



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 01:03 AM BST

PDB ID : 6OC5
Title : Lanthanide-dependent methanol dehydrogenase XoxF from *Methylobacterium extorquens*, in complex with Lanthanum
Authors : Fellner, M.; Good, N.M.; Martinez-Gomez, N.C.; Hausinger, R.P.; Hu, J.
Deposited on : 2019-03-21
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
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

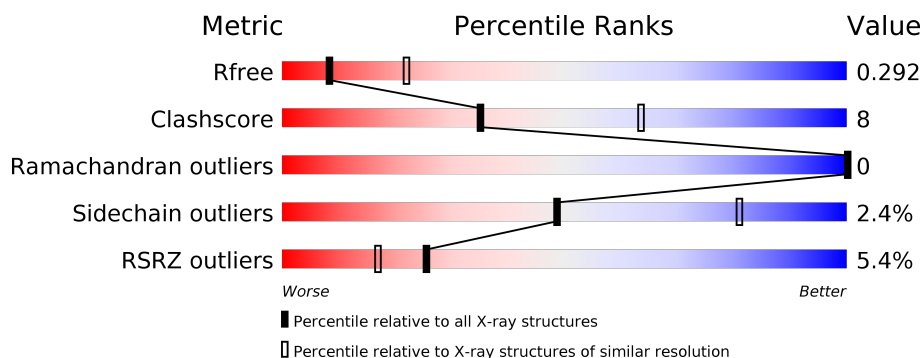
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	601	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>.</div> </div> </div>
1	B	601	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>.</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8433 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 Lanthanide-dependent methanol dehydrogenase XoxF.

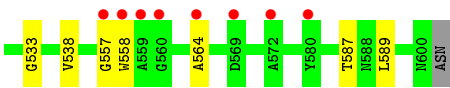
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	579	Total	C	N	O	S	0	0	0
			4242	2705	715	805	17			
1	B	579	Total	C	N	O	S	0	0	0
			4182	2663	707	795	17			

- Molecule 2 is LANTHANUM (III) ION (three-letter code: LA) (formula: La) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	La	0	0
			1	1		
2	A	1	Total	La	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	3	Total	O	0	0
			3	3		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.32Å 87.95Å 202.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 2.80 48.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.4 (48.61-2.80) 97.5 (48.61-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18rc1-3769	Depositor
R, R_{free}	0.249 , 0.280 0.257 , 0.292	Depositor DCC
R_{free} test set	1282 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8433	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
LA

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	0.31	1/4362 (0.0%)	0.51	0/5970
1	B	0.28	0/4299	0.50	1/5892 (0.0%)
All	All	0.29	1/8661 (0.0%)	0.50	1/11862 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	CYS	CA-CB	7.48	1.70	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	LYS	CA-CB-CG	-5.47	101.36	113.40

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	4242	0	3880	67	0
1	B	4182	0	3767	67	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	0	0
3	B	3	0	0	0	0
All	All	8433	0	7647	132	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 8.

All (132) 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:124:CYS:SG	1:A:125:CYS:N	2.50	0.84
1:B:125:CYS:HA	1:B:558:TRP:NE1	1.98	0.79
1:B:454:VAL:HG23	1:B:455:GLY:H	1.52	0.75
1:A:225:ASP:HB2	1:A:304:MET:HE1	1.70	0.73
1:B:500:THR:HG23	1:B:502:GLY:H	1.54	0.73
1:B:415:LYS:NZ	1:B:418:GLN:O	2.23	0.71
1:A:232:LEU:HD11	1:A:385:GLY:HA3	1.71	0.70
1:A:184:VAL:CG2	1:A:204:LEU:HD23	2.24	0.67
1:B:369:VAL:HG13	1:B:409:PRO:HD3	1.76	0.67
1:A:269:LEU:HD11	1:A:306:LYS:HE2	1.79	0.65
1:B:198:HIS:HA	1:B:214:TYR:HA	1.79	0.65
1:B:345:ARG:HB3	1:B:413:GLY:HA3	1.79	0.63
1:B:415:LYS:HD2	1:B:431:VAL:HG23	1.80	0.63
1:B:533:GLY:H	1:B:587:THR:HG21	1.64	0.62
1:A:181:LYS:NZ	1:A:301:ASP:OD1	2.33	0.62
1:A:298:ARG:HA	1:A:305:ALA:HA	1.82	0.60
1:B:494:TRP:HB2	1:B:510:LEU:HD11	1.84	0.59
1:B:126:ASP:HB2	1:B:557:GLY:O	2.03	0.59
1:A:198:HIS:HA	1:A:214:TYR:HA	1.85	0.59
1:A:404:SER:N	1:A:440:TYR:O	2.26	0.58
1:B:325:MET:HB3	1:B:340:LEU:HD11	1.85	0.57
1:B:124:CYS:SG	1:B:125:CYS:N	2.78	0.57
1:A:32:PRO:O	1:A:50:LEU:HD11	2.04	0.57
1:B:564:ALA:HA	1:B:589:LEU:HD21	1.87	0.56
1:B:125:CYS:HA	1:B:558:TRP:HE1	1.70	0.56
1:B:404:SER:N	1:B:440:TYR:O	2.30	0.56
1:A:328:THR:O	1:A:354:ARG:NH1	2.39	0.55
1:B:181:LYS:NZ	1:B:263:TYR:OH	2.37	0.55
1:A:132:LEU:HD22	1:A:139:ILE:CG2	2.37	0.54
1:B:41:ASP:OD2	1:B:45:THR:OG1	2.24	0.53
1:B:366:ASP:HB2	1:B:414:THR:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:ILE:HD12	1:B:483:ILE:HG12	1.91	0.53
1:A:222:LEU:HD21	1:A:241:SER:OG	2.09	0.53
1:B:518:ASP:HB3	1:B:522:GLY:H	1.73	0.53
1:A:216:ILE:HG22	1:A:250:TRP:HB2	1.90	0.53
1:B:278:SER:OG	1:B:279:THR:N	2.40	0.53
1:B:429:PHE:HB2	1:B:476:TRP:HB3	1.91	0.52
1:A:345:ARG:HB3	1:A:413:GLY:HA3	1.90	0.52
1:B:225:ASP:O	1:B:229:THR:HG23	2.09	0.52
1:A:51:ASP:N	1:A:51:ASP:OD1	2.44	0.51
1:A:366:ASP:HB3	1:A:369:VAL:HG23	1.92	0.51
1:A:518:ASP:HB3	1:A:522:GLY:H	1.75	0.51
1:A:41:ASP:OD2	1:A:45:THR:OG1	2.26	0.51
1:A:191:GLY:O	1:A:278:SER:HA	2.12	0.49
1:A:73:ARG:HH12	1:A:120:ILE:HG21	1.76	0.49
1:A:23:GLU:HA	1:A:26:LEU:HD12	1.95	0.49
1:A:130:ARG:NH2	1:A:174:THR:OG1	2.43	0.49
1:B:292:SER:O	1:B:310:GLN:NE2	2.41	0.49
1:B:434:ASN:ND2	1:B:492:SER:HB3	2.28	0.49
1:A:323:ASN:HB2	1:A:342:HIS:CE1	2.48	0.49
1:B:229:THR:HG22	1:B:305:ALA:O	2.12	0.49
1:B:362:ALA:HB3	1:B:377:LEU:HD11	1.94	0.49
1:A:126:ASP:HB2	1:A:557:GLY:O	2.12	0.49
1:B:126:ASP:OD2	1:B:557:GLY:N	2.46	0.49
1:B:176:THR:OG1	1:B:177:VAL:N	2.46	0.49
1:B:42:TYR:OH	1:B:179:PRO:O	2.20	0.49
1:B:256:CYS:O	1:B:275:GLY:N	2.46	0.49
1:A:176:THR:OG1	1:A:177:VAL:N	2.45	0.48
1:B:130:ARG:NH1	1:B:174:THR:OG1	2.46	0.48
1:B:415:LYS:CD	1:B:431:VAL:HG23	2.44	0.48
1:A:376:ASP:OD2	1:A:383:THR:OG1	2.24	0.48
1:A:193:PHE:HD1	1:A:452:PRO:HA	1.79	0.48
1:B:318:ASP:O	1:B:345:ARG:NH2	2.48	0.47
1:B:366:ASP:HB3	1:B:369:VAL:HG23	1.95	0.47
1:A:340:LEU:HB2	1:A:354:ARG:HB3	1.96	0.47
1:A:364:LYS:HD3	1:A:369:VAL:HB	1.96	0.47
1:B:257:THR:O	1:B:257:THR:OG1	2.31	0.47
1:B:323:ASN:HB2	1:B:342:HIS:CE1	2.49	0.47
1:B:494:TRP:CB	1:B:510:LEU:HD11	2.44	0.47
1:A:46:ARG:NE	1:A:497:ALA:O	2.35	0.47
1:A:240:SER:HB2	1:A:291:TRP:HE1	1.79	0.47
1:A:232:LEU:HD22	1:A:384:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ASN:N	1:B:57:ASN:OD1	2.48	0.46
1:A:429:PHE:HB2	1:A:476:TRP:HB3	1.97	0.46
1:B:95:ILE:HG12	1:B:112:GLU:HG3	1.98	0.46
1:B:25:VAL:O	1:B:29:VAL:HG23	2.15	0.46
1:A:443:PHE:HE2	1:A:457:THR:HG23	1.81	0.46
1:A:96:VAL:CG2	1:A:141:LEU:HD13	2.46	0.45
1:B:298:ARG:HA	1:B:305:ALA:HA	1.97	0.45
1:A:113:PRO:HG2	1:A:115:GLN:HE21	1.81	0.45
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.85	0.45
1:B:321:GLY:HA2	1:B:344:ASP:OD1	2.17	0.45
1:A:517:VAL:HG12	1:A:524:GLU:HA	1.97	0.45
1:A:73:ARG:HH11	1:A:127:THR:CG2	2.30	0.45
1:B:171:GLU:HB3	1:B:188:ILE:HD11	1.97	0.45
1:A:66:THR:OG1	1:B:529:LYS:O	2.33	0.45
1:A:184:VAL:HG21	1:A:204:LEU:HD23	1.98	0.45
1:A:223:ILE:O	1:A:304:MET:HA	2.17	0.45
1:A:546:LYS:NZ	1:A:598:LEU:O	2.40	0.45
1:B:414:THR:O	1:B:434:ASN:N	2.36	0.45
1:A:291:TRP:HB3	1:A:294:THR:HG21	1.99	0.44
1:A:25:VAL:O	1:A:29:VAL:HG23	2.17	0.44
1:A:339:LEU:HA	1:A:339:LEU:HD23	1.84	0.44
1:A:146:THR:O	1:A:164:ASN:N	2.37	0.44
1:A:65:TRP:CZ2	1:A:595:VAL:HG21	2.52	0.44
1:A:404:SER:HB2	1:A:440:TYR:HB3	2.00	0.44
1:A:211:TRP:CD2	1:A:303:GLY:HA3	2.53	0.44
1:B:216:ILE:HG22	1:B:250:TRP:HB2	1.98	0.44
1:B:471:GLY:HA3	1:B:492:SER:HA	1.99	0.44
1:B:236:ILE:HD12	1:B:240:SER:OG	2.17	0.44
1:A:50:LEU:CD2	1:A:542:GLU:HB2	2.48	0.43
1:A:193:PHE:CD1	1:A:452:PRO:HA	2.54	0.43
1:A:476:TRP:CZ2	1:A:481:GLY:HA2	2.54	0.43
1:A:98:ALA:O	1:A:108:VAL:N	2.42	0.43
1:B:225:ASP:H	1:B:229:THR:CG2	2.32	0.43
1:B:197:CYS:HB2	1:B:255:GLY:O	2.19	0.43
1:A:196:GLN:HG3	1:A:196:GLN:O	2.17	0.42
1:B:87:TYR:OH	1:B:153:ALA:O	2.34	0.42
1:B:476:TRP:CZ2	1:B:481:GLY:HA2	2.55	0.42
1:B:533:GLY:N	1:B:587:THR:HG21	2.34	0.42
1:A:214:TYR:CD2	1:A:221:GLN:HB2	2.55	0.42
1:A:540:THR:HA	1:A:549:VAL:HA	2.01	0.42
1:B:415:LYS:CD	1:B:431:VAL:CG2	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ARG:NH2	1:B:538:VAL:O	2.52	0.42
1:B:262:SER:OG	1:B:271:TYR:HB2	2.19	0.42
1:B:352:LEU:HG	1:B:359:VAL:HA	2.00	0.42
1:A:320:ASP:O	1:A:345:ARG:HG3	2.20	0.42
1:A:529:LYS:O	1:B:66:THR:OG1	2.37	0.42
1:A:61:LEU:HA	1:A:61:LEU:HD12	1.84	0.42
1:B:340:LEU:HB2	1:B:354:ARG:HB3	2.01	0.42
1:B:222:LEU:HD11	1:B:241:SER:HB2	2.02	0.41
1:A:290:LYS:HA	1:A:291:TRP:HA	1.64	0.41
1:B:162:VAL:HG11	1:B:207:GLY:O	2.21	0.41
1:B:320:ASP:O	1:B:345:ARG:HG3	2.21	0.41
1:A:185:ILE:HA	1:A:201:ALA:HA	2.03	0.41
1:B:500:THR:HG23	1:B:502:GLY:N	2.29	0.41
1:A:516:ALA:HB3	1:A:526:TYR:HB3	2.02	0.41
1:A:200:THR:OG1	1:A:212:ARG:NE	2.52	0.40
1:A:86:MET:HB2	1:A:101:LEU:HD21	2.03	0.40
1:A:323:ASN:ND2	1:A:343:PHE:O	2.53	0.40
1:B:269:LEU:HD21	1:B:306:LYS:HB2	2.04	0.40
1:B:339:LEU:HA	1:B:339:LEU:HD23	1.96	0.40

There are no symmetry-related clashes.

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	577/601 (96%)	544 (94%)	33 (6%)	0	100	100
1	B	577/601 (96%)	538 (93%)	39 (7%)	0	100	100
All	All	1154/1202 (96%)	1082 (94%)	72 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	410/484 (85%)	401 (98%)	9 (2%)	52	83
1	B	394/484 (81%)	384 (98%)	10 (2%)	47	80
All	All	804/968 (83%)	785 (98%)	19 (2%)	49	81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	TYR
1	A	68	SER
1	A	141	LEU
1	A	142	HIS
1	A	155	SER
1	A	161	SER
1	A	268	ASP
1	A	320	ASP
1	A	494	TRP
1	B	42	TYR
1	B	48	SER
1	B	78	SER
1	B	150	SER
1	B	155	SER
1	B	204	LEU
1	B	320	ASP
1	B	459	SER
1	B	486	SER
1	B	494	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	221	GLN
1	B	434	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	579/601 (96%)	0.36	24 (4%)	37 27	39, 66, 86, 95	0
1	B	579/601 (96%)	0.45	39 (6%)	17 10	39, 63, 101, 130	0
All	All	1158/1202 (96%)	0.41	63 (5%)	25 17	39, 65, 92, 130	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	280	TRP	5.2
1	B	253	GLY	4.8
1	B	440	TYR	4.4
1	B	558	TRP	3.8
1	B	501	ALA	3.6
1	A	124	CYS	3.6
1	B	385	GLY	3.5
1	B	414	THR	3.5
1	B	365	PHE	3.5
1	B	557	GLY	3.4
1	A	252	THR	3.4
1	A	375	VAL	3.4
1	B	420	ALA	3.4
1	B	580	TYR	3.1
1	B	443	PHE	3.1
1	A	253	GLY	3.0
1	B	191	GLY	3.0
1	B	560	GLY	3.0
1	B	381	SER	2.9
1	A	274	SER	2.8
1	A	449	PRO	2.7
1	A	194	GLY	2.7
1	B	332	PHE	2.7
1	A	291	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	572	ALA	2.7
1	B	281	ASN	2.7
1	A	357	GLY	2.6
1	B	559	ALA	2.6
1	B	252	THR	2.6
1	B	265	PRO	2.5
1	B	371	TRP	2.5
1	A	346	ASN	2.5
1	B	388	LEU	2.5
1	B	351	THR	2.4
1	B	319	PHE	2.4
1	B	318	ASP	2.4
1	A	197	CYS	2.4
1	A	217	GLY	2.3
1	B	343	PHE	2.3
1	B	436	VAL	2.3
1	A	245	TRP	2.3
1	A	368	VAL	2.2
1	B	396	GLU	2.2
1	A	440	TYR	2.2
1	B	258	TRP	2.2
1	A	319	PHE	2.2
1	A	280	TRP	2.2
1	A	254	GLY	2.2
1	B	362	ALA	2.2
1	B	409	PRO	2.2
1	A	313	PRO	2.2
1	A	407	ILE	2.1
1	A	445	VAL	2.1
1	B	413	GLY	2.1
1	A	356	THR	2.1
1	B	428	LEU	2.1
1	B	569	ASP	2.1
1	B	564	ALA	2.1
1	B	456	ALA	2.1
1	A	265	PRO	2.1
1	A	411	ALA	2.0
1	B	350	TYR	2.0
1	B	162	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

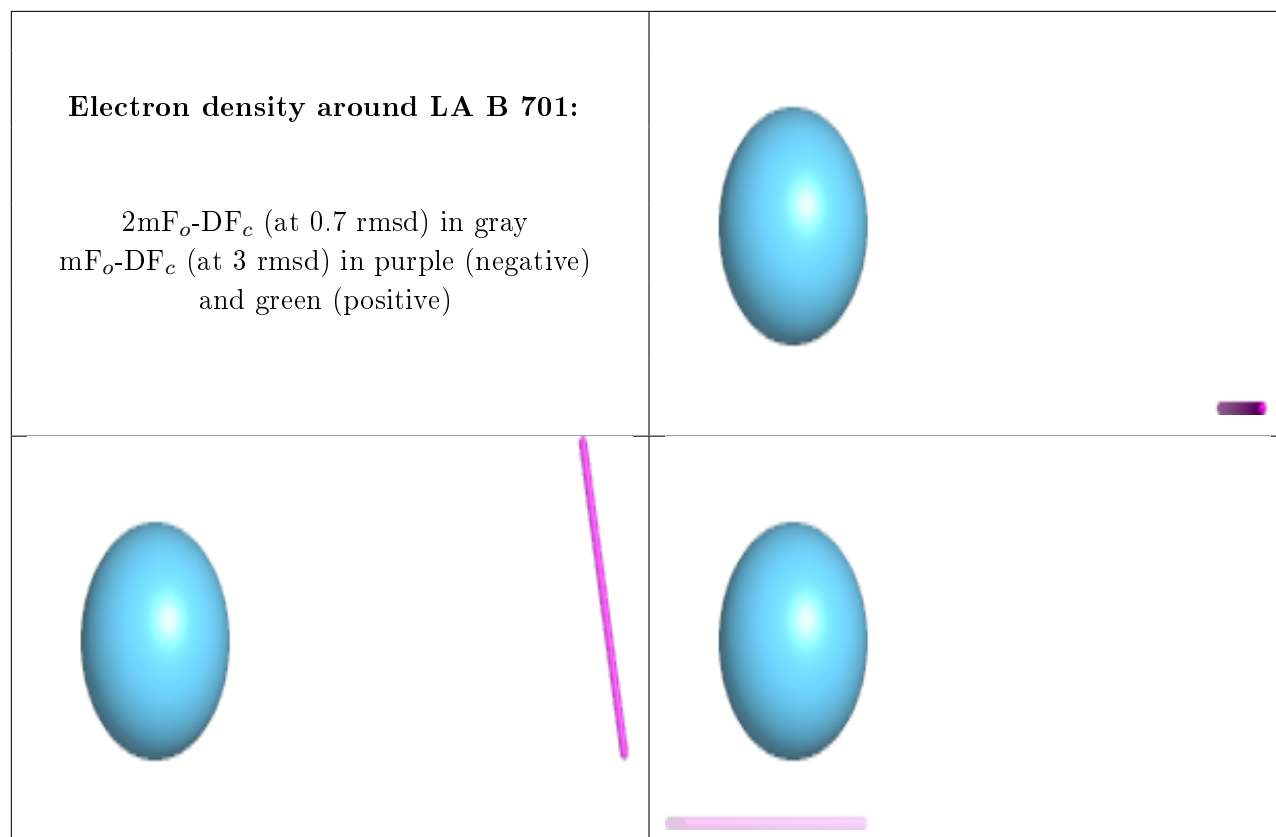
There are no monosaccharides in this entry.

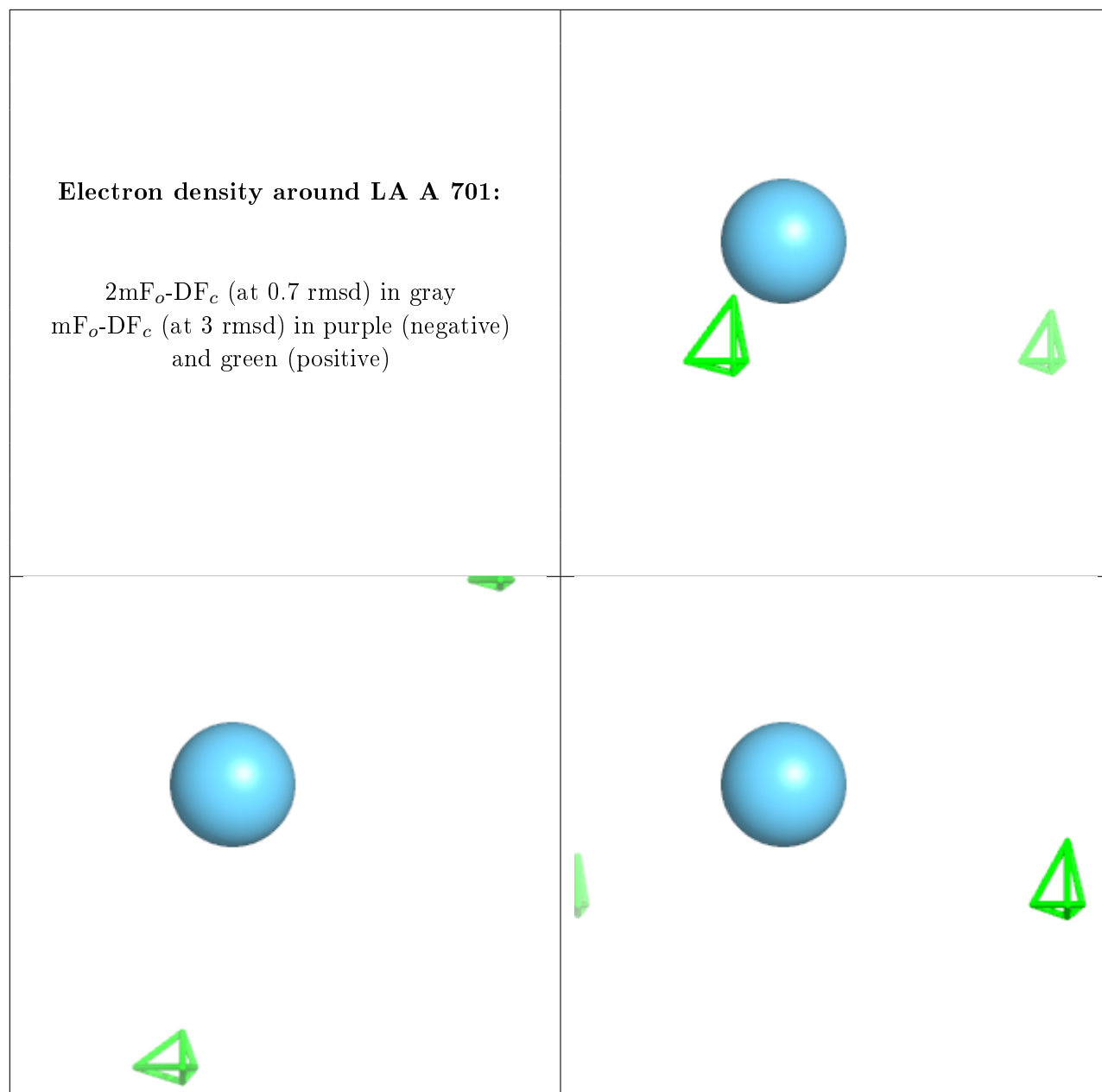
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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(\AA^2)	Q<0.9
2	LA	B	701	1/1	0.97	0.11	71,71,71,71	1
2	LA	A	701	1/1	0.99	0.15	65,65,65,65	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.