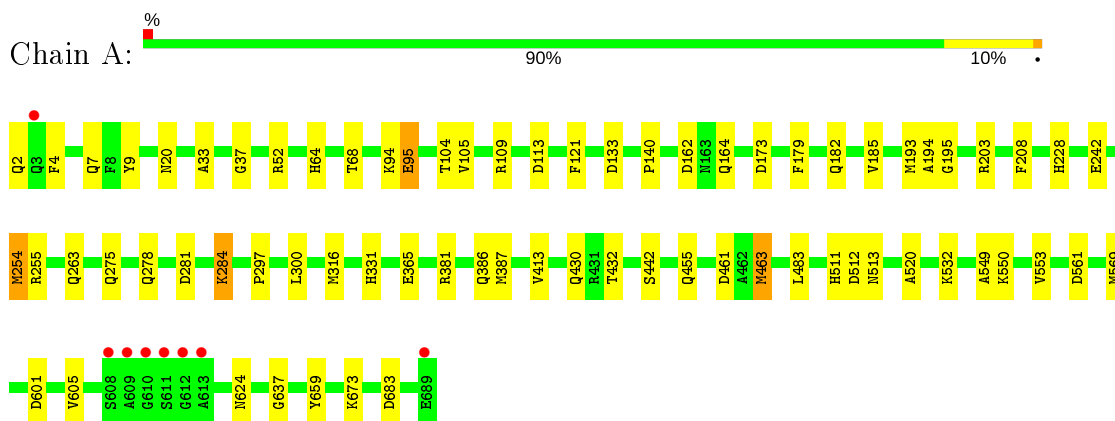
- Molecule 1: CATALASE

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.44Å 142.44Å 132.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	119.52 – 1.71 19.80 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.9 (119.52-1.71) 99.0 (19.80-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.3.0002	Depositor
R, R_{free}	0.129 , 0.154 0.139 , 0.162	Depositor DCC
R_{free} test set	8285 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	14.7	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.8	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12590	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MHO, MPD, NAG, F50, CA, O, HDD, ACT

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	0.90	2/5503 (0.0%)	0.86	5/7456 (0.1%)
1	E	0.90	2/5476 (0.0%)	0.87	8/7422 (0.1%)
All	All	0.90	4/10979 (0.0%)	0.87	13/14878 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	242	GLU	CB-CG	-7.50	1.37	1.52
1	A	242	GLU	CB-CG	-5.92	1.40	1.52
1	E	48	GLU	CD-OE2	5.36	1.31	1.25
1	A	95	GLU	CD-OE1	-5.12	1.20	1.25

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	631	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	162	ASP	CB-CG-OD1	6.69	124.32	118.30
1	E	36	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	E	79	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	683	ASP	CB-CG-OD2	6.03	123.73	118.30

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	5429	0	5242	67	0
1	E	5402	0	5205	57	2
2	B	28	0	25	3	0
3	A	44	0	31	1	0
3	E	44	0	31	1	0
4	A	42	0	39	9	2
4	E	28	0	26	0	0
5	A	1	0	0	0	0
5	E	1	0	0	0	0
6	A	2	0	0	0	0
6	E	4	0	0	0	0
7	A	20	0	15	1	0
7	E	32	0	24	9	0
8	A	5	0	4	0	0
8	E	10	0	8	0	0
9	A	8	0	14	6	0
10	A	774	0	0	25	3
10	E	716	0	0	15	2
All	All	12590	0	10664	135	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.

The worst 5 of 135 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLN:NE2	10:A:2463:HOH:O	1.81	1.12
1:A:68[A]:THR:HG21	1:A:255:ARG:HB3	1.33	1.07
4:A:1692:NAG:H82	10:A:2487:HOH:O	0.90	1.07
1:A:463:MHO:HE3	1:A:483:LEU:HD11	1.35	1.05
10:A:2697:HOH:O	7:E:1701:ACT:H2	1.55	1.04

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)
1:E:415:LYS:NZ	4:A:1693:NAG:O3[4_455]	1.74	0.46
1:E:129[B]:GLU:OE2	4:A:1693:NAG:O3[4_455]	1.76	0.44
10:A:2150:HOH:O	10:A:2723:HOH:O[2_665]	2.05	0.15

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2769:HOH:O	10:E:2457:HOH:O[4_565]	2.05	0.15
10:A:2156:HOH:O	10:E:2137:HOH:O[4_565]	2.13	0.07

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	692/688 (101%)	672 (97%)	20 (3%)	0	100	100
1	E	689/688 (100%)	672 (98%)	17 (2%)	0	100	100
All	All	1381/1376 (100%)	1344 (97%)	37 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	570/559 (102%)	567 (100%)	3 (0%)	88	83
1	E	567/559 (101%)	564 (100%)	3 (0%)	88	83
All	All	1137/1118 (102%)	1131 (100%)	6 (0%)	88	83

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	506	ASN
1	E	173	ASP
1	A	173	ASP
1	E	242	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	624	ASN
1	E	26	GLN
1	E	506	ASN
1	A	511	HIS
1	E	571	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)

10 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
1	MHO	E	316	1	7,8,9	4.72	2 (28%)	4,9,11	3.51	2 (50%)
1	MHO	A	316	1	7,8,9	4.75	2 (28%)	4,9,11	3.20	3 (75%)
1	MHO	A	569	1	7,8,9	4.32	2 (28%)	4,9,11	2.60	2 (50%)
1	MHO	E	254	1	7,8,9	2.49	1 (14%)	4,9,11	1.28	1 (25%)
1	MHO	E	569	1	7,8,9	4.72	3 (42%)	4,9,11	2.15	2 (50%)
1	MHO	A	254	1	7,8,9	5.12	2 (28%)	4,9,11	2.39	2 (50%)
1	MHO	A	193	1	7,8,9	4.78	2 (28%)	4,9,11	2.69	3 (75%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	MHO	E	193	1	7,8,9	4.93	2 (28%)	4,9,11	2.82	2 (50%)
1	MHO	E	463	1	7,8,9	4.56	2 (28%)	4,9,11	2.96	2 (50%)
1	MHO	A	463	1	7,8,9	4.53	3 (42%)	4,9,11	2.30	2 (50%)

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
1	MHO	E	316	1	-	2/6/7/9	-
1	MHO	A	316	1	-	1/6/7/9	-
1	MHO	A	569	1	-	2/6/7/9	-
1	MHO	E	254	1	-	0/6/7/9	-
1	MHO	E	569	1	-	2/6/7/9	-
1	MHO	A	254	1	-	1/6/7/9	-
1	MHO	A	193	1	-	1/6/7/9	-
1	MHO	E	193	1	-	1/6/7/9	-
1	MHO	E	463	1	-	1/6/7/9	-
1	MHO	A	463	1	-	1/6/7/9	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	MHO	OD1-SD	12.43	1.84	1.50
1	E	193	MHO	OD1-SD	12.35	1.83	1.50
1	A	316	MHO	OD1-SD	11.97	1.82	1.50
1	E	569	MHO	OD1-SD	11.83	1.82	1.50
1	A	193	MHO	OD1-SD	11.75	1.82	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	316	MHO	OD1-SD-CG	-6.54	88.00	106.03
1	A	316	MHO	CE-SD-CG	4.30	107.50	97.71
1	A	316	MHO	OD1-SD-CG	-4.26	94.28	106.03
1	E	463	MHO	OD1-SD-CG	-4.24	94.35	106.03
1	A	254	MHO	CE-SD-CG	4.15	107.16	97.71

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	569	MHO	CB-CG-SD-OD1
1	E	569	MHO	CB-CG-SD-OD1
1	A	193	MHO	CB-CG-SD-OD1
1	E	193	MHO	CB-CG-SD-OD1
1	A	463	MHO	CB-CG-SD-OD1

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	316	MHO	2	0
1	A	254	MHO	3	0
1	E	193	MHO	2	0
1	E	463	MHO	3	0
1	A	463	MHO	2	0

5.5 Carbohydrates (i)

2 monosaccharides 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	NAG	B	1	1,2	14,14,15	0.74	0	17,19,21	2.47	9 (52%)
2	NAG	B	2	2	14,14,15	0.76	1 (7%)	17,19,21	1.74	4 (23%)

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	NAG	B	1	1,2	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	2	2	-	<mark>2/6/23/26</mark>	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	O5-C1	-2.16	1.40	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C1-C2-N2	4.25	117.76	110.49
2	B	1	NAG	C4-C3-C2	-4.10	105.00	111.02
2	B	2	NAG	C4-C3-C2	-3.99	105.17	111.02
2	B	1	NAG	C1-O5-C5	3.63	117.11	112.19
2	B	2	NAG	C1-O5-C5	3.58	117.04	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	NAG	C1-C2-N2-C7
2	B	1	NAG	O5-C5-C6-O6
2	B	2	NAG	C1-C2-N2-C7
2	B	2	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	NAG	1	0
2	B	2	NAG	3	0

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 for Mogul analysis.

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	#$|Z| > 2$
8	F50	E	1705	-	3,4,4	2.08	1 (33%)	3,4,4	3.98	2 (66%)
7	ACT	E	1699	-	1,3,3	1.46	0	0,3,3	0.00	-
7	ACT	E	1712	-	1,3,3	1.68	0	0,3,3	0.00	-
4	NAG	E	1694	1	14,14,15	0.61	0	17,19,21	2.33	4 (23%)
7	ACT	E	1706	-	1,3,3	2.80	1 (100%)	0,3,3	0.00	-
7	ACT	E	1707	-	1,3,3	0.58	0	0,3,3	0.00	-
7	ACT	A	1702	-	1,3,3	2.01	1 (100%)	0,3,3	0.00	-
3	HDD	E	1691	1,5	38,52,52	1.75	6 (15%)	28,89,89	1.58	5 (17%)
4	NAG	E	1693	1	14,14,15	0.54	0	17,19,21	1.19	2 (11%)
7	ACT	A	1701	-	1,3,3	2.22	1 (100%)	0,3,3	0.00	-
4	NAG	A	1692	1	14,14,15	0.74	0	17,19,21	2.24	5 (29%)
8	F50	A	1699	-	3,4,4	2.22	1 (33%)	3,4,4	1.68	1 (33%)
7	ACT	A	1703	-	1,3,3	2.55	1 (100%)	0,3,3	0.00	-
7	ACT	E	1701	-	1,3,3	0.93	0	0,3,3	0.00	-
7	ACT	A	1698	-	1,3,3	1.41	0	0,3,3	0.00	-
3	HDD	A	1691	1,5	38,52,52	1.67	7 (18%)	28,89,89	1.73	9 (32%)
4	NAG	A	1694	1	14,14,15	0.40	0	17,19,21	1.47	2 (11%)
7	ACT	E	1703	-	1,3,3	1.92	0	0,3,3	0.00	-
9	MPD	A	1704	-	7,7,7	0.28	0	9,10,10	0.62	0
8	F50	E	1700	-	3,4,4	2.29	1 (33%)	3,4,4	1.18	0
7	ACT	A	1700	-	1,3,3	4.99	1 (100%)	0,3,3	0.00	-
7	ACT	E	1704	-	1,3,3	3.97	1 (100%)	0,3,3	0.00	-
4	NAG	A	1693	1	14,14,15	0.76	0	17,19,21	1.95	5 (29%)
7	ACT	E	1702	-	1,3,3	1.23	0	0,3,3	0.00	-

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
9	MPD	A	1704	-	-	1/5/5/5	-
8	F50	E	1705	-	-	0/0/2/2	-
8	F50	E	1700	-	-	0/0/2/2	-
3	HDD	E	1691	1,5	-	0/3/89/89	0/1/9/9

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1692	1	-	2/6/23/26	0/1/1/1
3	HDD	A	1691	1,5	-	0/3/89/89	0/1/9/9
4	NAG	E	1694	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1694	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1693	1	-	2/6/23/26	0/1/1/1
8	F50	A	1699	-	-	0/0/2/2	-
4	NAG	E	1693	1	-	2/6/23/26	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1700	ACT	CH3-C	4.99	1.55	1.48
3	E	1691	HDD	C3C-C2C	-4.55	1.34	1.40
3	A	1691	HDD	O1D-C3D	-4.32	1.39	1.46
3	A	1691	HDD	FE-ND	4.20	2.12	1.95
7	E	1704	ACT	CH3-C	3.97	1.53	1.48

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1694	NAG	C1-O5-C5	7.06	121.75	112.19
8	E	1705	F50	OXT-C-O	-5.16	117.91	124.14
3	A	1691	HDD	O1D-CGD-O2D	4.79	125.07	120.80
4	A	1692	NAG	C3-C4-C5	-4.75	101.77	110.24
8	E	1705	F50	OXT-C-CH3	4.53	119.42	111.09

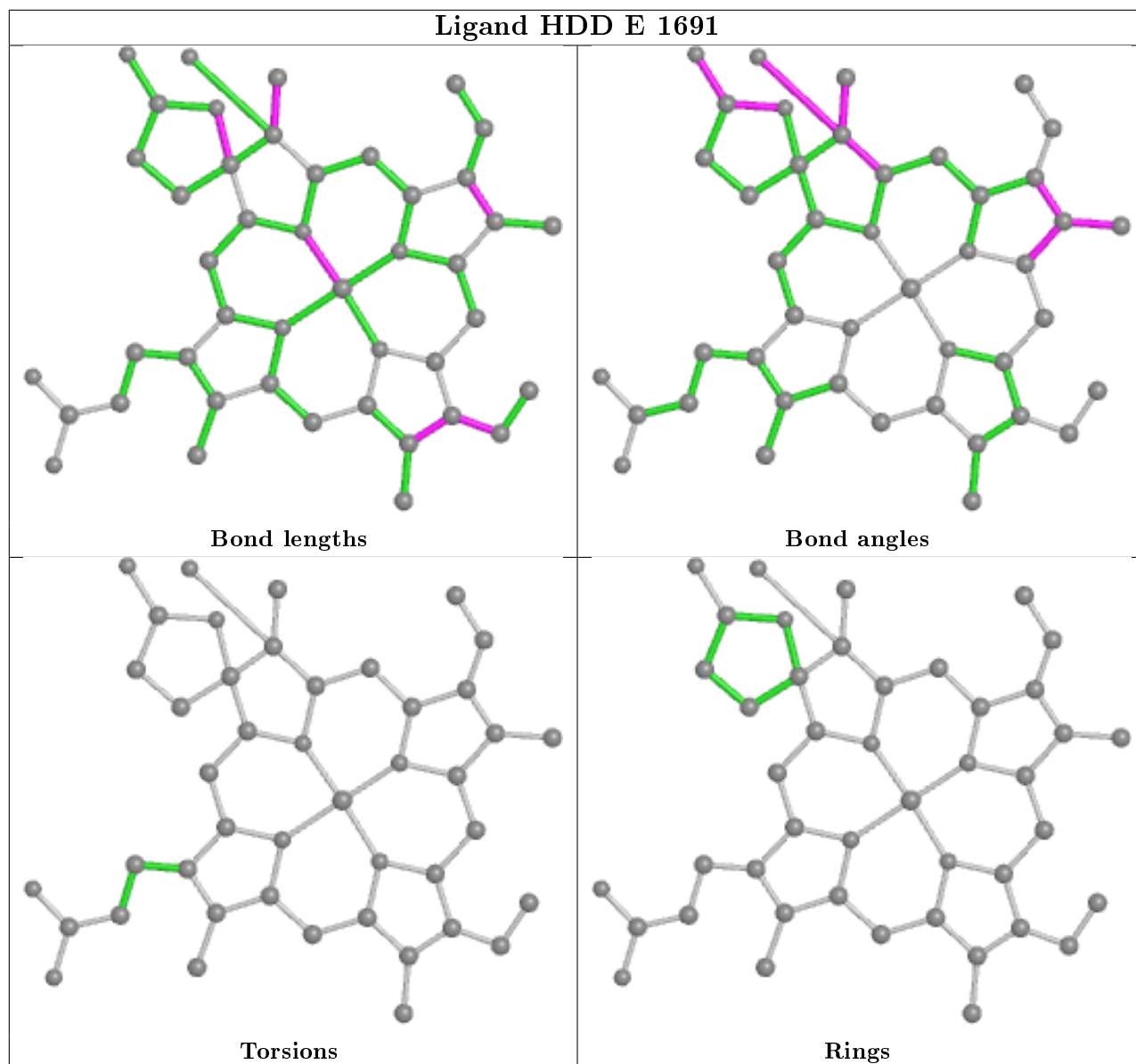There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	1704	MPD	C2-C3-C4-O4
4	E	1693	NAG	O5-C5-C6-O6
4	A	1693	NAG	C4-C5-C6-O6
4	E	1693	NAG	C4-C5-C6-O6
4	A	1692	NAG	C8-C7-N2-C2

There are no ring outliers.

8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	1707	ACT	5	0
3	E	1691	HDD	1	0
4	A	1692	NAG	4	0
7	E	1701	ACT	4	0
3	A	1691	HDD	1	0
9	A	1704	MPD	6	0
7	A	1700	ACT	1	0
4	A	1693	NAG	5	2

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 HDD E 1691

Bond lengths

Bond angles

Torsions

Rings

Ligand HDD A 1691

Bond lengths

Bond angles

Torsions

Rings
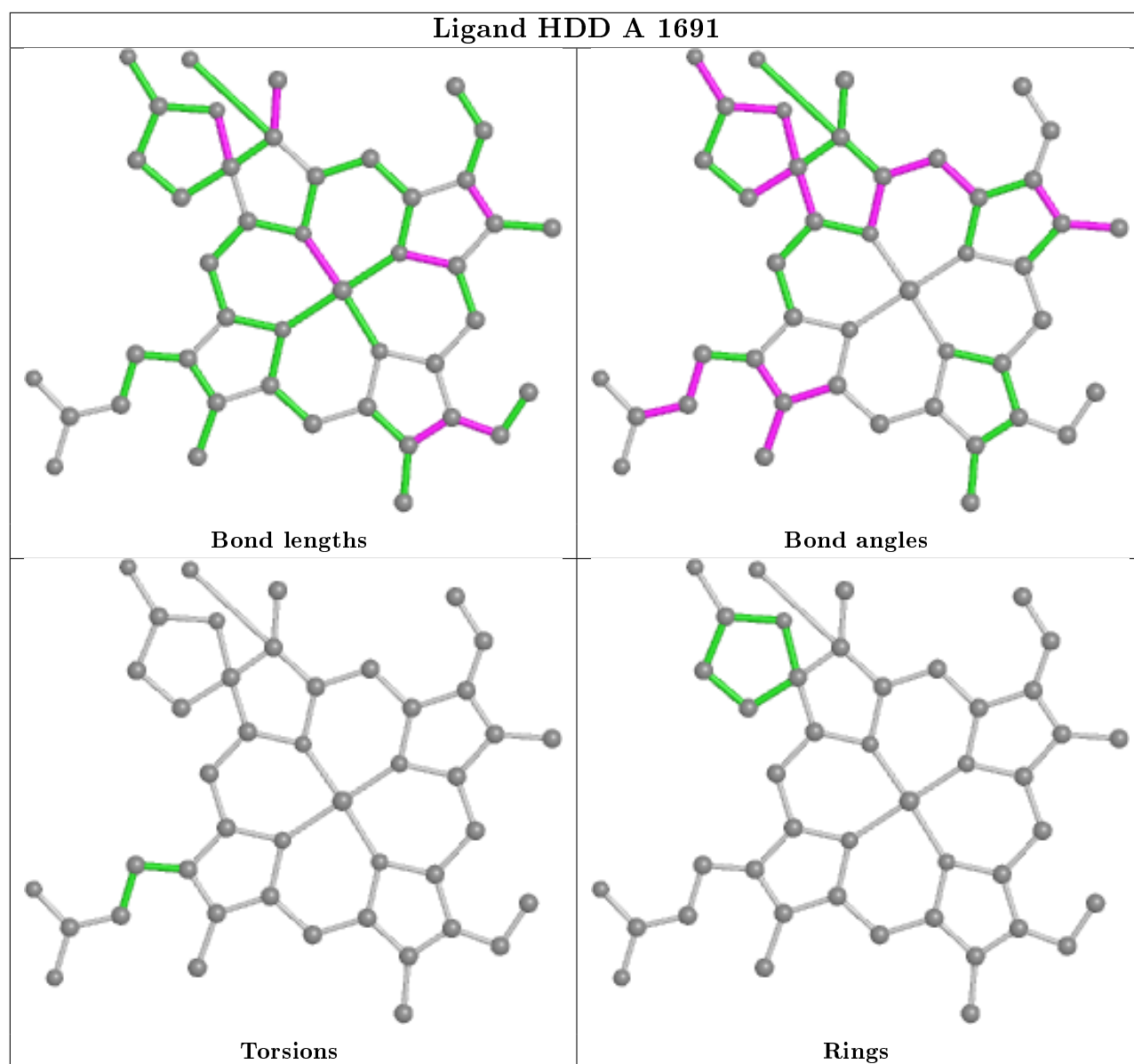
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	683/688 (99%)	-0.62	8 (1%)	79	83	8, 13, 22, 37	1 (0%)
1	E	683/688 (99%)	-0.54	10 (1%)	73	78	9, 14, 25, 45	0
All	All	1366/1376 (99%)	-0.58	18 (1%)	77	81	8, 13, 24, 45	1 (0%)

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	609	ALA	4.8
1	E	612	GLY	4.7
1	E	2	GLN	4.7
1	A	610	GLY	4.5
1	A	609	ALA	4.5

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	MHO	E	569	9/10	0.95	0.09	17,20,26,26	0
1	MHO	E	316	9/10	0.96	0.07	11,12,23,31	0
1	MHO	A	569	9/10	0.98	0.06	16,18,24,25	0
1	MHO	E	254	9/10	0.98	0.06	11,11,15,17	0
1	MHO	A	316	9/10	0.98	0.06	10,11,23,30	0
1	MHO	A	193	9/10	0.98	0.05	8,10,14,21	0
1	MHO	E	193	9/10	0.98	0.05	8,12,15,18	0
1	MHO	E	463	9/10	0.98	0.06	12,12,15,23	0
1	MHO	A	463	9/10	0.98	0.06	9,11,13,18	0
1	MHO	A	254	9/10	0.99	0.05	11,12,15,19	0

6.3 Carbohydrates (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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	NAG	B	2	14/15	0.67	0.27	31,37,39,40	14
2	NAG	B	1	14/15	0.73	0.25	36,42,49,50	0

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
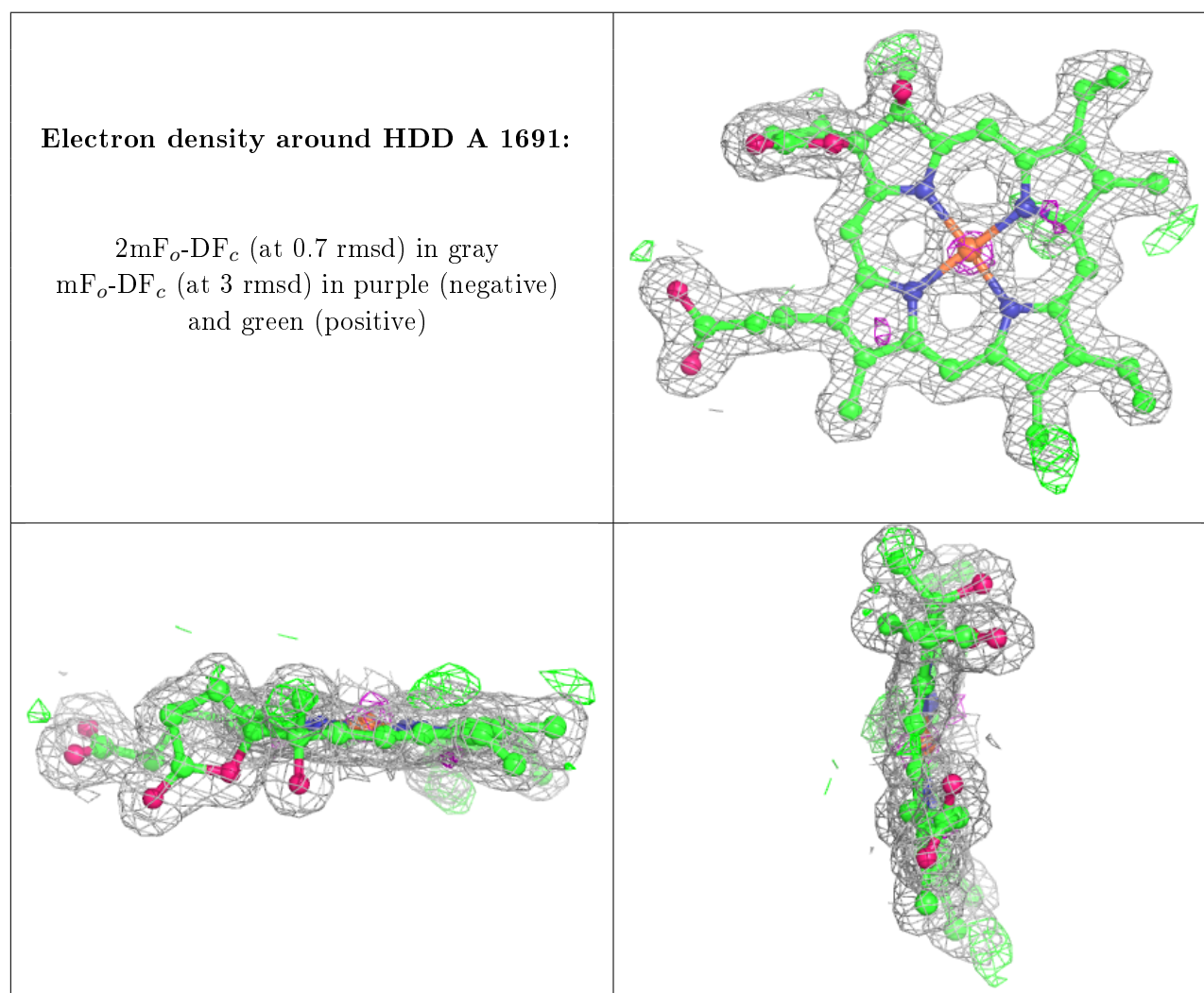
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
8	F50	E	1705	5/5	0.58	0.23	38,39,39,39	5
4	NAG	E	1694	14/15	0.63	0.40	45,50,54,54	0
7	ACT	E	1707	4/4	0.64	0.35	28,29,30,30	4
4	NAG	A	1694	14/15	0.69	0.42	45,52,55,56	0
4	NAG	A	1693	14/15	0.76	0.28	32,36,39,41	0
4	NAG	E	1693	14/15	0.78	0.33	50,57,59,61	0
7	ACT	A	1700	4/4	0.81	0.17	16,23,24,24	0
4	NAG	A	1692	14/15	0.81	0.21	30,36,43,44	0
7	ACT	E	1706	4/4	0.84	0.23	29,30,31,32	0
8	F50	A	1699	5/5	0.86	0.16	31,31,33,35	0
8	F50	E	1700	5/5	0.86	0.16	32,32,34,35	0
7	ACT	A	1701	4/4	0.88	0.31	26,28,29,29	0
7	ACT	E	1701	4/4	0.91	0.10	22,25,26,26	0
7	ACT	E	1702	4/4	0.91	0.25	28,28,29,29	0
9	MPD	A	1704	8/8	0.93	0.18	23,31,34,38	0
7	ACT	E	1704	4/4	0.93	0.16	22,23,24,25	0
7	ACT	E	1703	4/4	0.94	0.10	20,21,21,22	0
7	ACT	E	1712	4/4	0.95	0.11	46,46,46,46	0
7	ACT	A	1703	4/4	0.95	0.14	24,24,24,25	0
5	O	A	1695	1/1	0.97	0.08	12,12,12,12	0
7	ACT	E	1699	4/4	0.97	0.06	13,15,16,16	0
7	ACT	A	1702	4/4	0.97	0.06	17,18,19,19	0
5	O	E	1696	1/1	0.97	0.09	12,12,12,12	0
3	HDD	A	1691	44/44	0.97	0.07	8,11,14,16	0
3	HDD	E	1691	44/44	0.98	0.06	8,11,16,21	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	CA	E	1697	1/1	0.98	0.28	32,32,32,32	0
6	CA	E	1710	1/1	0.98	0.15	35,35,35,35	0
7	ACT	A	1698	4/4	0.98	0.04	13,14,15,15	0
6	CA	E	1711	1/1	0.98	0.23	29,29,29,29	1
6	CA	A	1696	1/1	0.99	0.19	23,23,23,23	0
6	CA	E	1698	1/1	0.99	0.11	21,21,21,21	0
6	CA	A	1697	1/1	1.00	0.10	19,19,19,19	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 HDD A 1691:

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 HDD E 1691:

$2mF_o-DF_c$ (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.