Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2023 – 07:18 pm BST

PDB ID	:	8A97
Title	:	ROOM TEMPERATURE CRYSTAL STRUCTURE OF THE COFACTOR-DEVOID 1-H-3-HYDROXY-4- OXOQUINALDINE 2,4-DIOXYGENASE (HOD) UNDER XENON PRESSURE (30 bar)
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Deposited on	:	2022-06-27
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

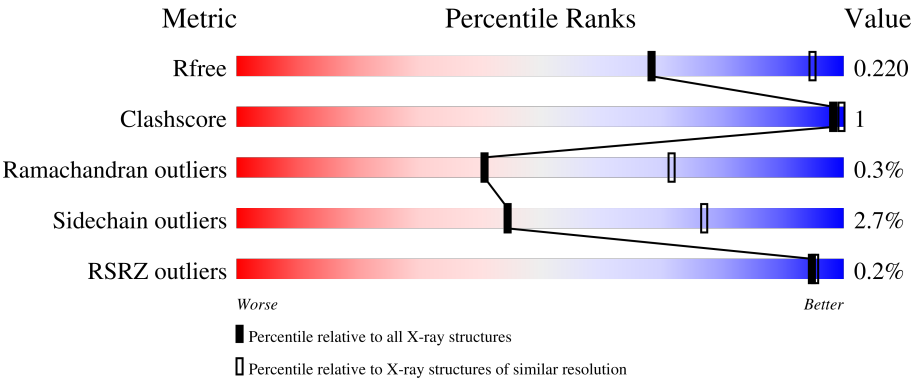
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	AAA	288	93% • 5%
1	BBB	288	93% • •
1	CCC	288	91% • • 5%
1	DDD	288	92% • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9096 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 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	275	Total	C	N	O	S	0	1	0
			2251	1436	393	413	9			
1	BBB	276	Total	C	N	O	S	0	1	0
			2257	1439	394	415	9			
1	CCC	275	Total	C	N	O	S	0	0	0
			2242	1431	392	410	9			
1	DDD	274	Total	C	N	O	S	0	1	0
			2243	1431	392	412	8			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-11	MET	-	initiating methionine	UNP O31266
AAA	-10	ARG	-	expression tag	UNP O31266
AAA	-9	GLY	-	expression tag	UNP O31266
AAA	-8	SER	-	expression tag	UNP O31266
AAA	-7	HIS	-	expression tag	UNP O31266
AAA	-6	HIS	-	expression tag	UNP O31266
AAA	-5	HIS	-	expression tag	UNP O31266
AAA	-4	HIS	-	expression tag	UNP O31266
AAA	-3	HIS	-	expression tag	UNP O31266
AAA	-2	HIS	-	expression tag	UNP O31266
AAA	-1	GLY	-	expression tag	UNP O31266
AAA	0	SER	-	expression tag	UNP O31266
AAA	69	SER	CYS	engineered mutation	UNP O31266
BBB	-11	MET	-	initiating methionine	UNP O31266
BBB	-10	ARG	-	expression tag	UNP O31266
BBB	-9	GLY	-	expression tag	UNP O31266
BBB	-8	SER	-	expression tag	UNP O31266
BBB	-7	HIS	-	expression tag	UNP O31266
BBB	-6	HIS	-	expression tag	UNP O31266
BBB	-5	HIS	-	expression tag	UNP O31266
BBB	-4	HIS	-	expression tag	UNP O31266

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	-3	HIS	-	expression tag	UNP O31266
BBB	-2	HIS	-	expression tag	UNP O31266
BBB	-1	GLY	-	expression tag	UNP O31266
BBB	0	SER	-	expression tag	UNP O31266
BBB	69	SER	CYS	engineered mutation	UNP O31266
CCC	-11	MET	-	initiating methionine	UNP O31266
CCC	-10	ARG	-	expression tag	UNP O31266
CCC	-9	GLY	-	expression tag	UNP O31266
CCC	-8	SER	-	expression tag	UNP O31266
CCC	-7	HIS	-	expression tag	UNP O31266
CCC	-6	HIS	-	expression tag	UNP O31266
CCC	-5	HIS	-	expression tag	UNP O31266
CCC	-4	HIS	-	expression tag	UNP O31266
CCC	-3	HIS	-	expression tag	UNP O31266
CCC	-2	HIS	-	expression tag	UNP O31266
CCC	-1	GLY	-	expression tag	UNP O31266
CCC	0	SER	-	expression tag	UNP O31266
CCC	69	SER	CYS	engineered mutation	UNP O31266
DDD	-11	MET	-	initiating methionine	UNP O31266
DDD	-10	ARG	-	expression tag	UNP O31266
DDD	-9	GLY	-	expression tag	UNP O31266
DDD	-8	SER	-	expression tag	UNP O31266
DDD	-7	HIS	-	expression tag	UNP O31266
DDD	-6	HIS	-	expression tag	UNP O31266
DDD	-5	HIS	-	expression tag	UNP O31266
DDD	-4	HIS	-	expression tag	UNP O31266
DDD	-3	HIS	-	expression tag	UNP O31266
DDD	-2	HIS	-	expression tag	UNP O31266
DDD	-1	GLY	-	expression tag	UNP O31266
DDD	0	SER	-	expression tag	UNP O31266
DDD	69	SER	CYS	engineered mutation	UNP O31266

- Molecule 2 is XENON (three-letter code: XE) (formula: Xe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total Xe 1 1	0	0
2	BBB	1	Total Xe 1 1	0	0
2	CCC	1	Total Xe 1 1	0	0

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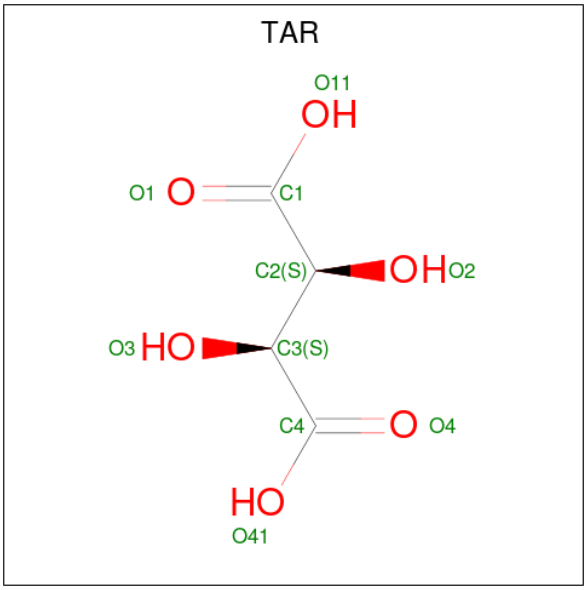
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	DDD	1	Total Xe 1 1	0	0

- Molecule 3 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: $C_4H_6O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 10 4 6	0	0
3	BBB	1	Total C O 10 4 6	0	0
3	BBB	1	Total C O 10 4 6	0	0
3	CCC	1	Total C O 10 4 6	0	0
3	DDD	1	Total C O 10 4 6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	14	Total O 14 14	0	0
4	BBB	13	Total O 13 13	0	0
4	CCC	9	Total O 9 9	0	0

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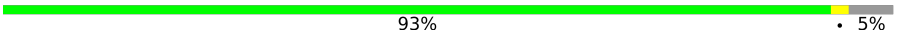
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	DDD	13	Total O 13 13	0	0

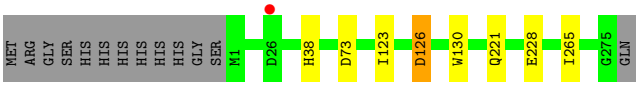
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase

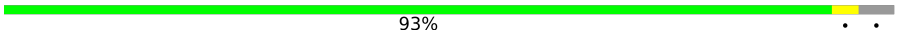
Chain AAA:





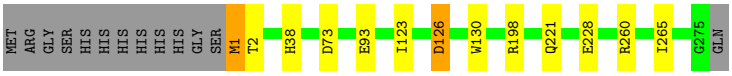
• Molecule 1: 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase

Chain BBB:



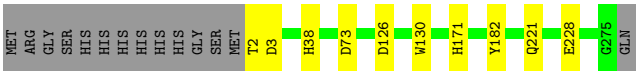
• Molecule 1: 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase

Chain CCC:



• Molecule 1: 1H-3-hydroxy-4-oxoquinaldine 2,4-dioxygenase

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	44.86Å 169.46Å 169.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.58 – 2.90 53.58 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (53.58-2.90) 98.8 (53.58-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.192 , 0.220 0.195 , 0.220	Depositor DCC
R_{free} test set	1483 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	69.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.428 for -h,l,k	Xtriage
Reported twinning fraction	0.524 for H, K, L 0.476 for -H, -L, -K	Depositor
Outliers	6 of 29382 reflections (0.020%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9096	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8885e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: XE, TAR

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	AAA	0.55	0/2322	0.59	0/3159
1	BBB	0.56	0/2328	0.60	0/3167
1	CCC	0.55	0/2313	0.60	0/3147
1	DDD	0.55	0/2314	0.59	0/3149
All	All	0.55	0/9277	0.59	0/12622

There are no bond length outliers.

There are no bond angle outliers.

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	AAA	2251	0	2142	1	0
1	BBB	2257	0	2147	3	0
1	CCC	2242	0	2137	4	0
1	DDD	2243	0	2130	3	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	10	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BBB	20	0	8	0	0
3	CCC	10	0	4	1	0
3	DDD	10	0	4	1	0
4	AAA	14	0	0	0	0
4	BBB	13	0	0	2	0
4	CCC	9	0	0	0	0
4	DDD	13	0	0	0	0
All	All	9096	0	8576	10	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 1.

All (10) 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:BBB:165:ASP:OD2	1:CCC:260:ARG:HD3	2.05	0.57
1:CCC:1:MET:O	1:CCC:2:THR:OG1	2.25	0.52
1:BBB:161:LEU:HD13	4:BBB:609:HOH:O	2.10	0.51
1:CCC:198:ARG:NH1	1:DDD:182:TYR:CE2	2.83	0.47
1:DDD:171:HIS:ND1	3:DDD:502:TAR:O11	2.30	0.47
1:BBB:112:GLU:HA	4:BBB:610:HOH:O	2.15	0.46
3:CCC:502:TAR:O1	3:CCC:502:TAR:O3	2.29	0.46
1:DDD:2:THR:O	1:DDD:3:ASP:HB2	2.21	0.41
1:AAA:123:ILE:HD12	1:AAA:265:ILE:HA	2.04	0.40
1:CCC:123:ILE:HD12	1:CCC:265:ILE:HA	2.04	0.40

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	AAA	274/288 (95%)	267 (97%)	6 (2%)	1 (0%)	34 66
1	BBB	275/288 (96%)	267 (97%)	7 (2%)	1 (0%)	34 66
1	CCC	273/288 (95%)	266 (97%)	6 (2%)	1 (0%)	34 66
1	DDD	273/288 (95%)	266 (97%)	7 (3%)	0	100 100
All	All	1095/1152 (95%)	1066 (97%)	26 (2%)	3 (0%)	41 71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	126	ASP
1	CCC	126	ASP
1	BBB	126	ASP

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	AAA	238/248 (96%)	232 (98%)	6 (2%)	47 78
1	BBB	239/248 (96%)	233 (98%)	6 (2%)	47 78
1	CCC	237/248 (96%)	229 (97%)	8 (3%)	37 71
1	DDD	237/248 (96%)	231 (98%)	6 (2%)	47 78
All	All	951/992 (96%)	925 (97%)	26 (3%)	44 77

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	38	HIS
1	AAA	73	ASP
1	AAA	126	ASP
1	AAA	130	TRP
1	AAA	221	GLN
1	AAA	228	GLU
1	BBB	38	HIS
1	BBB	73	ASP

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Mol	Chain	Res	Type
1	BBB	126	ASP
1	BBB	130	TRP
1	BBB	221	GLN
1	BBB	228	GLU
1	CCC	1	MET
1	CCC	38	HIS
1	CCC	73	ASP
1	CCC	93	GLU
1	CCC	126	ASP
1	CCC	130	TRP
1	CCC	221	GLN
1	CCC	228	GLU
1	DDD	38	HIS
1	DDD	73	ASP
1	DDD	126	ASP
1	DDD	130	TRP
1	DDD	221	GLN
1	DDD	228	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
3	TAR	BBB	502	-	9,9,9	1.05	0	12,12,12	0.94	0
3	TAR	BBB	503	-	9,9,9	0.95	0	12,12,12	1.05	0
3	TAR	AAA	502	-	9,9,9	0.96	0	12,12,12	1.00	0
3	TAR	DDD	502	-	9,9,9	1.08	0	12,12,12	0.93	0
3	TAR	CCC	502	-	9,9,9	1.10	0	12,12,12	0.87	0

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	TAR	BBB	502	-	-	2/12/12/12	-
3	TAR	BBB	503	-	-	4/12/12/12	-
3	TAR	AAA	502	-	-	6/12/12/12	-
3	TAR	DDD	502	-	-	4/12/12/12	-
3	TAR	CCC	502	-	-	10/12/12/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	DDD	502	TAR	O1-C1-C2-O2
3	DDD	502	TAR	O3-C3-C4-O4
3	CCC	502	TAR	C1-C2-C3-C4
3	BBB	502	TAR	O3-C3-C4-O4
3	BBB	502	TAR	O3-C3-C4-O41
3	BBB	503	TAR	O1-C1-C2-O2
3	BBB	503	TAR	O11-C1-C2-O2
3	BBB	503	TAR	O3-C3-C4-O4
3	BBB	503	TAR	O3-C3-C4-O41
3	CCC	502	TAR	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	CCC	502	TAR	O11-C1-C2-O2
3	CCC	502	TAR	O3-C3-C4-O4
3	CCC	502	TAR	O3-C3-C4-O41
3	DDD	502	TAR	O11-C1-C2-O2
3	DDD	502	TAR	O3-C3-C4-O41
3	CCC	502	TAR	C1-C2-C3-O3
3	CCC	502	TAR	O2-C2-C3-C4
3	CCC	502	TAR	O2-C2-C3-O3
3	AAA	502	TAR	O1-C1-C2-O2
3	AAA	502	TAR	O11-C1-C2-O2
3	AAA	502	TAR	O3-C3-C4-O4
3	AAA	502	TAR	O3-C3-C4-O41
3	CCC	502	TAR	O1-C1-C2-C3
3	CCC	502	TAR	O11-C1-C2-C3
3	AAA	502	TAR	C2-C3-C4-O4
3	AAA	502	TAR	C2-C3-C4-O41

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	DDD	502	TAR	1	0
3	CCC	502	TAR	1	0

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	AAA	275/288 (95%)	0.03	1 (0%)	92	93	45, 67, 92, 109	0
1	BBB	276/288 (95%)	0.06	1 (0%)	92	93	43, 67, 96, 114	0
1	CCC	275/288 (95%)	-0.03	0	100	100	42, 60, 90, 105	0
1	DDD	274/288 (95%)	0.01	0	100	100	46, 67, 95, 115	0
All	All	1100/1152 (95%)	0.02	2 (0%)	95	95	42, 65, 94, 115	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	26	ASP	3.3
1	BBB	275	GLY	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

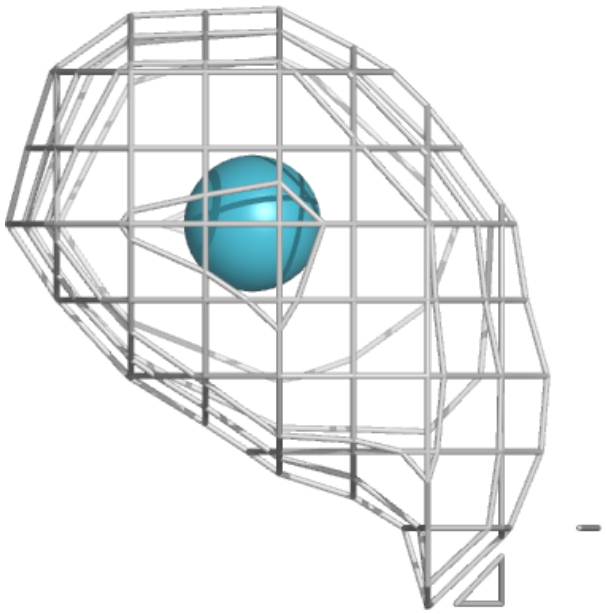
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

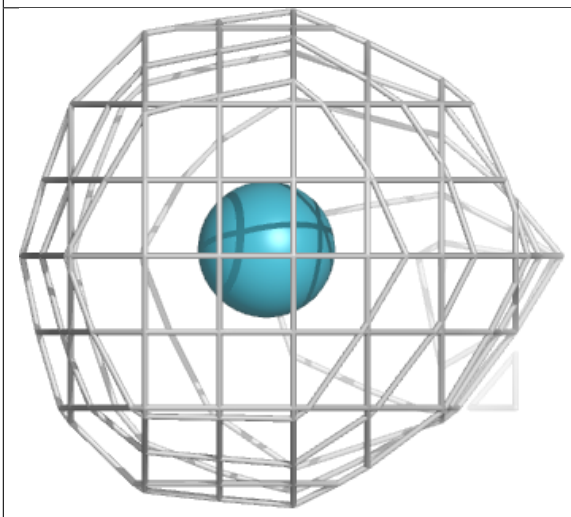
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	XE	DDD	501	1/1	0.89	0.10	89,89,89,89	1
3	TAR	BBB	503	10/10	0.92	0.14	54,59,62,63	0
3	TAR	AAA	502	10/10	0.93	0.20	64,66,70,75	0
3	TAR	BBB	502	10/10	0.94	0.23	62,65,69,71	0
3	TAR	CCC	502	10/10	0.94	0.17	45,49,50,51	0
3	TAR	DDD	502	10/10	0.96	0.10	49,53,55,55	0
2	XE	CCC	501	1/1	0.98	0.15	68,68,68,68	1
2	XE	BBB	501	1/1	0.99	0.10	81,81,81,81	1
2	XE	AAA	501	1/1	0.99	0.09	87,87,87,87	1

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 XE DDD 501:

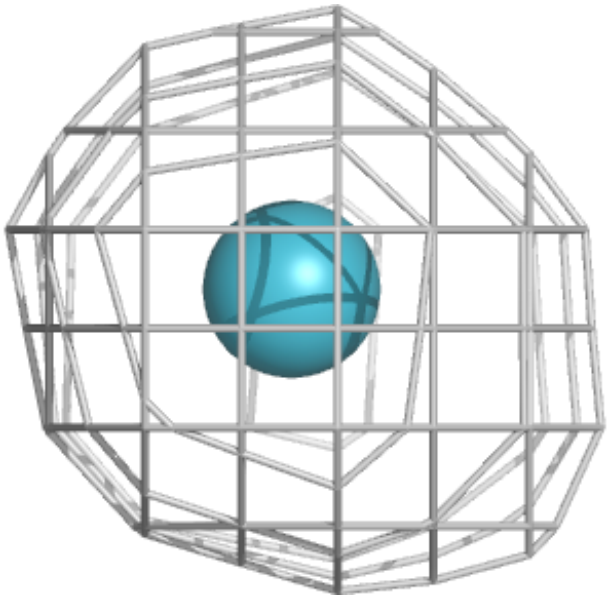
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

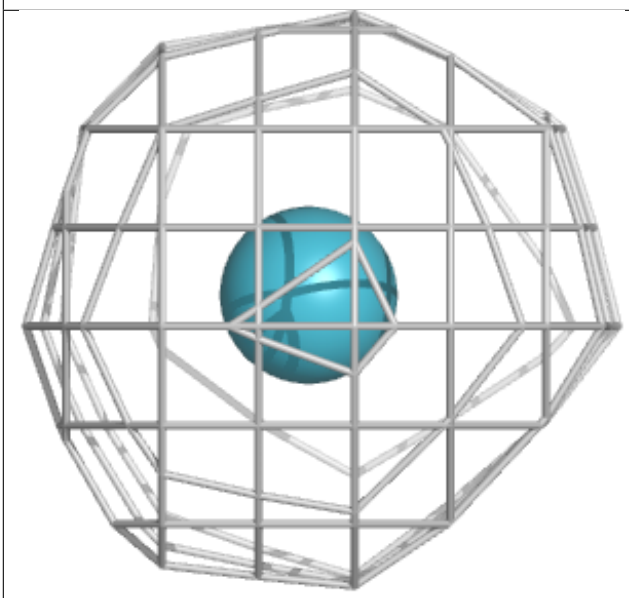


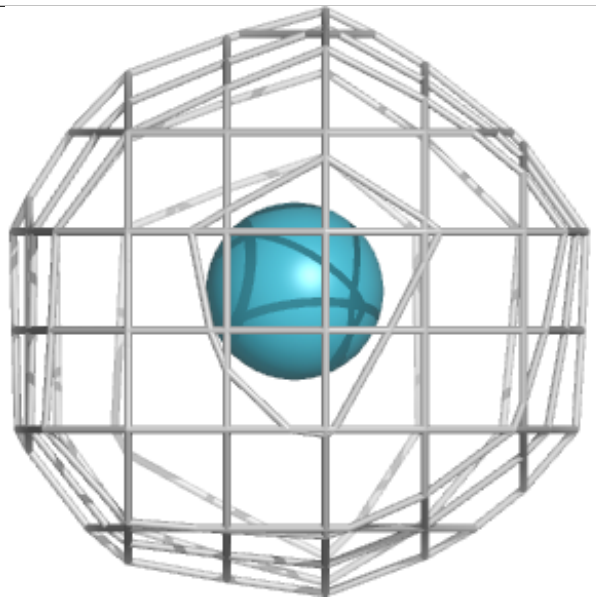


Electron density around XE CCC 501:

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

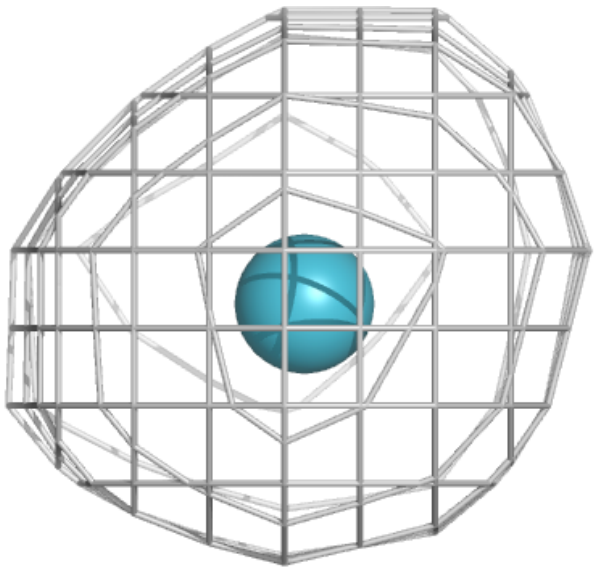


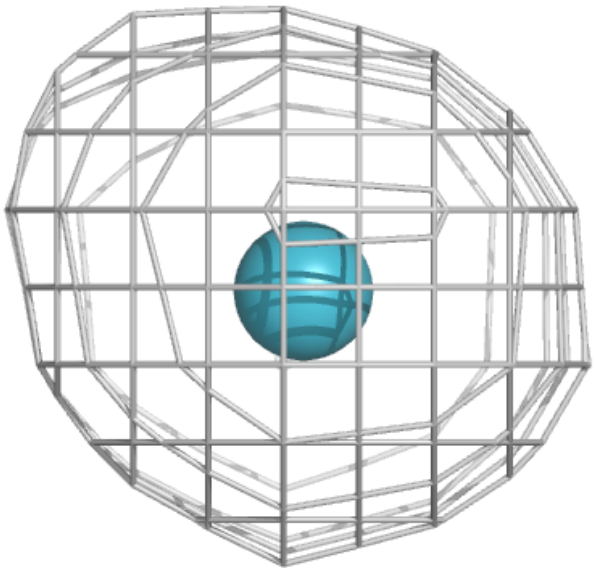


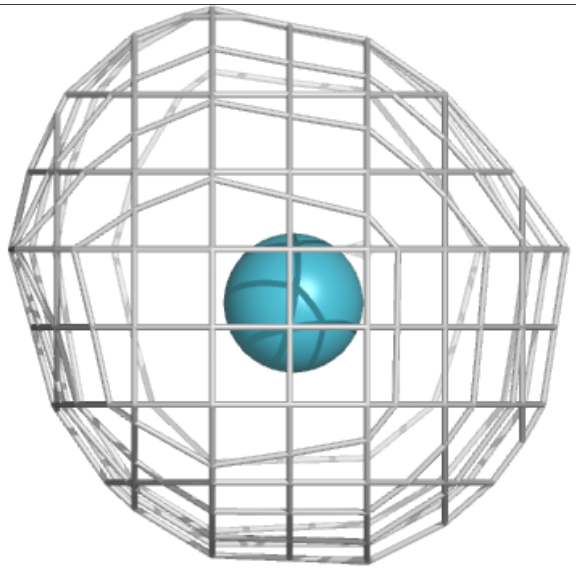


Electron density around XE BBB 501:

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

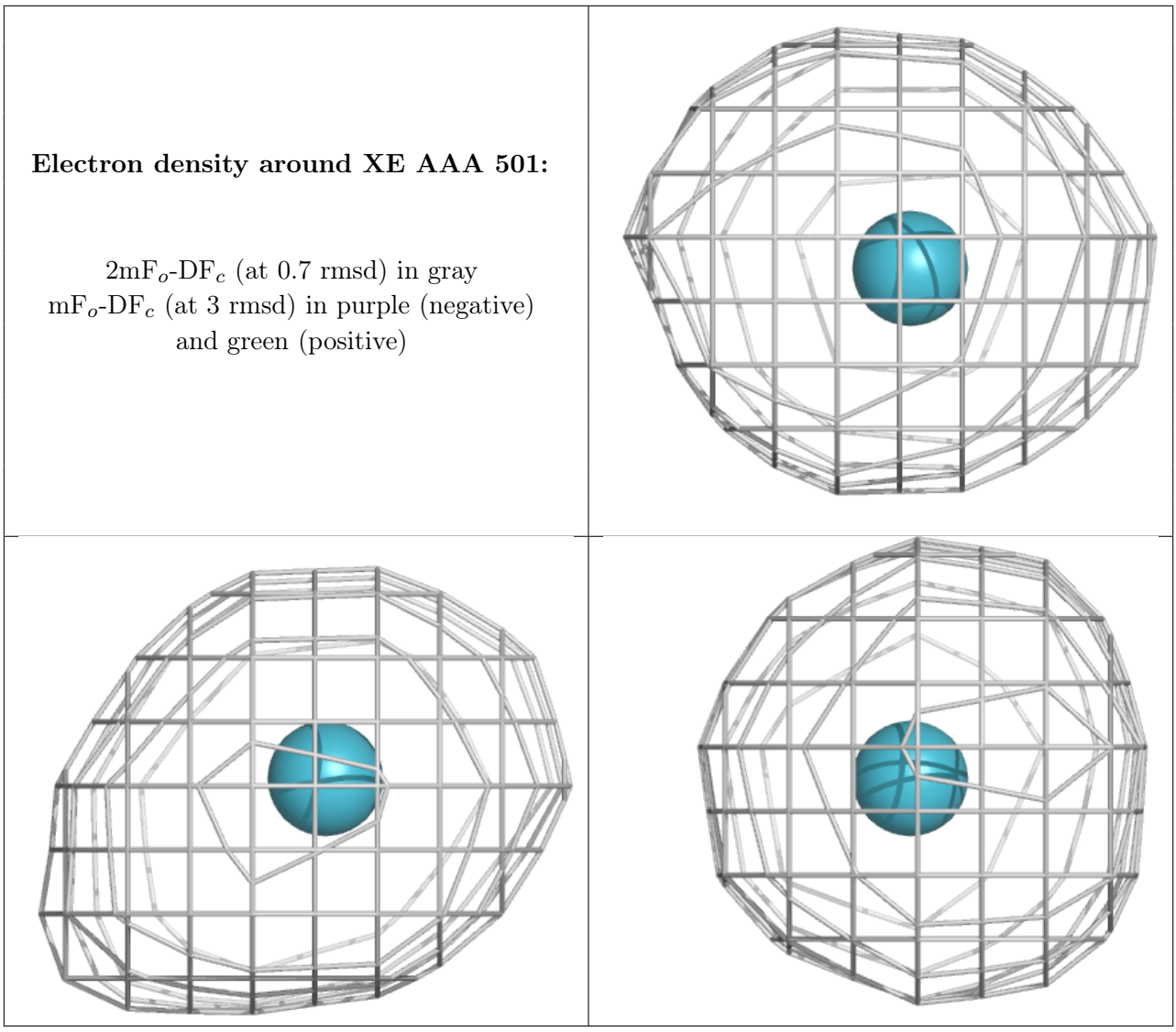






Electron density around XE AAA 501:

$2mF_o$-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.